A System-of-Systems Architecture Methodology to Evaluate Energy Systems Integration as a Pathway for the Energy Transition

A thesis submitted by

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For the Degree of

Doctor of Philosophy

School of Engineering

Newcastle University

June 2021

Abstract

One pathway for the energy transition is Energy Systems Integration (ESI), which aims to exploit synergies across the multiple energy vectors of electricity, gas and heat. This will create new interactions between different components of the energy system and increase the complexity involved. Existing studies focus on planning and operational models for ESI, but the literature lacks comprehensive studies around evaluation of ESI. This thesis develops a novel methodological framework for evaluating the effectiveness of ESI as a pathway for the energy transition. The framework provides a model to encompass stakeholders' perspectives in an indicator-based evaluation while reducing the complexity of the energy system architecture.

The framework is based on three main contributions presented in this research, drawn from the areas of sustainability assessments, sustainability transitions and systems engineering, respectively. Firstly, the framework exhibits principles identified to reflect a whole systems approach for evaluation being: multidimensional, multivectoral, systemic, systematic, futuristic, and applicable. Secondly, the framework operationalises an understanding of ESI in relation to the Multi-System Perspective for transitions, being conceptualised as a System-of-System (SoS). Thirdly, the framework combines systems engineering concepts and methods to (i) model the integrated energy system architecture as a SoS; (ii) identify the structural and functional relationships between its components and with its stakeholders at different levels of abstraction; and (iii) select indicators to measure the effectiveness of the energy system towards achieving its requirements.

The framework is validated using a test case study on the local energy system in Findhorn village and through a group interview with academic experts, whose feedback helped implement necessary improvements. From this, a Reference System Architecture Model that can be readily used as a standard approach for evaluation is developed. A full scale study is conducted on the North of Tyne energy system to demonstrate the framework applicability and usefulness.

Covid-19 Impact Statement

Some elements of this research have been disrupted by the Covid-19 pandemic outlined as follows. First, the experts' feedback workshop for validating the framework described in Chapter 5 was already planned to take place around March 2020. As the pandemic started, the workshop had to be moved to a virtual setting rather than face-to-face, and in addition a few invited experts were not able to attend anymore. Unfortunately, the recording of the live session discussions didn't work properly due to a technical issue out of our control. A contingency plan was followed in which a recorded presentation was sent to those who couldn't attend the live discussion along with a questionnaire to provide their feedback. All this meant that the value of the group interaction was not fully captured as planned and that the feedback was not provided uniformly by experts in a way that systematic reporting could be provided.

Second, the disruption has particularly affected the quantitative modelling efforts for the North of Tyne case study described in Chapter 7. These efforts are part of a collaborative work with other colleagues who had to work from home with lower computational power, in addition to being overwhelmed with their own caring responsibilities. This made the modelling stage progress more slowly than planned. In particular, the disruption to this stage affected the following:

- simulating more iterations of different scenarios for the case study was very demanding and time consuming
- including energy storage technologies in the energy system model was not possible as it requires additional computational effort that was not available to run the model at the time
- carrying out a sensitivity analysis of scenarios with different cost factors was not possible as it requires running the model again, which was also time consuming

Other Contributions to this Work

Some of elements of this research have been produced through collaborative work with colleagues from the Power Systems group in Newcastle University, namely Dr Hamid Hosseini and Dr Adib Allahham. Those relate to the work around the scenario formulation and quantitative modelling stages of the developed framework in the Findhorn case studies described in Chapter 5 and the quantitative modelling in the North of Tyne case study described in Chapter 7. This involves designing scenarios, developing the mathematical formulations for the model, implementing the model algorithms on MATLAB, running the model with different parameters for different scenarios, and any data analysis required to carry out those tasks.

First, in regards to the Findhorn case studies that were used initially for testing the developed framework in Chapter 5, the analysis was based on the scenarios and quantitative model developed by Dr Hosseini and Dr Allahham. Those are already published in peer-reviewed journals and are provided in Appendix B. The first test case study was based on the integrated energy network model and scenarios for delivering heat in Findhorn developed in (Hosseini, Allahham and Adams, 2021). The second case study was based on the integrated energy network model for Findhorn considering the impact of energy storage technologies and some of the scenarios developed in (Hosseini, Allahham, Vahidinasab, et al., 2021).

Second, in regards to the North of Tyne case study that was presented to demonstrate the full application of the developed framework in Chapter 7, the analysis was based on the quantitative model developed by Dr Allahham. This quantitative model is described in Appendix E and the full case study including the model description has been later published in (Berjawi, Allahham, et al., 2021).

Acknowledgments

I would like to start by acknowledging the School of Engineering at Newcastle University and the EPSRC National Centre for Energy Systems Integration (CESI) for this opportunity to do my PhD studies at their premises, which I took unreservedly around four years ago.

This work would not have been possible without my first supervisor Dr Sara Walker to whom I am grateful for her continuous support, confidence and motivation throughout this journey. I am also thankful for my second and third supervisors Dr Haris Patsios and Dr Hamid Hosseini for their help and insight. I would also like to thank Prof John Fitzgerald (NCL Computing), Dr Gareth Powells (NCL Geography), Prof Gordon Mackerron (SPRU Sussex), and Prof Raimund Bleischwitz (UCL ISR) for their valuable feedback and inspiration that helped shape the PhD at different stages. Thanks to all my colleagues at the Power Systems group for their cooperation, and a notable mention to Dr Adib Allahham who was my mentor throughout this journey since stepping in. I must also acknowledge the contributions of Dr Hamid Hosseini and Dr Adib Allaham for supporting my work with adjustments to their simulation models, which were used in the case studies presented in Chapters 5 and 7 of this thesis.

I would like to take this opportunity to offer gratitude to all those who stood with me during this journey. Special thanks to my parents, Hala and Hamza, whom without their unconditional love and encouragement, I would not have been doing this thesis in the first place. Thanks to my caring siblings, Marwa, Ahmad and Fatima, and to my extended family for their trust and support. I hope this milestone in my career rises up to their expectations and pride.

I would like to thank my 'support bubble' of friends in Newcastle who made the past four years bearable and enjoyable, especially during covid times. Thanks to all my friends in Lebanon and abroad for their patience and support during these difficult times our country is enduring. I would like to especially thank the soon-to-be Doctors Mohammed Muhieddine (Imperial College London), Hisham Hafez (Northumbria University), Ali Ayoub (ETH Zurich) and Dr Ali Kassem (Sussex University) for the endless conversations around PhD life and beyond.

Last but not least, all praise be to God for His greatest grace and many blessings, and the power He gave me to complete this work. God has made us humankind vicegerents on Earth and it is our duty to strive towards preserving nature and sustaining resources.

- and the Earth, We have spread it out, and cast in mountains standing firm, and grown in it everything in equilibrium. and We have provided in it sustenance for your and for those whom you do not support. (Qur'an 15:19-20)

I wish that this work is accepted in courtesy to the sacrifices of those who are Unknown on Earth but Known in the Sky, and in devotion to the return of the Awaited One.

- and say, 'O my Lord, increase me in knowledge. (Qur'an 20:114)

List of Publications

Journal Paper

Berjawi, A.E.H., Walker, S.L., Patsios, C. & Hosseini, S.H.R. (2021) An evaluation framework for future integrated energy systems: A whole energy systems approach. *Renewable and Sustainable Energy Reviews.* 145111163. **(Chapter 2 and 4)**

Book Chapter

Berjawi, A.E.H., Allahham, A., Walker, S.L., Patsios, C. and Hosseini, S.H.R. (2021). Whole Energy Systems Evaluation: A Methodological Framework and Case Study In: V. Vahidinasab and B. Mohammadi-Ivatloo, eds. *Whole Energy Systems Bridging the Gap via Vector-Coupling Technologies*. Springer International Publishing. Available from: https://www.springer.com/gp/book/9783030876524. **(Chapter 7)**

Conference Papers

Berjawi, A.E.H., Walker, S.L., Patsios, C. & Hosseini, S.H.R. (2020) Analysing energy systems integration: A socio-technical approach and a system architecture methodology. *Transformative Innovation Metrics Workshop, October 5-7.* **(Chapter 3)**

Berjawi, A.E.H., Walker, S.L., Patsios, C. & Hosseini, S.H.R., (2019). An evaluation framework for whole energy systems scenarios. In *Innovative Solutions for Energy Transitions, 11 International Conference on Applied Energy, August 12-15*. Available at: http://www.energy-proceedings.org/wp-content/uploads/2020/03/1190_Paper_0704103057.pdf

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Figures and Tables

Abbreviations and Acronyms

ACRE	Approach to Context-based Requirements Engineering
ASHP	Air-Sourced Heat Pump
CESI	National Centre for Energy Systems Integration
CHP	Combined Heat and Power
CS	Constituent System
DER	Distributed Energy Resources
DHN	District Heating Network
DSR	Demand-Side Response
ESI	Energy Systems Integration
EV	Electric Vehicle
GHG	Greenhouse Gas
GSHP	Ground-Sourced Heat Pump
HP	Heat Pump
ICT	Information Communication Technology
LULUCF	Land use, Land use change and forestry
MBSE	Model-Based Systems Engineering
MCA	Multi-Criteria Analysis
MLP	Multi-Level Perspective
moe	Measures of Effectiveness
MSP	Multi-System Perspective
NoT	North of Tyne
P2G	Power-to-Gas
P2X	Power-to-X
RES	Renewable Energy Sources
RSAM	Reference System Architecture Model
SGAM	Smart Grid Architecture Model
SoS	System-of-Systems
SysML	Systems Modelling Language
WES	Whole Energy Systems

Chapter 1 Introduction

This thesis aims to develop a novel methodological framework for evaluating the effectiveness of Energy Systems Integration (ESI) as a pathway for the energy transition. The framework addresses the need for a Whole Energy Systems (WES) approach for evaluation to embrace the complexity of future integrated energy systems and highlight the resulting interactions. Those systems could be increasingly employed in the future with the need for additional flexibility to the system, which can be provided by coupling the electricity, gas, heat and transport systems and exploiting synergies between them.

In this chapter the context for the topic this thesis aims to address is set out and the motivation for carrying out this work is outlined. The contributions of this thesis are outlined in the scope of the research gap, questions and objectives. The research strategy is accordingly discussed and an overview of the key multidisciplinary approaches this research is based on is provided.

The first section of this chapter provides the general context around the energy transition in the UK and the net-zero ambitions. Section 1.2 discusses the concept of ESI, its potential as a future pathway for the energy transition and its enabling technologies, in addition to an overview of previous work to realise the main literature gap. In Section 1.3, the research questions and objectives are presented. Section 1.4 discusses the research strategy and defines the key research areas involved in this project, namely the whole systems thinking, sustainability assessments, and sustainability transitions. Finally, Section 1.5 outlines the structure for the rest of the thesis.

1.1. Context

The UK, among other developed countries, has been planning for an energy transition in order to abide by its national and global commitments to deliver decarbonisation targets, while maintaining a secure and reliable energy supply and providing an acceptable and affordable energy (DECC, 2011), to address what is known as the energy policy trilemma. The UK has pledged to reduce its Greenhouse Gas (GHG) emissions by 100% below 1990 level by 2050, known as the net-zero target, under the Climate Change Act amendment in 2019. Delivering those targets is expected to have a significant impact on the current system architecture manifested by a shift in the planning and operations paradigms, the market structure and the regulatory framework (Singh et al., 2019).

While advancements have been achieved in terms of reducing carbon emissions from the electricity sector in past years, the transport and heating sectors are yet to see major reductions.

Figure 1.1 shows the GHG emissions trend by sector between 1990 and 2018 in the UK and Figure 1.2 shows the percentage of emissions from each sector (CCC, 2020).

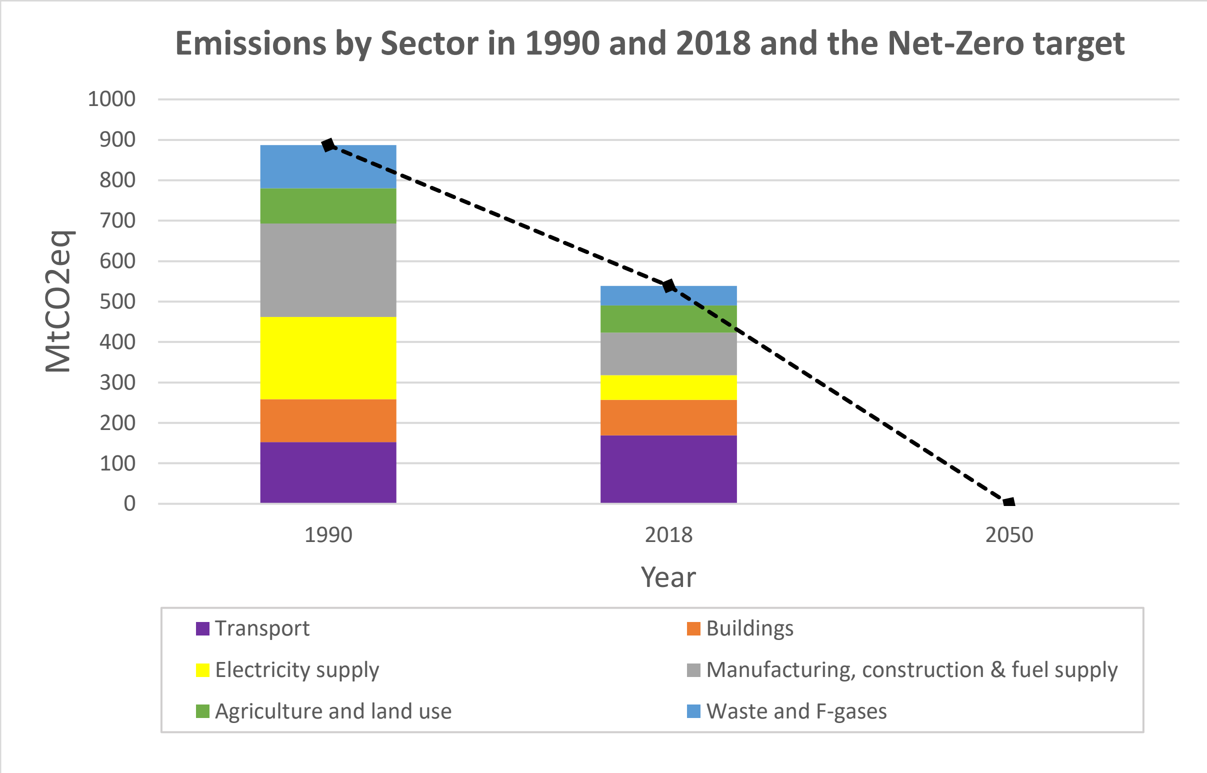


Figure 1.1 GHG emissions by sector in 1990 and 2018
Redrawn from (CCC, 2020)

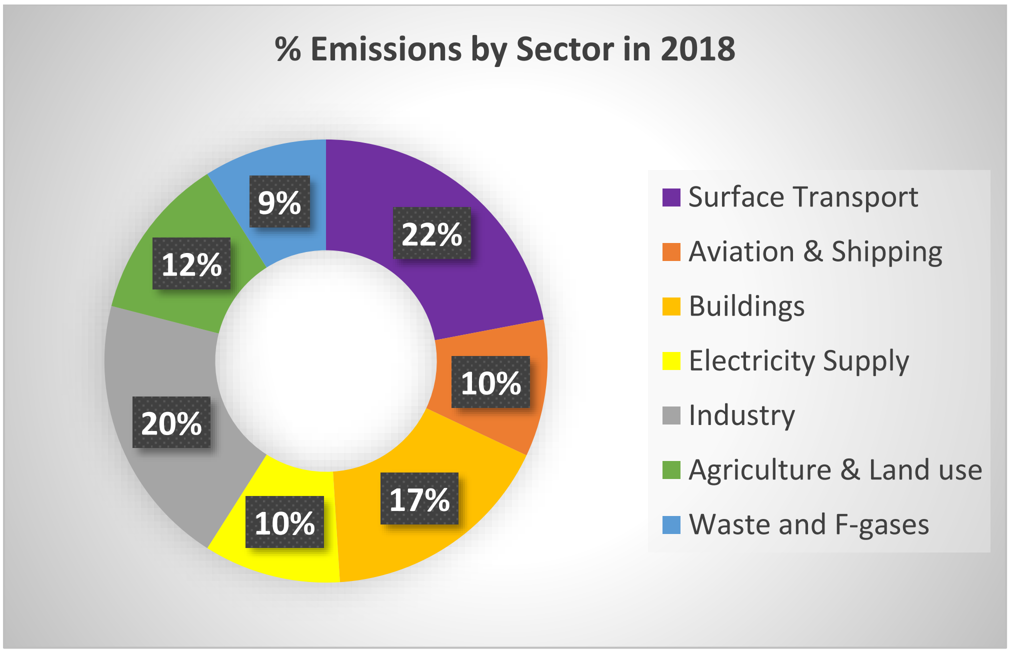


Figure 1.2 Emissions breakdown by sector in 2018

While the electricity and industry sectors have encountered significant reductions from the 1990 levels, it can be seen from Figure 1.1 that the level of emissions from transport and buildings are still largely unchanged. Note that the emissions from buildings are mainly attributed to space and water heating in residential and commercial settings, in addition to cooking. Figure 1.2 shows that surface transport is the largest single contributor in 2018 to the UK total GHG emissions with 22%, followed by industry with 20% and buildings with 17%. This poses a challenge for decarbonising the heat and transport sectors, being classified as hard-to-abate sectors. One possible solution is the electrification of heat and transport through Heat Pumps (HPs) and Electric Vehicles (EVs) technologies, respectively, supplied by low-carbon electricity. Another solution is the use of different energy vectors, such as hydrogen or district heating enabled by Power-to-X (P2X) and Combined Heat and Power (CHP) technologies, respectively (BEIS, 2018).

Moreover, the increasing shares of Renewable Energy Sources (RES) used to generate electricity and Distributed Energy Resources (DER) giving more control to consumers, mean that there is a need for more flexibility to manage uncertainties and maintain the balance between the energy supply and demand across time and space (Energy Systems Catapult, 2019). The future energy system therefore needs new and extended functionalities, to flexibly and cost-effectively manage uncertainties and to address the need for coordination across the energy systems, namely electricity, gas, heat and transport (IET, 2016b). In this context, one possible technical pathway proposed to drive the energy transition flexibly and cost-effectively is Energy Systems Integration (ESI), also known as sector coupling, of electricity, gas, heat and transport.

1.2. Energy Systems Integration

ESI aims to capture and exploit interactions and diversity across multiple energy vectors, by connecting energy systems physically and virtually across infrastructures and markets. ESI is perceived as a potential solution as it provides the required system flexibility by diversifying input and output energy streams, and allowing peak in demand or production to be shifted from one system to another by conversion between vectors (O'Malley et al., 2016; Hanna et al., 2018; Jamasb and Llorca, 2019). ESI is thus enabled by technologies that allow for energy vector conversion across multiple energy systems and at different levels. These technologies include CHP, P2X, HPs and EVs (Guelpa et al., 2019).

In the context of ESI, flexibility is defined as the ability of the integrated energy system to adjust generation or consumption in response to changes, such as fluctuations in RES or deviations in voltage and frequency in the electricity system and pressure in the gas system, without violating operational conditions or technical limits of the integrated energy networks (Hosseini et al., 2020). Flexibility can be considered to address short-term stability challenges and long term seasonal fluctuations (Witkowski et al., 2020). Other forms of flexibility provision include curtailment or variation in energy supply, interconnectors, energy storage technologies in different forms, and Demand-Side Response (DSR) techniques (Lund et al., 2015).

ESI has developed as an overarching concept that may encompass other modern concepts such as smart grids and smart cities, but goes beyond the limited spatial scale provided by those concepts (O'Malley et al., 2016). Integration can take place at various scales, linking different energy sources, technologies and services, from a building level to the community, regional, national and international levels (Hanna et al., 2018). Therefore, ESI may be defined differently depending on the level, scale and scope of integration. For instance, two distinctions can be made here. First, the scope of integration that can take place across energy end-use sectors (residential, industrial, transport, etc.) all supplied by electricity, or across energy vectors (electricity, gas, heat, etc.) (Ramsebner et al., 2021). A generic definition of scope can be otherwise provided to involve a range of options including the co-production, combined use, conversion and substitution of different energy supply and demand forms (Ramsebner et al., 2021).

Second, the level of analysis that could range from the technology level, such as the energy hub concept (Mohammadi et al., 2017; Aljabery et al., 2021), to the system level in which networks and infrastructure are of main interest (Hosseini et al., 2020). In this research, the focus is on the integration between multi-vector energy networks including the electricity, gas and heat networks. Transport is outside the scope of this research but is included in some of the discussions throughout the thesis for its relevance to ESI, as it is expected to have an impact on the future energy system with the increased electrification of transport modes.

Despite some discrepancy in the definition of ESI, it is generally perceived as a holistic consideration of the energy system covering multiple energy vectors and spanning different stages of the energy supply chain (Kriechbaum et al., 2018). Accordingly, the aim of ESI is to exploit synergies horizontally and vertically across the integrated energy system (Cambini et al., 2020). In summary, the concept of ESI originates from a holistic theoretical approach that considers the WES (Jamasb and Llorca, 2019), which is comprised of:

- multiple energy vectors: electricity, gas, heat
- the energy supply chain span from generation to end-use, through infrastructure and markets

- the system environment embracing different stakeholders with multiple perspectives and objectives, including the technical, environmental, economic, political and social aspects

In addition to providing flexibility through energy vector shifting, ESI presents other potential benefits to the WES as summarised in the literature (Kroposki et al., 2012; Abeysekera et al., 2016; Hanna et al., 2018) to include :

- reducing carbon emissions by enabling the integration of RES
- reducing the use of primary energy
- reducing costs by improving overall efficiency through increased resource utilisation and sharing of assets across energy systems
- increasing system security and resilience given the greater flexibility and diversity of energy resources provided
- deferring investments such as for networks expansion
- enabling the effective analysis, design and control of the system interactions and interdependencies along the technical, economic, environmental, political, and social dimensions

However, challenges facing the implementation of ESI involve spanning multiple energy vectors, crossing siloed institutional and market structures of different energy sectors, the significant technical complexity, sharing of data among several stakeholders, the development of new modelling and simulation tools, and the multidisciplinary expertise needed for research and development (IET, 2016b; Abeysekera et al., 2016; Hanna et al., 2018).

1.2.1. Enabling Technologies

ESI is enabled by technologies that allow for energy vector conversion across multiple energy systems and at different levels. These technologies include CHP, P2X, HPs, and EVs (Guelpa et al., 2019). Moreover, energy storage in different forms enables long-term storage, for instance by transforming electricity into thermal or chemical energy, with the latter allowing long-distance transportation (Guelpa et al., 2019). Figure 1.3 shows possible lines of integration across the different energy systems linked through various enabling technologies, also known as coupling components.

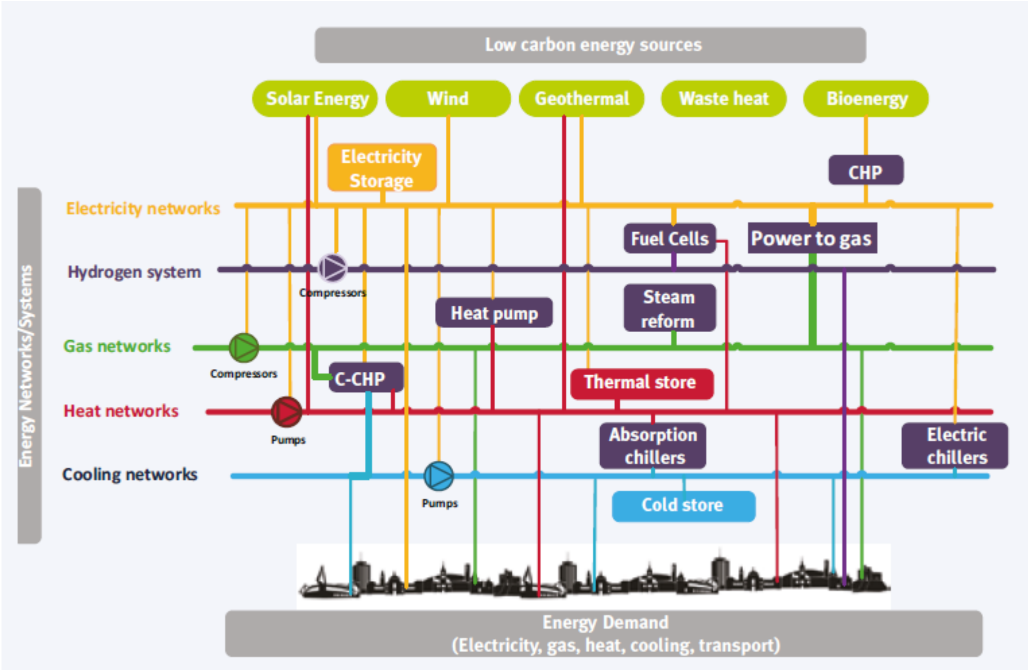


Figure 1.3 Possible areas of integration between different energy systems
Source: (Abeysekera et al., 2016)

ESI can support the decarbonisation of heat and transport, through (i) direct electrification of heat and transport (via HPs and EVs) accompanied by integration of RES; or (ii) the emergence of new energy carrier systems such as district heating and hydrogen (using CHP and P2X). The second approach involving cross-vector integration would reduce or delay the costs for electricity networks reinforcement required for electrification (Erbach, 2019).

CHP systems generate electricity and heat and can be connected to the electricity grid at different levels and to district heating networks at different scales. CHP systems can provide a number of flexibility services to the electricity system by increasing or decreasing electricity generation while maintaining the level of heat generation (Wang et al., 2019). Another advantage of CHP is in its higher overall energy efficiency compared to the separate production of electricity and heat (Raven and Verbong, 2007). The use of CHP could also provide savings through avoided transmission and distribution system upgrades (Hanna et al., 2018).

P2X systems involve converting electricity, ideally surplus from RES, into hydrogen through electrolysis as a first stage. The hydrogen produced can be then stored for a short or long time (seasonal storage) for later use. In terms of end-use, the produced hydrogen can follow several pathways into different forms of energy (electricity, gas, heat) or to be used for different purposes (mobility, industrial, feedstock). P2X provides flexibility in coupling energy systems whereby more RES can be absorbed and converted into other forms of energy for different end-uses (Mazza et al., 2018). Figure 1.4 describes several P2X pathways of electricity conversion into different end-uses. P2X is used as a generic term where X can refer to any of the different end-uses, one of which is methane gas, thus the term Power-to-Gas (P2G). P2X and P2G are used interchangeably in the scope of this thesis.

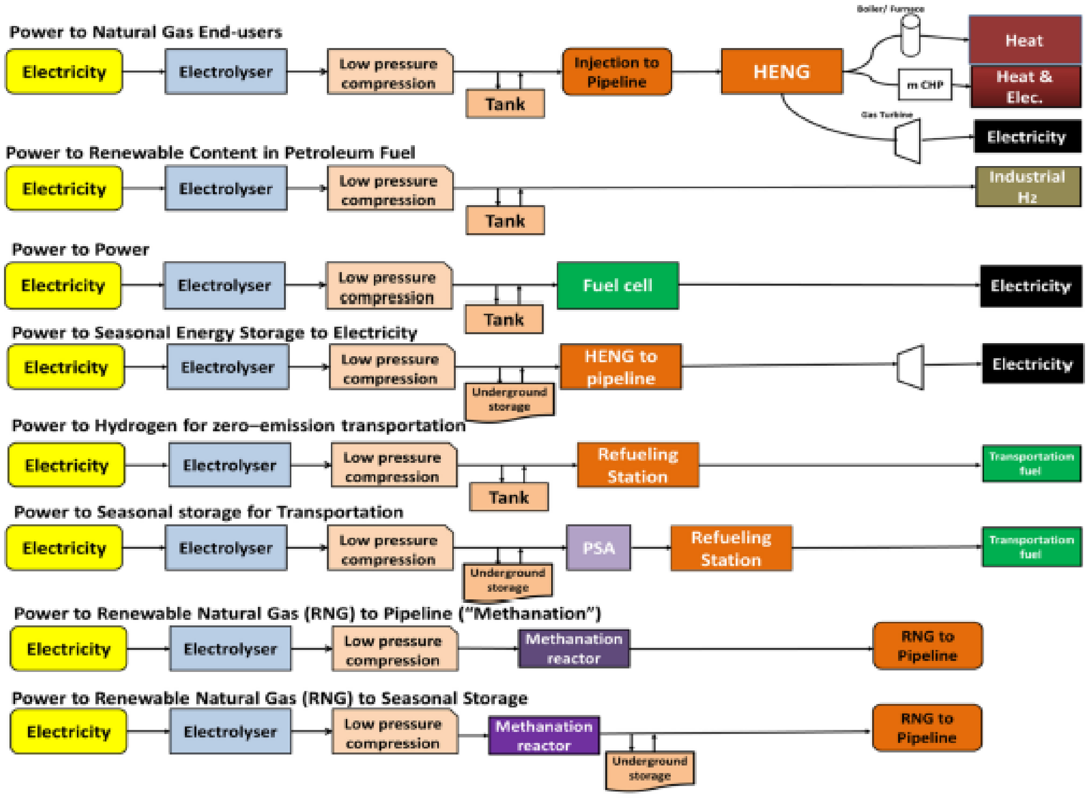


Figure 1.4 Different P2X pathways
Source: (Maroufmashat and Fowler, 2017)

Using hydrogen produced from RES can support the decarbonisation of heat and transport. Similarly, HPs and EVs allow the direct electrification of heat and transport, respectively. These solutions are based on a holistic view that looks at different energy systems simultaneously to provide opportunities for flexibility and more RES integration (Lund et al., 2015). The use of electricity for heating (sometimes referred to as Power-to-Heat) through, for example, the use of HPs also provides flexibility to the energy system by energy vector shifting, allowing for more RES integration (Witkowski et al., 2020). In addition, HPs support the transition to district heating networks and the coupling between the electricity and heat systems (Leitner et al., 2019).

1.2.2. Literature Gap

Previous work has been presented in recent years to explore ESI in terms of the overall concept and potential benefits (Kroposki et al., 2012; Mancarella, 2014; O'Malley et al., 2016; Abeysekera et al., 2016; Hanna et al., 2018; Ramsebner et al., 2021), modelling for planning and operation of integrated energy systems (Kriechbaum et al., 2018; Hosseini et al., 2020;

Heendeniya et al., 2020), enabling technologies (Guelpa et al., 2019), flexibility provision (Lund et al., 2015; Wang et al., 2017; Witkowski et al., 2020), and economics and policy (Jamasb and Llorca, 2019; Cambini et al., 2020). This is a selection of papers that summarise the state of the art in different areas of ESI research.

In terms of evaluation of ESI, previous reviews on ESI have identified gaps around evaluation and suggested research recommendations. Specifically, while ESI provides an opportunity to improve the system performance in terms of the energy trilemma there is still a need for (i) more quantified evidence to validate this claim and support decision making in this direction; (ii) new tools and metrics to identify the full range of benefits of ESI under different situations; and (iii) comprehensive assessment methodologies to capture the interdependencies across energy systems and the emergent complexity of the whole system (Mancarella, 2014; O'Malley et al., 2016; Abeysekera et al., 2016; Hanna et al., 2018). Evaluation has been since considered in some studies yet not in a holistic manner; that is focusing on particular technologies (Leitner et al., 2019; Hosseini, Allahham and Adams, 2021) or looking at a limited scope of indicators (Mancarella et al., 2018; Moslehi and Reddy, 2018). Therefore, the literature still lacks methodologies that address the identified gaps in the evaluation of ESI as a pathway to achieve the energy transition objectives. In this regard, a WES approach for evaluation is needed to evaluate the overall system benefits and drawbacks, identify the interdependencies among the different energy systems, and adapt to future changes.

1.3. Research Questions and Objectives

Based on the identified literature gap regarding evaluation of ESI, this research is carried out with the main objective of developing a methodological framework to evaluate the effectiveness of ESI as a pathway to achieve the energy transition objectives and addressing the following research question:

- **RQ1:** What is the value of Energy Systems Integration for a sustainable energy transition?

The first research question is broken down to understand the issues involved and specify the research gaps. Three research questions are thus posed to tackle the main research objective and address the first research question:

- **RQ2:** What is a Whole Energy Systems approach for evaluation?
- **RQ3:** How does Energy Systems Integration drive the energy sustainability transition?
- **RQ4:** How to identify and analyse future structural and functional interactions across integrated energy systems?

To answer the research questions the following research objectives are set:

- Define principles of the Whole Energy Systems approach for the evaluation of integrated energy systems
- Provide a conceptualisation of Energy Systems Integration from a sustainability transitions perspective
- Develop a methodological framework to address the defined evaluation principles and capture future structural and functional interactions across integrated energy systems
- Demonstrate the applicability and usefulness of the developed evaluation framework

Hence, in this thesis, the WES approach from which the concept of ESI originates is examined and applied to evaluation. The developed WES evaluation[1] principles are used to examine the fitness of existing energy sustainability assessment frameworks for evaluating integrated energy systems. ESI is also conceptualised as a transition pathway using a socio-technical sustainability transitions approach. This understanding of ESI provides the theoretical ground to develop the evaluation framework using concepts and methods from systems engineering in a System-of-Systems (SoS) Architecture Methodology. The SoS architecture methodology allows the future structural and functional interactions across integrated energy systems to be conceptually identified and analysed. This conceptual modelling of the integrated energy system is linked with scenario formulation and quantitative modelling in a methodological framework for quantification and assessment. The evaluation framework is tested, validated, and finally applied to a case study to demonstrate its applicability and usefulness to provide evidence around the effectiveness of ESI in achieving a sustainable energy transition.

1.4. Research Strategy

This research project provides an interdisciplinary analysis of ESI and aims to provide conceptual, methodological, and empirical contributions to the knowledge by addressing the research questions. The research strategy followed in this project involves the use of both inductive and deductive approaches. The inductive approach refers to the use of available data to derive theoretical or conceptual constructs allowing research findings to emerge from frequent, dominant or significant themes in the literature (Thomas, 2006). The inductive approach is used in the first part of this thesis (Chapters 2, 3, 4) to derive principles for the WES approach for evaluation (RQ2), conceptualise ESI as a transition pathway (RQ3), and develop a methodological framework for evaluation of ESI (RQ4), respectively, through an exploration of the literature. On the other hand, the deductive approach refers to the use of a theory to derive

[1] The terms evaluation and assessment are used interchangeably in this thesis

logical conclusions, which need to be verified or confirmed (Thomas, 2006). This can be done in a case study where theoretical propositions are tested for applicability and validated for consistency (Saunders et al., 2009). In this research, the deductive approach is used to test and demonstrate the developed evaluation framework through case studies to eventually address RQ1 (Chapters 5 and 7).

This project is aligned to the vision and objectives of the EPSRC National Centre for Energy Systems Integration (CESI) (CESI, 2017), and has been supported by the resources made available through CESI. The overall vision includes employing a whole systems approach to address the challenges and risks associated with delivering a fully integrated energy system in the future. In addition, a bottom-up approach is considered with analysis based on real-life demonstrators for local energy systems. Those are used as case studies in the scope of this research. The quantitative models used for the analysis in the case studies are also a research product of CESI colleagues. Finally, the developed framework is validated through eliciting feedback from experts who are academics from multiple disciplines involved in ESI research with CESI.

This research draws on theories, concepts, and methods from the areas of whole systems thinking, sustainability assessments and sustainability transitions, with a focus on integrated energy systems. Figure 1.5 highlights the intertwined contributions this research makes in relation to those areas, with the common aim of developing a methodological framework to evaluate the effectiveness of ESI as a pathway for the energy transition.

In the following subsections, an overview of the key areas this research is based on is provided, in addition to the reasoning for the case study approach.

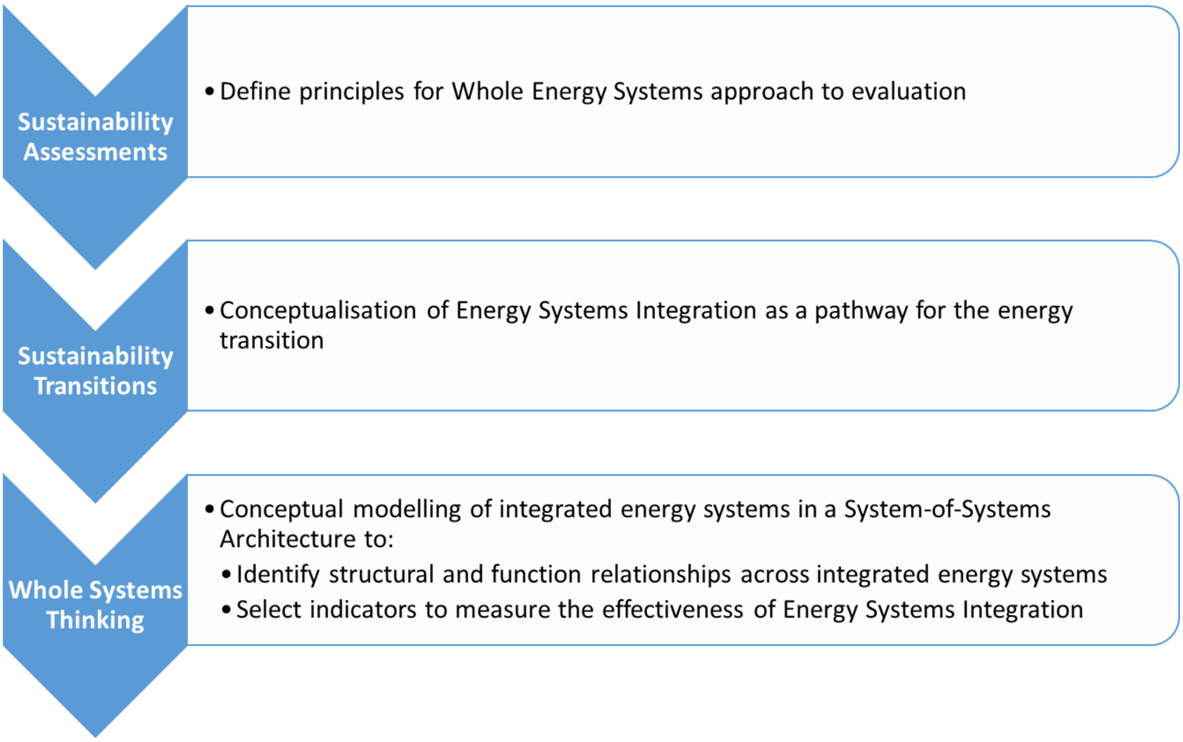


Figure 1.5 Key research contributions and research areas

1.4.1. Whole Systems Thinking

A multidisciplinary approach is required to investigate ESI and to achieve the energy transition to a net-zero carbon society (Abeysekera et al., 2016; Hanna et al., 2018; Guelpa et al., 2019; Jamasb and Llorca, 2019). One approach for multidisciplinary research is based on systems thinking that addresses complexity in systems with multiple and interacting factors (Neely et al., 2021). Systems thinking is a broad set of principles spanning diverse fields of physical and social sciences, engineering and management useful for considering interrelationships between system elements and their effect on the wider system behaviour (Energy Systems Catapult, 2019). A number of tools and techniques use a systems thinking approach to solve complex problems such as those developed in systems engineering, which itself is a discipline that integrates multiple disciplines to enable the realisation of successful systems across its lifecycle (Energy Systems Catapult, 2019). Given the complexity of the energy system, a systems thinking approach is valuable to understand system change and reflect the interactions between its heterogeneous elements (Bale et al., 2015).

Going one step beyond is the notion of whole systems thinking, which extends the systems thinking to look at interrelationships within and between systems due to the increasing prospects of systems integration (Bale et al., 2015). Accordingly, the concept of SoS has emerged to study large scale interdisciplinary problems that span multiple, distributed systems (Energy Systems Catapult, 2019). The concept of whole systems thinking has been recently endorsed by the UK government as a rigorous approach to reveal interdependencies, synergies and trade-offs between policy decisions in all areas that affect the delivery of the net-zero emissions target by drawing on systems engineering principles (UK Government, 2020).

Systems thinking also provides an interdisciplinary approach for the evaluation of systems (Mangoyana et al., 2013). This can be used to inform planning and decision-making whilst ensuring that the evaluation is not focused on a single aspect of the system (Energy Systems Catapult, 2019). In this project, a WES approach for evaluation is considered as it is closely related to the concept of ESI. Such an approach is not clearly defined in the literature, and it is therefore one of the objectives of this research to define principles for a WES approach for evaluation. The principles are derived inductively based on the literature review. Moreover, concepts and methods from systems engineering are used in this research, mainly the SoS and system architecture, to develop a methodological framework for ESI evaluation.

1.4.2. Sustainability Assessments

Sustainability assessment is a complex appraisal method used in different domains to evaluate progress towards sustainable development and support decision making. It is a structured procedure that involves multidisciplinary analytical methods for measurement and evaluation (Sala et al., 2015). It is a form of impact assessment but goes beyond its scope and has a specific imperative to sustainability (Bond et al., 2012). A guiding approach for designing and implementing sustainability assessments known as the BellagioSTAMP outlines high level principles covering the content and process of assessment. Those include (i) having a guiding vision to assess progress towards sustainability; (ii) considering the social, economic and environmental aspects and the interactions between them; (iii) having an adequate temporal and spatial scope; (iv) be based on a conceptual framework that identifies evaluation criteria and relates indicators with targets; (v) and ensuring a transparent, effective, participatory and replicable assessment (Pintér et al., 2012).

Sustainability assessment requires integrated, interdisciplinary frameworks that take a holistic view on the diverse scales, interactions and uncertainties involved (Sala et al., 2015). At the same time, sustainability assessment frameworks need to be generic and transparent to adapt to different contextual and methodological challenges (Grunwald and Rösch, 2011; Büyüközkan and Karabulut, 2018). Most sustainability assessment frameworks are based on indicators, which are recognised as a useful tool for conveying information, highlighting trends and supporting decision making (Singh et al., 2012). Therefore, selecting indicators is a core part of the assessment where a number of considerations are needed including making indicators relevant for purpose, validating the indicators in context, and ensuring a balance between complexity and simplicity for measurement, handling and communication of indicators (Mace and Baillie, 2007).

A systems-based approach that considers a holistic view on the complex and interacting systems affecting sustainability has been called for to derive comprehensive indicator sets for assessment. That is, identifying the relationships between systems and their contributions to performance of other components and the overall system, and identifying corresponding indicators that represent those contributions (Bossel, 2002). A set of indicators as such can provide a reduced view of the complex system as a whole including interrelations among various dimensions (Rovere et al., 2010). One approach for sustainability assessment that uses multiple indicators is Multi-Criteria Analysis (MCA) that integrates the multiple considerations of sustainability while managing trade-offs (Bond et al., 2012). The main advantage of MCA is the diversity of criteria, which are related to defined objectives and represent perspectives of different stakeholders (Mainali and Silveira, 2015). In this context, it is important to include multidimensional evaluation criteria beyond only the techno-economic to reflect the different needs of local actors that might have conflicting objectives (Bush and Bale, 2019).

However, sustainability issues are considered wicked problems defined by a complex of interconnected factors in a pluralistic context. This poses a challenge for the methodological organisation of sustainability assessment frameworks and the knowledge required to conduct them. Thus, there is a need for problem structuring to proceed sustainability assessments (Dijk et al., 2017). Several problem structuring methods have been used in conjunction with MCA including systems thinking approaches (Marttunen et al., 2017). Such an approach supports incorporating complexity into the evaluation by describing the context, identifying stakeholders, highlighting interrelationships, and bringing a holistic whole systems perspective (Marttunen et al., 2017). It also supports a bottom-up participatory approach to develop indicators (Reed et al., 2006).

In the context of energy, sustainability assessments consider multidimensional concepts such as the triple bottom line (Mainali and Silveira, 2015), the energy trilemma (WEC, 2019), energy security (Sovacool and Mukherjee, 2011) and energy sustainability (Santoyo-Castelazo and Azapagic, 2014). Moreover, sustainability goals can be translated into engineering practice for the energy systems throughout its lifecycle (design, assessment, operation, planning) and supply chain (generation, networks, consumption) (Moslehi and Reddy, 2019).

The evaluation in this thesis is carried out using a methodological framework developed in this research, which entails an indicator-based sustainability assessment, particularly a MCA approach supported by a whole systems thinking approach for problem structuring. In addition to the general guidelines for sustainability assessment outlined in this section, the framework shall exhibit the WES principles to evaluate the effectiveness of ESI as a pathway for the energy transition.

It is worth noting here the distinction in the terminology used in the systems engineering literature between performance and effectiveness. In this scope, performance describes what the system does, while effectiveness describes what a system does in a relevant context or scenario. Thus, the term measures of effectiveness (moe) is used for metrics or indicators that assess changes in system behaviour or capability, and measures the attainment of an end state or achievement of an objective. Evaluating effectiveness is considered appropriate for SoS level analysis (Jamshidi, 2017).

1.4.3. Sustainability Transitions

Sustainability transitions have been a focus area of research in innovation studies. In particular, there is an interest in understanding the dynamics of transitions for socio-technical systems towards sustainability. Those are typically large systems made up of artefacts (technology, infrastructure), institutions (rules, knowledge) and networks of actors, interacting to provide services for the society (Markard et al., 2012). This applies to the energy transition that involves a co-evolution of the physical infrastructure, consumers, business models and governance frameworks (Eyre et al., 2018). The energy transition can have different trajectories where it can be driven by structural change (fundamental changes to global markets and infrastructures and radical shifts in production and consumption) or systemic change (incremental change targeted at interdependencies of technologies and relationships in complex systems) (Scoones et al., 2020). Therefore, a socio-technical understanding in addition to a whole systems approach can offer valuable insights into the potential and challenges for the energy transition (Eyre et al., 2018).

Evaluating transitions requires setting normative objectives to be met in addition to understanding the depth and scope of the system changes involved (Turnheim et al., 2015). In this context, an overarching concept from the sustainability transitions research that allows better understanding of the transition processes and the opportunities for intervention is the concept of transition pathways. It is defined as unfolding socio-technical patterns of change in systems leading to new ways of achieving societal functions (Turnheim et al., 2015). A typology of pathways for transitions is developed to explain several mechanisms of systemic change due to different types and timings of interactions. Those include transformation, technological substitution, de-alignment and re-alignment, and reconfiguration (Geels and Schot, 2007). Conceptualising transition pathways can support mapping possible futures, planning interventions, learning about change processes, bridging diverse perspectives, and communicating about potential choices and trade-offs (Rosenbloom, 2017).

Recent efforts are shifting the focus in this research area from historical analysis of transitions to realise patterns of change, towards bridging socio-technical perspectives with quantitative modelling to inform future transition pathways (Rosenbloom, 2017). Bridging is required between the different approaches needed to study the transitions due to its co-evolutionary nature. For instance, these include the techno-economic (focus on energy flows and conversion processes, coordinated through energy markets), socio-technical (focus on technological change, driven by knowledge, practice and networks associated with energy technologies), and political (focus on change in policies which affect energy systems towards transition) (Cherp et al., 2018). Therefore, modelling is becoming part of the toolkit used for studying energy transitions and bridging perspectives. A model can have different connotations in different disciplines, but it is generally a simplified and formalised representation of reality. It can be formulated in different ways including, for example, conceptually, mathematically, graphically or as a computer code (Holtz et al., 2015).

In this research, ESI is first conceptualised as a transition pathway based on the sustainability transitions perspective. A conceptualisation of ESI as such has not been presented previously in the literature. The conceptualisation is carried out inductively by comparing relevant concepts from the sustainability transitions literature, such as the pathways typology, with the features of ESI. Although the conceptualisation is based on the socio-technical understanding of the energy system, the focus of this research is on the physical system architecture including technologies and infrastructure. This means that the technical couplings created by ESI are considered the trigger for the co-evolutionary changes at the social level. Moreover, in the scope of this research, the temporal dynamics of change through ESI as a transition pathway are not considered. The conceptualisation of ESI is followed by the evaluation of ESI through the developed methodological framework, which incorporates conceptual system modelling, quantitative system modelling and scenario formulation. The evaluation is demonstrated using a case study approach.

1.4.4. Case Study Approach

A case study approach is taken for the testing and application of the developed framework, as opposed to the use of generic or standard energy network models. A case study is a research strategy that allows a deep level of investigation into a given phenomenon within its real life context (Saunders et al., 2009). A case study can be valuable for testing the applicability of a theoretical proposition and illustrating a conceptual contribution (Siggelkow, 2007; Saunders et al., 2009). In addition to context, complexity can be incorporated through a case study approach that considers multiple variables (Bolton and Hannon, 2016). The choice to use this approach in this research is based on two factors. First, the importance of contextual factors surrounding the energy system especially at a local level (Basu et al., 2019) and, as will be explained later in this thesis, the developed framework is context-based. Second, the demonstration resources available and the bottom-up approach outlined by CESI guided this research in this direction.

The case studies presented in this thesis are based on local and regional energy systems. This is based on the trend of decentralisation and localisation of energy systems. This assumption has not been investigated closely in this research, but there are growing evidence on the value of local energy systems (Ford et al., 2021). This doesn't mean that local or regional energy systems are considered in isolation. On the contrary, to reach the net-zero targets the interaction with the national energy system has to be maintained for technical support and large scale decarbonisation (Arabzadeh et al., 2020). This is also the case given the socio-economic implications and the socio-political decision-making processes on energy and climate issues at the national level. This research is focused on the energy system in the UK context, but the developed framework is flexible to be applied in different contexts.

Both the case study approach and the use of generic models are common in the research areas of the literature studies considered in this research. For instance, in the scope of energy sustainability assessments, most studies reviewed in Chapter 2 are based on real-life applications (60%) most of which are on a national level, while some others are either applied to generic energy systems (20%) or have not been applied (20%). Most studies in the sustainability transitions literature, such as those presented in Chapter 3, are based on case studies given the focus of this area on historical analyses (Papachristos, 2014; Zolfagharian et al., 2019). On the other hand, most of the studies around multi-vector energy networks modelling reviewed in (Hosseini et al., 2020) use standard or generic network models of integrated systems (70%) and some use real case study networks (30%). While there is no standard integrated multi-vector network model, studies tend to use ad hoc network models through coupling separate standard electricity and standard gas network models or coupling real case networks (Marcos et al., 2017).

1.5. Thesis Outline

The thesis consists of eight chapters. In addition to the introduction, the rest of the thesis is structured as follows.

Chapter 2 – Energy Sustainability Assessments

Chapter 2 addresses the second research question (RQ2) by defining the principles for the sustainability assessment of integrated energy systems based on the WES approach. This chapter starts by discussing the drivers of change of the energy transition and the need for flexibility. ESI is proposed as a potential pathway to deliver the additional flexibility required. Accordingly, the impacts that ESI would have on the energy system architecture are identified. The WES approach for evaluation is then defined through a set of principles that energy sustainability assessment frameworks should exhibit for ESI evaluation. The principles are used to qualitatively appraise existing frameworks to conclude with gaps in the evaluation of integrated energy systems. A version of this chapter has been published in the peer-reviewed journal *Renewable and Sustainable Energy Reviews* along with Chapter 4 (Berjawi, Walker, et al., 2021).

Chapter 3 – Energy Sustainability Transitions

Chapter 3 addresses the third research question (RQ3) by providing a conceptualisation of ESI from a socio-technical sustainability transitions perspective. This chapter starts with an overview of the key theories from the sustainability transitions research area before focusing on the relevant concepts to the scope of ESI. In particular, concepts related to multi-system interactions and whole systems reconfiguration are compared with ESI features to conceptualise ESI as a transition pathway for the energy transition. In line with this, it is proposed that integrated energy systems are conceptualised as a SoS. This paves the way for developing a methodological framework based on systems engineering concepts and methods, which operationalises the proposed conceptualisation and provides methodological contributions to the sustainability transitions research.

Chapter 4 – Developed Methodological Framework

Chapter 4 addresses the fourth research question (RQ4) and provides the means to address the first research question (RQ1) by developing a methodological framework for the evaluation of ESI. The framework is described in terms of its design and implementation. The framework is based on the SoS architecture methodology that addresses the WES principles identified in Chapter 2 and operationalises the SoS approach proposed in Chapter 3. The SoS architecture methodology combines concepts and methods from systems engineering for the development of a conceptual system model that describes the integrated energy system context, stakeholders, structural and functional relationships, requirements and measures of effectiveness. The conceptual model is coupled with scenario formulation and quantitative system modelling for quantification and evaluation of alternative system configurations. The dashboard approach used to graphically represent the results of the evaluation is discussed. Applying the developed evaluation framework should then provide an answer to the first research question. A version of this chapter has been published in the peer-reviewed journal *Renewable and Sustainable Energy Reviews* along with Chapter 2 (Berjawi, Walker, et al., 2021).

Chapter 5 – Framework Testing and Validation

In Chapter 5, the developed framework is tested through two case studies on the local energy system in Findhorn village, Scotland, with different heating technologies and different energy storage technologies, respectively. Challenges to the framework implementation are identified. Moreover, preliminary findings from the test case studies are presented to academic experts in energy research from multiple disciplines in an online group interview to elicit their feedback for validation and improvement of the framework. Accordingly, improvements have been implemented to the framework and later applied to the case study in Chapter 7.

Chapter 6 – Reference System Architecture Model

Chapter 6 builds on the proposed methodology and the learnings of Chapter 5 to present a Reference System Architecture Model (RSAM) that describes a comprehensive configuration of the integrated energy system including the electricity, gas and heat systems, coupled by a range of ESI technologies. The RSAM supplements the developed framework whereby it is used as a standard conceptual system model for the first stage of the framework implementation. The RSAM can be used as a flexible, modular approach whereby relevant elements are added or omitted for different applications. It can also support further architectural analysis in addition to supporting the WES analysis and evaluation.

Chapter 7 – Case Study: North of Tyne Region

Chapter **7** finally implements the improvements to the framework based on the testing and validation with a full case study application to demonstrate the applicability and usefulness of the developed framework. This chapter addresses the first research question (RQ1) by providing evidence on the effectiveness of ESI adopted at the regional level to achieve the energy transition objectives. The case study is based on the local energy system of the North of Tyne region in England and involves comparing different integrated system configurations (combinations of networks and technologies), under different conditions of supply and demand. The usefulness and limitations of the framework are discussed in this chapter in the scope of the case study, in addition to the empirical findings. A version of this chapter has been accepted for publication as a book chapter (Berjawi, Allahham, et al., 2021)**.**

Chapter 8 – Conclusion

Chapter 8 concludes with a summary of the research findings and contributions, a discussion of the limitations of this research, and suggestions for future work.

Chapter 2 Energy Sustainability Assessments

This chapter reviews the literature around multi-criteria sustainability assessments of energy systems and aims to identify the gaps with existing assessment frameworks in the scope of future integrated energy systems. The frameworks are critically reviewed against a set of principles developed in this research to reflect a Whole Energy Systems (WES) approach for evaluation.

The chapter starts by an investigation of the energy transition drivers and the need for flexibility (Section 2.1). This is followed by a consideration of the wider system implications of Energy Systems Integration (ESI) leading to a new energy system architecture (Section 2.2). The underpinning WES approach for ESI is examined and is translated into principles for the evaluation of integrated energy systems (Section 2.3). Existing literature around energy sustainability assessment frameworks is then reviewed and frameworks are appraised against the identified principles for WES evaluation. Accordingly, the chapter closes with the research gap related to WES evaluation, which is addressed in this thesis (Section 2.4).

2.1. Drivers of Change

The energy system is constrained by a policy requirement to achieve the energy trilemma objectives in terms of environmental sustainability, social and economic acceptability, and technical energy security. In this sense, the energy trilemma itself is considered the main driver for the energy transition since the current energy system arrangements are considered insufficient to achieve it (Ruth and Kroposki, 2014). A shift from conventional technological and market paradigms, regulatory frameworks, consumption patterns and social practices is therefore likely to be able to fulfil the trilemma objectives (Singh et al., 2019). Those changes create uncertainties related mainly to the mismatch between the energy supply and demand, which require additional flexibility to the energy system to maintain the balance (Lund et al., 2015). As discussed in Chapter 1, looking beyond traditional paradigms of separate energy systems planning and operation and due to the increased need to coordinate between multiple energy vectors, ESI is a possible solution to provide the required flexibility by diversifying input and output energy streams and shifting between vectors (Hanna et al., 2018).

This transition in the energy system is driven by technological and market changes attributed to three D's: Decarbonisation, Decentralisation and Digitalisation (IET, 2016a). These changes can be across the energy system. On the supply side, change is driven by the increased use of Renewable Energy Sources (RES) for decarbonisation, both large and small scale, and decentralisation of energy generation and storage technologies. On the demand side, change is driven by electrification of transport and heat to drive decarbonisation through greater deployment of Electric Vehicles (EVs) and Heat Pumps (HPs). Furthermore, digitalisation of the system is governing the interaction of smart appliances, smart meters and demand-side response (DSR) with varying tariffs. These drivers have an impact on the current energy system structure and dynamics (Farid et al., 2016). Moreover, new market opportunities are emerging for established and new actors to provide a range of aggregated energy services as a result of these drivers (IET, 2016b).

Decarbonisation, using RES, creates a technical challenge related to their supply intermittency and the effect on the balance between supply and demand over time and space, for the electricity system in particular (Hanna et al., 2018). Decarbonisation can also have a significant impact beyond the electricity system, with the rise of new energy carrier systems such as district heating and hydrogen, and a greater interconnectedness between energy vectors due to the electrification of transport and heat (Abeysekera et al., 2016; Energy Systems Catapult, 2017). Electrifying transport and heat is considered vital for their decarbonisation but presents new and unfamiliar challenges to the energy system. For instance, electrified transport would lead to an increase in electric demand and investment for charging infrastructure, while it could provide flexibility for better integration of RES if vehicle-to-grid technologies are adopted (Lund et al., 2015).

Decentralisation of energy generation is facilitated by RES since it can be implemented at smaller scales and at or closer to the point of consumption. This allows energy consumers to also be producers, i.e. prosumers, giving them more control over their energy use based on real-time network conditions and dynamic energy prices (Farid et al., 2016). Consequently, supply-side and demand-side decisions will be variably interdependent, creating additional uncertainty over the mismatch between energy supply and demand (Mittal et al., 2015; Energy Systems Catapult, 2017). The heat system can encounter a similar shift from hierarchical large scale towards distributed infrastructures (Guelpa et al., 2019).

Digitalisation of the energy system supports the energy transition by enabling smart operation and control strategies of multiple energy systems, supported by advanced data collection and analysis capabilities (Ruth and Kroposki, 2014; Guelpa et al., 2019). This improves the reliability on the supply side by better predicting, responding and adapting to the intermittency of RES. On the network level, digitalisation enables automated control and response with smart meters and flexibility options, while allowing more active participation of end-users on the demand side (Hanna et al., 2018).

The uncertainties the energy transition is expected to bring, mainly over the balance between energy supply and demand, can be managed through additional flexibility (Kondziella and Bruckner, 2016). Flexibility is an important mechanism for protection against uncertainties in the structure and functioning of the future energy system particularly with unpredictable supply and demand patterns (Hanna et al., 2018). Additionally, there is a need arising from the electrification of transport and heat to coordinate the increasingly interconnected energy vectors. Changes to the energy system are therefore expected to involve increasing complexity and interconnectedness between its components. Thus, a holistic view of the WES considering the interactions and interdependencies within is needed in planning, operation and evaluation of future integrated energy systems. This makes ESI a possible solution, beyond the traditional paradigms, to provide the required flexibility to drive the decarbonisation transition cost-effectively.

2.2. Impacts of Energy Systems Integration

Adopting ESI as a pathway for the energy transition will impact the structure and function of the energy system. First, ESI creates new interactions and interdependencies between the different energy systems, making it more complex to manage the WES. New interactions could be related to physical, commercial or informational flows between different components across energy systems. Second, integrating different energy systems brings together multiple actors with different objectives and motivations. This leads to a change in the market structure with the emergence of new actors and new business models, in addition to new policy and governance frameworks.

Traditionally, energy systems and associated networks are designed and operated separately with limited interactions between them. However, ESI enables approaches that expand the system boundaries beyond one sector. Thus, energy systems are expected to be more interconnected through ESI. This creates new interactions and further interdependencies between the different energy systems. Interactions include, for example, having a shortfall in energy available in one network being met by energy carried by another one, or one network providing its surplus energy to another to help with constraints across networks (Olczak and Piebalgs, 2018). This consequently brings new perspectives to energy systems analysis to find innovative solutions to the different constraints (Mancarella, 2014).

Due to the greater interconnection and new interactions between energy systems, ESI would make the management and operation of the whole system more complex. Greater interconnection means that solutions in one system can have implications on the others. For instance, electrification in the transport sector through deployment of EVs would lead to an increase in electricity demand, which may compete for supply under a constrained system (KPMG, 2017). Moreover, interactions lead to emergent behaviour that could be harmful or beneficial for the energy system, and can affect the reliability performance of integrated energy systems (Lei et al., 2018). For instance, interdependencies between energy systems make the whole system vulnerable to disruptions occurring in one system. This can create new failure models such as cascading failure, where an infrastructure system is impacted by the failure in an interdependent system (Erdener et al., 2014). On the other hand, the emergent flexibility provided by shifting energy vectors across networks, facilitated by ESI technologies, improves the resilience of the system. For example, at times of high wind energy output and constraints on the electricity system, wind energy can be converted to gas rather than being curtailed, and injected into a gas network (Blanco and Faaij, 2018). Thus, new planning and operational paradigms need to be designed to manage and control the energy system accounting for such emerging interactions.

On the market level, new opportunities would develop upon ESI for partnerships between separate energy businesses, each of whom has an independent market structure and regulatory framework (Abeysekera et al., 2016). This would bring together actors and stakeholders from different energy systems that did not necessarily need to communicate with each other previously. ESI provides an opportunity for more collaboration among stakeholders in planning and decision making to have a cohesive energy strategy to deliver the energy policy trilemma objectives (KPMG, 2017). Actors in each energy system tend to act in ways that maximise value for their domain, but not necessarily for the WES. If this is to change, actors should coordinate and collaborate while having a common understanding of each other's objectives, incentives and information they have access to (O'Malley et al., 2016). Looking at a future integrated energy system, actors need to acknowledge the relationships between their business models, processes and technologies in practice (Energy Systems Catapult, 2017). Figure 2.1 shows a schematic of the whole energy system moving from (a) separate configuration with independent planning and operation; to (b) an integrated system with interactions and combined actors.

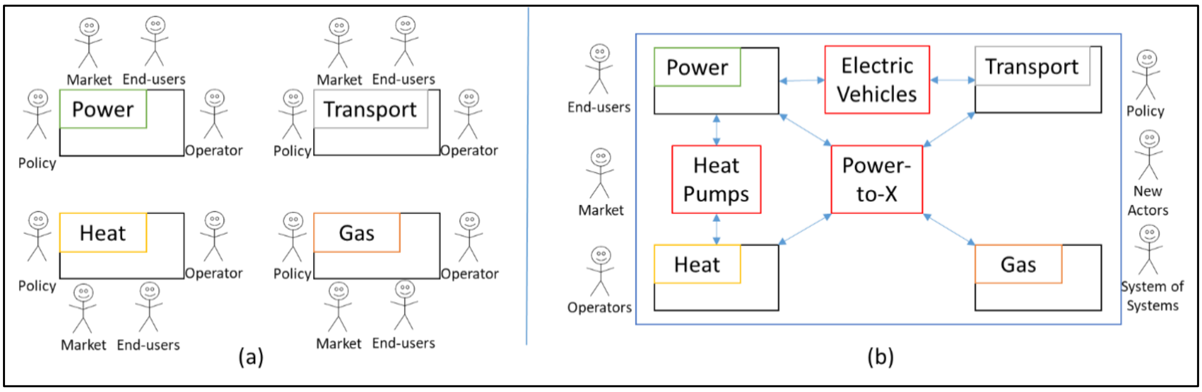


Figure 2.1 Possible configurations for (a) Separate energy systems; (b) Future integrated energy system

Actors in the energy system have divergent views of what the future energy system will look like and what impact this would have on how they manage or operate energy technologies and infrastructure (Winskel et al., 2019). Actors such as generators and storage operators, distribution and transmission network operators, suppliers, intermediaries and service providers can see their roles and relationships to each other and to end-users changed in an integrated energy system (Jamasb and Llorca, 2019). New actors could also emerge upon integrating energy systems. These include aggregators, mobility-as-a-service companies, EV charging infrastructure companies, local energy companies making use of distributed energy resources, cities and municipalities, and new service providers for services such as flexibility and smart homes (IET, 2017e).

Furthermore, ESI can create new markets for emerging services and products. Potentially, this would foster the market competition across various energy sectors, adding value to the end-user and allowing additional revenue stream for energy companies through diversification of their products or services (Abeysekera et al., 2016). For instance, ESI can provide business opportunities moving towards a model of providing energy as a service such as heat, light or mobility, rather than providing a commodity (Jamasb and Llorca, 2019). The heat-as-a-service model can make use of the value propositions provided by ESI through heat electrification, district heating networks, and the use of hydrogen, and in turn drive the decarbonisation of heat (Britton et al., 2021). Similarly, new business models and innovative arrangements can be implemented to draw advantages from ESI. For instance, the integration of the electricity and hydrogen systems through P2X could facilitate collaboration between the electricity and transport sectors to boost the uptake of hydrogen vehicles (Abeysekera et al., 2016). This can make way for new forms of energy services companies, including multi-utility service companies, that may be better suited for the net-zero carbon transition and with the evolution of the energy system (Hannon et al., 2013).

Thus, market and regulatory structures must be redesigned to capture the benefits emerging from ESI. Those structures should be adapted to new planning and operational paradigms, changing network features, incorporated Information and Communication Technologies (ICT) systems, and flexible end-use technologies (O'Malley et al., 2016). A change in market arrangements is also needed in a way to reward new and different types of flexibility services supporting ESI, such as energy vector conversion and storage technologies (Hanna et al., 2018). Moreover, market arrangements should create incentives for new opportunities that could facilitate the emergence of new types of firms (Jamasb and Llorca, 2019).

In summary, to realise ESI and exploit its potential, new technologies and innovations should be adopted to enable the physical integration and interactions between energy systems and components. Moreover, ICT infrastructure and advanced collaborative control techniques are required to maintain interoperability between the different integrated components (Farid et al., 2016). This includes looking at data flows and cyber-physical interfaces. Additionally, appropriate market structures and regulatory frameworks are needed to define actors' roles and relationships and reward and incentivise new forms of flexibility provided by ESI, such as energy vector conversion. This essentially means a new energy system architecture, which defines the principles governing the system structure and functions, the relationships between its components and with its environment, and how it will meet its requirements.

2.3. Evaluation Principles for Whole Energy Systems

The evaluation of integrated energy systems needs to account for the increasing interactions, interdependencies, and emergent behaviour in the WES. This is necessary to have an overall understanding of the mutual influences and the potential benefits and impacts of integration between the different energy systems at all levels (Guelpa et al., 2019). ESI has a variety of potential benefits and impacts, including the technical, economic, environmental, regulatory and social aspects. A thorough evaluation of ESI would help policymakers make informed decisions to support this pathway.

However, there is a gap in comprehensive assessment methods and indicators targeting the performance of integrated energy systems (Mancarella, 2014; Abeysekera et al., 2016; Hanna et al., 2018). While there has been progress since the gap was initially identified in developing specific indicators for integrated systems (Mancarella et al., 2018; Moslehi and Reddy, 2018) or focusing on particular technologies (Leitner et al., 2019; Hosseini, Allahham and Adams, 2021), the gap is still applicable when considering holistic sustainability assessment frameworks for those systems. Such frameworks are required to capture the whole system interactions, quantify interdependencies, and identify the benefits particularly attributed to integration, while considering the trade-offs between the various aspects. The gap is highlighted by a critical literature review of existing evaluation frameworks in Section 2.3.1. Prior to that, a set of evaluation principles is defined below, to which the literature is qualitatively appraised against. Those principles represent a WES approach to the evaluation of integrated energy systems. The evaluation principles are drawn from the definition of the WES approach and from examples in the literature presented in Sections 2.3.2-2.3.7.

In order to evaluate the effectiveness of integrated energy systems towards achieving designated targets, evaluation frameworks should be able to reflect the changes discussed earlier. In particular, the framework should account for the WES approach defined in Chapter 1, to capture the interdependencies involved. In this context, the WES approach is defined by three axes corresponding to the system components and the system environment. The first axis relates to the multiple dimensions of the WES environment representing the technical, economic, environmental, regulatory, and social aspects. The second axis represents the multiple energy vectors of the WES, such as electricity, gas, heat, and potentially transport. The third axis involves a systemic view of the WES supply chain from generation to end-use, through infrastructure, markets and policies. Accordingly, the three principles representing the WES approach that any evaluation for ESI should exhibit are multidimensional, multivectoral and systemic (Figure 2.2). Three supplementary principles, related to the nature of the framework itself, are futuristic, systematic, and applicable. In the rest of the thesis, the six principles are referred to as the WES evaluation principles for convenience.

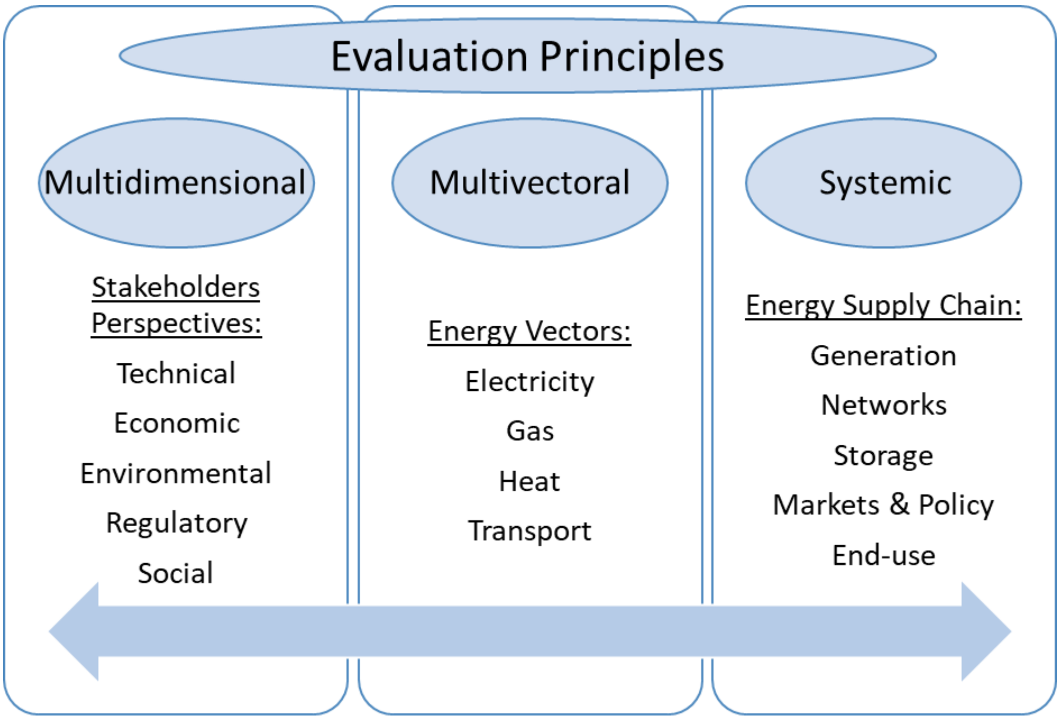


Figure 2.2 Whole energy systems approach for evaluation of future integrated energy systems

These six principles are identified in this research as insightful for a thorough evaluation of future integrated energy systems, where:

- A *multidimensional* framework is necessary to consider the multiple perspectives and objectives of the different stakeholders involved in ESI. This permits one to ask if the energy system is heading towards achieving the various objectives and whether those objectives can be achieved synergistically or require trade-offs.
- The framework should be *multivectoral* to consider the interactions and influences between the coupled energy vectors and the interdependencies across different energy systems.
- A *systemic* framework is needed to span the energy system from generation to end-use, through networks and markets. This is important to capture properties emerging from interactions at the whole system level such as flexibility and resilience.
- The framework should also be *futuristic* in the sense of being able to evaluate major changes to the structure and function of the energy system expected in the future. Such changes would alter the way the system is planned and operated, and consequently the way the system performance is evaluated.
- The framework should be *systematic* in terms of procedures for the derivation and interpretation of evaluation criteria and indicators. This is important for transparency, validity and replicability in different contexts.

- It is important for the framework to be *applicable* to prove its usefulness in supporting decision-making.

The proposed principles are different from the Bellagio STAMP principles for sustainability assessments discussed in Chapter 1 (guiding vision, essential considerations, adequate scope, framework and indicators, transparency, effective communication, broad participation, continuity and capacity). However, the two sets of principles are not to be seen in tension but rather complimentary with some overlaps as well. The WES principles are specific to the case of integrated energy systems, whereas the Bellagio STAMP principles apply broadly to any sustainability assessment. The Bellagio STAMP principles have been also used to appraise energy evaluation frameworks in the context of sustainable development (Gunnarsdottir et al., 2020).

Section 2.3.1 summarises the literature of existing evaluation frameworks based on the identified principles. Sections 2.3.2-2.3.7 explain in more detail each of those principles with relevant examples from the literature.

2.3.1. Existing Evaluation Frameworks Appraisal

The identified principles are used to qualitatively appraise the ability of existing evaluation frameworks to capture the changes and complexity involved in future integrated energy systems, and consequently their adequacy for evaluating the performance of such systems.

Table 2.1 presents a review of a number of existing evaluation frameworks for energy systems against the set of principles required for ESI evaluation. Evaluation frameworks that satisfy at least one of the following WES approach principles (multidimensional, multivectoral, systemic) are included in this review. In fact, a large number of multidimensional evaluation frameworks can be found targeting different energy systems or different parts of the energy system (Martín-Gamboa et al., 2017). Most of them aim to compare energy generation technologies including RES using different methods (Evans et al., 2009; Troldborg et al., 2014). Multidimensional frameworks that present unique methods and relevant insights to the WES approach are included in the analysis and are discussed in the subsequent sections.

This review focuses on the frameworks setup and application based on the identified evaluation principles rather than on the individual indicators adopted. A review of indicators for energy systems evaluation can be found in a number of references (Neves and Leal, 2010; Sovacool and Mukherjee, 2011; Ibáñez-Forés et al., 2014; Narula and Reddy, 2015; Azzuni and Breyer, 2018), and a survey of the indicators used in some of the reviewed frameworks is provided in Appendix A.

Table 2.1 Comparative assessment of existing energy systems evaluation frameworks

Framework	Reference	Multidimensional	Multivectoral	Systemic	Futuristic	Systematic	Applied
Energy Matrix	(Kisel, 2017)	✓	✓	✓	✗	✗	✗
Sustainable Energy Security	(Narula and Reddy, 2016)	✓	✓	✓	✗	✓	✗
Renewable power & heat	(Dombi et al., 2014)	✓	✓	✗	✗	✓	✓
Hybrid Energy Systems	(Afgan and Carvalho, 2008)	✓	✓	✗	✗	✓	✓
Multi-feed Multi-product	(He and Feng, 2012)	✓	✓	✗	✗	✓	✓
Energy transition index	(Singh et al., 2019)	✓	✗	✓	✓	✓	✓
Security Interdependencies	(Osorio et al., 2017)	✓	✗	✓	✗	✓	✓
Decentralised energy	(Karger and Hennings, 2009)	✓	✗	✓	✓	✓	✓
Biofuels systems	(Mangoyana et al., 2013)	✓	✗	✓	✗	✓	✗
Multi-criteria analysis of energy scenarios	(Witt et al., 2020)	✓	✗	✓	✓	✓	✓
EU low-carbon energy security	(Gracceva and Zeniewski, 2014)	✗	✓	✓	✓	✓	✓
UK Energy Security Future	(Watson et al., 2018)	✗	✓	✓	✗	✗	✓
Irish Energy System	(Glynn et al., 2017)	✗	✓	✓	✗	✓	✓
Integrated energy security assessment	(Augutis et al., 2017)	✗	✓	✓	✗	✓	✓

Energy Security under decarbonisation	(Jewell et al., 2014)	✗	✓	✓	✓	✓	✓
Environmental Sustainability	(Hadian and Madani, 2015)	✗	✗	✓	✗	✓	✓
World Energy Council Energy Trilemma Index	(WEC, 2019)	✓	✗	✗	✗	✓	✓
World Economic Forum Energy Architecture Performance Index	(WEF, 2017)	✓	✗	✗	✗	✓	✓
Energy Justice Metric	(Heffron et al., 2015)	✓	✗	✗	✗	✗	✓
Realising Transition Pathways	(Chilvers et al., 2017)	✓	✗	✗	✗	✓	✓
Energy Security	(Sovacool et al., 2011)	✓	✗	✗	✗	✓	✓
UK Energy Security	(Cox, 2016)	✓	✗	✗	✗	✓	✓
Aggregated Energy Security Performance Indicator	(Martchamadol and Kumar, 2013)	✓	✗	✗	✗	✓	✓
Sustainable Energy Development Index	(Iddrisu and Bhattacharyya, 2015)	✓	✗	✗	✗	✓	✓
Sustainability Assessment	(Santoyo-Castelazo and Azapagic, 2014)	✓	✗	✗	✗	✓	✓
Swiss Energy Pathways	(Volkart et al., 2017)	✓	✗	✗	✗	✓	✓

Table 2.1 shows the review of existing evaluation frameworks, and it is clear that no framework from those reviewed addresses all the required principles for effective ESI evaluation. Notably, only a few frameworks consider major changes to the energy system in the future, such as electrification, decentralisation and digitalisation of the system, but not particularly ESI. Most frameworks tend to focus solely on the electricity system, without linking it with other energy systems such as gas, heat or transport, and hence are not multivectoral. Also, within the electricity system the focus is typically on primary energy resources and electricity generation technologies, rather than the whole system span from supply to demand, which limits the extent to which these are systemic. While most frameworks reviewed are applied, only three are not. Accordingly, existing frameworks seem to have gaps and are considered unfit for evaluating future integrated energy systems, lacking one or more of the principles required for the appropriate evaluation of WES. The principles are discussed in further detail below along with their applications, or the lack thereof, in the literature.

2.3.2. Multidimensional

Evaluation should be multidimensional, in terms of the dimensions with which energy systems are evaluated. Dimensions represent the objectives and perspectives of different stakeholders involved. A multidimensional evaluation permits one to ask if the energy system is heading towards achieving the various objectives and whether those objectives can be achieved synergistically or require trade-offs. Table 2.2 summarises the dimensions used in the literature under various multidimensional conceptual frameworks to evaluate energy systems (Sovacool and Mukherjee, 2011; Santoyo-Castelazo and Azapagic, 2014; Kisel, 2017).

Table 2.2 Multidimensional conceptual frameworks for energy system evaluation

Energy Trilemma	Energy Security	Energy Sustainability
Affordability Environmental Sustainability Security of Supply	Availability Accessibility Affordability Acceptability Reliability Environmental Sustainability Efficiency Governance Generation and Grid Adequacy Supply and Demand Flexibility Geopolitics and Terrorism	Environmental Social Economic Institutional Technological Educational Security

Energy system evaluations presented in the literature range from being one-dimensional to multidimensional. Examples of one-dimensional studies include for instance those focusing on security of supply (Jewell et al., 2014; Gracceva and Zeniewski, 2014; Glynn et al., 2017;

Augutis et al., 2017; Watson et al., 2018), or the environmental and social sustainability of energy technologies (Gallego Carrera and Mack, 2010; Hadian and Madani, 2015). On the other hand, multidimensional studies include those adopting the energy trilemma (Heffron et al., 2015; Kisel, 2017; Chilvers et al., 2017; WEF, 2017; WEC, 2019; Singh et al., 2019); in addition to energy security (Sovacool et al., 2011; Martchamadol and Kumar, 2013; Cox, 2016; Osorio et al., 2017) and energy sustainability (Afgan and Carvalho, 2008; Karger and Hennings, 2009; Santoyo-Castelazo and Azapagic, 2014; Dombi et al., 2014) as used in their broad definitions. Those concepts stem from the wider concept of the triple bottom line that emphasises a balanced approach to the economic, environmental, and social aspects for sustainability (Habib et al., 2020). Note here that there are overlaps in the terminology used for the different dimensions and frameworks. It is also worth mentioning that energy sustainability challenges are context-specific and priorities could vary between developed and developing countries (Mainali and Silveira, 2015; Iddrisu and Bhattacharyya, 2015; Shaaban and Scheffran, 2017).

The variety of conceptual frameworks and dimensions used for energy systems evaluation reflects two aspects. First, the variety indicates that evaluation could mean different things in different contexts. Previous research has shown that there exists diverse perspectives forwarded by various experts and stakeholders from different domains in the energy sector, and accordingly different criteria are prioritised for evaluation (Sovacool et al., 2011; Cox, 2016). Secondly, it shows that a multidimensional evaluation is necessary in order to include the different criteria considered important for evaluation regardless of what is prioritised (Narula and Reddy, 2015; Larsen et al., 2017). In comparison, evaluation by single metrics in isolation would provide an incomplete and often misleading assessment (Sovacool et al., 2011; Gracceva and Zeniewski, 2014; Singh et al., 2019).

Thus, a multidimensional framework includes a multitude of perspectives reflecting the diversity of stakeholders. In this context, a participatory approach is needed to accompany the multidimensional principle to ensure an equitable and transparent representation of all relevant stakeholders in the evaluation process. This drives collaboration to understand the implications of different pathways and support decision making (Voinov and Bousquet, 2010). A participatory evaluation framework might be resource intensive to implement, but it provides a robust and democratic procedure that addresses uncertainties, acknowledges multiple perspectives and encourages social learning (Kowalski et al., 2009).

It is not only important to consider multiple dimensions for evaluation, but also to be able to identify trade-offs between them. This allows designing alternative strategies that could maximise synergies and improve all objectives (Sovacool and Mukherjee, 2011; Gracceva and Zeniewski, 2014). In this context, ESI has a role in exploiting those synergies across energy systems, as it provides an opportunity for more collaboration among stakeholders in planning and decision making to have a cohesive energy strategy.

Some of the techniques previously used to highlight the trade-offs are:

- cross impact analysis, scatter plots and influence diagrams of the degree of interrelation between the different dimensions (Osorio et al., 2017)
- a balance score associated with the trilemma index (WEC, 2019)
- a ternary diagram to plot each of the energy trilemma dimensions (Heffron et al., 2015)
- a dashboard of indicators without aggregation (Cox, 2016)
- a radar chart to plot each of the energy sustainability dimensions (Iddrisu and Bhattacharyya, 2015)
- multi-criteria decision analysis techniques (Santoyo-Castelazo and Azapagic, 2014)
- scenario analysis coupled with multi-criteria analysis (Volkart et al., 2017; Witt et al., 2020)

On the other hand, the trilemma dimensions have been assessed separately using life cycle analysis, risk assessment and cost minimisation models (Chilvers et al., 2017) and have been presented in separate matrices (Kisel, 2017) without making any relationship between them.

2.3.3. Multivectoral

Evaluation of ESI should also be multivectoral so that the multiple energy vectors of the WES are considered and the interdependencies involved upon integration are accounted for. As evident from the examples in Section 2.2, coupling energy vectors would create additional interactions and interdependencies between energy systems. Other examples include using hydrogen to power vehicles, with electrolysers offering grid balancing and storage services while increasing the electricity demand and affecting the gas network (KPMG, 2017). Also, through integration, energy systems with low storage capacities could access the benefits of storage available in other systems. Hence, sharing of assets is another way in which ESI can reduce whole system costs (Hanna et al., 2018). A framework that can capture such integration links and their impacts is necessary for the evaluation.

Most of the existing frameworks tend to focus the evaluation around the electricity system, while a few include other systems such as gas, heat and transport (Gracceva and Zeniewski, 2014; Jewell et al., 2014; Dombi et al., 2014; Narula and Reddy, 2016; Kisel, 2017; Glynn et al., 2017; Augutis et al., 2017; Watson et al., 2018). However, those studies do not capture the interactions and interdependencies between the different energy systems as in the case of ESI. They simply expand the boundaries of the evaluation to show indicators specific for each respective system separately. Other studies consider hybrid energy systems with multiple input and output streams of energy (Afgan and Carvalho, 2008; He and Feng, 2012). However, the focus of those studies is on the generation technology level, and thus they do not consider interactions beyond that point, particularly at the network level which is of interest in the scope of ESI.

2.3.4. Systemic

Evaluation of ESI should consider the whole energy supply chain from generation to end-use, through networks, storage, markets and policy. It is important to reflect systemic properties of the WES, particularly features emerging from interactions between the different system components upon integration. For instance, energy security is considered a property of the whole system rather than its individual components (Hoggett, 2014; Narula and Reddy, 2016), and a result of the interactions and interdependencies across the whole system (Gracceva and Zeniewski, 2014; Lund et al., 2015). However, previous studies tend to focus on security from the supply side, particularly in terms of primary energy resource availability and energy generation diversity (Sovacool et al., 2011; Gracceva and Zeniewski, 2014). Similarly, flexibility has a different connotation in a WES context, where it reflects the capacity of energy vector conversion and shifting energy between different systems. Consequently, resilience defined as the adaptive capacity of the energy system would be enhanced by this form of flexibility (Molyneaux et al., 2016).

In the scope of ESI, the whole system would be more than its parts due to the emergence of system characteristics or performance at the WES level, resulting from interactions within the system (Mittal et al., 2015; Chicco et al., 2020). This is highlighted by the requirements of future systems to provide resilience and flexibility due to the uncertainties involved in the energy transition (Hoggett, 2014; Kondziella and Bruckner, 2016). Systemic features such as resilience and flexibility will arise as a result of the interaction of the different components of the integrated energy system (Bale et al., 2015; Hanna et al., 2018). Therefore, evaluation should be able to reflect those features and properties at the whole system level. In this context, a systemic approach to evaluation would support accounting for interdependencies across different components and pathways within the energy system (Gracceva and Zeniewski, 2014; Cox, 2016).

A systemic approach is applied to the evaluation of energy security considering the contribution of different components of the whole system, namely the supply, conversion and distribution, and demand subsystems (Narula and Reddy, 2016). The evaluation presented acknowledges the dynamic complexity of the energy system and its interacting components to realise properties for the system as a whole. However, the framework looks at current national energy systems for developing countries without considering future prospects of structural changes, such as with ESI. On the contrary, some frameworks, although multidimensional, would focus only on a particular component of the energy system, such as power generation (Rovere et al., 2010; Onat and Bayar, 2010), the demand subsystem (Narula et al., 2017), or energy policy (Cosmi et al., 2015).

Furthermore, a systemic approach is adopted for sustainability assessments of different energy systems in considering their own supply chain stages or lifecycle phases. For instance, a systemic approach is proposed for the evaluation of biofuel systems to consider the interactions at different levels of its supply chain (Mangoyana et al., 2013). This approach is chosen to identify properties of the whole biofuel system emerging from interrelationships and feedbacks between the different system components. However, the framework design is only described but is not applied. Similarly, a systemic approach is proposed for the holistic evaluation of waste-to-energy (Chong et al., 2016) and hydrogen (Afgan et al., 2007) systems throughout their lifecycles.

Moreover, frameworks are proposed for energy security with systemic properties defined at different system levels (such as adequacy of generation and grid, and flexibility of supply and demand) (Osorio et al., 2017), and within different time horizons (i.e., stability, flexibility, resilience, adequacy and robustness) (Gracceva and Zeniewski, 2014). On the other hand, a systemic approach is used to evaluate the environmental sustainability of energy supply technologies regarding the impact on the climate, water, land and economy as system environments (Hadian and Madani, 2015). Additionally, the market structure, business environment, policy framework and the society are considered as variables affecting the energy system security (Watson et al., 2018; Singh et al., 2019).

2.3.5. Futuristic

Evaluation of future energy pathways is important to anticipate the impact of different energy policies and technologies on the energy transition and the impact of the transition on the performance of the WES (Martchamadol and Kumar, 2013). Therefore, evaluation frameworks specifically targeting future energy systems should be sufficiently generic to be valid for energy systems totally different from existing ones (Jewell et al., 2014). This is particularly essential for the evaluation of ESI given the magnitude of the expected changes to the energy system architecture discussed in Section 2.2. It is therefore important to understand the impact of the future state of the system and its evolving architecture on the evaluation (Konrad et al., 2008; Turnheim et al., 2015).

Although several evaluations are conducted on future scenarios for the energy system (Santoyo-Castelazo and Azapagic, 2014; Cox, 2016; Chilvers et al., 2017), these have not considered major changes or reconfigurations that would totally transform the system. Future scenarios evaluated in those studies were focused around the different technological composition for electricity supply, while leaving out the potential impacts of structural changes in the energy system (Jewell et al., 2014). On the other hand, the field of energy sustainability transitions that aims to understand radical system transformations falls short when it comes to using evaluation methods for future-oriented analyses (Zolfagharian et al., 2019). This is discussed further in Chapter 3.

A few exceptions can be found in the literature investigating the impacts of future system changes. However, none of those studies have specifically considered the impact of ESI on the WES. For instance, the impact of decentralisation and digitalisation is considered using scenarios analysis coupled with multi-criteria analysis (Karger and Hennings, 2009; Witt et al., 2020). The two studies highlight the importance of setting the boundaries and how this could affect the evaluation. Another study looks at the risks imposed from decentralisation and electrification on the energy security using scenario analysis (Gracceva and Zeniewski, 2014). The authors identify increasing risks to the stability and resilience of the system but suggest that further analysis is still needed. Furthermore, the energy system readiness for the transition is assessed in relation to the energy system structure, financial and human capital, regulation and political commitment, institutions and governance, consumer participation, and the business environment and infrastructure (Singh et al., 2019).

2.3.6. Systematic

The evaluation framework should be systematic in terms of procedural derivation and interpretation of evaluation criteria and indicators. This is important for replicability under different circumstances as there is no definitive set of indicators. Indicators must be context-specific to accommodate for different conditions and priorities. This is evident by the multifaceted concept of energy security, which is manifested in different ways according to the different context in which it is being used (Narula and Reddy, 2016). This characteristic is also important for the clarity and transparency of the evaluation, which improves its validity and credibility (Niemeijer and de Groot, 2008). Thus, systematic evaluation frameworks should be inherently comprehensive and flexible to cover the different aspects involved in different situations (Mancarella, 2014; O'Malley et al., 2016).

As mentioned earlier, a participatory approach to the evaluation is needed to include different stakeholders. In practice, this should be part of the systematic principle with different methods and considerations in place to map the relevant stakeholders, elicit their corresponding views, and eventually incorporate them in the evaluation framework (Voinov and Bousquet, 2010; Salter et al., 2010). The communication could go the other way round to receive feedback from the stakeholders on the outcome of the evaluation as well (Vaidya and Mayer, 2016).

Most frameworks reviewed are noted as systematic with a few exceptions. Frameworks indicated as systematic are those that present the lead up and derivation of the appropriate evaluation criteria or indicators they use. This could be through systems analysis techniques (Afgan and Carvalho, 2008; He and Feng, 2012; Mangoyana et al., 2013; Gracceva and Zeniewski, 2014; Narula and Reddy, 2016; Witt et al., 2020), experts interviews or surveys (Karger and Hennings, 2009; Sovacool and Mukherjee, 2011; Cox, 2016), or a literature review with selection principles to filter indicators (Iddrisu and Bhattacharyya, 2015; WEF, 2017; Singh et al., 2019; WEC, 2019). The strength of systems analysis is in providing a holistic approach to problem solving for complex systems (Afgan and Carvalho, 2008). Some of the systematic frameworks also conduct additional analysis of the results beyond quantification of indicators (Jewell et al., 2014; Osorio et al., 2017; Volkart et al., 2017). On the other hand, frameworks not indicated as systematic just list the indicators used without an explicit justification.

2.3.7. Applied

The evaluation framework should be applicable in practice to prove its usefulness and contribute to decision-making. The application should also be part of the testing and validation for any framework (Bautista et al., 2019). Validity could have different interpretations, and thus different methods, in different contexts. This is discussed in the scope of this research in Chapter 5. While most of the frameworks reviewed are applied to systems using existing data or with future scenarios, a different approach has been taken in (Kisel, 2017). In their study, the author develops an ideal set of indicators for policymakers considering the separate trilemma dimensions without relying on existing data. However, the indicator set presented has not been tested due to the data being unavailable, which is one of the main challenges generally for evaluation. Data availability could also pose a challenge for validation (Holtz et al., 2015). Hence, it is important to be able to get relevant data from energy models resembling future scenarios.

2.4. Summary and Research Gap

In summary, the energy transition aims at achieving the energy policy trilemma objectives, and is also driven by decarbonisation, decentralisation and digitalisation of the energy system. The transition is creating uncertainties related to the mismatch between the energy supply and demand, and increasing the complexity of the whole system with the need to coordinate between multiple energy vectors. Additional flexibility can address the increasing uncertainty and complexity to help manage the energy system, and can be provided by Energy Systems Integration (ESI). ESI aims to capture and exploit interactions and diversity across multiple energy vectors, by connecting energy systems physically and virtually across infrastructures and markets.

The concept of ESI originates from a Whole Energy Systems (WES) approach that holistically considers integrating energy vectors to achieve horizontal synergies and efficiencies at all levels. A WES approach to planning and operation of energy systems is a holistic approach that looks at:

- multiple energy vectors: electricity, gas, heat
- energy supply chain span from generation to end-use, through infrastructure and markets
- the system environment comprising different stakeholders with multiple perspectives and objectives, including the technical, environmental, economic, regulatory and social aspects

Similarly, there is a need for a WES approach to the evaluation of integrated energy systems. This approach has been translated into three principles that the evaluation framework should exhibit. These are summarised as follows:

- Multivectoral, accounting for the interactions between multiple energy vectors and interdependencies between coupled energy systems
- Systemic, reflecting whole system properties emerging from system interactions at different levels

- Multidimensional, considering multiple perspectives and objectives and potential trade-offs or synergies among them

Three further principles are considered useful for the evaluation framework, which are:

- Futuristic, adapting to major future changes to the energy system structure and function
- Systematic, being flexible to be replicated and adopted in different contexts
- Applicable, proving its usefulness in supporting decision making

These principles represent the WES domains and the changes to the energy system, which are necessary for an appropriate evaluation framework. Considering existing frameworks against those principles, gaps are identified making them inappropriate for evaluating future integrated energy systems. None of the reviewed frameworks simultaneously exhibit the six principles required for the evaluation of ESI. While it is common to find *multidimensional*, *systematic* and *applicable* evaluation frameworks, existing frameworks mainly fail in reflecting *systemic* attributes emerging at the whole system level particularly those related to *multivectoral* interactions and interdependencies across energy systems. Moreover, existing frameworks generally neglect major structural and functional changes to the energy system in a *futuristic* evaluation.

Accordingly, in this project, a new methodological framework addressing the identified principles is developed and applied to evaluate the effectiveness of ESI as a future pathway for the energy transition. Next, the conceptualisation of ESI as a pathway for the energy transition using a sustainability transitions approach is presented in Chapter 3. Later, the evaluation framework design and implementation are explained in Chapter 4, the framework is tested and validated through a case study in Chapter 5, while its full-scale application is demonstrated through a second case study in Chapter 7.

Chapter 3 Energy Sustainability Transitions

In the scope of the socio-technical systems and sustainability transitions literature, integration has been identified as one of the multi-regime interactions that could occur within or across socio-technical systems. The concept of multi-regime interactions extends from the Multi-Level Perspective (MLP) theory, moving to a Multi-System Perspective (MSP) that highlights the fact that interactions between multi-regimes across systems, rather than within systems, are of main interest. In this chapter, the MSP is used to conceptualise ESI as a pathway for the energy transition, where interactions occur between the multi-regimes (generation, networks, demand) of its different integrated systems (electricity, gas, heat, transport). A System-of-Systems (SoS) conceptualisation of ESI is proposed. This conceptualisation unlocks concepts and methods used in systems engineering to analyse SoSs. Those concepts and methods are employed in this research to operationalise the understanding presented in this chapter and answer the research questions, through the methodological framework developed in Chapter 4.

This chapter starts by providing an overview of the sustainability transitions framework, in particular the MLP and its extensions in Section 3.1, as a foundation to the later discussion. Section 3.2 provides an understanding of ESI as a pathway for the energy transition using the MSP and proposes a conceptualisation of the integrated energy system as a SoS. Section 3.3 discusses the methodological contributions of this conceptualisation and the proposed methodology in comparison to other methods, in terms of operationalising the MSP, as a means of representing co-evolutionary dynamics of change in ESI, and as a bridge between analytical methods for sustainability transitions research. Finally, Section 3.4 summarises the concepts discussed in this chapter.

3.1. Sustainability Transitions Approach

The field of sustainability transitions research starts from the definition of socio-technical systems, which are composed of actors and institutions, in addition to technological artefacts and knowledge, interacting to provide services for the society (Markard et al., 2012). Note that institutions in this context refer to rules, both formal (law, regulations, etc.) and informal (customs, habits, etc.), rather than organisations (Papachristos et al., 2013). One example of socio-technical systems is the energy system, along with other infrastructure systems such as water, transport, and communication systems. Those socio-technical systems can see fundamental, long-term shifts along different dimensions including the technological, material, organisational, institutional, political, economic and socio-cultural (Markard et al., 2012). This happens through a set of processes conceptualised as a socio-technical transition, which include the coevolution of technological transformations as well as changes in user practices and institutions, and the emergence of new functionalities (Elzen et al., 2004). Hence, sustainability transitions are socio-technical transitions to more sustainable modes of production and consumption, typically associated with sustainability targets and guided by public policies (Markard et al., 2012).

The energy system, as a socio-technical system, is undergoing a transition to achieve the energy policy trilemma objectives of delivering decarbonisation, while maintaining a secure and reliable energy supply, and providing acceptable and affordable energy (Araújo, 2014). Accordingly, the energy transition has been explored within the field of sustainability transitions. Transitions in such large, complex systems typically occur gradually with incremental changes adding up to major reconfigurations. For instance, RES technologies were first introduced to modern energy systems to solve a particular problem as low-carbon alternatives for conventional electricity generation technologies. Since then, RES technologies have led to gradual system changes due to their emerging functional characteristics, such as their flexible and decentralised operation (Elzen et al., 2004). Therefore, socio-technical systems frameworks have been developed to conceptualise and understand such large scale, complex, and co-evolutionary processes of technology and social change (Papachristos et al., 2013).

In the following subsections, an overview of the key framework to understand sustainability transitions and its extensions is presented. The most relevant concepts to the scope of this research are identified and later projected to the case of ESI in Section 3.2.

3.1.1. The Multi-Level Perspective

The MLP is a key theory in the literature to understand the dynamics of sustainability transitions. The MLP and its extensions are the focus of this section as they are more aligned than other transition frameworks to the scope of this research. In particular, the MLP allows to focus on the different linkages between the systems elements at the regime level, both social and technical. Conversely, other transition frameworks such as the Transition Management and Technological Innovation Systems, focus more on the governance of innovation policy and the institutional aspects affecting technology development at the niche level, respectively (Geels, 2005; Markard et al., 2012). Additionally, the MLP builds on the concept of Large Technical Systems while being more comprehensive and explicit on incorporating the broader aspects of technological transitions (Paredis, 2011).

The MLP distinguishes between three levels for the transitions of socio-technical systems, highlighting the multidimensionality and multiplicity of actors involved (Rohracher, 2018). The first level is the niche-innovations level where radical novelties emerge in protected spaces acting as an engine for change. The second is the socio-technical regime level which constitutes the institutional structuring of existing systems providing stable structures and selection environment for innovations. This includes the set of rules embedded in technological artefacts and social networks, in addition to the rules related to intermediary activities (e.g., distribution, market transactions, policy making) and user activities (Raven and Verbong, 2007). The third is the socio-technical landscape (deeply entrenched cultural norms and values) where exogenous developments that affect niche and regime activity take place. The three levels of the MLP and the interactions between them are described in Figure 3.1.

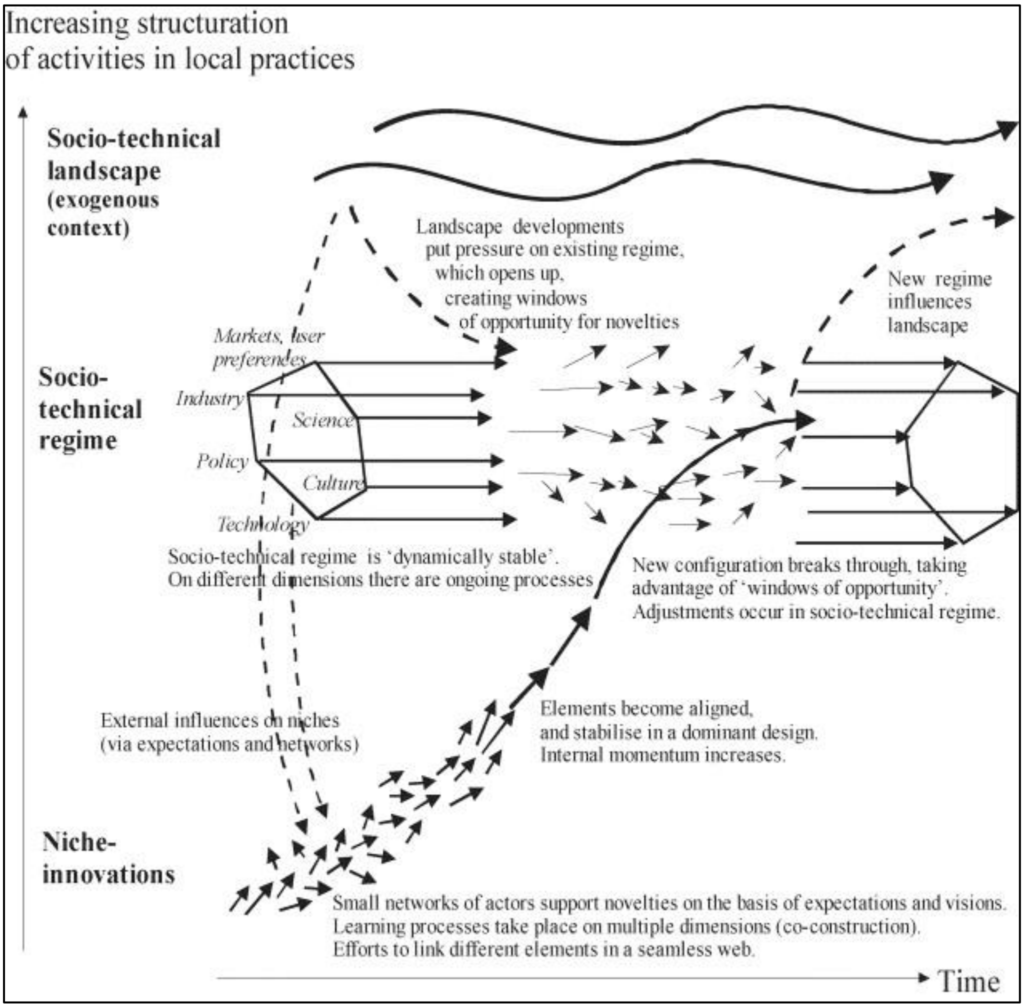


Figure 3.1 The Multi-Level Perspective on socio-technical transitions
Reproduced with permission; Source: (Geels and Schot, 2007)

According to the MLP, transitions happen as a result of interactions between processes at the three levels. Typically, niche-innovations pick up momentum internally through learning processes while changes at the landscape level create pressure on the regime. At some point the regime gets destabilised creating an opportunity for niche-innovations to be adopted (Geels, 2005). Different types and timings of interactions between the multiple levels lead to different types of transition pathways, namely transformation, technological substitution, de-alignment and re-alignment, and reconfiguration, as described in Table 3.1 (Geels and Schot, 2007).

Table 3.1 MLP transition pathways topology

Transition Pathway	MLP conditions	Outcome
Transformation	• Moderate landscape pressure • Niche-innovations not sufficiently developed • Regime shift in the direction of development and innovation efforts	• New regimes grow out of old regimes through cumulative adjustments and reorientations. • Regime actors survive, although some changes may occur in social networks. • Regime actors may import external knowledge if the 'distance' with regime knowledge is not too large. • Such symbiotic niche-innovations add to the regime and do not disrupt the basic architecture.
Technological Substitution	• Much landscape pressure (specific shock, avalanche change) • Niche-innovations developed sufficiently	• Innovations breakthrough to replace existing regime
De-alignment and Re-alignment	• Large and sudden landscape change • Increasing regime problems causing regime actors to lose faith • If niche-innovations are not sufficiently developed, then there is no clear substitute.	• De-alignment and erosion of the regime. • Space is created for the emergence of multiple niche-innovations that co-exist and compete for attention and resources. • Eventually, one niche-innovation becomes dominant, forming the core for re-alignment of a new regime.
Reconfiguration	• Innovations developed in niches are initially adopted to solve local regime problems • They subsequently trigger further adjustments in the basic regime architecture	• The new regime grows out of the old regime • Substantial changes in the regime architecture • Regime actors survive in this path, but competition and tensions occur among component suppliers

The reconfiguration pathway is of particular interest in the scope of this research. Reconfiguration happens when, for instance, an innovation is initially adopted to solve a local regime problem, but leads to an adjustment in the system architecture (Papachristos et al., 2013). This pathway concerns socio-technical systems that function through the interplay of multiple technologies where transitions are caused by a sequence of multiple component-innovations rather than a breakthrough of one technology (Geels and Schot, 2007). In this context, configurations are defined as the alignment between a heterogeneous set of elements shaped to work together in practice to fulfil a specified function (Geels, 2005). This definition highlights the inherent linkages between technical and social aspects. Hence, under the circumstances outlined for this reconfiguration pathway, regimes may transform into fundamentally new configurations, leading to new interrelations of technologies, institutions, actor networks, and social practices (Rohracher, 2018).

The reconfiguration pathway relates to the concept of architectural innovations that alter the architecture of a system without changing its components by reconfiguring an established system to link existing components in a different way (Henderson and Clark, 1990). However, although reconfigurations and architectural changes are of interest in the scope of ESI, the MLP as initially described focuses on breakthroughs of singular innovations and the transition pathways in Table 3.1 only describe the interactions between the different levels of the MLP.

3.1.2. Multi-Regime Interactions

An extended version of the MLP accounts for interactions between multi-regimes and multi-niches. Multi-regime interactions are interactions between fairly well defined and separated systems of production, intermediation and use (Raven and Verbong, 2007). For example, multiple regimes exist and interact in the transport system such as auto-mobility, bus, rail and cycling (Geels, 2018). Similarly, in the electricity system multiple regimes typically include generation, networks and consumption (McMeekin et al., 2019). Different types of multi-regime interactions leading to a system reconfiguration are identified namely, competition, symbiosis, and integration (Geels, 2018). In this case, the transition pathway becomes a whole system reconfiguration, which is recognised as a system reconfiguration due to multiple change mechanisms rather than breakthroughs of singular disruptive innovations. These mechanisms comprise not only the adoption of niche-innovations within existing regimes, but incremental regime improvements, changes in the relative size of regimes, or new combinations between niche and regime elements that alter the system architecture (Geels, 2018). This understanding of multi-regime interactions attempts to overcome the hierarchical separation between the MLP levels and enables the interpretation of the dynamic, parallel process of change taking place concurrently (Laakso et al., 2021). Figure 3.2 shows the multi-regime interactions in the MLP.

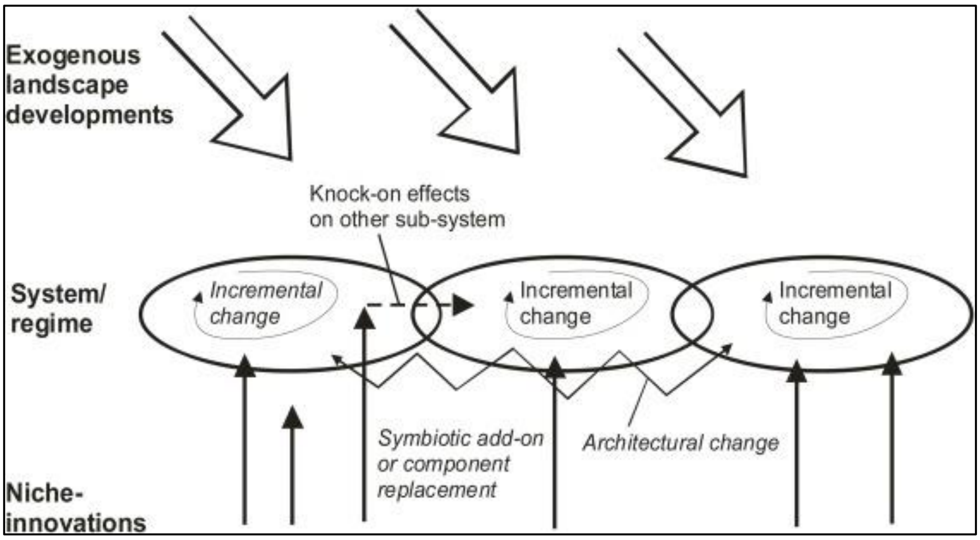
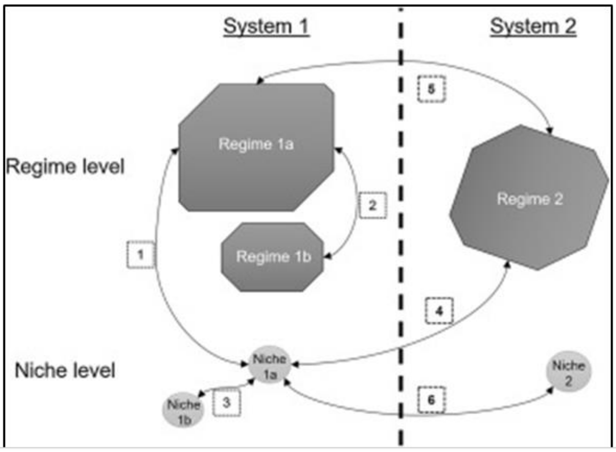


Figure 3.2 MLP multi-regime interactions
Reproduced with permission; Source: (McMeekin et al., 2019)

A new whole system architecture is expected as a result of reconfiguration since linkages between subsystems are changing (McMeekin et al., 2019). This opens up a stream of research around whole systems from a socio-technical perspective with greater attention to the system architecture and the linkages between its constituents (Geels, 2018). As discussed in Chapter 2, there have been calls for a whole systems approach to energy, which haven't been always fully implemented. The same applies to the field of sustainability transitions. For example, studies looking at the electricity system tend to focus either on the generation side or the consumption side, with single niche-innovations such as individual electricity generation technologies or specific consumption practices (McMeekin et al., 2019). Furthermore, there isn't an agreement in the literature to what a WES approach exactly is. For some, this approach takes into account all technologies and energy flows in the energy system (techno-economic perspective), while for others a socio-technical perspective is involved considering actors and institutions as well (McMeekin et al., 2019).

3.1.3. The Multi-System Perspective

The MSP builds on the concept of multi-regime interactions. While this is not yet a fully established terminology, the MSP is distinguished by focusing on interactions between multiple regimes *across* systems, rather than multiple regimes *within* the same system (Rosenbloom, 2020), as illustrated in Figure 3.3. For instance, in the context of ESI, rather than looking at the interactions within the multiple regimes of the electricity system (generation, networks, consumption), the interest is in the interactions across the different energy systems (electricity, gas, heat) each of which has their multiple regimes within. This can be expanded to other utility sectors such as water and telecom (Konrad et al., 2008). It is therefore essential to clearly define the boundaries of the systems under study to identify what are the internal and external influences (Papachristos et al., 2013). It is increasingly expected that radical innovations will cross traditional boundaries, where separated regimes start cooperating and new linkages are established between different parts of multiple regimes (Raven and Verbong, 2007). For example, CHP linking the electricity, gas and heat systems, EVs linking transport and electricity systems, and biofuels linking the energy, transport, and agriculture systems (Papachristos et al., 2013).



#	Interaction	Illustrative case
Within system		
1	Niche-regime	Interactions between the distributed solar niche and conventional power regime in the electricity system
2	Regime-regime	Interactions between radio and recording regimes in the music system
3	Niche-niche	Interactions between the battery electric and hydrogen vehicle niches in the transport system
Across system		
4	Niche-regime	Interactions between the conventional power regime in the electricity system and the electric vehicle niche in the transport system
5	Regime-regime	Interactions between the conventional power regime in the electricity system and the natural gas-based heating regime in the heat system
6	Niche-niche	Interactions between early biofuel experiments in the agri-food and transport systems

Figure 3.3 MSP Interactions within and across systems
Reproduced with permission; Source: (Rosenbloom, 2020)

According to Papachristos et al. (2013), the MSP provides an extension to the MLP as a conceptual framework to describe the involvement of external entities (regimes, niches) in systems transitions. This suggests an additional type of transition pathways, which is the emergence pathway, where a new system emerges initially as a niche from the interaction between two or more systems. This pathway is driven by reinforcing interactions, that is interactions that can be absorbed by existing regimes rather than being disruptive. Those interactions should happen at a time when interacting systems are under pressure (e.g. landscape pressure) and have sufficiently developed complementary capabilities to contribute successfully to the niche emergence.

Taking a MSP approach opens up different directions for sustainability transitions research, which include expanding the scope of analysis, capturing the pervasiveness of change, and considering opportunities for acceleration (Köhler et al., 2019). In particular, the focus of the MSP is on identifying three aspects. First, the functional and structural interlinkages between the systems. Second, the system interactions patterns and their implications for sustainability transitions. Third, the emerging interfaces where interactions take place. Identifying interfaces is particularly important as it helps understand how the system architecture could be shaped upon a transition and how system boundaries may be accordingly redefined (Rosenbloom, 2020).

According to the MSP, four types of multi-regime interactions are identified as summarised in Table 3.2 (Raven and Verbong, 2007; Geels, 2018; Rosenbloom, 2020).

Table 3.2 MSP multi-regime interactions typology

Interaction type	**Description**	**Example**
Competition	Regimes compete in delivering similar functions, which could lead to substitution effects or increasing variety in delivery	The electricity and gas systems competing to deliver power and heat service
Symbiosis	Regimes cooperate in delivering a societal function, which might result in stronger and more stable ties between regimes or generate innovative activities	Natural gas suppliers having a market in electricity generators, and electricity generators securing the required fuel
Integration	Regimes become integrated to become one or form a new entity for delivering a societal function; integration could be partial	Electricity and gas distribution companies merging; CHP technology coupling the electricity and gas systems
Spill-over	Elements from one regime are taken up within another (transfer of rules)	Liberalisation of the telecom market which served as an exemplar for the liberalisation of energy markets

The four types of interactions are not necessarily exclusive. Regimes can be competing while having aspects of symbiosis at the same time (Raven and Verbong, 2007). The system interactions are also characterised by the MSP as being *diverse* because socio-technical systems tend to share a range of different connections, *layered* stretching across regime and niche levels at multiple geographic scales, and *evolving* with system boundaries and objectives changing over time (Rosenbloom, 2020).

There is still a limited, yet growing literature considering case studies of the MSP. The diffusion of CHP in the Netherlands is considered as a case study of a technology that would create multi-regime interactions between distinct systems (electricity and gas), to demonstrate that transitions would possibly cross traditional regime boundaries and conceptualise multi-regime interactions across systems (Raven and Verbong, 2007). Another study considers the interactions between the different energy systems in the case of electrification of heat and transport in Ontario, Canada, highlighting the importance of multi-system interactions in shaping the energy transition (Rosenbloom, 2019). However, the latter study focuses on the changing relationships between the actors involved due to the multi-system interactions, which is important to understand the political implications of the transition.

Other relevant studies have looked at case studies of multi-regime interactions between the energy and waste systems (Raven, 2007), energy and agriculture systems (Sutherland et al., 2015), electricity and mobility through EVs (Haley, 2015; Mazur et al., 2015), electricity and ICT systems for smart grid development (Hiteva and Watson, 2019), energy services and buildings (Lazarevic et al., 2019), and energy and transport through biogas (Forbord and Hansen, 2020). However, most of those case studies focus on governance, organisational arrangements and the role of actors in the transition. In contrary, this research starts from a technical standpoint with the technical regimes as an entry point to discuss the transition, as will be discussed in the next section.

Moreover, most of the case studies available in the literature are focused on historical analysis of multi-regime interaction patterns. Nevertheless, it is argued that an approach investigating multi-regime interactions across systems is needed for future-oriented analysis of transformations to sustainable sector structures with different degrees of systemic change. This is demonstrated through looking at the interlinkages within and between utility systems (telecom, electricity, gas, water, sewage) and the potential future architectural changes that would gradually add up into a reconfiguration rather than a complete regime shift (Konrad et al., 2008). A similar call to explore future system changes through considering different possible system architectures is suggested, however, the study is focused on the electricity system (Hojčková et al., 2018). Hence, this research aims to make use of the socio-technical approach discussed in this chapter to provide future-oriented evaluation of the energy transition, while focusing on ESI.

In the rest of this chapter, the focus turns to conceptualising ESI from a sustainability transitions perspective considering the relevant multi-regime interactions across systems and the whole system reconfiguration as the appropriate transition pathway. The conceptualisation is followed by proposing a methodology to operationalise it and fill the identified gap in the sustainability transitions literature, and to also answer the main research question of this research related to evaluation.

3.2. Conceptualising Energy Systems Integration

The MSP is applied to understand the dynamics between the multiple regimes across socio-technical systems. In particular, we are interested in looking at the concepts of multi-regime integration and whole system reconfiguration. Furthermore, a SoS conceptualisation for ESI is proposed in line with the MSP.

3.2.1. A Multi-System Perspective for Energy Systems Integration

ESI involves multiple energy systems, namely the electricity, gas, heat and transport systems. The systems are technically linked by coupling components such as CHP, P2X, HPs, and EVs. These technologies enable energy vector conversion or electrification of end-use sectors, as discussed in Chapter 1. Each of the energy systems has multiple regimes, responsible for generation, networks and consumption. Interactions occur between multiple regimes across different systems. For instance, CHP couples the electricity and heat systems at the generation level, both being fed by the same energy source. In the case where the energy source is natural gas, the coupling would include the gas system as well. On the other hand, P2X couples the different energy systems at the networks level. HPs and EVs can relate energy system on both the networks and consumption levels, depending on their scale.

First of all, the five characteristics to which understanding multi-regime dynamics is pertinent are considered. Below each of those characteristics the relevant ESI features are discussed. According to Konrad et al. (2008), multi-regime dynamics are relevant and applicable when and if:

- *Similarly structured regimes are considered*

In the scope of this research and in the context of ESI, three systems are considered, the electricity, gas and heat systems. The three energy systems have similarly structured regimes mainly the generation/supply, the networks for transmission and/or distribution, and the consumption/end-use.

- *Transformations relate to all regimes fulfilling a specific societal function including competing and complementary relations*

The three energy systems fulfil a specific societal function of delivering energy services, in the form of electricity or heat. In the context of ESI, the three systems are envisaged to have complementary relations to make use of potential synergies.

- *Radical innovation creates linkages to different regimes*

ESI technologies (CHP, P2G, HPs, EVs) are adopted as technological innovations that create linkages between different regimes across energy systems.

- *Strong couplings via a third regime exists between otherwise separated regimes*

ESI technologies create linkages between the currently separated regimes across energy systems. Referring to the emergence pathway, those technologies may be adopted first as niche technologies but later develop into a system. In this context, we virtually group those technologies into one 'coupling system' as will be described in the next subsection.

- *Future transformation of regime structures are in the focus of analysis*

The focus of the analysis in this research is around the future energy transition through ESI, which is expected to mainly affect regime structures and reconfigure the WES, as described in Section 2.2.

After demonstrating the relevance of multi-regime interactions to the case of ESI, we look at another set of characteristics for system interactions in the MSP. Those are being *diverse* because socio-technical systems tend to share a range of different connections, *layered* stretching across regime and niche levels at multiple geographic scales, and *evolving* with system boundaries and objectives changing over time (Rosenbloom, 2020). In this context, ESI resonates to those characteristics being a concept that originates from the holistic WES approach that is defined in Chapter 2, setting out three key principles: multidimensional, systemic, and multivectoral. Accordingly, the three MSP characteristics and the three WES principles are complimentary, considering the *diverse, multidimensional* relations and connections between the various system components and stakeholders, the *layered, systemic* span of the energy system across the supply chain from generation through infrastructure and markets to end-use, and the *evolving* boundaries changing due to the new *multivectoral* couplings.

Looking closer at the multi-regime interactions across systems defined in Table 3.2, it is clear that ESI falls under the integration type. This is when regimes are integrated to become one or form a new entity for delivering a societal function. It is worth noting that integration could be partial where multi-regime settings do not necessarily disappear. Integration can take place at the actors and institutional level or take a hard form with technological integration (Raven and Verbong, 2007). Both forms of integration are expected in ESI, which will involve a whole system reconfiguration leading to a different system architecture.

The concept of the system architecture has been stressed in the literature around multi-regime interactions and the MSP. The system architecture is considered a comprehensive unit of analysis for this type of study spanning the whole system while focusing on the linkages and interfaces between the different system components (McMeekin et al., 2019; Rosenbloom, 2019). It is clear in this scope that a transition does not have to be a full-fledged regime shift, but a systemic change that involves some elements of a regime and particularly affecting the system architecture (Konrad et al., 2008).

As discussed in Chapter 2, a new energy system architecture is expected as a result of ESI. On the technological level, ESI will create new interactions and interdependencies between the different energy systems beyond the traditional boundaries. Thus, new planning and operation paradigms are needed to manage for the emergent complexity involved. On the markets and institutional level, ESI will bring together multiple actors with different objectives and motivations. New opportunities would develop upon ESI for partnerships between separate energy businesses, each of whom has an independent market structure and regulatory framework. In addition, new actors could emerge with new business models developed to take advantages of ESI. This could lead to a new market structure and regulatory framework.

The electricity system in the UK has already seen a whole system reconfiguration through spatial reconfiguration of the network to accommodate additional RES, the increase of distributed generation and the emergence of electricity prosumers, and the digitalisation of the electricity network with smart meters and smart grids. Those three changes affect the system architecture and the linkages between the three regimes of the electricity system (McMeekin et al., 2019). More changes to the system architecture are expected in the future whereby the regime become more tightly coupled and operate in different paradigms induced by, for example, intelligent load management, DSR, storage, and smart appliances (McMeekin et al., 2019). Radically different architectures could be proposed to solve a particular problem or as an outcome of a transition. For instance, the future electricity system could see three distinct transition end-points being set up as a super-grid, smart-grid, or off-grid. The three alternatives are different in terms of the level and type of connectedness between its constituents (Hojčková et al., 2018). However, they have all built momentum through similar co-evolutionary process including technology development, actors' mobilisation, networks formation and institutional work, and linking up with the existing regime. Each alternative architecture shows different benefits and drawbacks. Hence, there is a value in monitoring, understanding and evaluating the architectural developments by looking at the structural links between system components enabling or hindering the reconfigurational transition (Hojčková et al., 2018).

3.2.2. Integrated Energy System as a System-of-Systems

Integration of socio-technical regimes involves coupling previously separated regimes to form a new entity, but doesn't necessarily mean that parent systems would disappear (Raven and Verbong, 2007). We conceptualise this new entity for the case of ESI as a System-of-Systems (SoS). A SoS is defined as an integration of independent systems that act jointly towards a common goal, through synergies, to collectively offer emergent functionality that cannot be provided by constituent systems (CSs) alone (Nielsen et al., 2015). A SoS has distinctive characteristics of autonomy, independence, distribution, evolution, interdependence, and interoperability of its CSs, in addition to emergence as a result of synergistic collaboration of the CSs (Table 3.3) (Nielsen et al., 2015).

Table 3.3 Characteristics of SoS

Characteristic	**Descriptions**
Independence	- Capacity of the CSs to operate when detached from the rest of the SoS - CSs may offer a range of behaviours, some related to its role in a SoS and others independent of it
Autonomy	- Extent to which a CS behaviour is governed by its own rules rather than by others external to the constituent - Constituents that are conceived as parts that exhibit no autonomy are really enabling elements of the SoS, rather than CSs in their own right
Distribution	- Geographical distribution and network connection between its CSs - Extent to which constituent systems are dispersed so that some form of connectivity enables communication or information sharing
Evolution	- Coping with evolution caused by changes or upgrades to the CSs
Dynamic Reconfiguration	- Capacity of an SoS to undertake changes to its structure and composition, typically without planned intervention
Emergence	- Refers to the behaviours that arise as a result of the synergistic collaboration of CSs - Delivery of a higher functionality than what is delivered by the CSs separately
Interdependence	- Refers to the mutual dependency that arises from the CSs having to rely on each other in order to fulfil the common goal of the SoS - SoS requires trade-offs between the degree of independence in the CSs and the interdependence required to reach the common goal
Interoperability	- Ability of the SoS to incorporate a range of heterogeneous CSs - Refers to the integration of capabilities and adaptation of interfaces and standards

Hence, a SoS is mainly characterised by operational and managerial independence, geographical distribution, evolutionary development, and emergence. The SoS features apply to ESI where different utility companies are independently responsible for operating, managing and developing the CSs, which are naturally geographically dispersed, and emergent behaviour resulting from interacting components between the CSs (Mittal et al., 2015). In this case, each CS can maintain their autonomous management, objectives, and resources while collaborating within the SoS to meet the overall objectives (Energy Systems Catapult, 2019).

The CSs of an integrated energy system defined in this research are the electricity, gas and heat systems. In addition, energy vector conversion technologies are defined as the coupling system. The integrated energy system can therefore be characterised as a SoS with its CSs having the following features (Maier, 1998; Mittal et al., 2015):

- Managerial independence, where each CS performs its own function under its own rules being currently managed by various utility companies
- Operational independence, with the capacity of CSs to continue to operate normally when detached from the SoS
- Evolutionary independence, where each CS is continuously upgraded and has its own lifecycle
- Geographic distribution, where CSs are typically geographically dispersed in the form of networks
- Emergent behaviour, resulting from interacting components between the CSs
- Having a collective purpose as a SoS, in this case improving the overall efficiency, reliability and resilience, and reducing overall costs and emissions of the whole energy system

The emergent behaviour of integrated multi-vector energy systems due to the multisystem interactions and shifting across vectors has been mathematically verified. More flexibility is provided by the integration of energy systems compared to the aggregation of traditional means of flexibility in the separate operation of energy systems (Chicco et al., 2020).

Conceptualising integrated energy systems as a SoS enables the use of concepts and methods used in systems engineering to analyse SoS. Those are explained in detail in Chapter 4. Here, a brief overview from the literature on the relevance and usefulness of a systems engineering approach to transitions studies is presented.

Systems engineering is an interdisciplinary approach which aims to analyse and design large scale, complex systems (Davis et al., 2013). One of the focus areas of systems engineering is system integration, which refers to the integration of components, elements, subsystems, or human interactions to realise a system that accomplishes specific objectives. Traditional systems engineering considers integration as a technical process to satisfy system requirements, architecture, and design with a focus on interfaces between technical elements that facilitate interoperability (Rajabalinejad et al., 2020). However, multiple levels of integration are identified. On the SoS level, integration occurs between two or more systems with a focus on functional, operational, and managerial aspects. Another level is the socio-technical systems integration that focuses on the integration of a SoS with societal needs and compliance with existing institutions to ensure the optimal delivery of its services (Rajabalinejad et al., 2020).

It is suggested that systems engineering offers multiple benefits in understanding socio-technical systems and transitions in a systemic, traceable, and consistent way. This is provided through making the problem space explicit, exploring the solution space, and evaluating the potential contribution of technologies on future systems (Kirkels et al., 2021). Moreover, systems engineering can be effective in providing an integrated systems view of the multidimensional aspects and processes of sustainability transitions, and supporting those transitions through the focus on tools for monitoring and measurement (Davis et al., 2013). However, an adapted systems engineering approach may be needed to consider the particular challenges associated with studying socio-technical integration and socio-technical transitions (Rajabalinejad et al., 2020).

There is a growing direction in the research area of complex systems to study the multidimensional characteristics of sustainability transitions of socio-technical systems. The concept of system architecture is again relevant here, this time as a methodological approach. As a methodological approach in systems engineering, the system architecture is a holistic system-level approach that links what is desired to what is feasible. It outlines the structure and function of the system, as well as with the interfaces between constituents and with its environment (Davis et al., 2013). The architecting process allows for changes in objectives over time and does not necessarily pursue an optimal solution but rather supports integrated decision making and systems thinking. In this context, architectural frameworks include prescriptions for developing views to describe the system architecture, which can be represented textually or graphically. Since the outcome of the transition cannot be predefined, the proposed architectural framework should support iterations to describe the evolving changes in the system architecture. It is also important that an architecture outlines how the system integrates with people, products, processes and organisational systems (Davis et al., 2013). Thus, systems engineering and system architecture stand out as promising approaches to study the complexity of socio-technical systems transitions.

Hence, a SoS architecture methodology is proposed to operationalise the MSP in the context of ESI and understand the interactions across the integrated energy systems. An overview of this methodology is presented in the next section along with its contribution to the sustainability transitions literature. The methodology is developed in full elaboration in Chapter 4 as part of the overall methodological framework for evaluation.

3.3. The System-of-Systems Architecture Methodology

A SoS architecture methodology is proposed to operationalise the described conceptualisation of ESI. An overview of this methodology is first presented along with its merits compared to other similar methods. The methodology is described briefly in this section but is explained in detail in Chapter 4 in terms of design and implementation. This is followed by discussing the contributions of this methodology in tackling the methodological challenges for the MSP specifically and the sustainability transitions field generally. Finally, a closer look to the methodology is considered in the context of the MSP research focus and as a bridge between different analytical approaches for the sustainability transitions research.

3.3.1. Proposed Methodology

The SoS architecture methodology is proposed as an appropriate method to operationalise the MSP conceptualisation of ESI described in this chapter, as well as to address the principles for WES evaluation identified in Chapter 2. The SoS architecture methodology can be briefly described as a comprehensive mapping and traceability method for the different system components. The integrated energy system in this case, which is conceptualised as a SoS, is decomposed into its different CSs at different levels of abstraction. Structural and functional interactions between the different CSs and different system levels are highlighted. This process is outlined by a new architectural framework tailored for the purposes of this study. The ultimate goal of this method in the scope of this research is to facilitate the evaluation of ESI as a pathway for the energy transition using a set of indicators, which are deduced through the systems analysis. In other words, it complements multi-criteria energy sustainability assessments as a problem structuring method, as described in Section 1.4.2.

This method provides a socio-technical approach for evaluation by incorporating stakeholders' requirements and the technical components and functions into the energy system architecture (described as a conceptual model). The conceptual system model is coupled with scenario formulation and quantitative system modelling for a full representation of the system and a future-oriented sustainability assessment, to address the main research question for this project. Feedback between the three implementation stages (conceptual modelling, scenario formulation, quantitative modelling) is envisaged as well as iteration within each stage. As mentioned earlier, the system architecture is evolving with different configurations and interactions taking place across different system components. Thus, the system architecture methodology is a flexible means to represent different future conditions of the system including structural and functional aspects.

To the best of my knowledge, only one effort to directly use such a method from systems engineering for studying socio-technical transitions is found in the literature. The study develops an architectural framework in line with transition frameworks, such as the MLP, to support the planning and execution of sustainable technology projects (Davis et al., 2013). The need and utility of the architectural approach is demonstrated theoretically and through case studies. However, the architectural framework developed is restricted to the classical MLP approach described earlier in this chapter, and thus doesn't consider multi-regime interactions as in the case of the MSP. Furthermore, the architectural framework developed by Davis et al. (2013) is limited to a textual description of the system architecture as opposed to the approach developed in this research where a graphical representation is produced. This is important to illustrate the structural and functional interactions between the different system components. The graphical representation is created using the Systems Modelling Language (SysML) as will be elaborated in the following chapters.

This methodology has not been widely adopted outside its origin in systems engineering where it is used, for instance, in applications related to software engineering, enterprise information systems and military defence systems (Davis et al., 2013). However, similar approaches related to the concept of system architecture are receiving increased attention in the energy research community (Lubega and Farid, 2016; Energy Systems Catapult, 2017; ENA, 2018; Uslar et al., 2019). In comparison with other methods, the proposed SoS architecture methodology combines multiple merits as it allows:

- describing functional relations (behavioural influences) between different system components, similar to the System Dynamics method (Bautista et al., 2019; Papachristos, 2019)
- representing structural relations and flows between different system components, similar to system visualisation methods such as the Sankey Diagram (Liu and Mancarella, 2016)
- tracing the relations between high-level goals and lower level requirements, similar to the Strategy Map used in strategic management (Lea et al., 2018)

- facilitating participatory modelling involving stakeholders, similar to the Collaborative Conceptual Modelling method (Neely et al., 2021)

A unique feature that distinguishes the SoS architecture methodology is the ability to represent and analyse SoS specifically, which is the entry point to choose this approach. Another important feature of this methodology is the ability to include measures of effectiveness, or in other words the evaluation criteria and indicators, as part of the conceptual system model. While other methods show the above merits, they do not necessarily link to the evaluation, which is the main objective of this research.

3.3.2. Methodological Contributions

The contributions of the proposed methodology are discussed in the scope of the methodological challenges for the MSP and the sustainability transitions field realised from the literature review.

Contribution 1: Utilising a WES approach in MSP

A drawback of the whole system reconfiguration framework is the loss of some granularity, which makes it difficult to analyse micro-struggles, changing perceptions, individual strategies, and specific debates (Geels, 2018). This is partially remedied by considering a WES approach that incorporates a span of social and techno-economic dimensions. The WES approach is reflected in the proposed methodology by exhibiting the principles for evaluation defined in Chapter 2. This is discussed further in Chapter 4.

Contribution 2: Utilising conceptual level abstraction for system boundary considerations

Despite broadening the unit of analysis to the whole system, linkages outside the traditional electricity system still need to be accounted for, in particular the gas, heat and transport systems which are expected to become increasingly coupled with multi-regime interactions crossing traditional boundaries (Raven and Verbong, 2007; McMeekin et al., 2019). This raises the second challenge, which is around drawing the system boundaries. It is thus suggested that boundaries be drawn depending on the density and strength of couplings between the elements of socio-technical configurations (Konrad et al., 2008). This is when couplings between constituent elements (actor networks, technologies, institutions) are stronger within a specific regime than outside it. Two types of couplings are identified: functional couplings refer to input-output relations between different regime elements (relations within a value chain), and structural couplings refer to elements which are conjointly used by two regimes (Konrad et al., 2008).

A similar challenge relates to the appropriate conceptual level to describe the systems or the regimes under study. This stays a subjective selection depending on the objectives of the study and the scale of change involved (Davis et al., 2013). In this context, abstraction is a key concept in the proposed methodology where the system is considered at different conceptual levels with the aim of reducing the complexity of the system. Lower level challenges and extensive levels of details should still be considered. For instance, to consider technical aspects quantitative models are used in conjunction for evaluation to ensure technical feasibility of future system configurations.

Contribution 3: Technical standpoint for whole system reconfigurations (ESI as a trigger)

Thirdly, while there is a growing interest in studying whole system reconfigurations, within and across systems, most studies consider the relations between multiple niche and regime actors and changing practices as the crux of the reconfiguration. Starting from an innovation studies point of view, those studies consider the main interaction in a reconfiguration occurring between niche actors who develop and supply new components and technologies, and regime actors selecting and supporting the innovations (Laakso et al., 2021). A different approach is considered in this research, where the focus is on the new structural and functional couplings created by ESI technologies as the trigger for the whole energy system reconfiguration. This provides a technical standpoint for the socio-technical analysis. As described earlier, the technological reconfiguration would then be manifested as new market structures and regulatory frameworks affecting the relations between actors. This co-evolutionary dynamic is articulated in Section 3.3.3.

Contribution 4: Future-oriented analysis

The fourth challenge is identified with regards to the transitions literature in general, including MSP studies. This is around the focus of the transitions research area on historical analysis of transition patterns rather than presenting a future-oriented analysis (Zolfagharian et al., 2019). Therefore, there is a need to extend the methodological tools used in this research area to provide future-oriented analyses on how to achieve sustainability transitions successfully, such as the use of scenarios analysis and modelling techniques (Konrad et al., 2008). In Chapter 4, the full evaluation framework developed in this project is presented including scenario formulation and quantitative modelling to enable a futuristic assessment.

Contribution 5: Evaluation of system architecture change

Fifth, in line with the need for future-oriented analyses, there is a need to monitor architectural developments that enable or hinder transitions, and evaluate the benefits and drawback of possible transition pathways (Hojčková et al., 2018). This can be done by coupling sustainability transition studies with sustainability assessments that are adequately set up to accommodate complexity and diversity (Konrad et al., 2008; Kirkels et al., 2021). In fact, this is the overarching objective of this research, to develop an evaluation framework for ESI as a pathway for the energy transition that addresses the gaps in the energy sustainability assessment literature discussed in Chapter 2. In this context, it is important to beware of the evolving system architecture that could change the way it is evaluated (Turnheim et al., 2015), which is also one of the premises (futuristic principle) for the evaluation as discussed in Chapter 2.

Contribution 6: A method to bridge qualitative and quantitative analysis

Finally, there is a need for combining different analytical approaches for studying sustainability transitions in general, for instance, quantitative and qualitative approaches, given that transitions cannot be reduced completely to quantitative models (Zolfagharian et al., 2019). This can be fostered by developing new bridging methods and through the mutual learning and cooperation between modellers and other researchers in the field (McDowall and Geels, 2017). This challenge is discussed elaborately in Section 3.3.4.

3.3.3. Operationalising the Multi-System Perspective

The SoS architecture methodology is proposed to operationalise the MSP theory in line with the SoS conceptualisation presented earlier. The affinity of this methodology to the MSP is discussed in the scope of the three focus areas of MSP brought forward by Rosenbloom (2020):

- the structural and functional interlinkages between the systems
- the system interaction patterns and their implications for sustainability transitions
- the emerging interfaces where interactions take place

The three focus areas can be addressed by the proposed methodology. In fact, the co-evolution between three architectural layers can be explored using this methodology in line with the typical sustainability transition dynamics.

Prior to describing how this is achieved, it is worth mentioning that in this research we adopt the distinction between three layers of the energy system architecture as defined by (Energy Systems Catapult, 2017). The first is the physical layer focused on physical interactions, dependencies, and constraints. The second is the market layer focused on policy, regulation, and commercial interactions between actors. The third is the ICT layer focused on arrangements that enable communication within and between actors and components, in addition to interoperability and cyber security.

In relation to the MSP focus areas, first, the structural and functional interlinkages between the different components within and across the integrated energy systems are identified and visualised in the system architecture model using appropriate tools from systems engineering, such as model-based systems engineering. Second, the implications of the technological reconfiguration resulting from the technical multi-regime interactions on the market layer and the relationships between actors are similarly explored. Third, the technical interfaces are already examined in the physical architecture layer, while the socio-technical interfaces are studied by looking at both the physical and market layers. The cyber-physical interfaces required for interoperability are finally analysed on the ICT layer. Since the focus in the rest of the thesis is on the physical system architecture, the demonstration of analysing the co-evolutionary dynamics between the three layers is considered as future work.

3.3.4. Bridging Method for Sustainability Transitions Research

Based on multiple reviews for methodological challenges in the sustainability transitions literature (Holtz et al., 2015; McDowall and Geels, 2017; Köhler et al., 2019; Zolfagharian et al., 2019), there has been a direction to diversify the toolkit of methods used to study transitions, for instance, through theoretical bridging (Hansmeier et al., 2021). Due to its co-evolutionary nature, different theoretical approaches are needed to study the energy transition. For instance, these include the techno-economic (focus on energy flows and conversion processes, coordinated through energy markets), socio-technical (focus on technological change, driven by knowledge, practice and networks associated with energy technologies), and political (focus on change in policies which affect energy systems towards transition) (Cherp et al., 2018). In practice, a linking strategy between different analytical approaches has been proposed (Turnheim et al., 2015). This includes the following steps: alignment (developing a shared problem formulation and framing) and bridging (exchange of data and metrics, pathways evaluations, views on their delivery), in a continuous iterative cycle (techno-economic and socio-political feasibility checks). This linking strategy enables a multi-dimensional evaluation of transitions as they unfold, informing governance decisions and practices (Turnheim et al., 2015).

Similarly, in the energy modelling research community, there have been calls to incorporate socio-technical aspects and capture human behaviour (Pfenninger et al., 2014). On one hand, existing energy models focus on techno-economic feasibility with limited consideration of societal actors, socio-political dynamics, and the co-evolutionary nature of technological change (Bolwig et al., 2019). On the other hand, socio-technical transitions frameworks that address those aspects are difficult to operationalise in quantitative analyses that are useful for supporting policy making. Thus, the two approaches have a potential to provide complementary insights for studying future energy transitions (Li et al., 2015).

Multiple objectives are sought from combining the two approaches, including finding solutions to energy and climate challenges, increasing realism in models and theories, and enabling interdisciplinary learning between the two scholarly communities (Hirt et al., 2020). Specifically, models can be used in transition studies to scrutinise narratives or explore transition dynamics (Holtz et al., 2015). It is believed that simulation models are essential to understand sustainability transitions and provide timely and robust policy recommendations as they provide a suitable method to address the complexity of transitions and explore future trajectories. Moreover, simulation models can serve as a mediating instrument between the real world and the highly abstract world of theory (Papachristos, 2014). Furthermore, energy models provide a tool for systematic, quantitative and forward-looking analysis to investigate the co-evolution of technology, the economy and the environment, and quantify the associated uncertainties (Hirt et al., 2020).

Models, however, are not without limitations. Those could be specific depending on the model dimensions including the model purpose, method applied, level of abstraction, epistemological foundations, application context, and data requirements and availability (Holtz et al., 2015). When combining different analytical approaches, this might create validation issues, such as with over determination of outcomes or over dependency on existing data. To overcome some of those limitations, better cooperation and stronger interaction between modellers and other scholars and stakeholders is needed (McDowall and Geels, 2017). Moreover, modellers should make sure to convey the complexity of the model and the uncertainty associated with its results, especially if they are used as input for decision support (Holtz et al., 2015).

The proposed SoS architecture methodology can act as a bridging method between different analytical approaches for studying sustainability transitions (Figure 3.4). In essence, this methodology is proposed to operationalise a conceptual, qualitative framework for understanding multi-regime interactions across systems (the MSP), but it is also developed as the core of an evaluation framework that leads to a sustainability assessment of integrated energy systems in conjunction with quantitative energy models.

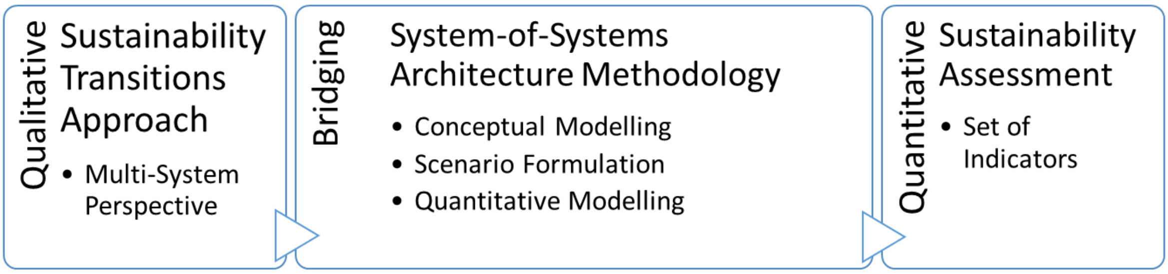


Figure 3.4 Bridging analytical approaches for sustainability transitions

The evaluation, as will be explained further in the next chapter, combines three methodological stages: scenario formulation, conceptual modelling and quantitative modelling, in an iterative process of feedback between them. First, the scenario formulation describes the system under study in terms of system configurations, conditions of energy demand and supply, and any other assumptions. Second, the conceptual system modelling represents the system architecture at different levels of abstraction and decomposes the system into its different components. The conceptual system model shows the system stakeholders and constituents, the structural and functional relationships, and measures of effectiveness. Finally, the quantitative system modelling includes the mathematical formulations representing the system topology and technical feasibility.

This integrated methodological framework fits the three requirements for socio-technical energy models (Li et al., 2015). The first requirement is incorporating techno-economic detail including technology cost and performance bounded with operational or resource constraints. This is fulfilled mostly by the quantitative modelling. The second is being explicit about actor heterogeneity with differentiated preferences and behaviours and involving actors that possess agency to shape transitions. This is fulfilled mostly by the conceptual modelling which is based on stakeholders' requirements. Thirdly, reflecting the transition pathway dynamics that include the assessment of normative goals, sufficient time horizons, and radical alternative reconfigurations. This is fulfilled by the overall approach of this research starting with the sustainability transitions conceptualisation leading to the sustainability assessment of integrated energy systems.

3.4. Summary

In summary, this chapter presents both a conceptual understanding of Energy Systems Integration (ESI) from a sustainability transitions research perspective and a methodological approach to operationalise this understanding. In particular, the Multi-System Perspective (MSP), which is a conceptual framework extending from the Multi-Level Perspective (MLP) used to understand multi-regime interactions across systems is applied in the context of ESI.

ESI is thus conceptualised as a pathway for the energy transition comprising a whole system reconfiguration that involves the integration of separate energy systems (electricity, gas, heat). Integration is facilitated by vector-coupling technologies, which in this conceptual analysis are considered niche-innovations that create linkages between the energy systems, but later emerge as one virtually grouped coupling system.

A System-of-Systems (SoS) architecture methodology is proposed to operationalise this understanding, where the integrated energy system is defined as a SoS. This methodology is further developed and applied in the following chapters to evaluate the effectiveness of ESI as a pathway towards achieving the energy transition objectives. The proposed methodology combines the strengths of other similar methods as it allows for describing and visualising structural and functional relations between different system components, tracing the relations between system requirements at different levels, and facilitating a participatory modelling that involves stakeholders and provides a socio-technical evaluation. This is done through abstraction at different levels, decomposing the system into its different components, and mapping stakeholders' requirements to the different system functions. This process is guided by an architectural framework developed in this research. The proposed methodology contributes to the sustainability transitions research by addressing a number of methodological challenges. This includes supporting a whole (energy) systems approach for studying (energy) transitions, providing a tool to analyse the co-evolutionary dynamics between the different system architectural layers, extending existing methods to explore future transition pathways through scenario analysis and sustainability assessments, and acting as a bridge between qualitative and quantitative methods for studying transitions.

Since the scope of this project has been limited to the energy system, future work could explore the application of the proposed methodology on other socio-technical systems. Moreover, since the focus in this project is on the physical system architecture, the analysis of the co-evolutionary dynamics between the physical, market and ICT system architecture layers is considered as future work. Future work should also examine if the proposed methodology is compatible with other sustainability transition frameworks besides the MSP.

Chapter 4 Developed Methodological Framework

In this chapter, a novel methodological framework to evaluate the effectiveness of Energy Systems Integration (ESI) as a future pathway towards achieving the energy transition objectives is developed. The developed framework aims to address the identified gaps and exhibit the six principles for whole energy systems (WES) evaluation described in Chapter 2, and operationalise the socio-technical transitions approach for ESI described in Chapter 3. The framework is based on the System-of-Systems (SoS) architecture methodology to develop a conceptual system model, which is coupled with scenario formulation and quantitative system modelling for evaluation.

The methodological framework is explained in two parts in this chapter:

- The framework design, including the underlying concepts and methods of the evaluation framework (Section 4.1)
- The framework implementation, including the stages whereby the framework can be applied for evaluation (Section 4.2)

The developed framework is first tested on the local energy system of Findhorn village, Scotland, in Chapter 5. Preliminary findings from the test case studies are used for the framework validation through a group interview with academic experts, whose feedback helped implement necessary improvements. From this, a Reference System Architecture Model that can serve as a standard conceptual model used for the first stage of the evaluation framework is developed. This is presented in Chapter 6. A full-scale study conducted on the case study of the North of Tyne region, England, to demonstrate the framework applicability and usefulness is presented in Chapter 7.

4.1. Framework Design

The framework design is based on concepts and methods from systems engineering related to the SoS architecture methodology. These are:

- System architecture, includes principles and guidelines governing the system structure, functions, the relationships between its components and with its environment, and how the system will meet its requirements (Section 4.1.1);
- System requirements, which refer to the functions and capabilities that the system needs to fulfil or acquire, and are mainly related to the needs of stakeholders (Section 4.1.2);
- System-of-systems (SoS), which is defined as integration of independent systems that act jointly towards a common goal, through synergies, to collectively offer emergent

functionality that cannot be provided by Constituent Systems (CSs) alone, employed here as an architectural modelling approach (Section 4.1.3);

- Model-based systems engineering (MBSE), is the formalised application of modelling to support system design, architecture, analysis and evaluation (Section 4.1.4);
- Architectural framework, is a structured prescription specifying the system views required to describe a system architecture (Section 4.1.5).

In addition, the evaluation is conducted using an indicator-based approach (Section 4.1.6). Figure 4.1 describes how the concepts and methods mentioned are related within the proposed framework. Each of those concepts and methods is investigated in further details in subsequent sections. Figure 4.1 also shows what concepts and methods fulfil the evaluation principles identified in Chapter 2. The evaluation principles are summarised again as follows:

- Multidimensional, considering trade-offs and synergies between multiple perspectives and objectives
- Multivectoral, accounting for interactions between multiple energy vectors
- Systemic, spanning the whole energy supply chain to capture emerging properties at different system levels
- Futuristic, adapting to major future changes to the energy system structure and function
- Systematic, being flexible and transparent to be replicated and adopted in different contexts
- Applicable, proving its usefulness in practice

The main aim of adopting those concepts and methods is to develop a conceptual system model of the energy system, whereby the system structure, functions, requirements, and measures of effectiveness are identified and combined into a system architecture[2] description. This is done through abstraction and decomposition of the integrated energy system into its different components at different levels. The framework provides a socio-technical approach for evaluation by incorporating stakeholders' requirements (stakeholders' needs and objectives) and the energy system technical components in a system architecture model. This is carried out by tracing the system requirements to the relevant functionalities delivered by the system and the capabilities it acquires. The conceptual modelling facilitates the deduction of appropriate evaluation criteria and indicators that represent the level of satisfaction of the system

[2] The terms 'conceptual system model' and 'system architecture model' are used interchangeably.

requirements through systems analysis. This delivers on the evaluation principles identified for being multidimensional and futuristic.

Using a SoS modelling approach allows the evaluation to be multivectoral and systemic, where the energy system is modelled at different system levels and decomposed into different CSs. This highlights the interactions, interdependencies and emergent behaviour between the different energy vectors (electricity, gas, heat) and the respective system components (supply, networks, storage, demand).

MBSE is the technique used to develop conceptual models that represent the system architecture, including its structure, functions, requirements and measures of effectiveness. MBSE is supported by the Systems Modelling Language (SysML), which is a graphical modelling language for designing and analysing complex systems. An architectural framework is needed to systematically guide the system modelling in order to capture different perspectives and viewpoints critical for the analysis. The architectural framework incorporates the designated system architecture such as the SoS.

The evaluation is conducted using an indicator-based approach, where indicators are the final means for the evaluation. The conceptual model needs to be coupled with a quantitative model to quantify indicators (Section 4.2). Thus, the applicability principle of the evaluation mainly depends on the availability and suitability of the data and quantitative model used.

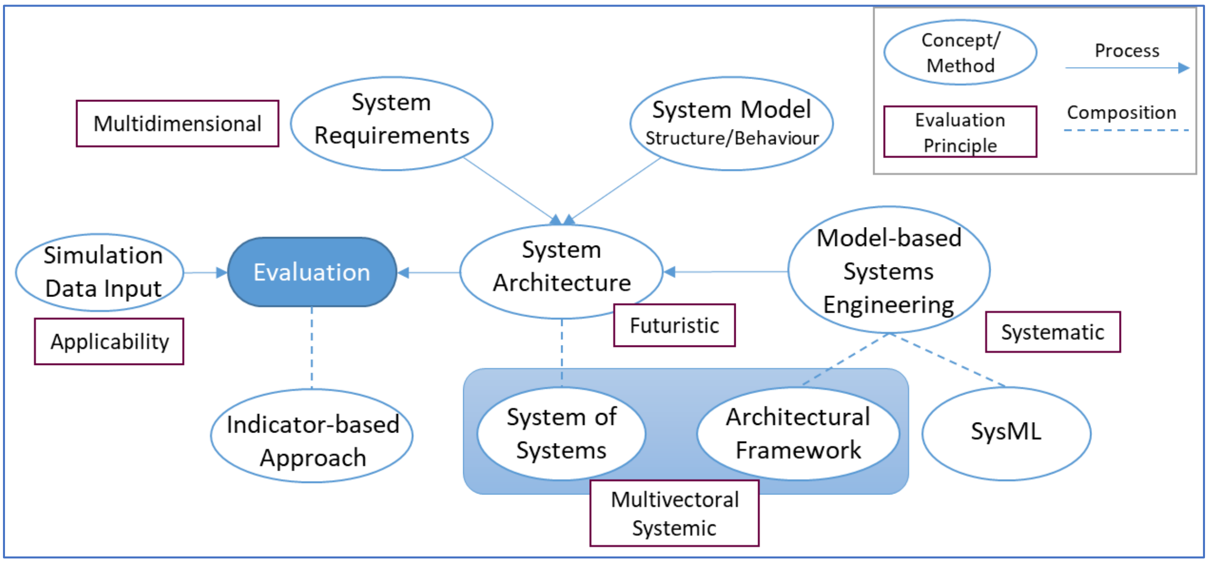


Figure 4.1 The proposed framework design for whole energy systems evaluation

4.1.1. System Architecture

As discussed in Sections 2.1 and 2.2, the future changes to the energy system are expected to transform the system and alter its architecture, where the whole system must evolve to recognise the new interfaces created by new interactions, while satisfying the system requirements. The system architecture is defined as the highest-level conception of a system in its environment. A system architecture generally includes the guiding principles for the system design and evolution and the fundamental organisation of the system, including its structure, functions, the relationships between its components and with its environment, and how the system will meet its requirements (Tang et al., 2004; Ingram et al., 2014).

The energy system architecture can be accordingly described in three layers. The first is the physical layer focused on physical interactions, dependencies, and constraints. The second is the market layer focused on policy, regulation, and commercial interactions between actors. The third is the ICT layer focused on arrangements that enable communication within and between actors and components, in addition to interoperability and cyber security (Energy Systems Catapult, 2017). In this project, the focus is on the physical system architecture of integrated energy systems, which can serve as a basis for further understanding and analysis of the market and ICT architectures. The physical layer comprises the energy infrastructure used to generate, transform, and transport energy. This includes networks and storage technologies for different vectors, and energy vector conversion technologies such as CHP, P2G, and HPs (Guelpa et al., 2019).

Accordingly, the system architecture concept is used as a structured method that facilitates the development and evaluation of potential future conditions of a system. This is performed through abstraction and breaking down the system into multiple interacting perspectives with different system components (Energy Systems Catapult, 2017). In this project, the system architecture of integrated energy systems is modelled as a SoS, having the features discussed in Section 3.2. This approach satisfies the principle of the evaluation being futuristic given the versatility in considering future changes to the system architecture.

Some systems architecture principles and examples are presented in further details by (COMPASS et al., 2014; Ingram et al., 2014; Energy Systems Catapult, 2017).

4.1.2. System Requirements

System requirements refer to the high-level goals and capabilities that the system should deliver or acquire to satisfy stakeholders' needs (Geyer and Buchholz, 2012). A stakeholder represents the role or set of roles of anyone or anything that has a vested interest in the project. Hence, requirements analysis is an exercise where requirement specifications are captured and analysed to support the system architecture and give evidence on its fitness for the required needs and capabilities. The process starts by identifying stakeholders and eliciting their requirements (Holt and Perry, 2013).

Requirements can be captured from various sources including: (Holt, S.A. Perry, et al., 2012)

- formal and informal conversations, interviews and workshops with stakeholders
- documentation of systems design and specifications
- standards and laws
- existing systems and best practice

For the development of the system architecture model in this research, a range of stakeholders' perspectives are derived through requirements in the literature. Literature review is a common approach for setting evaluation criteria as mentioned in Section 2.3.6 and is also common for identifying stakeholders' requirements. The latter is discussed further in Chapter 6. For a specific application of the architecture, requirements would ideally be elicited from stakeholders directly through a participatory approach.

There are two types of system requirements: (i) Functional requirements that relate to the system performing a desired functionality and are usually described by action verbs such as do, provide, deliver, produce, etc.; and (ii) Non-functional requirements that represent a constraint to another system requirement, including quality, implementation and solution-specific requirements. For example, this could be meeting a standard, complying with a legislation, using a particular technology, or ensuring a specific performance level, in addition to size and operations constraints (Holt, S.A. Perry, et al., 2012). This distinction is useful for the conceptual system modelling procedure and the deduction of evaluation criteria described in Section 4.2.

Requirements also form a basis for traceability, contractual agreements, and evaluation. Therefore, in this framework, requirements are used as a benchmark to evaluate the system effectiveness in achieving the stakeholders' objectives. System requirements and requirements engineering are extensively discussed in (Holt, S.A. Perry, et al., 2012).

4.1.3. System-of-Systems as a Modelling Approach

As discussed in Chapter 3, the integrated energy system is conceptualised, and accordingly modelled, as a SoS with all the properties and analytical approaches which SoS enables. System-of-Systems Engineering, a subfield of systems engineering, has evolved to understand and design complex and interdependent systems, with a focus on the boundaries and interactions between different systems (Nielsen et al., 2015). The SoS concept is considered an approach that is appropriate for modelling and analysing complex systems, with multiple actors, which can be decomposed into different levels (Pruyt and Thissen, 2007). This approach is primarily used to understand interfaces, manage interoperability between integrated systems, and capture emergent behaviour (Uslar et al., 2019). Furthermore, the SoS approach provides a holistic way to look at quantitative models in perspective with a wider context (Pruyt and Thissen, 2007). The SoS modelling approach is chosen in this framework because it meets the WES evaluation principles of being multivectoral and systemic.

While the SoS approach is not very common in energy systems evaluation, the new paradigm of ESI can drive analyses in the energy field into this direction. ESI is based on a WES approach that aims to find innovative solutions beyond one energy system and make use of possible interrelations between different energy systems to collectively achieve a greater outcome (Mendes et al., 2011). A SoS approach can be therefore employed for the improved evaluation of emerging features and functionalities expected upon ESI (Mittal et al., 2015). For instance, it has been mathematically verified that ESI offers additional flexibility compared to the separate operation of energy systems (Chicco et al., 2020). In fact, an integrated energy system lends itself to a SoS approach since its comprising subsystems can be characterised by the distinctive SoS features of operational and managerial independence, geographical distribution, evolutionary development and emergence, as discussed in Section 3.2.2.

The SoS approach can capture the complexity and variety involved in integrated energy systems since it can (DeLaurentis and Callaway, 2004; Williams and Imam, 2007; Otto et al., 2014; Hall et al., 2016):

- support multidisciplinary understanding and evaluation of systems
- help understand the way a system is performing by exploring interdependencies
- deal with complexity and consider dynamics of change
- enable the provision and validation of emerging behaviour
- prevent unintended consequences by considering the interactions between the CSs and with the system environment

By using a SoS approach, a broader, integrated and more holistic approach to evaluation is enabled. This approach will better capture the value of emergent properties such as flexibility and resilience across the whole system, describe the system interactions, and relate indicators to each other and to strategic goals and objectives.

Such an approach is recommended in the evaluation of complex and interdependent fields such as infrastructure provision systems (Otto et al., 2014; iBUILD, 2018; Saidi et al., 2018), water management (Pires et al., 2017), energy and climate policy (Agusdinata and Dittmar, 2009), and sustainable development (Bell and Morse, 2003; Phillis et al., 2010). The SoS approach has been also employed on a wider analysis of national infrastructure networks and services including energy (Hall et al., 2016). The study considers the integration of infrastructure sectors at the planning level and seeks to evaluate the outcomes for each sector on the operational level, by simulating coupled system models. This research differs from Hall et al. (2016) in that it looks at integration within the energy sector rather than across different infrastructure sectors.

4.1.4. Model-Based Systems Engineering

MBSE is the formalised application of modelling to support system design, architecture, analysis, verification and evaluation. MBSE is a rigorous, iterative process to develop conceptual models that coherently represent a system and its operating domain. Thus, the main artefact of MBSE is a system model that is at the core of all the consequent systems engineering activities (Holt et al., 2015). The system model in this case is an abstract description of the system architecture that typically represents its structure, behaviour, requirements and parameters, and takes into account the system concepts, constraints and trade-offs (Ramos et al., 2012; COMPASS et al., 2014). A survey that reviews the state of the art of SoS modelling and architectural description within the area of MBSE is presented by Nielsen et al. (2015).

MBSE techniques are used to produce structured, conceptual models of complex systems comprising input from different stakeholders, to support understanding of critical components, interfaces and processes of these systems. This allows different stakeholders to consider the system in their perspective of interests, without losing internal consistency across the range of viewpoints (Topper and Horner, 2013). The aim is to have a system architecture capable of satisfying the system requirements. Accordingly, developing a system architecture model involves collecting information from different stakeholders, understanding the relationships between the CSs, translating capability objectives into requirements, and evaluating the system performance against the system requirements (Lane and Bohn, 2013).

MBSE is suited for modelling SoSs as it provides a common language for interdisciplinary understanding by the different counterparts involved (Ramos et al., 2012). MBSE is supported by SysML, which is a graphical modelling language used as a standard tool to abstract and visualise systems and their interactions (Saidi et al., 2018). SysML offers rigor and flexibility along with breadth of diagrams that could be used to comprehensively represent SoS (Topper and Horner, 2013). SysML diagrams of interest in this project are both structural and behavioural and are summarised as follows: (Holt, S.A. Perry, et al., 2012; Geyer and Buchholz, 2012; COMPASS, 2014)

- Block definition diagram: to define the system structure, composition, relationships and properties
- Internal block diagram: to describe the internal structure and flows in the system
- Requirement diagram: to define and describe system requirements and their relationships
- Use case diagram: to link the system requirements to actors or CSs, showing requirements in application context
- Parametric diagram: to define calculations for parameters (measures of effectiveness) used for evaluation

These diagrams are used to develop the conceptual system model, including the context, structure, functions, requirements and measures of effectiveness. The exact use of SysML diagrams in this framework is further discussed in the Section 4.2.1. The relevant SysML notation is summarised below.

4.1.4.1. SysML Notation

The figures in this section describe the different SysML diagrams and the notation used to develop them. The figures are retrieved from (Holt and Perry, 2013). Figures 4.2-4.6 show the structural diagrams while Figures 4.7 and 4.8 show the behavioural diagrams.

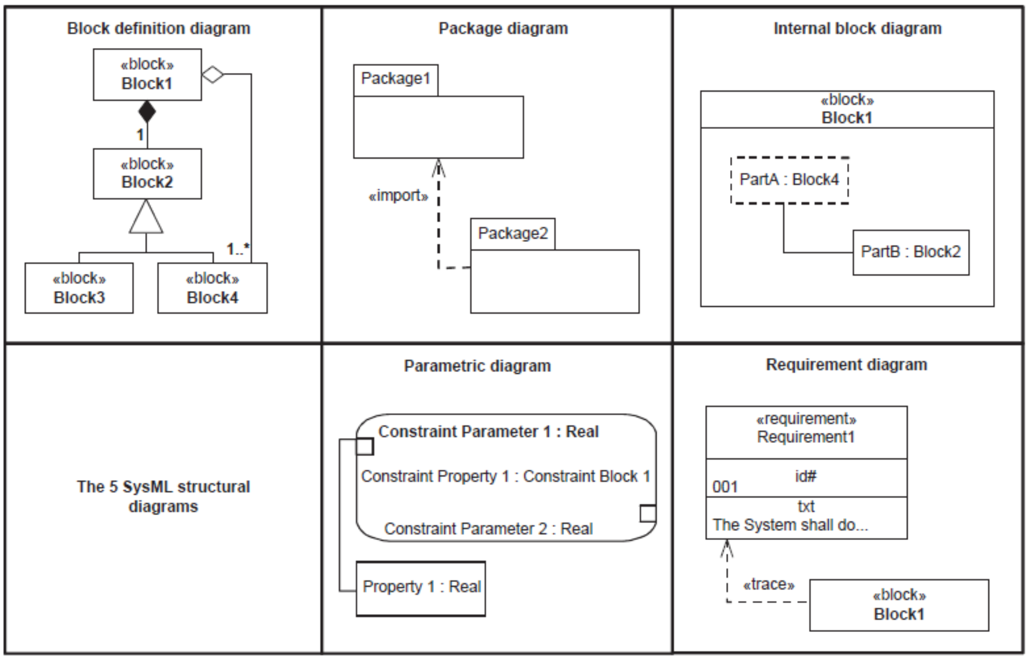


Figure 4.2 Summary of SysML structural diagrams
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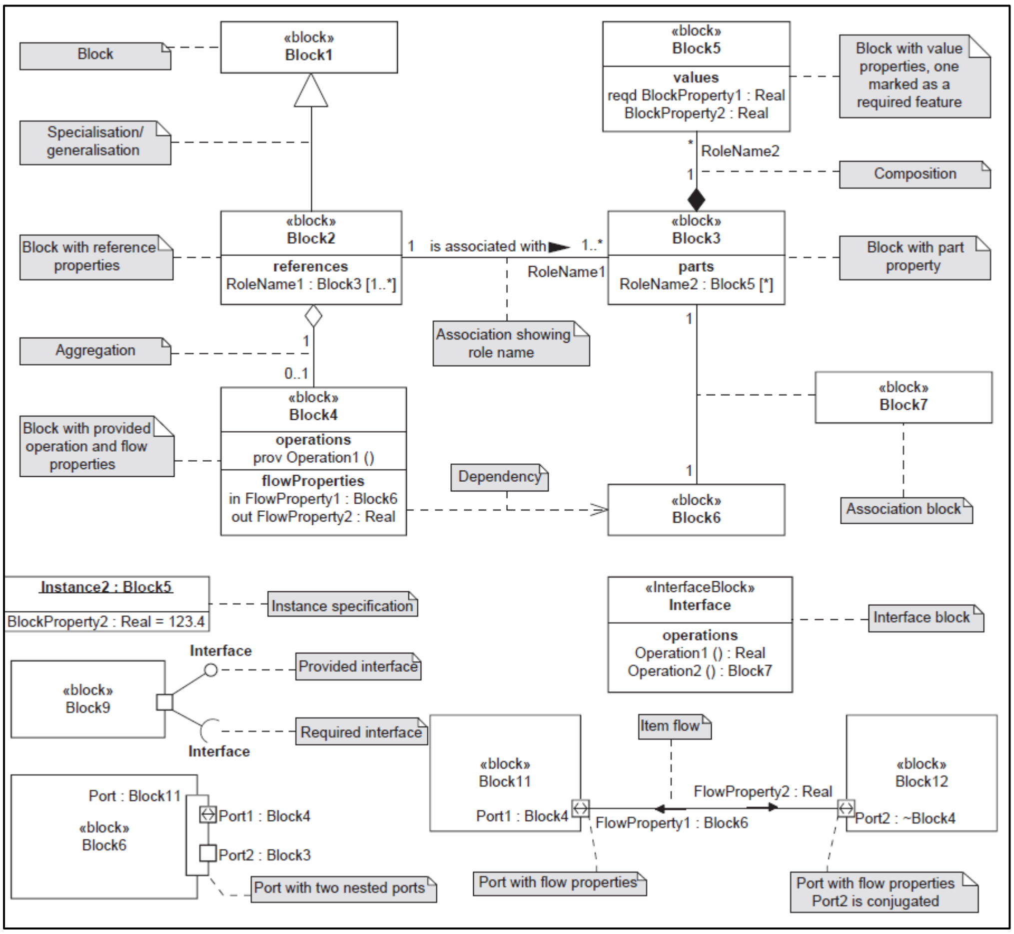

Figure 4.3 Block definition diagram notation
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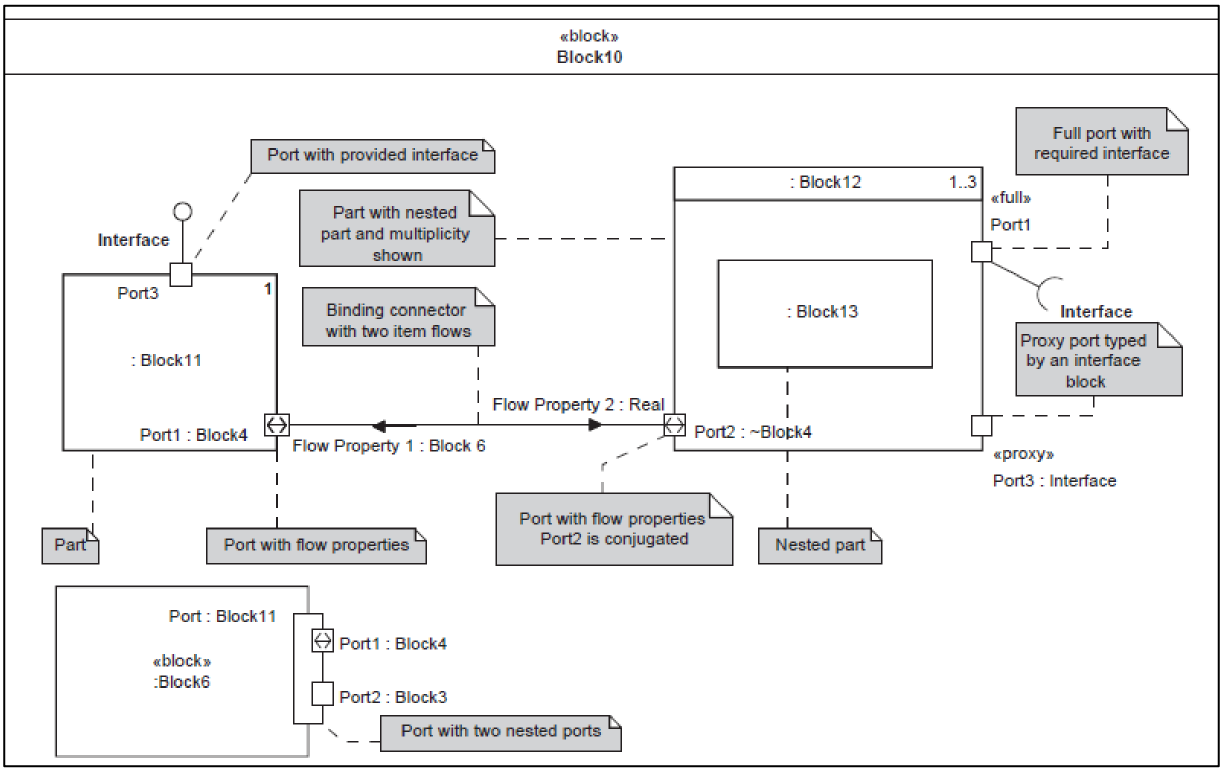

Figure 4.4 Internal block diagram notation
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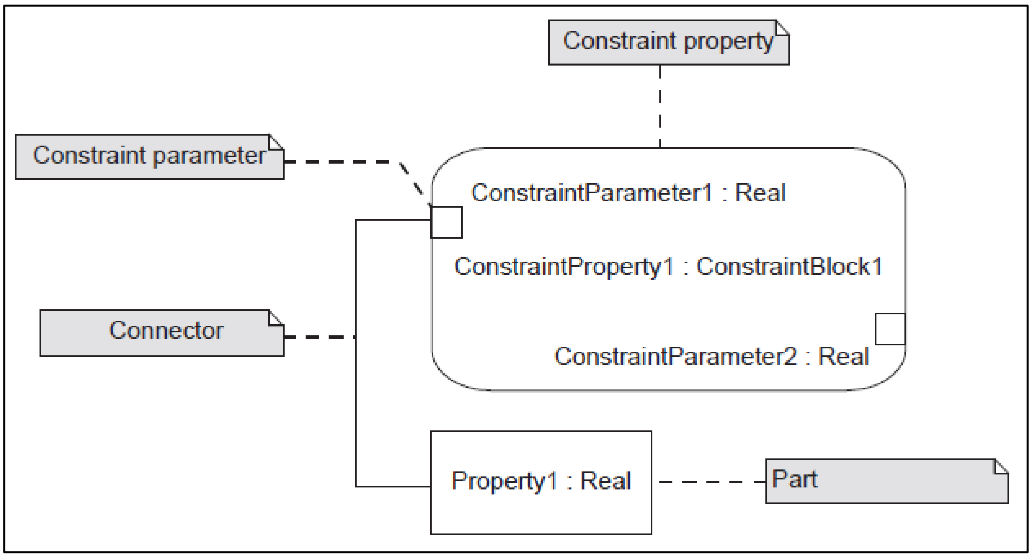

Figure 4.5 Parametric diagram notation
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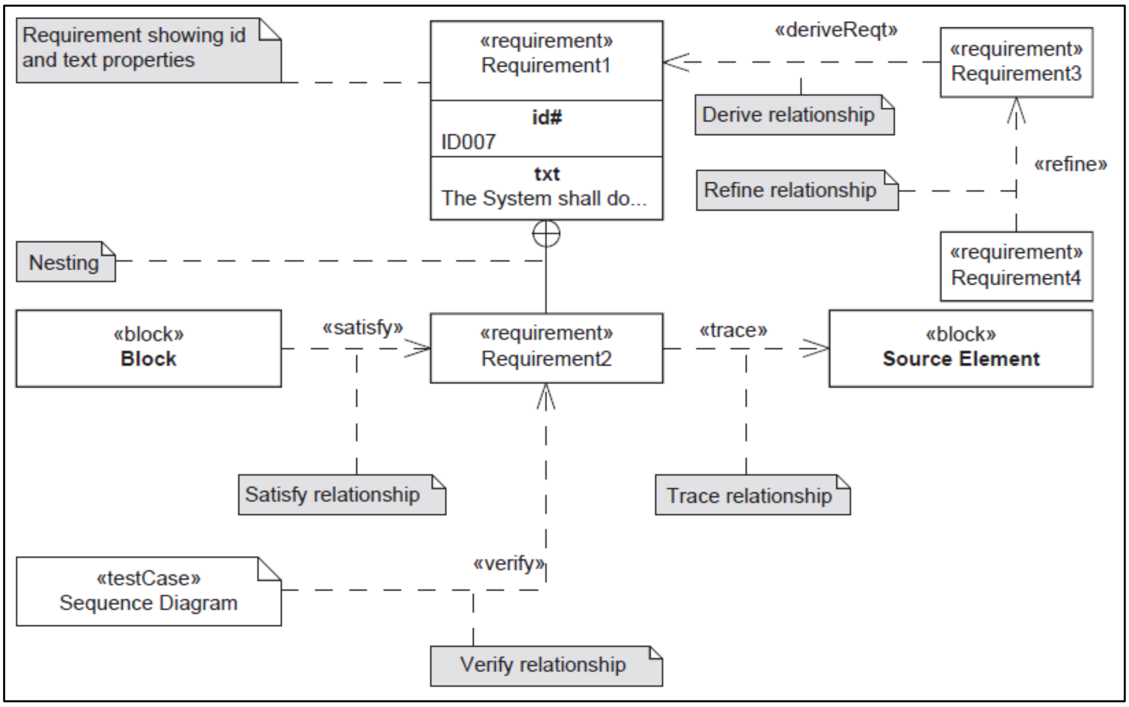

Figure 4.6 Requirement diagram notation
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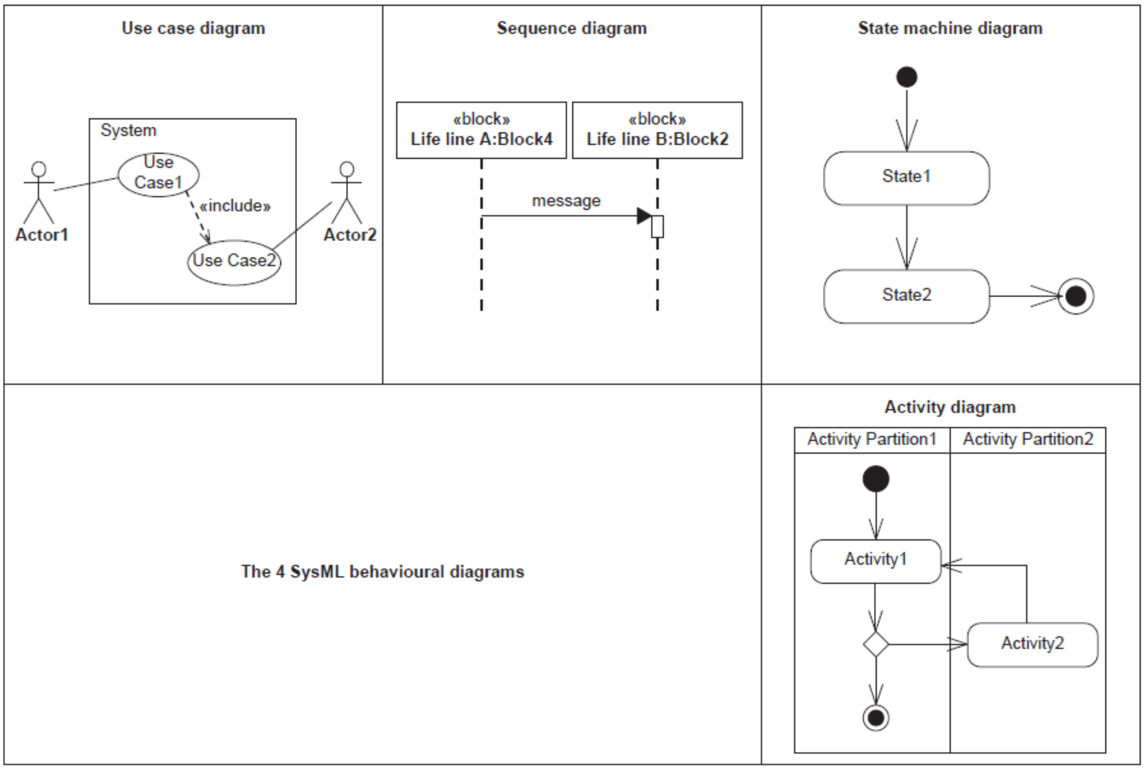

Figure 4.7 Summary of SysML behavioural diagrams
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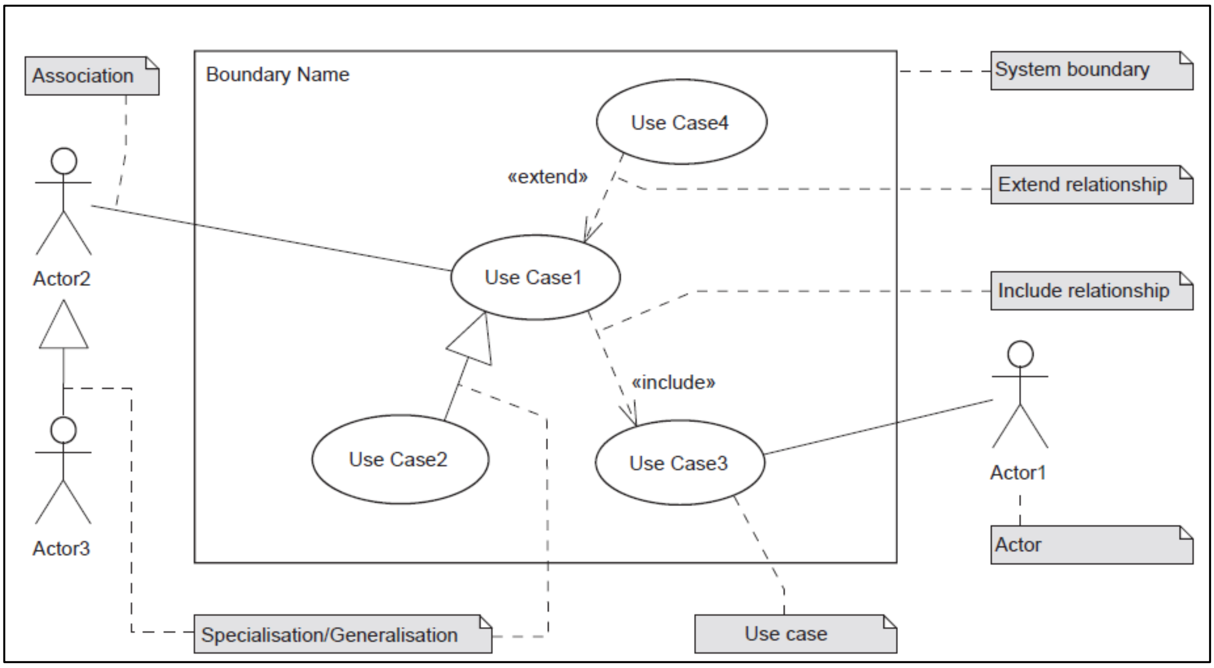


Figure 4.8 Use case diagram notation
Reproduced with permission; Source: (Holt and Perry, 2013)

4.1.5. Architectural Frameworks

An architectural framework provides a systematic and consistent approach for creating system architecture models. Architectural frameworks are based on high level abstractions called system views, with different viewpoints representing different perspectives of the system model (Tang et al., 2004; Perry and Holt, 2014). The architectural framework and the respective viewpoints are selected based on the objectives intended from the system architecture (Tang et al., 2004). The most widely used architectural frameworks include defence frameworks, such as MODAF[3], DODAF[4] and NAF[5], used for enterprise management; in addition to the TOGAF[6] and Zachman frameworks used to develop IT-based enterprise architectures. However, these are not particularly suitable for SoS architectures (Perry and Holt, 2014; Nielsen et al., 2015).

In this context, there are three key differences between SoS and other systems, which means there is a need for a multi-level framework. First, the notion of independence, where system capabilities should be assigned to either requirements for the SoS or one of the CSs. This necessitates that requirements are analysed at both levels. Second, the concept of emergent behaviour at the SoS level resulting from the interaction between CSs. Finally, the concept of system evolution that applies to both levels as well (Holt, S. Perry, et al., 2012).

To model the system architecture for integrated energy systems, an architectural framework adapted from the System-of-Systems Approach to Context-based Requirements Engineering (SoS-ACRE) architectural framework is followed. The adapted framework is presented in detail in Section 4.2.1. The SoS-ACRE framework is a model-based approach to requirements engineering tailored for SoS, where the system model is built around system requirements (Holt, S. Perry, et al., 2012). Accordingly, the system model considers requirements in the context of different points of view. This supports understanding and managing the complexity of requirements while maintaining consistency between the different system views (Holt, S. Perry, et al., 2012). Here, a participatory approach for evaluation is realised where the conceptual system model, which is facilitating the evaluation, is created around contextual stakeholders' requirements (as the name of the architectural framework suggests) and evaluation criteria and indicators eventually reflect those requirements.

The SoS-ACRE framework has a three-fold objective. First, it allows understanding of the context at both the SoS and CSs levels. Second, it facilitates understanding the relations, interactions, and interfaces between the SoS and its CSs. Finally, it aims to define verification and validation criteria to ensure the SoS satisfies its requirements (Holt et al., 2015). Therefore, the main features of this architectural framework support the purposes of this research in highlighting the interactions within and across CSs and with the SoS as a whole. In addition, the architectural framework provides a traceability view that maps requirements with system

[3] The British Ministry of Defence Architecture Framework
[4] The Department of Defense Architecture Framework
[5] NATO Architecture Framework
[6] The Open Group Architecture Framework

components, functions, and measures of effectiveness at different levels leading up to the evaluation.

Table 4.1 presents the architectural views defined by the SoS-ACRE framework (Holt et al., 2015). Not all views need to be realised, but the essential ones according to Holt et al. (2012) are the requirement description view, context definition view and requirement context view. The SoS-ACRE is based on the original ACRE framework but has additional views specific to SoS. These are the context interaction view and the validation interaction view. In the context interaction view, the interactions between the SoS and its CSs are identified by mapping the SoS requirements to the underpinning CSs requirements (Holt et al., 2015). In particular, the CSs requirements that are needed to support the SoS are represented. This link, among others, is captured on the traceability view (Holt, S. Perry, et al., 2012).

Table 4.1 SoS-ACRE architectural views

View	Description
Source Element	includes all relevant source information used to identify system requirements
Requirement Description	includes descriptions of each system requirement, goal, and capability
Rule Set Definition	includes rules that could be applied to each requirement definition
Requirement Context	puts requirements in context by considering them from a specific point of view
Context Definition	defines the points of view considered in the Requirement Context View
Validation	demonstrates how requirements are met or complied with
Traceability	shows explicit traceability links between different elements of the system model
Context Interaction	illustrates the relationships between the Requirement Context Views of all CSs and the SoS
Validation Interaction	combines the Validation Views for several related use case scenarios

4.1.6. Indicator-based Evaluation

The developed framework uses an indicator-based approach for evaluation. In this framework, evaluation criteria and indicators are systematically deduced from the conceptual system model developed and are examined in a Multi-Criteria Analysis (MCA). MCA is both a conceptual framework and a set of techniques, with varying complexity, designed to evaluate different options and guide decision making in line with stakeholders’ preferences (Qureshi et al., 1999). This approach supports the aforementioned systems engineering concepts and methods in delivering the required evaluation principles in practice and is typically used in energy sustainability assessments (Wang et al., 2009; Kumar et al., 2017).

Indicators are a typical means used to facilitate evaluation and aid decision making, as they can convey a complex message in a simplified informative manner, and have an international recognition (Mangoyana et al., 2013). Indicators are trusted for highlighting problems, identifying barriers, and providing insights into the dynamics of the energy system. However, indicators must evolve over time to fit different conditions, priorities and capabilities (Narula and Reddy, 2016). In this context, systems thinking can provide theory for the changes and emergence of system characteristics, which would make relevant evaluation criteria seem redundant later (Williams and Imam, 2007). On the other hand, a limitation for the use of energy indicators as policy instruments is their partial view and simplification of complexity, which would hide multiple dynamic vulnerabilities of the energy system, such as security (Gracceva and Zeniewski, 2014). In this regard, combining a plenitude of indicators with a SoS approach can resolve this limitation, by capturing the variety and complexity involved at different levels of the whole system.

Identifying principles for selecting the appropriate indicators sits at the heart of the process of developing an indicator set. A rigorous and transparent selection process of indicators allows for the conceptual validation and increases the credibility of the evaluation framework (Niemeijer and de Groot, 2008). Selection principles commonly used in literature include measurability, analytical robustness, scientific reliability, validity, policy relevance and sensitivity to changes, exhaustiveness, comparability and data availability (Niemeijer and de Groot, 2008; Patlitzianas et al., 2008). Too few indicators might not be sufficient for the proper evaluation, and too many indicators would be difficult to handle and draw conclusions from (Van Cauwenbergh et al., 2007). In this regard, a systemic approach provides a good conceptual basis to tackle the challenging task of identifying a coherent set of essential indicators but requires extensive knowledge of the whole system.

MCA is a formal approach for evaluation using criteria and indicators (Witt et al., 2020). It is a universal and versatile tool for evaluation that can be utilised as a generic assessment tool for different sustainability issues (Van Cauwenbergh et al., 2007). In line with the holistic SoS approach, MCA can be applied as an evaluation technique that can capture the diversity of perspectives and complexity involved (Troldborg et al., 2014). It provides a multidisciplinary, participatory and transparent framework for policy evaluation (Munda, 2005), and is well suited for supporting decision making when several considerations are of interest, such as in energy policy and planning (Løken, 2007). MCA is considered particularly suitable to examine multi-vector energy systems due to its ability to capture synergies between multiple systems (Løken, 2007). Similarly, it can support understanding the plurality involved in sustainability transitions (Scoones et al., 2020).

MCA can be used either to close down a discussion by aggregation and ranking, or to open it up by a disaggregated set of indicators (Trutnevyte et al., 2012). Upon quantification, indicators can be aggregated into a weighted index or displayed as a set of disaggregated measures. Indices can be easy to interpret and would provide a uniform scale for comparison (Iddrisu and Bhattacharyya, 2015). However, indices are not always robust and different indices addressing the same concept can show inconsistent evaluations (Munda, 2005; Narula and Reddy, 2015). Indices can also mask trade-offs by compensation of bad performance in one dimension by good performance in another (Larsen et al., 2017). Moreover, aggregation requires weighting preferences of different stakeholders', which could pose a political challenge favouring some perspectives and a technical challenge with some of the complex methods used (Cox, 2016). On the other hand, presenting indicators in a disaggregated form such as a dashboard, enables decision makers to realise trade-offs between the different indicators when comparing different scenarios (Hall et al., 2016). Nevertheless, the use of dashboards could be daunting if a large number of indicators is presented (Iddrisu and Bhattacharyya, 2015). In this framework, indicators are presented in a disaggregated form such as a dashboard as it better presents trade-offs and leaves any outcome open for discussion. The approach for representing the results of the evaluation in this research is discussed further in Section 4.2.4.

4.2. Framework Implementation

In order to implement the framework for the evaluation of integrated energy systems, three stages of different methodological activities are coupled in an iterative process of feedback between them (Figure 4.10). The first stage is the conceptual modelling described in Section 4.2.1, the second stage is the scenario formulation described in Section 4.2.2, and the third stage is the quantitative modelling described in Section 4.2.3. The approach followed for the graphical representation of results is discussed in Section 4.2.4.

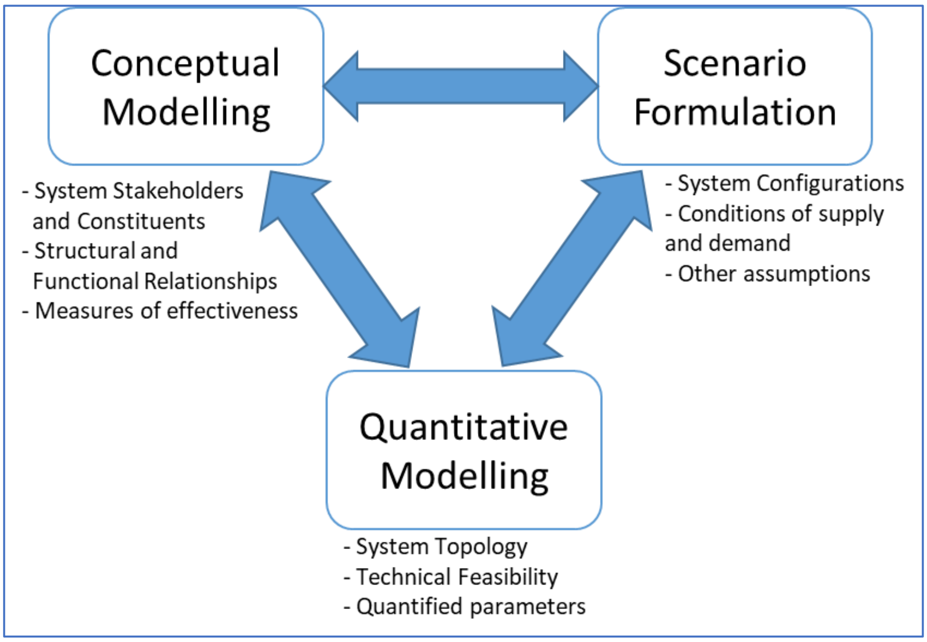


Figure 4.9 Evaluation framework implementation stages

The first stage of the framework implementation is the conceptual system modelling and involves developing a system architecture model using the concepts and methods for the SoS architecture methodology described in Section 4.1. That is, the conceptual system model is developed following a newly established architectural framework, applying a SoS modelling approach, and using MBSE techniques. The conceptual modelling stage comprises creating context, structural and functional diagrams of the system, in addition to identifying the system requirements and measures of effectiveness. The conceptual system model portrays the WES through its stakeholders and CSs, the structural and functional relationships within and across CSs, and the evaluation criteria and indicators.

The first stage is the novel contribution of this research where the WES is reduced in complexity to an abstract representation that facilitates system evaluation as a problem structuring methods. It also embodies the sustainability transitions approach for ESI conceptualised in Chapter 3. Evaluation reflects both contextual objectives at the SoS level and the functional requirements at the CSs level. This shows the performance of the energy systems in delivering capabilities independently and as a whole with respect to stakeholders' requirements. This approach enables evaluation considering different system levels and multiple perspectives. Thus, this stage identifies the relationships and indicators required for the evaluation, through tracing the different requirements to the system functions that fulfil it and components to which the level of fulfilment can be measured.

The second stage of the framework implementation involves scenario formulation, which describes the system under study bearing in mind the scope and objective of the evaluation.

This includes specifying the system configurations (combination of energy networks and technologies), the conditions of energy supply and demand, in addition to any other assumptions to the energy system environment such as for policies, markets, demographics and behavioural changes. Thus, the scenario formulation activity provides the description of the system that is modelled conceptually and quantitatively. This stage can take place before or in parallel with the conceptual modelling stage.

The final stage of the framework implementation is the quantitative system modelling, which combines inputs from the two previous stages with the system topology and physical constraints in mathematical terms and the existing data. The quantitative model demonstrates the technical feasibility of scenarios and provides quantified output parameters assigned in stage 1. Indicators are finally shown in a dashboard to present findings with respect to multiple dimensions without masking trade-offs. Evaluations of different scenarios are compared and analysed to examine whether the targets and objectives can be achieved synergistically or whether they require trade-offs.

The framework implementation is an iterative process with feedback loops between the three stages. For instance, during the conceptual modelling, scenarios could be modified to ensure variability between scenarios while maintaining comparability. Also, scenarios could be modified if rendered infeasible in the quantitive model. Essentially, assumptions across the three stages should be checked for compatibility. Moreover, the feedback between the conceptual model and the quantitative model is mainly around the input and output parameters required to calculate the indicators. This could be affected by the data available, the exogenous variables set to the quantitative model, and the nature of the model itself. Therefore, early communication between the two models is essential to ensure common understanding of what is available and possible and what changes might need to be implemented.

4.2.1. Stage 1: Conceptual Modelling

The first stage of the evaluation framework presented in Figure 4.10 involves developing the conceptual system model, which includes contextual, structural and functional representations of the system, using the systems engineering concepts and methods described in Section 4.1. The conceptual system model portrays the WES through its stakeholders and CSs, the structural and functional relationships within and across its CSs, and the measures of effectiveness for evaluation.

Appropriate evaluation criteria are deduced based on the systems analysis and corresponding indicators are assigned to measure the state of the criteria. The evaluation criteria are related to system requirements at different levels and are traced to the relevant system components or functions that contribute to its satisfaction or fulfilment. Indicators are then assigned by considering what parameters are indicative to measure this extent of satisfaction. Indicators are the measures of effectiveness used eventually for the multidimensional evaluation.

The process starts by identifying an architectural framework guiding the modelling process and the system requirements as inputs to the SoS architecture methodology (Figure 4.11). The architectural framework describes the system views that are needed to develop the conceptual model, which facilitates the evaluation through abstraction and decomposition feeding into the next stages. In this case an architectural framework tailored for the purposes of this research is used.

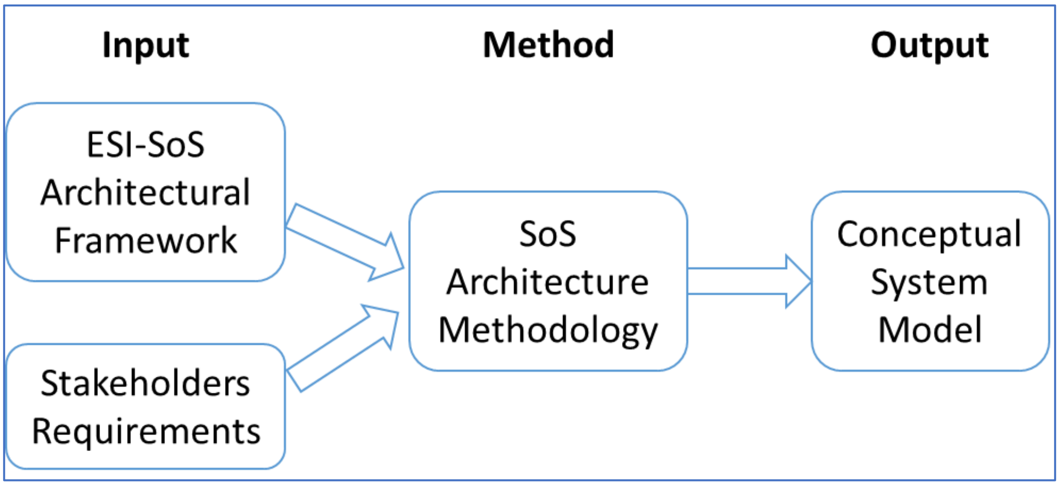


Figure 4.10 Conceptual modelling stage

The ESI-SoS framework, an adapted version of the SoS-ACRE framework described in Section 4.1.5, is established in this research and used to develop the system architecture model for integrated energy systems. The ESI-SoS framework is described in Table 4.2. The relevant views adopted from the SoS-ACRE framework are the context definition, requirement description, requirement context, context interaction, and traceability views. However, additional views that show the structure and composition of the system are added, in addition to a view showing the measures of effectiveness (i.e. indicators). These views are added to clearly show the physical relationships between CSs and system components, since the focus is on the physical system architecture and integration between CSs. Moreover, the additional views support the traceability and evaluation of the system effectiveness in relation to system components as well as requirements. The SysML diagram used to develop each system view is also indicated in Table 4.2.

Table 4.2 ESI-SoS architectural framework

Level	**View**	**Diagram**
Context	Context Definition: Constituent Systems and Stakeholders	Block Definition
System-of-Systems	**Structure**	Internal Block
	Requirements Description	Requirements
	Requirements Context	Use Case
Constituent Systems	**Composition**	Block Definition
	Structure	Internal Block
	Requirements Context Interaction	Use Case
Whole System	Traceability	Requirements
	Measures of Effectiveness	Parametric

The ESI-SoS framework explicitly divides the conceptual system model into four levels. These are the Context, SoS and CSs levels, in addition to a cross-cutting level called the whole system level. At the context level, the CSs and the stakeholders of the SoS are defined (Section 4.2.1.1). At the SoS level, the structure is defined, whereby the relationships between CSs, presented as black boxes, are shown. Moreover, the requirements at this level are defined and put in context using the requirement description and requirement context views, respectively (Section 4.2.1.2). Similarly, the composition and the structure of the CSs are defined at the CSs level. The composition defines the system elements making up each of the CSs and the structure shows the relationships between the system elements across the CSs (Section 4.2.1.3). Lastly, the whole system level includes two views (Section 4.2.1.4). The first view is the traceability view where requirements at both the SoS and CSs levels are related to different system components and functions at different levels. The relations include tracing back the requirements to the component where it could be measured or to the functionality that satisfies it. The final view shows indicators used to measure the system effectiveness in satisfying the system requirements defined in the requirements description view.

Although the system views are presented in a specific sequence from a higher system level to a lower one, the process of developing those views is iterative. One might move from one system view and one system level back to another to make the whole system model complete and consistent. Each level is further described in the following subsections, but is demonstrated case study applications in the coming chapters.

4.2.1.1. Context Level

The first step in the ESI-SoS architectural framework presented in Table 4.3 is setting the context and defining the system to be evaluated. At the context level, the system boundaries are specified in order to identify what is considered inside and outside of the system, thus its CSs and the stakeholders composing its environment. This enables the identification of the system requirements corresponding to the stakeholders' needs. Block definition diagrams are used to show the composition of the system and its stakeholders. At this level also, the perspectives to be considered are identified. These could be for instance the technical, economic, environmental, regulatory, and social aspects.

For example, the focus of the evaluation could be the physical system architecture of ESI. In this case, the boundaries would mainly include the physical aspects of the energy system. Accordingly, the CSs would be the electricity, gas, heat, and transport physical systems involved, in addition to integration enablers or coupling components, such as CHP, P2X, HPs and EVs. On the other hand, the system environment would include stakeholders affecting or affected by the system, in other words, having some control on the system or requirements from it. This typically includes actors from policy, environment, markets, and society, and therefore reflect the political, environmental, economic and social perspectives.

4.2.1.2. System-of-Systems Level

The second step is developing system views for the SoS level, where the structure and requirements of the system as a whole are shown, i.e. showing each CS as a black box. The structure at this level follows from the composition shown at the context level, but with a closer look at how the CSs are linked. This is carried out using an internal block diagram, showing the relationships and flows between the different CSs. Flows could be generally physical, commercial or informational.

At this SoS level, requirements are related to the perspectives introduced in the context level. Requirements are first defined in the requirements description diagram and are then shown in relation to stakeholders in the requirements context view. Requirements could be technical features that are expected from the system as a whole, such as resilience, flexibility and interoperability. For instance, the whole system resilience is resilience across CSs, since it is enhanced by operational flexibility which could be fulfilled through structural and organisational interoperability of different CSs, where interactions typically involve exchange of energy and information. Furthermore, requirements of stakeholders reflecting other perspectives can be considered as contextual objectives of the energy system as set by external actors. These could be objectives or constraints related to political concerns, environmental regulations, economic considerations, and social acceptability. Hereby, multiple dimensions such as those presented in Table 2.2 can be accounted for in this framework.

At this level, requirements refer to functions or capabilities that the SoS should deliver or acquire to satisfy the needs of the corresponding stakeholders. Requirements are thus presented in a use case diagram that shows the desired functions or features of the SoS which are linked to external stakeholders, showing the SoS capabilities from different users' perspectives. Requirements can be also linked to one another with some requirements constraining others or being an extension to others. Use cases provide context to requirements by showing how the system can be used, and help understand SoS functions, requirements and capability gaps. In this framework, requirements at the SoS level are mainly non-functional requirements.

4.2.1.3. Constituent System Level

The next level is the CS level. First, the composition of each CS is defined in terms of its system elements using a block definition diagram. For instance, the electricity system can be further broken down at this level to include the components for primary energy resources, generation, transmission, distribution, and storage. Then, the system structure at this level is shown using an internal block diagram. This is similar to the structure diagram at the SoS level but shows the interrelationships between the system elements across CSs.

Additionally, the requirements context interaction is described in a use case diagram. Requirements at this level relate to the independent functionality of each CS, in addition to the functionalities supported by the CSs that contribute to achieving the requirements the SoS has to deliver. Accordingly, requirements at this level are associated with other CSs and with the SoS as a whole. Those contributions mainly emerge from the interaction between the different CSs. For instance, the coupling system comprising ESI technologies can deliver flexibility to the SoS through energy vector shifting between the different CSs. Moreover, using CHP and HPs is expected to reduce the overall energy use. Using P2X can also provide networks services by relieving network constraints across vectors, and thus could delay network upgrades and reduce costs and losses. Therefore, in this framework, the requirements at the CS level are predominantly functional requirements.

A lower system level that is not included in the ESI-SoS architectural framework can be modelled if needed, where each of the CS elements is further decomposed into different technologies. For instance, within the electricity system, various primary energy resources exist (gas, uranium, wind, solar radiance etc.) and accordingly different generation technologies are applied, such as gas-fired turbines, nuclear reactors, wind turbines and solar PV. Therefore, the composition of the different CSs and the properties of their system elements could also be viewed using block definition diagrams. This could be relevant if particular technologies are of interest, where each of those technologies have different attributes that impact higher levels of the system in a different way. In this framework, however, a technology agnostic approach is taken when it comes to the system element level. For instance, looking at the components of the coupling system, different technologies exist for heat pumps (air-sourced and ground-sourced) and P2X (types of electrolysers and pathways) as discussed in Section 1.2. The same applies to storage technologies for the other CSs. The variations of those are not directly considered in this project.

4.2.1.4. Whole System Level

Finally, two views including components from both the SoS and CSs levels are presented at the whole system level. The first view is the traceability view where requirements at both the SoS and CSs levels are related to different system components and functions at different levels. The relations include tracing back the requirements to the component where it could be measured or to the functionality that satisfies it. The traceability view can therefore support the realisation of possible trade-offs and synergies between the different system components. Accordingly, the final view shows indicators used to measure the system effectiveness in satisfying the system requirements defined in the requirements description view. This includes parameters and indicators used to measure the level of satisfaction of the system requirements defined in the requirement description view. The traceability and measures of effectiveness views are developed using requirements and parametric diagrams, respectively.

A pool of potential suitable indicators can be retrieved from the literature (e.g. Appendix A), but the choice of the exact indicators depends partially on the two other stages. Depending on how the scenarios are formulated, indicators could be relative or absolute; and depending on the data availability and the quantitative models output, different indicators could be measured or calculated. At this point, the process could involve iteration; going back and forth to the data available and the simulation models used to check what could actually be measured or computed.

4.2.2. Stage 2: Scenario Formulation

The scenario formulation stage describes the system under study bearing in mind the scope and objective of the evaluation. This includes specifying the system configurations (combination of energy networks and technologies), the conditions of energy supply and demand, in addition to any other assumptions to the conditions surrounding the energy system such as for policies, markets, demographics and behavioural changes. Thus, the scenario formulation stage provides the description of the system that is modelled conceptually and quantitatively.

It is a challenging task to identify the best types of scenarios suitable for the developed evaluation framework given the diverse typology of those. In the following, some distinctions between scenario types identified in the literature are presented, before explaining where the developed framework can be of most value.

One taxonomy for energy system scenarios is distniguishing between three types: (Kowalski et al., 2009)

- Extrapolatory scenarios that aim to forecast the future based on past trends
- Normative scenarios that aim to investigate the actions required to achieve a specific target
- Exploratory scenarios that aim to explore the possible future space of options

Exploratory scenarios can typically combine qualitative features through a storyline and quantitative features through indicators for evaluation. This combination facilitates understanding how energy systems work and evolve more comprehensively to inform decision making (Kowalski et al., 2009).

Another taxonomy presents a different categorisation of energy scenarios based on different methodological approaches: (Hughes & Strachan, 2010)

- Trend based studies, with scenarios developed around different combinations of broad, high level extrapolated trends, sometime arranged within a 2x2 matrix.
- Technical Feasibility studies, with scenarios based around demonstrating the technical feasibility of the energy system in meeting energy demands and other constraints such as decarbonisation targets. Those studies typically include normative scenarios.
- Modelling Studies, with scenarios being directly related to model runs as inputs or outputs, and usually focus on the whole energy system. In some cases, the scenarios are coupled with elaborative, qualitative storylines, and could be normative or explorative.

It is worth noting that the above categorisations are not discrete and overlaps are encountered in many studies. For instance, scenarios could have both exploratory and normative features for different aspects. Moreover, modelling studies include investigations of technical feasibility (Hughes & Strachan, 2010).

The developed evaluation framework is theoretically compatible to any type of scenario, given that scenarios are consistent and comparable. However, due to the ability of the conceptual system modelling, which makes up the core of the framework, to capture future structural and functional changes and interactions, and the embodied representation of the sustainability transitions approach (whole system reconfigurations) described in Chapter 3, the value of the framework is mostly exploited when comparing scenarios with different system configurations.

In line with the WES approach, scenarios developed for modelling studies, which show both normative and explorative features, could be the most suitable for the evaluation framework. For instance, scenarios could explore the impact of employing energy systems integration under exogenous constraints such as achieving net-zero emission targets, or under different supply and demand conditions. The latter could be influenced by changes to the RES capacity or variations to the peak demand levels.

Note that the type of scenarios formulated can dictate the choice of evaluation criteria and indicators. For instance, criteria can typically be objective focused (translation of objectives into criteria) or alternative focused (highlighting strengths and weaknesses of each alternative) (Trutnevyte et al., 2012). In this framework, criteria will highlight both approaches by reflecting the transition objectives and system requirements identified in the first stage at the different levels, and the variation between alternative system configurations through the scenario formulation. Thus, the system is evaluated against both: (i) the contextual objectives manifested as non-functional requirements at the SoS level and (ii) the functional requirements identified in the first stage at the CS level. This shows the performance of the integrated energy systems in delivering capabilities independently and as a whole. In line with this, indicators are grouped thematically into broader dimensions (e.g. the energy trilemma) to link them with objectives and monitor progress (Narula and Reddy, 2016).

4.2.3. Stage 3: Quantitative Modelling

Stage 3 of the framework implementation presented in Figure 4.10 involves quantitative system modelling through, for example, energy simulation models. At this stage, inputs from the two previous stages are combined with the system topology and physical constraints in mathematical terms and existing system data, to identify the technical feasibility and provide quantified output parameters.

Scenarios should be translated from narrative storylines to a set of quantitative input parameters to quantitative models. This process is again iterative and includes many simplifications and assumptions depending on the energy model capabilities and on the data availability. Storylines can reflect aspects such as the exogenous context of the system environment, exogenous modelling assumptions, or aspirational targets for the future energy system. Accordingly, multiple diverse models may be needed to address the various aspects outlined in the storyline

(Trutnevyte et al., 2014). It is therefore important in this case to consider the type of modelling used in the analysis at the stage of scenario formulation.

Several types of energy quantitative models have been identified in the literature. These are mainly divided around two dichotomies. First, the distinction between simulation and optimisation models. Simulation models aim primarily to provide forecasts of how the system may evolve, while optimisation models aim primarily to provide scenarios of how the system could evolve. Second, the distinction between operational and planning models. Operational models aim to calculate energy flows and dispatching in different networks while ensuring that networks meet the energy demand without violating operational constraints. On the other hand, planning models consider investment planning of different assets, such as generation capacity expansion and network upgrades, in terms of size, cost and location (Pfenninger et al., 2014; Hosseini et al., 2020).

It is common to associate simulation models with operational models and optimisation models with planning models. However, this is not always the case, as there are models that involve different combinations. For instance, optimal dispatch models that consider the optimal operational scheduling of the energy system with a minimum operational cost as the objective function, while ensuring that operational constraints are not violated (Hosseini et al., 2020). Furthermore, there are hybrid models that combine planning and operational perspectives into one model or through soft linking (Pfenninger et al., 2014; Mancarella, 2014). Note that this discussion applies to both independent electricity system modelling and integrated energy systems modelling.

Essentially, the decisive factor for the suitability of which type of quantitative energy models with the developed framework is the purpose of the evaluation. Different energy models serve different purposes and timescales, and eventually provide information to different decision makers (Hughes and Strachan, 2010). Therefore, it is only possible to judge on the suitability of models with the developed framework in the scope of the evaluation objective. A discussion on the best suitable type of quantitative modelling in the case of this project, where the objective is to evaluate the effectiveness of ESI in achieving the energy transition objectives, is presented upon testing and demonstrating the framework in Chapters 5 and 7.

Findings of different scenarios are finally compared and analysed to examine whether objectives can be achieved synergistically upon ESI or whether they require trade-offs. The performance of integrated systems can be evaluated either against set targets or as improvements relative to a baseline scenario, for example one with no integration between energy systems.

4.2.4. Representation of Results

Upon quantification, a graphical representation (visualisation) of the results is created. The main goal of this is to facilitate the analysis and interpretation of the indicators and the effective communication of the outcome of the evaluation (Lea et al., 2018), in line with one of the BellagioSTAMP principles described in Chapter 1. A balance between oversimplification of a complex issue and the problematic complexity in analysis and communication is provided by a dashboard representation of indicators involving a manageable number of indicators that are not weighted or aggregated into an index (Cox, 2016). The dashboard approach is also in line with the multidimensional and systematic WES principles whereby a diverse set of indicators is incorporated and a transparent and replicable evaluation is enabled.

In this research, indicators are presented in a dashboard, i.e. without aggregation. This approach is followed for two reasons as discussed in Section 4.1.6. First, to be able to understand trade-offs and synergies between different indicators, which are otherwise masked through aggregation. This has been discussed as part of the multidimensional principle in Chapter 2. Second, to use the indicators and the evaluation as supporting evidence to open up the socio-political discussion about future pathways and alternative configurations, rather than closing it down with a clear cut ranking.

A dashboard approach is typically used for performance evaluation but does not require rigid causal or hierarchical relationships among the indicators in its setup (Lea et al., 2018). However, this is complemented in this framework by the traceability view of the conceptual system model, which is a graphical representation of the structural and functional relationships between different system components, requirements (evaluation criteria), and measures of effectiveness (indicators). Thus, the traceability view, which can be considered a condensed summary of the conceptual system model, drives the different diagrams used in the visualisation. This is demonstrated in practice in Chapter 7.

The proposed dashboard that is used later in Chapter 7 includes first a tabular representation of indicators in their original units for all scenarios under study. This allows investigating the progress of individual indicators and their variability across scenarios, if required. The second part is presenting all indicators for all scenarios in a radar chart to ease comparison. A radar chart, also known as spider, web or amoeba chart, visualises multiple variables with each variable plotted on its own axis resulting in a polygon. All axes are arranged radially, starting at the centre with equal distances between one another, and have the same scale (Döbler and Großmann, 2020). Thus, indicators in this case are normalised. A radar chart has been used in similar energy evaluation studies such as in (Agusdinata and Dittmar, 2009; Frangopoulos and Keramioti, 2010; Hadian and Madani, 2015; Iddrisu and Bhattacharyya, 2015; Mainali and Silveira, 2015). It is suggested to display no more than 10 indicators on a single radar chart and to display each variable in a separate plot as well to maintain clarity (Döbler and Großmann, 2020). The radar chart is therefore associated with bar or line plots of individual indicators, or multiple indicators in relation to each other as required. The latter are mainly chosen based on the relations in the traceability diagram.

4.3. Summary

A methodological framework is developed to address the gaps previously identified in evaluating future integrated energy systems and to operationalise the socio-technical transitions approach for ESI. The framework is designed based on concepts and methods from systems engineering enabled by the SoS conceptualisation of ESI. Those are combined for a methodological framework that addresses the WES evaluation principles. First, the system architecture description of the technical components of the energy system and future system conditions, and the system requirements representation of stakeholders' perspectives deliver on the principles for being multidimensional and futuristic. Second, the SoS modelling approach decomposing the system into its different levels and components allows the evaluation to be multivectoral and systemic. Finally, MBSE and an architectural framework provide a systematic guide for conceptual modelling, while applicability relies mainly on the data availability and quantitative models suitability for measuring indicators.

The framework is implemented by coupling three methodological stages: conceptual system modelling, scenario formulation, and quantitative modelling. The implementation involves iterations and feedback within and between the three stages. The first stage is the conceptual system modelling stage where the system stakeholders, constituent systems, structure, requirements, and measures of effectiveness are described. This stage includes the deduction of evaluation criteria and indicators. Criteria reflect stakeholders' requirements and indicators are assigned to measure the level of satisfaction of those requirements. This is done by tracing the system requirements to the relevant functionalities delivered by the system and the capabilities it acquires, and to the components from which indicators are measured.

The conceptual modelling is based on the SoS architecture methodology and is guided by the ESI-SoS architectural framework developed in this research. This enables the creation of diagrams that show:

- the SoS structure and composition in terms of CSs (e.g. electricity, gas, heat, coupling technologies)
- the CSs composition in terms of system elements (e.g. generation, networks, individual technologies)
- the systems stakeholders involved (e.g. local government, local community, system operators, end-users, prosumers)
- system requirements reflecting the non-functional relationships between stakeholders and the SoS (e.g. energy trilemma objectives)
- system requirements reflecting the functional relationships among the CSs and with the SoS (e.g. delivering energy, transforming energy, providing network services, etc.)
- the tracing of the system functions, components, requirements and indicators

The second stage is the scenario formulation in which alternative system configurations, varying conditions of energy supply and demand, and other assumptions related to the system environment are specified. The third stage is the quantitative modelling that represent the same system topology and conditions to quantify the performance and relationships, and consequently the indicators for evaluation.

As a result, the developed framework provides a method to encompass stakeholders' perspectives in evaluating the effectiveness of a socio-technical pathway that involves multi-systems interactions towards achieving the transition objectives. The evaluation is conducted using metrics that hold behind it a reduced representation of the complex system architecture, including structural and functional interlinkages.

The developed framework is tested and validated through a case study and feedback from experts in Chapter 5. Improvements are accordingly implemented, of which mainly is presenting a standard approach to use the framework for evaluation flexibly and without the need to develop a conceptual model from scratch. This is provided through a Reference System Architecture Model (RSAM) presented in Chapter 6, which provides a modular template to use in stage 1 of the framework. Finally, a full-scale application of the evaluation framework and the RSAM on another case study is presented in Chapter 7.

Chapter 5 Framework Testing and Validation

In this chapter, the evaluation framework described in Chapter 4 is tested using an operational model for the local energy system in Findhorn village, Scotland. Two case studies are presented to consider different system configurations with various heating and energy storage technologies under different supply and demand conditions. The first case study is based on the integrated energy network model and scenarios for delivering heat in Findhorn developed in (Hosseini, Allahham and Adams, 2021). The second case study is based on the integrated energy network model for Findhorn considering the impact of energy storage technologies and some of the scenarios developed in (Hosseini, Allahham, Vahidinasab, et al., 2021). The model algorithms and parameters for the two case studies are presented in Appendix B.

The two case studies have a number of limitations that are discussed later in this chapter. Hence, the aim is to present the gradual testing of the evaluation framework stages and the learning encountered earlier in the project, rather than a full case study application. The objectives of the two test case studies presented in this chapter are summarised as follows:

- Apply the conceptual modelling approach for different combinations of integrated energy technologies (stages 1 and 2 of the framework implementation)
- Observe patterns to develop a generalised conceptual system model (‘Reference System Architecture Model’) of integrated energy systems for standard use in stage 1 of the framework implementation
- Trial the application of stage 3 of the framework implementation with quantitative models
- Demonstrate the evaluation framework application for the expert’s validation workshop

After testing, the evaluation framework is validated in terms of its design, output and end-use, through feedback received from experts in a virtual group interview, which is based on the preliminary findings from the test case studies presented in this chapter. Learnings from the case studies and the validation workshop have been used to implement necessary improvements to the framework in a full case study presented in Chapter 7. This mainly relates to the development of a consistent, standardised way to the application of the framework through a Reference System Architecture Model (RSAM) for stage 1 described in Chapter 6. Additional improvements have been made to the framework implementation description including the interaction between the three stages, and the suitable types of scenarios and quantitative models, as currently presented in Chapter 4 (Figure 5.1).

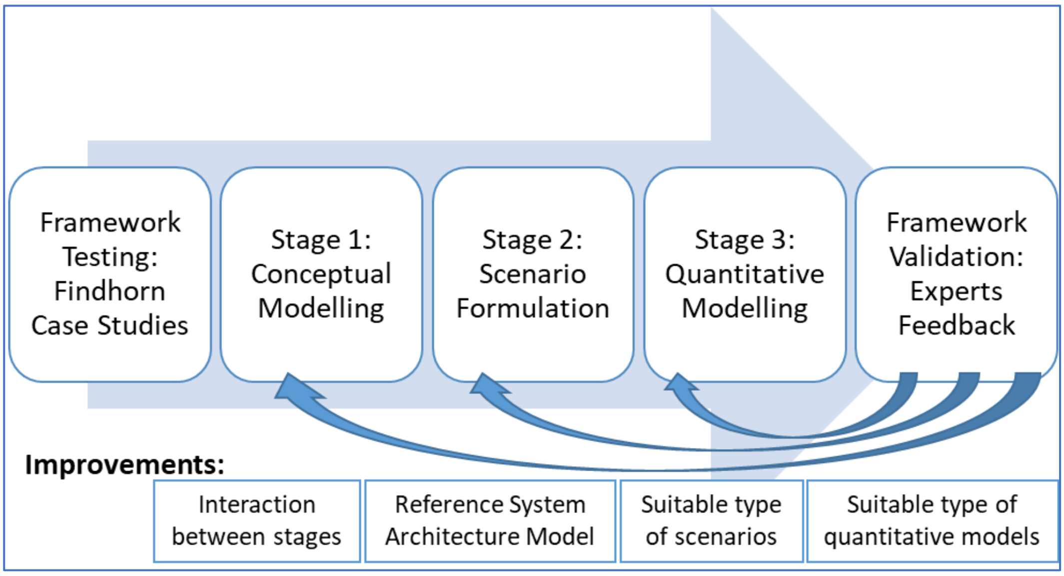


Figure 5.1 Framework testing and validation

The outline for the rest of this chapter is as follows:

- Case Study Description (Section 5.1)
- Findhorn Heat Case Study (Section 5.2)
- Findhorn Storage Case Study (Section 5.3)
- Framework Validation (Section 5.4)
- Summary (Section 5.5.)

5.1. Case Study Description

5.1.1. Energy System Overview

Findhorn is a small ecovillage located in Moray, Scotland, with around 300 residents and 120 dwellings. The village serves as a rural area demonstrator for research and real-world case studies in CESI. In terms of energy, the village is connected to the electricity distribution network and also benefits from electricity generated by a small community-owned wind farm (675 kW) and dispersed rooftop solar PV (75 kW). However, the village is not connected to a gas distribution network. Hence, the heat load is met by a mixture of technologies including gas boilers, electric heaters, air-sourced and ground-sourced heat pumps, and biomass-fired district heating.

The data available for the village include electricity and heat loads, and wind and solar generation in 5-min time steps for a typical winter week (w/c 23rd February 2015). The data include both domestic and commercial buildings. The load and generation profiles are presented in Figure 5.2. Those are used as a baseline for the analysis.

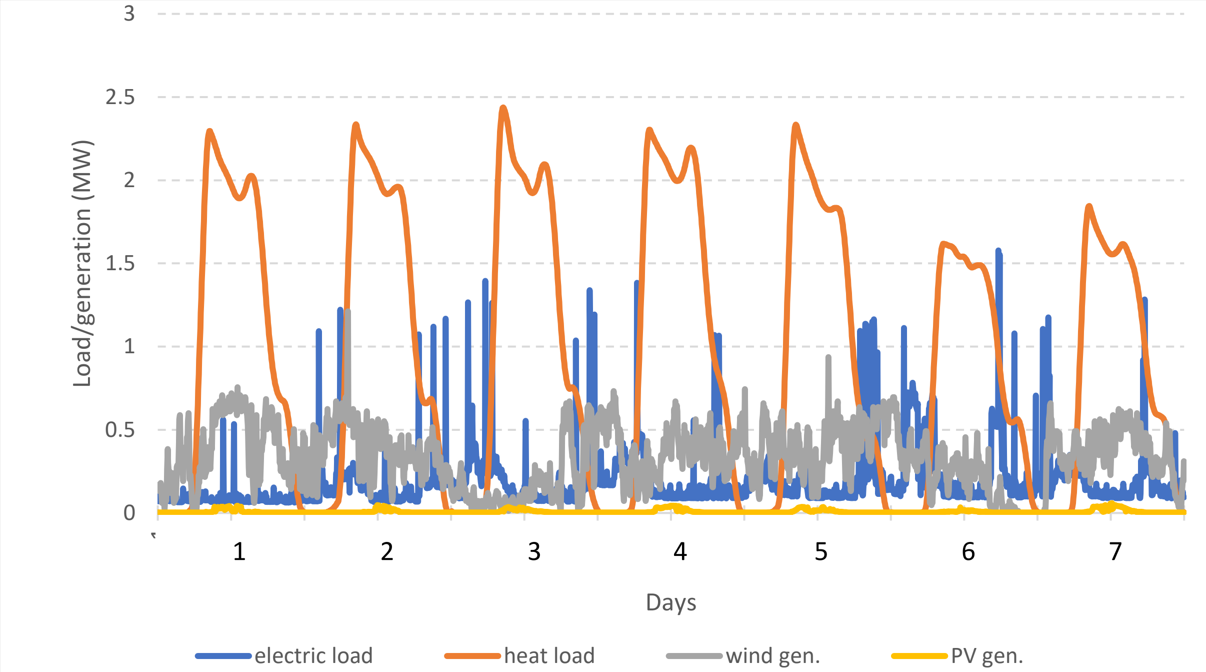


Figure 5.2 Baseline load and generation profiles for a typical winter week in Findhorn

The integrated network model used for this analysis is an operational simulation model for energy (power, gas, heat) flow analysis. For this simulation model, the village is divided into 6 zones, each of which corresponds to a final electricity and heat load point. The total electricity and heat loads for each zone is considered as a lumped load of the zone. For each zone a node/bus is considered and the lumped load is placed in correspondence. Note that a hypothetical gas distribution network was designed and added to the model to consider in the scenario analysis. For this, a gas node was considered for each zone and the gas load, which was calculated based on the heat load, was placed on the node (Hosseini, Allahham, Vahidinasab, et al., 2021). A schematic of the integrated energy network for the heat and storage case studies is provided in Figure 5.3.

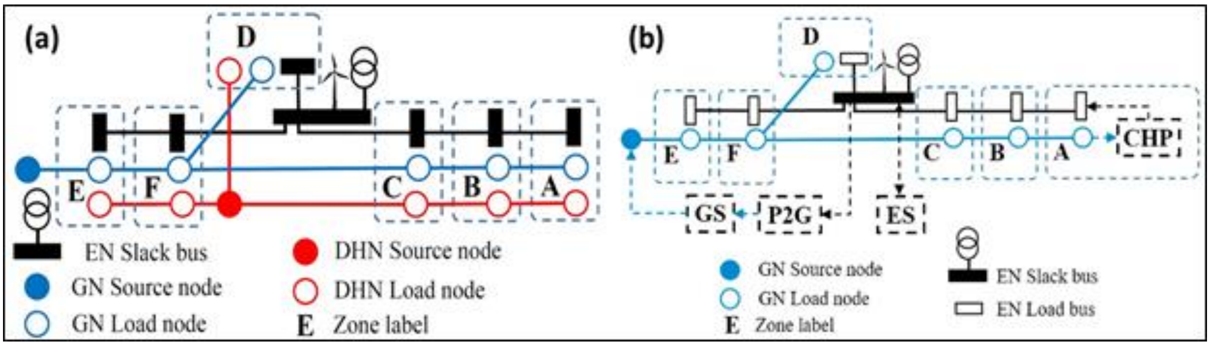


Figure 5.3 Schematic of the integrated energy network in Findhorn for the (a) heat and (b) storage case studies; Abbreviations: EN: Electricity Network, GN: Gas Network, DHN: District Heating Network; Sources: (Hosseini, Allahham and Adams, 2021; Hosseini, Allahham, Walker, et al., 2021) *Reproduced with permission*

Based on the available model and data, two case studies are carried out on the Findhorn local energy system. The first examines different system configurations and technologies to deliver heat, described briefly in Section 5.1.2. The second examines different system configurations with energy storage technologies, described briefly in Section 5.1.3. The two case studies are analysed to include a range of different energy technologies and coupling technologies at different levels. This constitutes the scenario formulation stage of the evaluation framework. Limitations to the two case studies are discussed in Section 5.1.4. The full evaluation framework implementation as outlined in Chapter 4 for the two case studies is demonstrated in Sections 5.2 and 5.3, respectively.

5.1.2. Heat Case Study

In the first case study, different system configurations and technologies to deliver heat to the end-users are considered, as described in Table 5.1. Scenarios are formulated as a combination thereof, as presented in Table 5.2, all under baseline conditions for supply and demand. The simulation model parameters and algorithms used for this case study are presented in (Hosseini, Allahham and Adams, 2021) and given in Appendix B. Those are summarised as follows. The model inputs include the network topology, load and generation profiles, performance factors for energy technologies, and unit factors for cost and emissions. The model runs a number of mathematical equations representing the flows in each energy network along with the representations for the different energy technologies and connections involved, to provide the operational costs, carbon emissions, and energy flow values as outputs.

Table 5.1 Findhorn heating technologies and networks

Heating Technology	Networks meeting heat load
Gas Boiler	Gas Network
Electric Heater	Electricity Network
Air-sourced Heat Pump (ASHP)	Electricity Network
Ground-sourced Heat Pump (GSHP)	District Heating Network (DHN)
Combined Heat and Power	DHN

Table 5.2 Findhorn heat case study scenarios

Scenario	Technologies meeting heat load	Networks meeting heat load
1	All gas – Gas Boilers	Gas Network
2	All electric – Electric Heaters	Electricity Network
3	Gas & electric – Gas Boilers and ASHP	Gas and Electricity Networks
4	GSHP with Electric Heaters at DHN source	DHN
5	CHP	DHN
6	GSHP and Electric Heaters at final load	Electricity and DHN
7	GSHP and Gas Boilers at final load	Gas and DHN

5.1.3. Storage Case Study

In the second case study, energy storage technologies are incorporated into the integrated energy network, including single-vector storage for electricity and gas, and cross-vector storage through P2G technology. In addition to P2G, CHP is considered in this case study as a coupling component between the electricity and gas networks. Scenarios are formulated as a combination of those technologies to understand the impact of storage on the integrated energy system, with various supply and demand conditions, as summarised in Table 5.3.

A total of 16 scenarios are generated as a combination of the four different configurations and the four varying supply and demand conditions. The load increase or decrease indicate a 20% change in value from the baseline case, while the change in RES supply indicates a 100% increase or decrease in value.

Table 5.3 Findhorn storage configurations and supply and demand conditions

No.	System Configuration	No.	Supply and Demand Conditions	
			RES Supply	**Load**
1	No integration / No storage	1	Baseline	Baseline
2	No integration / Electric storage	2	Baseline	20% increase
3	Integration via CHP & P2G / No storage	3	100% decrease	20% increase
4	Integration via CHP & P2G / Electric storage	4	100% increase	20% decrease

The model used for this case study is similar to the one used for the heat case study except with the addition of energy storage technologies. Hence, the model incorporates inputs related to energy storage performance factors, mathematical formulations representing energy storage management, and outputs related to the energy flow through storage technologies. The model parameters and algorithms used for this case study are presented in (Hosseini, Allahham, Vahidinasab, et al., 2021) and given in Appendix B.

5.1.4. Limitations

A number of issues exist that make the Findhorn case studies presented in this chapter limited in value beyond testing of the framework. First, the size of the existing energy networks in Findhorn is sufficient to accommodate any reasonable changes relative to the existing load and generation profiles with minimal impact. Thus, the value of ESI could not be captured under conditions of system stress. Second, the quantitative model used for the analysis in the two case studies show some limitations in the scope of the evaluation. As mentioned, this has been used for testing the developed framework based on the available resources at the time and to trial the different possible options.

The model is an operational model as opposed to a planning model. Therefore, the model only accounts for operational costs with no capital costs. Accounting for capital costs is relevant to the evaluation when comparing different investment options for different system configurations in the implementation of ESI. Moreover, the operational model uses assumptions on the capacity sizes of energy generation and storage assets and coupling components, which might not be based on optimal decisions. Furthermore, the model used is a simulation model that doesn't necessarily make optimal choices on the energy dispatch but rather ensures the system operates properly (within constraints) under a set of exogenous values. Therefore, any reflection of the capacity values or the exogenous constraints in the evaluation is not necessarily indicative. Similarly, the scenarios have not been initially designed for the purpose of this evaluation but are used here to consider different options for the framework application.

The aforementioned limitations imply that the two case studies described in the following subsections are carried out to fulfil the objectives outlined at the beginning of this chapter. Thus, as a gradual testing and learning process to demonstrate and validate the evaluation framework stages without focusing on the empirical soundness of results. Accordingly, the heat case study presented in Section 5.2 aims to demonstrate stages 1 and 2 of the framework implementation, where the conceptual system model is developed for different combinations of heating technologies. Additionally, it aims to get the first glimpse of the issues and data exchanges that need to be considered for the coupling of the conceptual model with quantitative models. Those issues are then carried to the storage case study, in order to try and address them. Therefore, the storage case study presented in Section 5.3, in addition to presenting the conceptual system model for different combinations of storage technologies, aims to show more of stage 3 of the framework with results for different scenarios. Those tasks led to:

- demonstrating the framework application to the experts' validation workshop (Section 5.4)
- creating the RSAM (Chapter 6)
- developing a clearer view on coupling the conceptual system model with scenario formulation and quantitative models for the framework implementation, and the suitable types thereof (Section 4.2)
- using the learnings and feedback to improve the framework and apply it to a full case study (Chapter 7)

5.2. Findhorn Heat Case Study

Two scenarios for the Findhorn heat case study are selected to demonstrate the conceptual modelling and scenario formulation stages of the evaluation framework presented in Figure 4.10. Those are scenarios 1 and 7 from Table 5.2. Scenario 1, which represents the baseline scenario, involves a separate operation of the electricity and gas networks, while scenario 7 includes the electricity, heat and gas systems, in addition to the coupling system. The conceptual system model is developed for the two scenarios following the ESI-SoS architectural framework in Table 4.2. The system views at each level are presented in conjunction to ease comparison between the two scenarios. The conceptual system model diagrams are developed using SysML stencils in Microsoft Visio and colour coding is used to ease the navigation between diagrams.

5.2.1. Context Level

Stage 1 of the evaluation framework is the conceptual modelling stage. This stage starts with defining the system in terms of its CSs and stakeholders at the context level. For scenario 1, the electricity and gas systems are the only systems available (Figure 5.4), while for scenario 7, the CSs include the electricity, gas, heat and coupling systems (Figure 5.5). The system stakeholders are the same across all scenarios and are identified in this case study to be the local council, local community, network operators, and end-users (Figure 5.6).

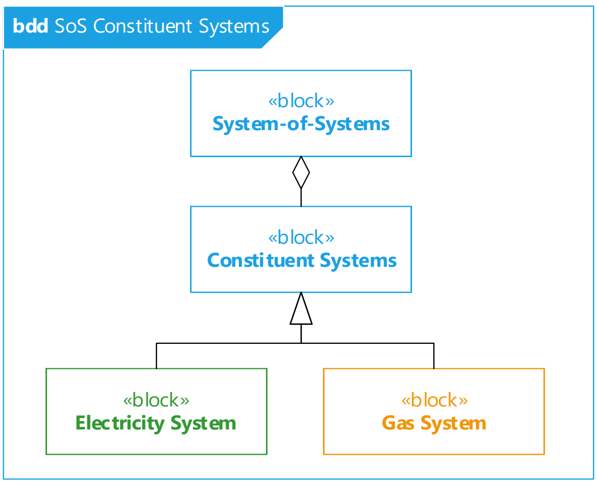


Figure 5.4 Constituent systems: Findhorn heat scenario 1

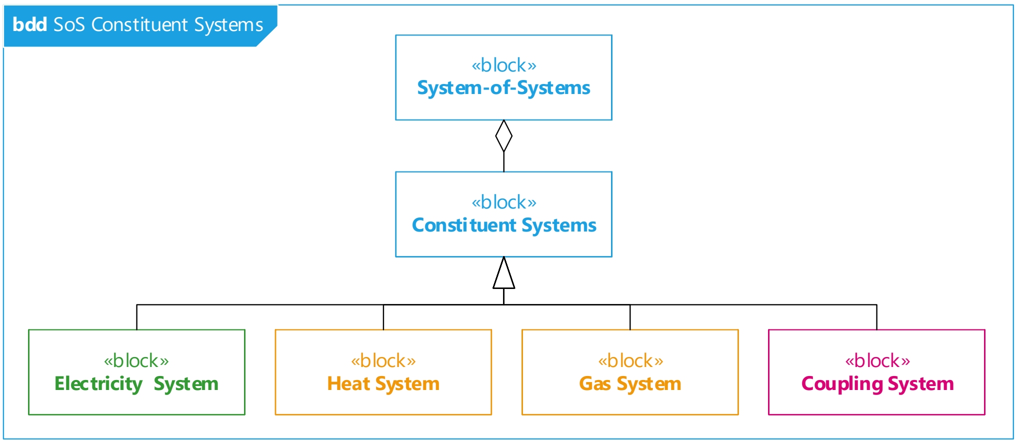


Figure 5.5 Constituent systems: Findhorn heat scenario 7

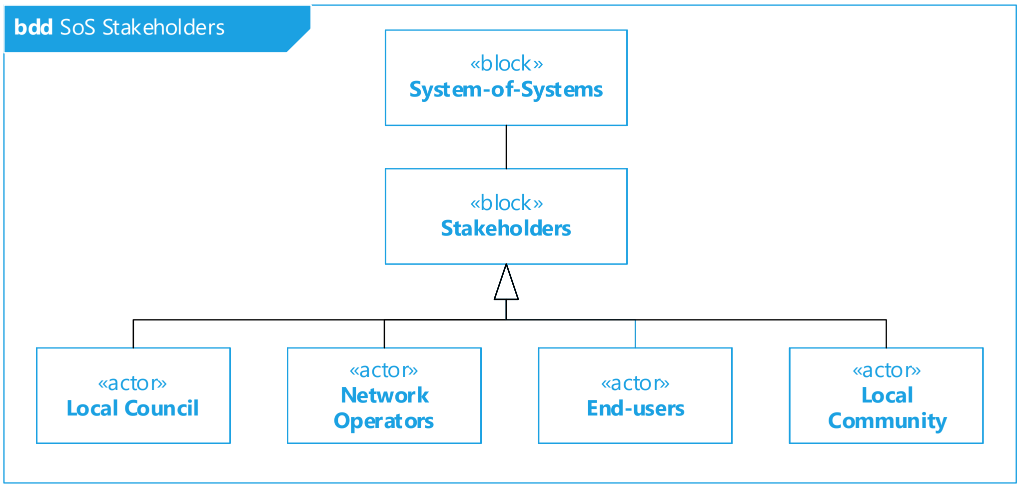


Figure 5.6 Stakeholders: Findhorn heat scenarios

5.2.2. System-of-Systems Level

The next level in the ESI-SoS architectural framework is the SoS level, where the structure and requirements of the system are identified. Figures 5.7 and 5.8 show the system structure at the SoS level for scenarios 1 and 7, respectively. For scenario 1, it can be seen that the electricity and gas systems are not connected, but rather each is operated separately to satisfy the energy demand. In comparison, the structure view for scenario 7 shows that the electricity and heat systems are coupled, while the gas system is physically separate.

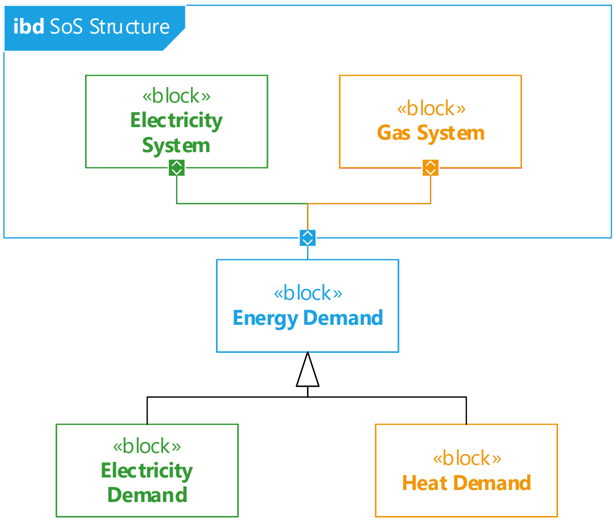


Figure 5.7 SoS structure: Findhorn heat scenario 1

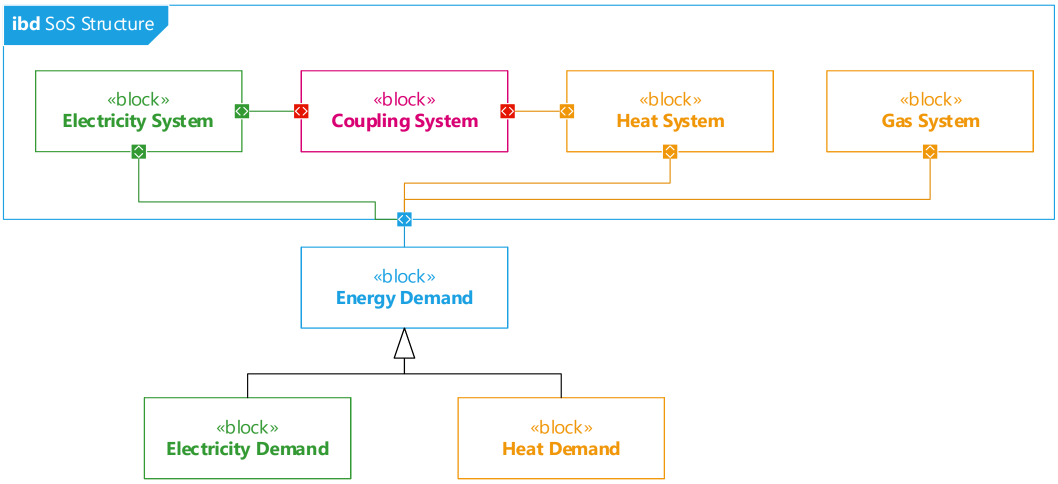


Figure 5.8 SoS structure: Findhorn heat scenario 7

The system requirements for all scenarios are defined in the requirements description diagram in Figure 5.9 and are then related to the corresponding stakeholders in Figure 5.10. The requirements follow from the energy trilemma notion, including objectives for environmental sustainability, social and economic acceptability, and technical energy security. These objectives are requirements sought by the local council representing the government, the local community pushing for environmental and social values, the network operators working to maintain a secure energy system, and end-users aiming for an affordable and reliable service. The requirements at this level are the same across all scenarios given that the same system stakeholders are maintained.

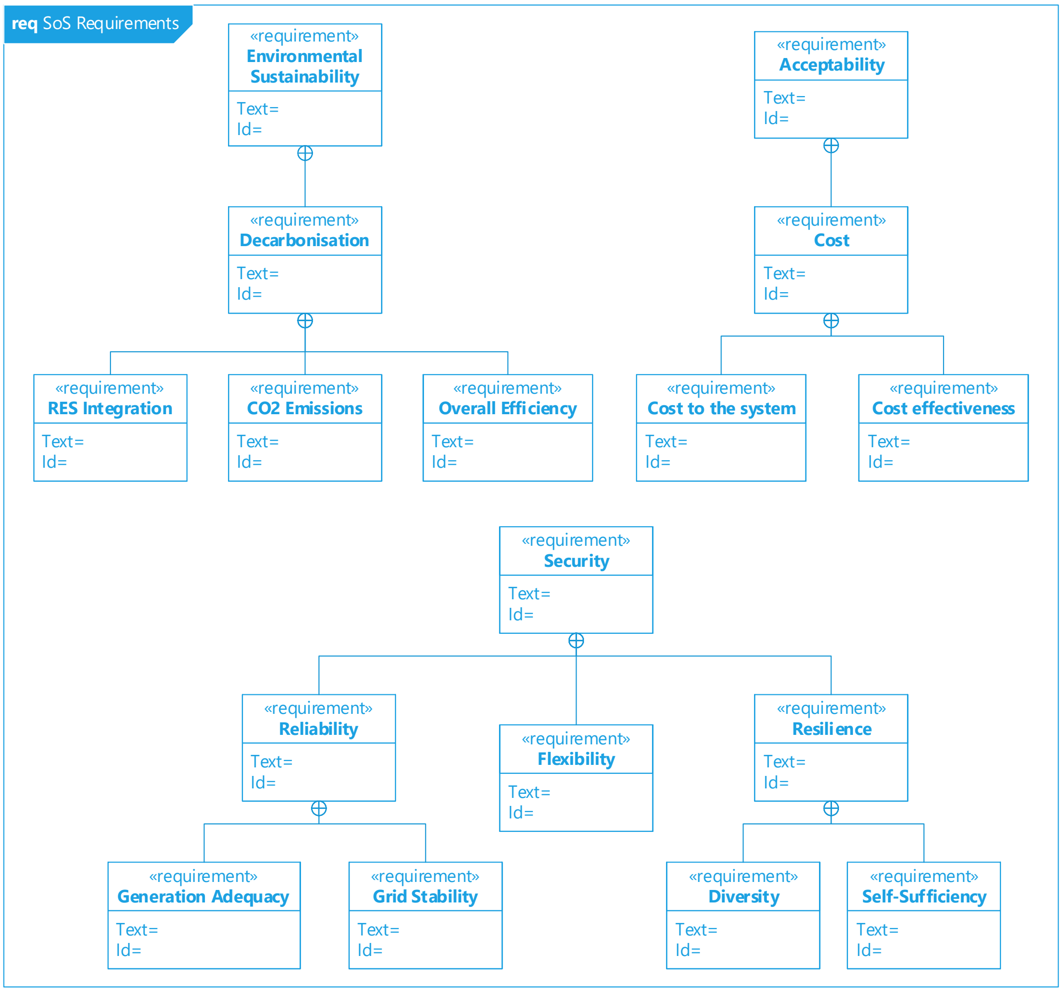


Figure 5.9 SoS requirements description: Findhorn heat scenarios

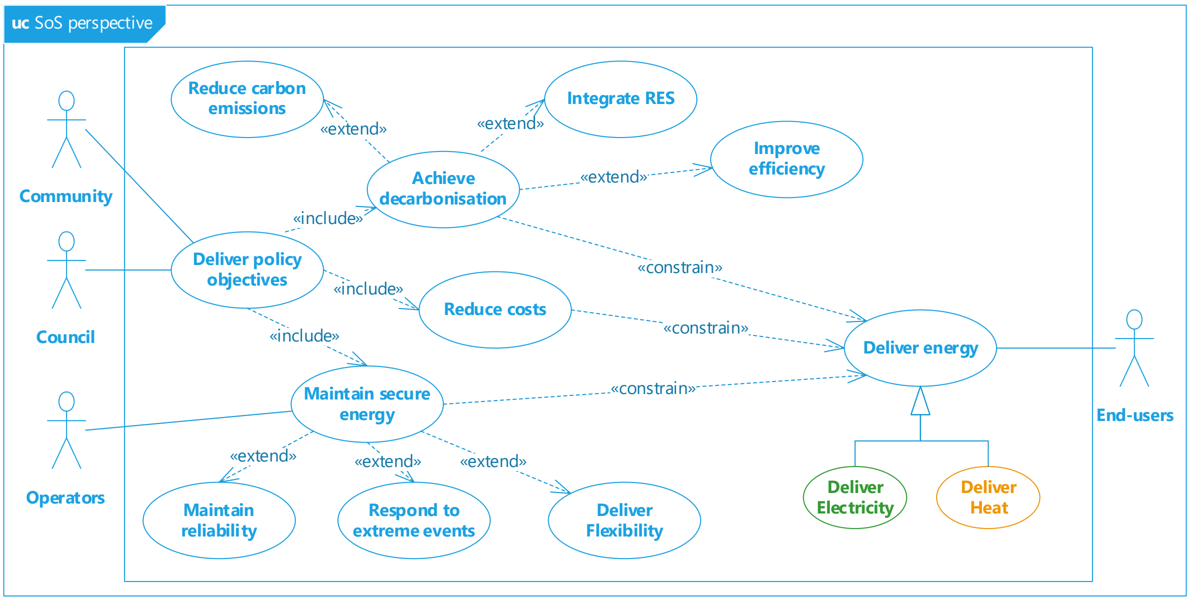


Figure 5.10 SoS requirements context: Findhorn heat scenarios

5.2.3. Constituent Systems Level

The main differences between scenarios start to appear at the CS level with different composition, structure and requirements. Figure 5.11 shows the composition of the two CSs of scenario 1. The electricity system is fed by two components, the upstream network where energy is imported into the local system and the downstream network which is fed by generation from the nearby wind farm and rooftop solar PV. Similarly, the gas system is made up of energy imports from the upstream network, the local distribution network, and gas boilers at the end-user point to deliver heat. On the other hand, Figure 5.12 shows the composition for the four CSs in scenario 7. The electricity and gas systems have the same composition as in scenario 1. The heat system is made up of a distribution network and a geothermal source, while the coupling system in this case consists of a GSHP. Note that some demand-side technologies, such as gas boilers, are shown in the composition because of the case study focus on delivering heat. This implies that for scenarios 2 and 6 for example, electric heaters are included as a component of the electricity system to deliver heat.

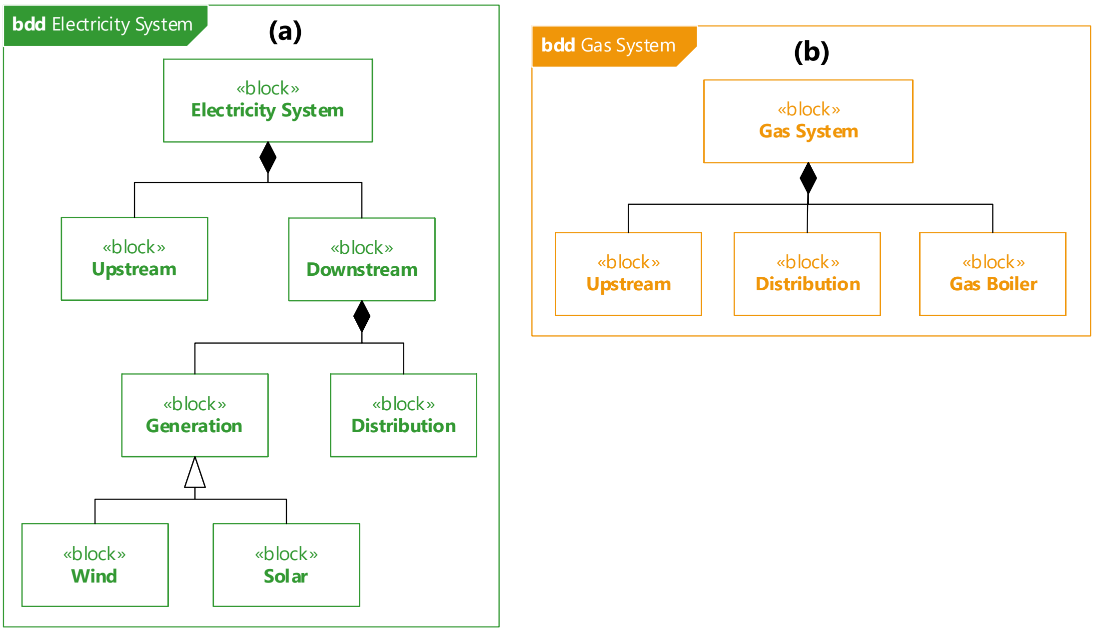


Figure 5.11 Findhorn heat scenario 1: CS level composition for (a) electricity and (b) gas systems

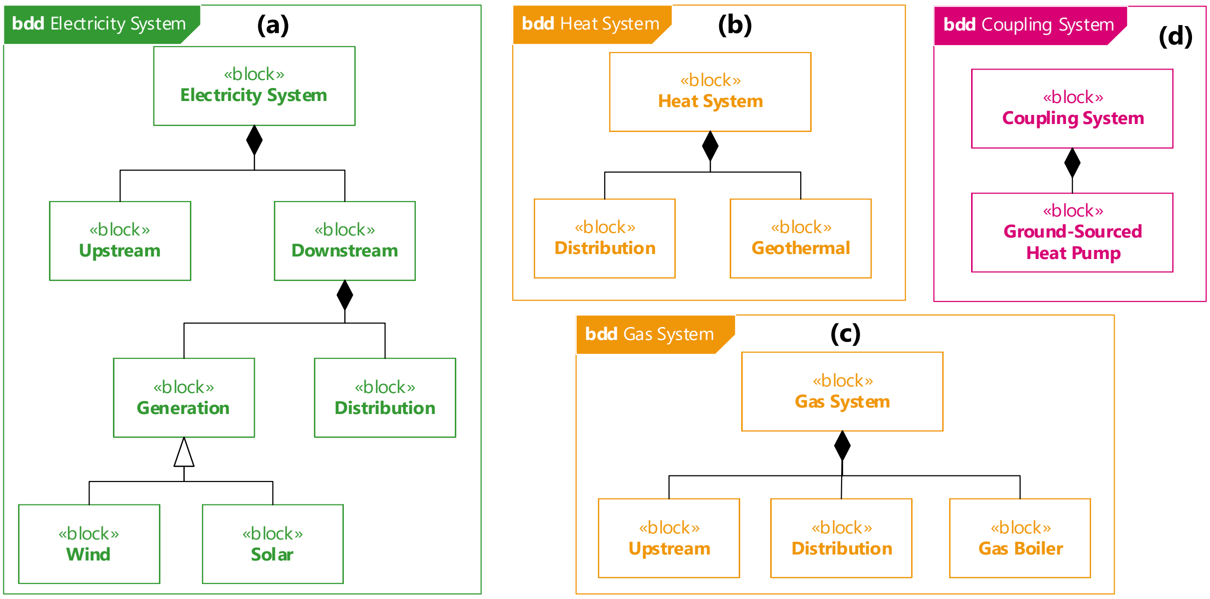


Figure 5.12 Findhorn heat scenario 7: CS level composition of (a) electricity; (b) heat; (c) gas; and (d) coupling systems

The system structure at the CS level is intended to show the structural relations between components identified in Figures 5.11 and 5.12, within CSs and across CSs, in line with the structure at the higher SoS level. However, in scenario 1, the two CSs are operated separately and thus Figure 5.13 shows no relations across systems. Conversely, it can be seen in Figure 5.14 that for scenario 7, the heat demand is satisfied by the gas and heat systems, where the heat system is supported by the electricity system through the GSHP to exploit the geothermal heat source, while the gas system has no interaction with other systems.

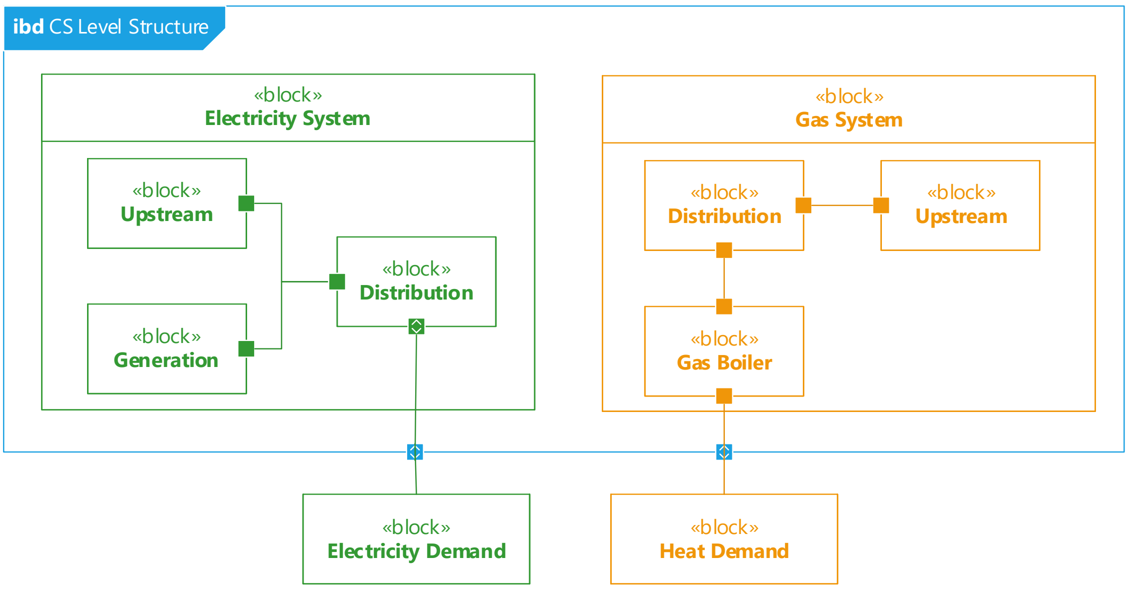


Figure 5.13 CS level structure: Findhorn heat scenario 1

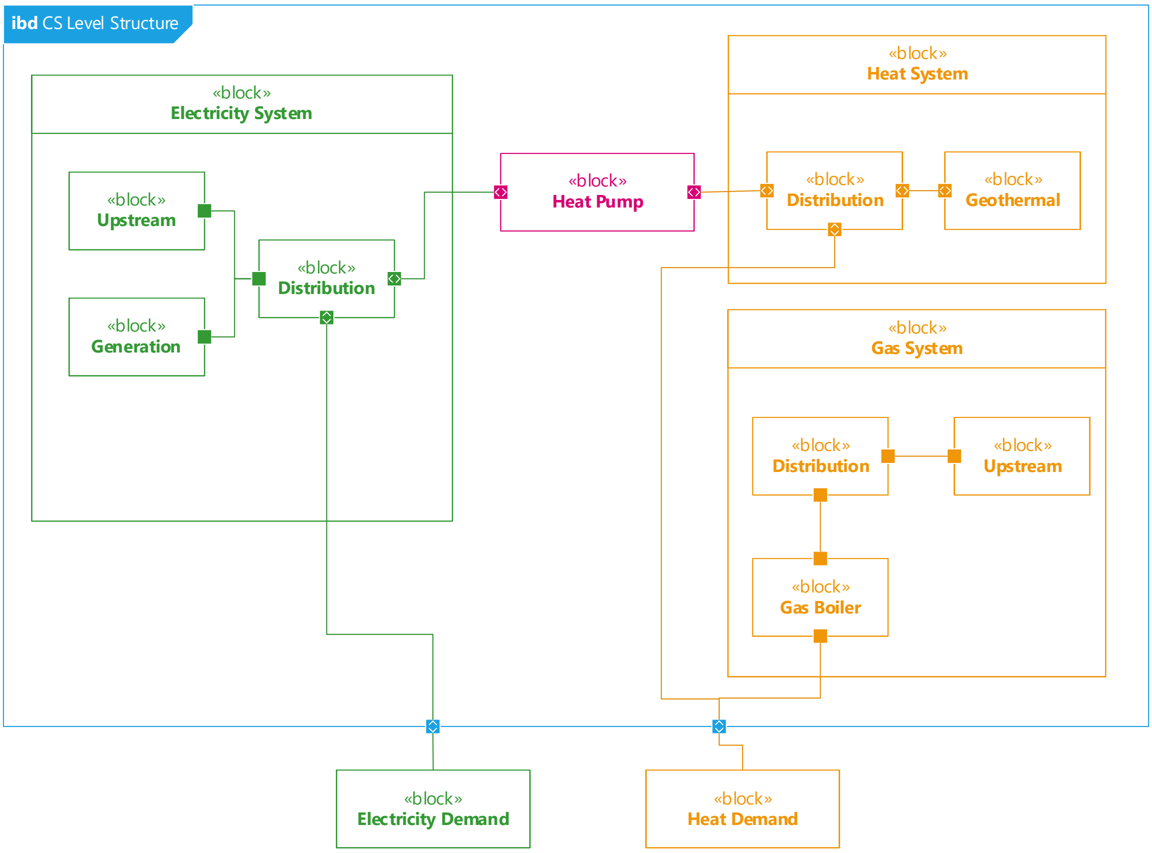


Figure 5.14 CS level structure: Findhorn heat scenario 7

The requirements context interaction view is meant to show the functional interactions between CSs and with the SoS. However, since the two CSs are separate in scenario 1, requirements in Figure 5.15 are limited to those of delivering energy by each CS to the SoS. This doesn't necessarily mean that there is no provision of security functions within each system, but the focus of this research is on the functions emerging from interactions between CSs that contribute to the whole system.

The view in Figure 5.16 is different for scenario 7, compared to scenario 1. The gas and heat systems deliver heat to the SoS to satisfy the end-users heat demand. Similarly, the electricity system delivers electricity to the SoS to satisfy the end-users demand, in addition to the coupling system to drive the GSHP. In return, the coupling system provides grid services to the electricity system if DSR is provisioned. The coupling system also coverts the electricity to heat to support the heat system in satisfying its requirement to deliver heat, which provides flexibility to the SoS, and satisfies the SoS of improving the overall system efficiency by reducing the final energy use.

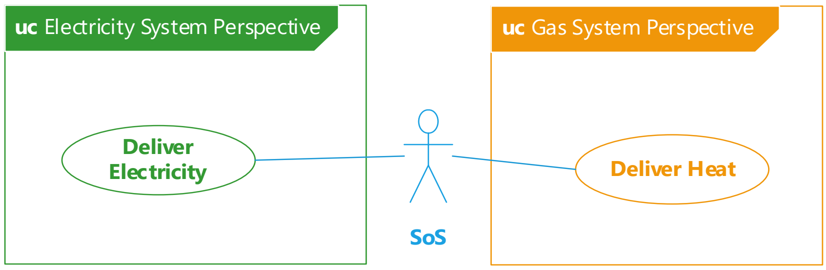


Figure 5.15 CS level requirements: Findhorn heat scenario 1

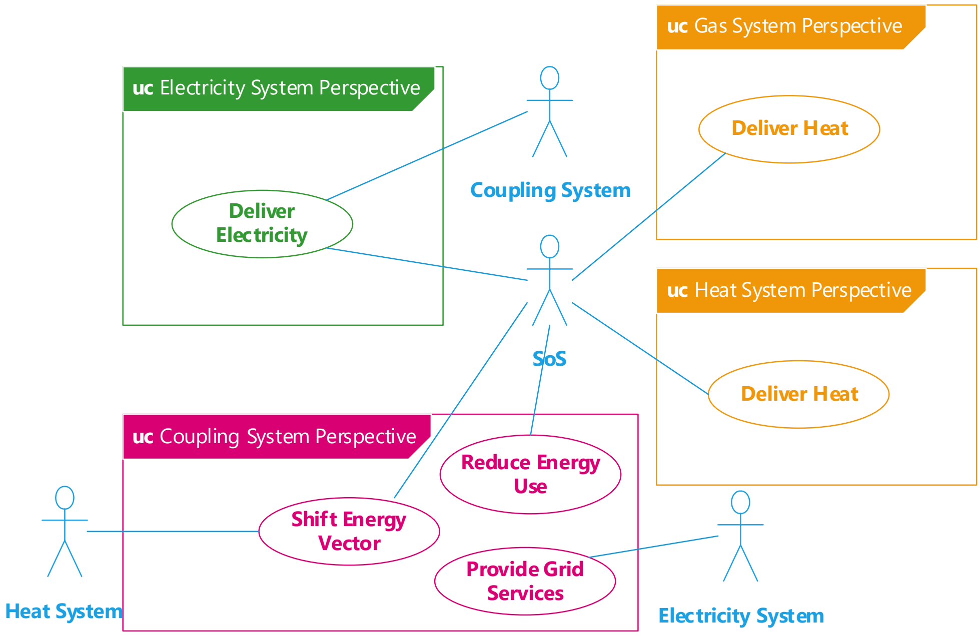


Figure 5.16 CS level requirements: Findhorn heat scenario 7

5.2.4. Whole System Level

Finally, on the whole system level, the traceability and measures of effectiveness views are presented. The traceability view combines different system components and functions from different levels to trace the relationships between them in fulfilling the system requirements. This is presented in Figures 5.17 and 5.18 for scenarios 1 and 7, respectively. Accordingly, measures of effectiveness are shown in Figure 5.19 and 5.20 for the two scenarios, including simple relationships to calculate the indicators. The difference between the two scenarios is mainly around the coupling system components and the contributions of its functional requirements. Note that in scenario 1, system flexibility cannot be traced to any system component or function as shown in Figure 5.17, with no coupling components, energy storage, or DSR. Hence, no indicator was included for flexibility in Figure 5.19.

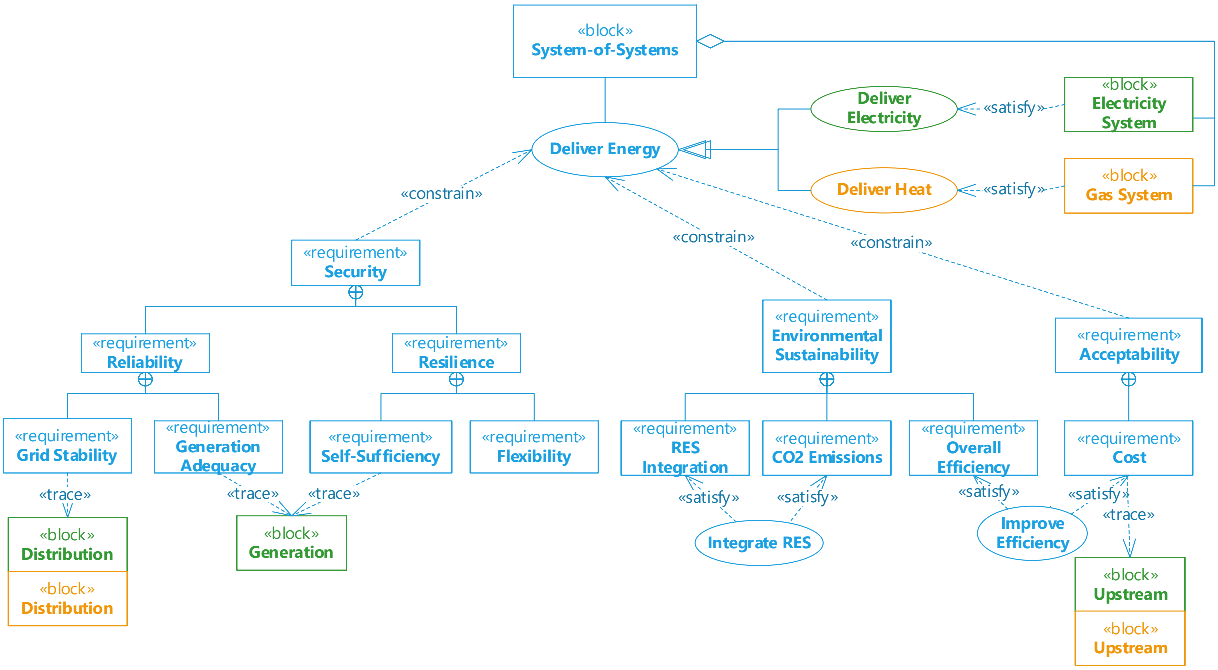


Figure 5.17 Traceability view: Findhorn heat scenario 1

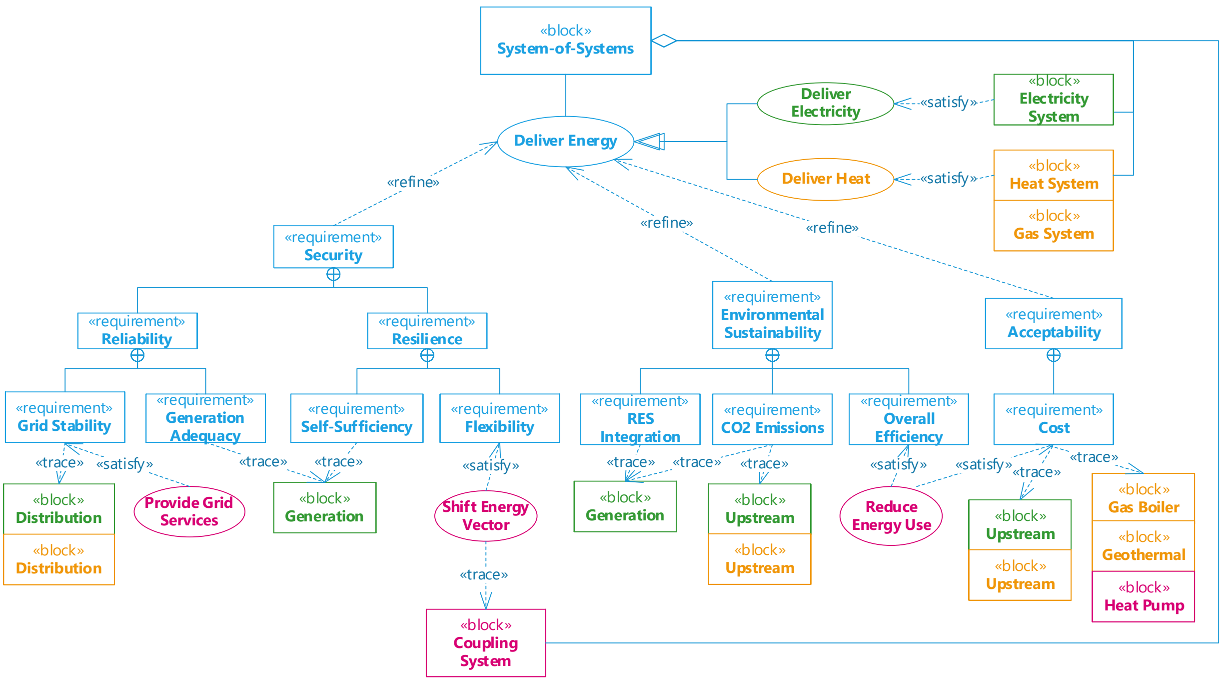


Figure 5.18 Traceability view: Findhorn heat scenario 7

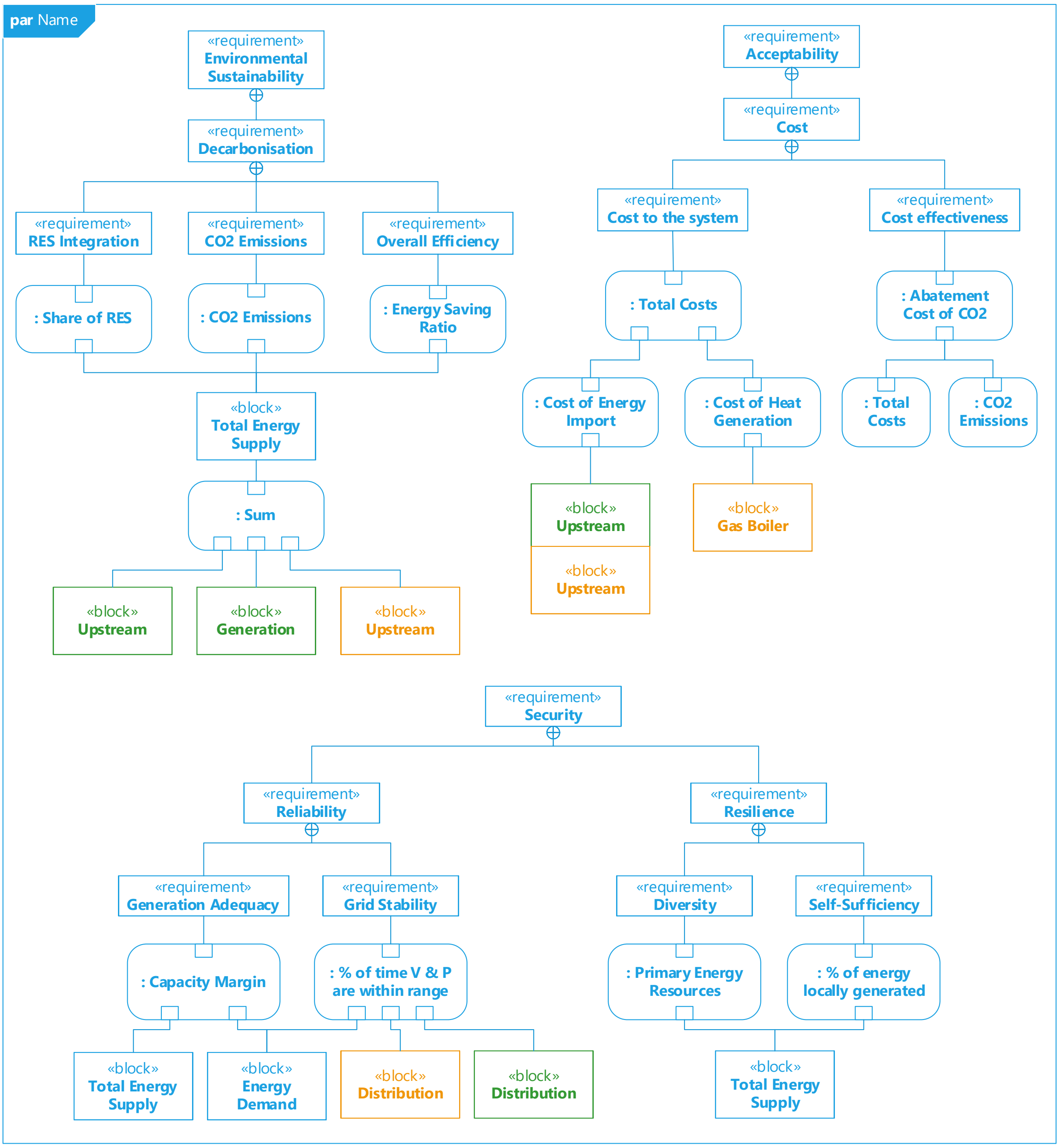


Figure 5.19 Measures of effectiveness: Findhorn heat scenario 1

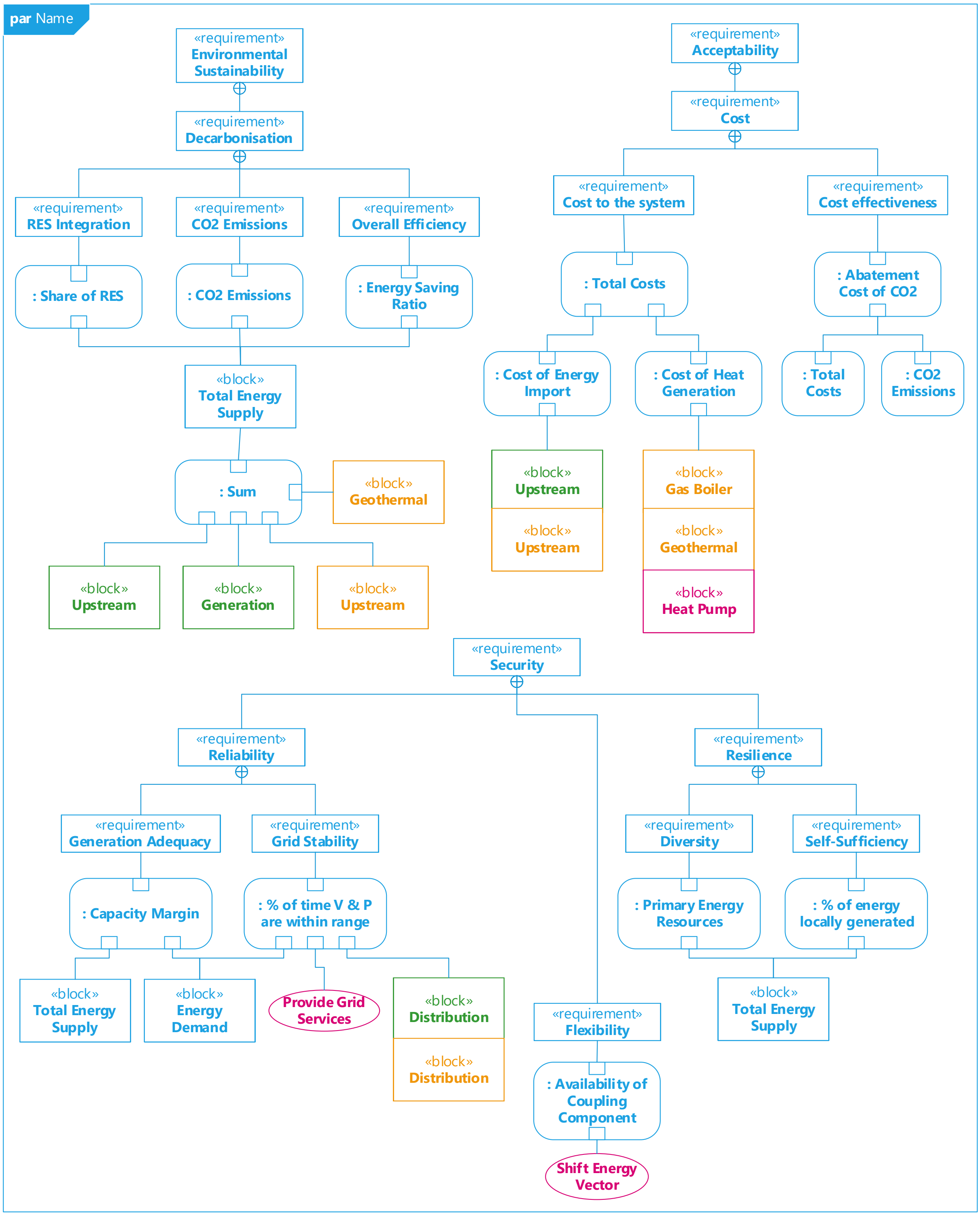


Figure 5.20 Measures of effectiveness: Findhorn heat scenario 7

5.2.5. Discussion

The Findhorn heat case study illustrates the first two stages of the framework implementation, which involve conceptual modelling and scenario formulation. As mentioned previously in Chapter 4, the two stages can take place simultaneously. The outcome of the two stages is a set of indicators for evaluation of different system configurations. It is worth mentioning here that indicators are chosen based on the relations identified in the traceability view but also based on the data available. This highlights the feedback loops between the framework stages and the iterations involved, as depicted in Figure 4.10. Stage 3 of the evaluation framework is the quantitative modelling where the assigned indicators are quantified, and results are compared for all scenarios.

At this point of the project, the communication with the quantitative modelling had not been fully established and thus complete results had not been reached. Hence, this case study is used as a starting point to test the framework and learn from the gaps and challenges faced, particularly for stages 1 and 2. Additionally, it has been used to demonstrate the approach, the rationale and the flow of the framework developed in this project to the experts for validation, as discussed in Section 5.4.

The gaps and challenges realised during this case study raise the following questions:

- What data outputs are needed from the quantitative models?
- How to deal with incomplete results?
- How to maintain comparability across scenarios?
- What is the impact of P2G and energy storage?

Those questions are carried to the Findhorn storage case study to be resolved.

5.3. Findhorn Storage Case Study

For the purpose of demonstration, the conceptual system model is shown only for configuration 4 of the storage case study, which actually includes all the components included in other configurations. This configuration comprises integration through CHP and P2G in addition to electric and gas storage, as described in Table 5.3. Note that diagrams similar to those of the heat case study are indicated but are not reproduced to avoid redundancy.

For stage 3 of the evaluation framework, the results for the 16 scenarios presented in Section 5.1.3 are generated and provided in Appendix C, without further interpretation. However, the results are discussed in the scope of the process involved in stage 3 including the exchange with the quantitative model and the concerns identified in the heat case study.

5.3.1. Context Level

The CSs for this configuration include the electricity, gas, heat, and coupling systems, as shown in Figure 5.21. The stakeholders, however, are the same as those shown in Figure 5.6: the local council, local community, network operators, and end-users.

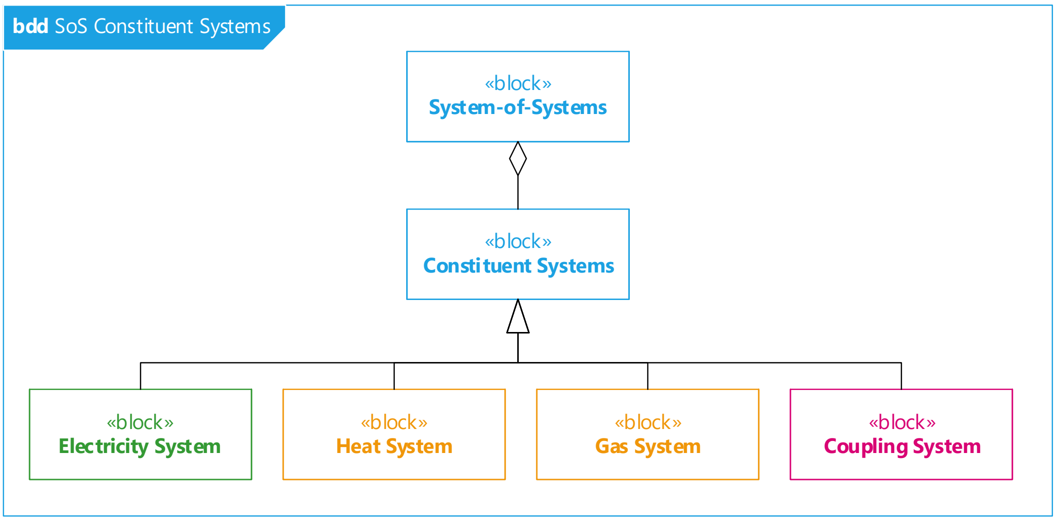


Figure 5.21 Constitutent Systems: Findhorn storage configuration

5.3.2. System-of-Systems Level

The structure at the SoS level is shown in Figure 5.22. The diagram shows that the CSs are linked through the coupling system in this case, while each CS still also operates separately to satisfy energy demand. Given that the system stakeholders are the same as those in the heat case study, requirements at this level are also unchanged from Figures 5.9 and 5.10.

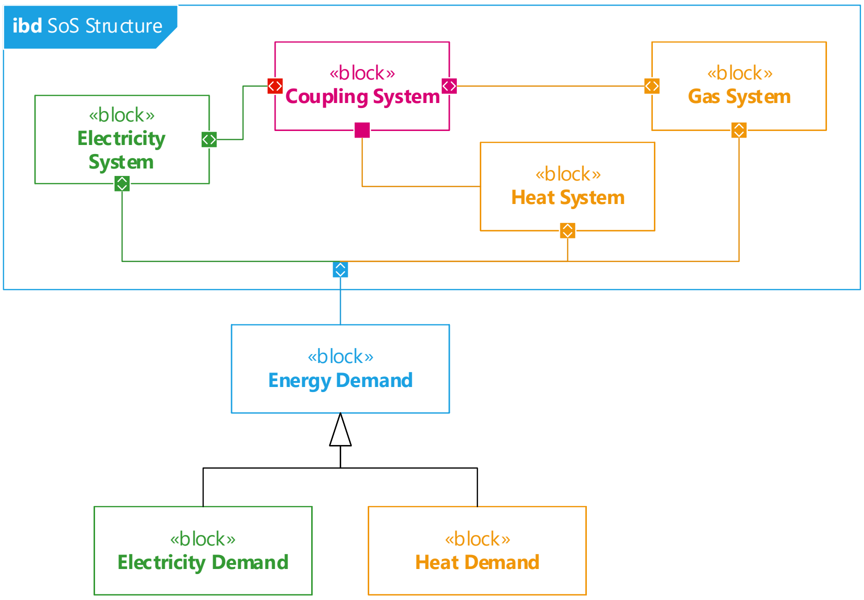


Figure 5.22 SoS level structure: Findhorn storage configuration 4

5.3.3. Constituent Systems Level

At the CSs level, the system composition, structure and requirements are shown in more details. The system composition is first presented in Figure 5.23. In this case, the electricity and gas systems include storage, while the heat system consists only of the district heating network. Two types of coupling components are considered in this case, those are the CHP and P2G.

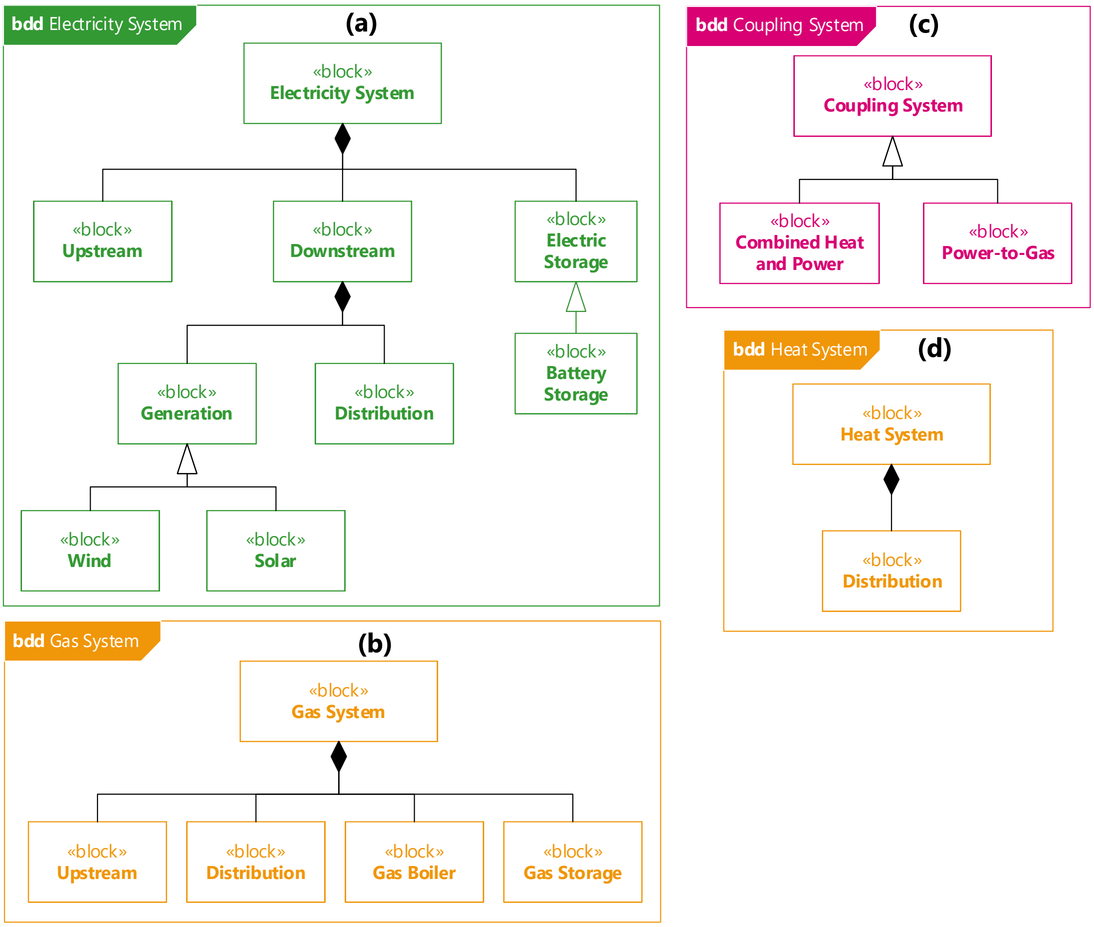


Figure 5.23 Findhorn storage configuration 4: CS level composition of the (a) electricity; (b) gas; (c) coupling; and (d) heat systems

The structural relationships between the CSs elements are shown in Figure 5.24. CHP connects the electricity, gas and heat systems, where it takes gas as an input from the gas system and provides electricity and heat to the respective systems as output. On the other hand, P2G couples the electricity and gas systems by converting electricity into gas. Note that the interactions in this case take place at the distribution level since the local energy system in Findhorn is the one modelled.

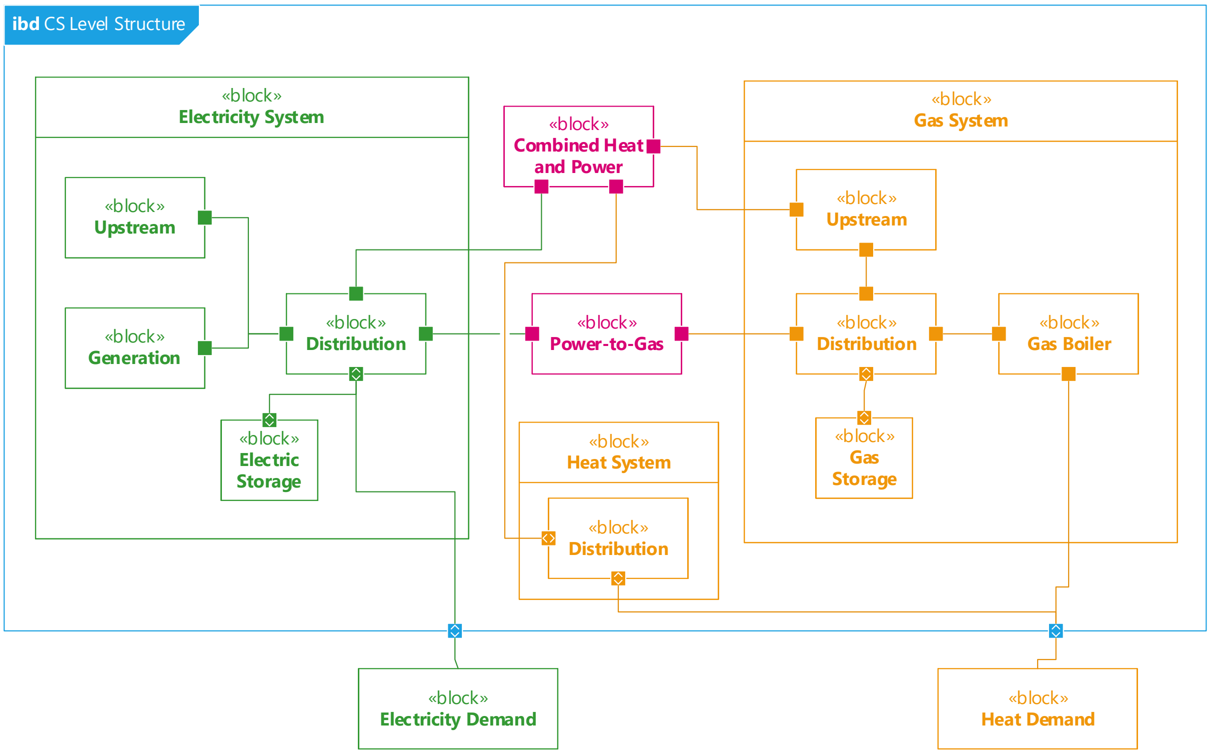


Figure 5.24 CS level structure: Findhorn storage configuration 4

The requirement context interaction view for the CS level is presented in Figure 5.25. This diagram shows the functional interactions between the CSs and with the SoS to fulfil the system requirements. The electricity, gas and heat systems mainly have the requirement to deliver their respective services to satisfy energy demand. Additionally, the electricity and gas systems provide storage services that support the SoS security requirement of reliability, resilience and flexibility. The coupling system receives electricity and gas as inputs from the other CSs, as mentioned previously for CHP and P2G, and in return provides functions that support the SoS requirements. These include improvement to the overall system efficiency through reduced total energy use, providing grid services that supports the system reliability, and shifting energy vectors that provides flexibility to the whole system.

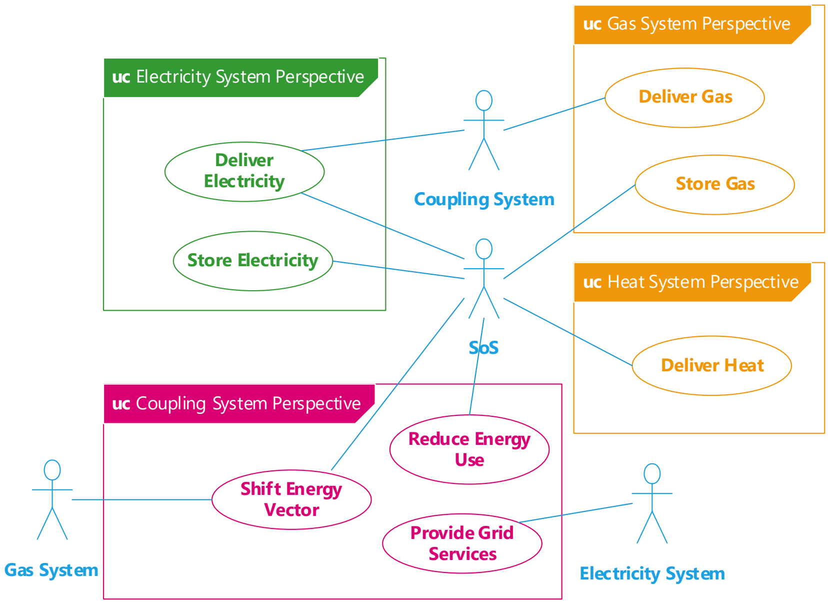


Figure 5.25 CS level requirements: Findhorn storage configuration 4

5.3.4. Whole System Level

The traceability view for configuration 4 is presented in Figure 5.26 and the measures of effectiveness are presented in Figure 5.27. As discussed earlier, the traceability view relates the different system requirements, components, and functions at different system levels. Measures of effectives are accordingly chosen to measure the level of satisfaction of the relevant requirement from the component it is traced to or the function that satisfies it.

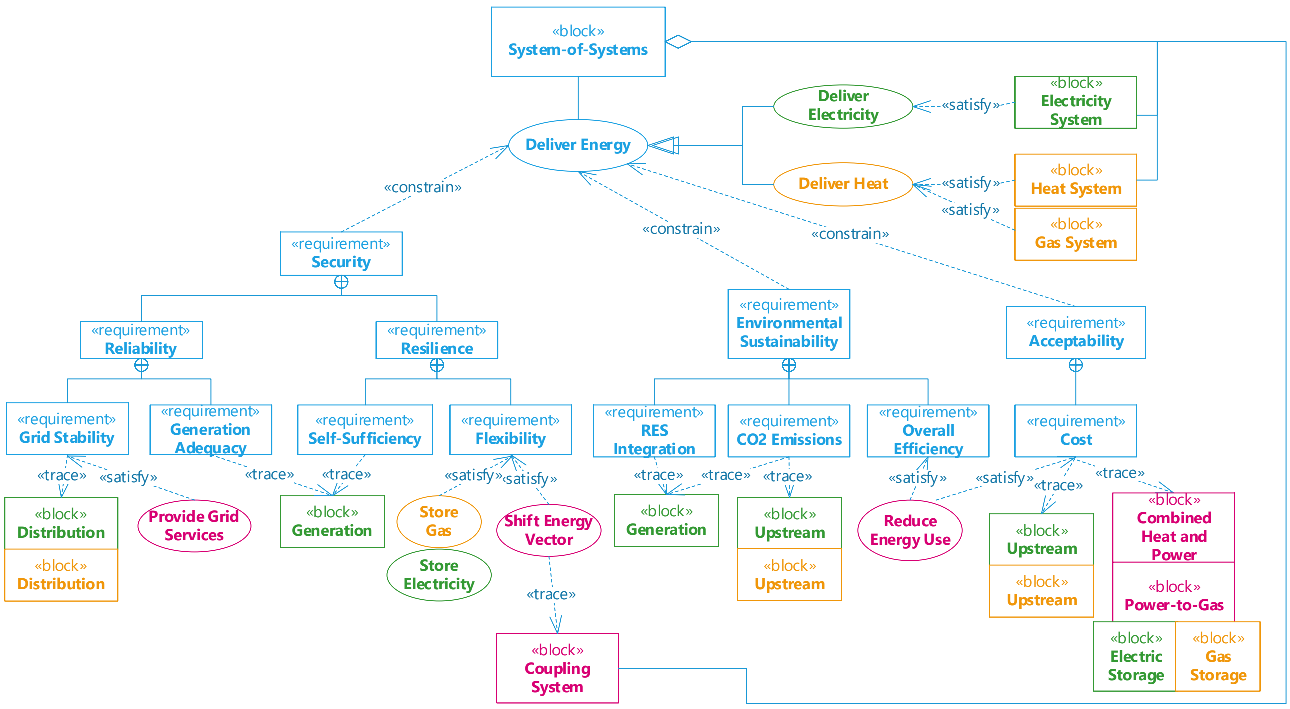


Figure 5.26 Traceability view: Findhorn storage configuration 4

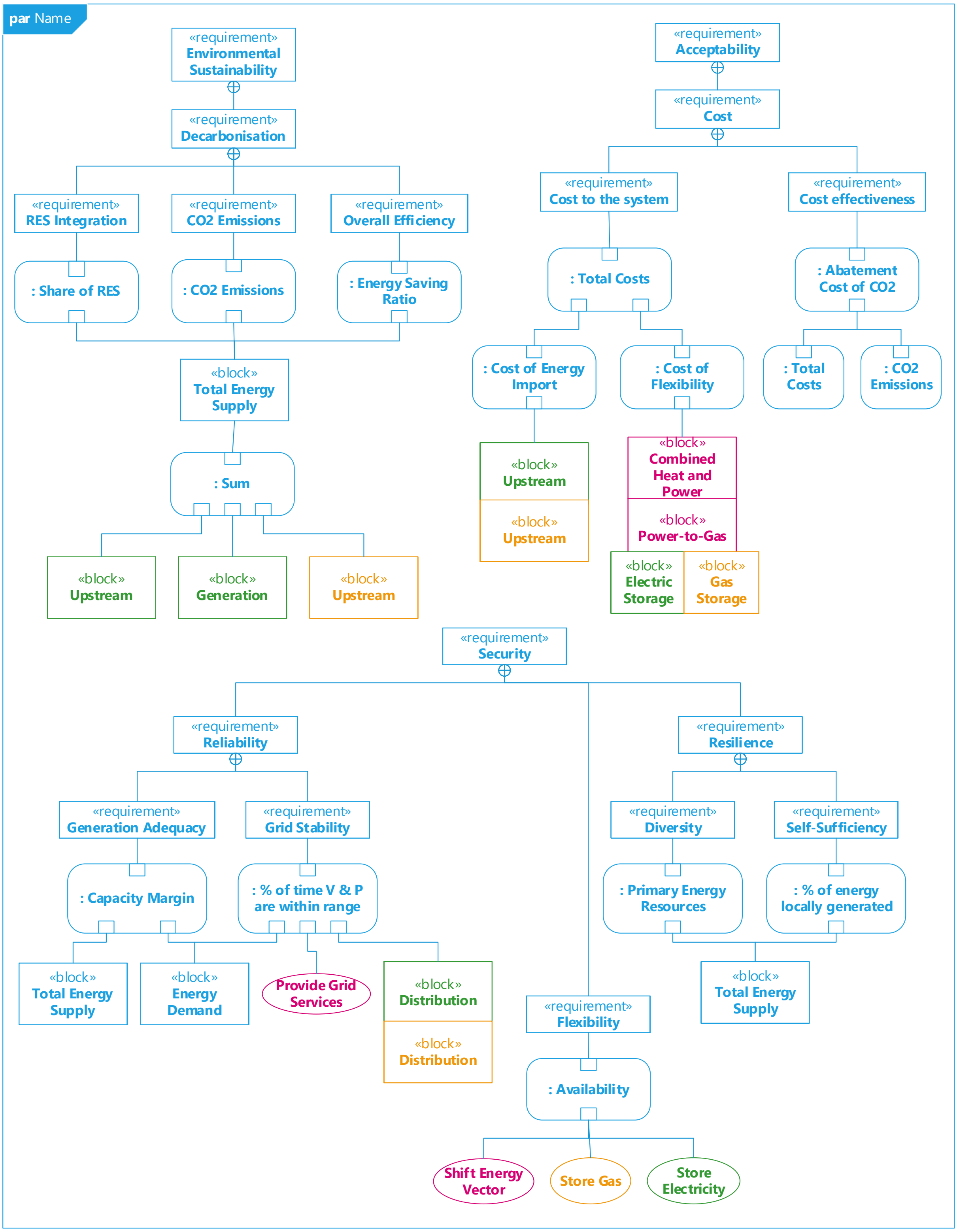


Figure 5.27 Measures of effectiveness: Findhorn storage configuration 4

5.3.5. Scenario analysis

The conceptual system model is developed for all configurations, although not shown here, and the scenarios are implemented in the quantitative simulation model to quantify the identified indicators. The results for the 16 scenarios are shown in Appendix C for demonstration purposes only. A large number of scenarios has been developed to consider different system configurations of multiple combinations of energy technologies. Although more challenging with higher number of scenarios, the analysis would provide a better understanding of the wide range of alternatives. The values are calculated from the simulation model output parameters including the amount, cost and emissions of the upstream energy imports, the amount of energy generation from local and RES sources, the losses incurred across the system components, the total energy input to the system, the total energy load, and the peak energy load.

Other parameters assumed include the levelised cost of flexibility assets (coupling components and energy storage) to calculate the cost of flexibility and add to the operational cost of energy import. Moreover, the capacity values of those assets are used to calculate the flexibility indicator (% of flexible capacity to the peak load), being assumed in the model as mentioned earlier.

5.3.6. Discussion

In the Findhorn storage case study, the challenges identified in the heat case study are tackled. First, data outputs from the simulation model are understood through the communication with the modellers. Iterations between the framework stages are required to consider the data available to calculate the identified indicators, as discussed in Chapter 4. Second, some indicators that could not be calculated are further examined. For instance, reliability indicators are not available, and this is due to the nature of the simulation model (operational model). Reliability is a condition for model convergence, and therefore does not vary across different scenarios. This has to be made clear when communicating the results. Different methods may be needed to evaluate reliability, but it is still included as a requirement in the conceptual system model for completion. Third, there is a need to maintain comparability across scenarios for the evaluation. This can be dealt with at the time of the scenario formulation and when specific indicators are assigned. Scenarios should be designed in a comparable way and indicators should be comparable across scenarios. This again highlights the importance of iteration across the evaluation framework stages. Finally, P2G and energy storage have been included in the conceptual system model developed in this case study after being dismissed in the heat case study.

However, limitations still exist with this case study. The first evident limitation particular to this case study is the number of scenarios. While this is useful to investigate different combinations of system configurations and conditions, it makes the interpretation and presentation of results more challenging with a higher number of scenario. This prompts the question: what is the ideal number of scenarios, and what type of scenarios is the evaluation framework best suited to deal with. This is addressed by initially designing the case study and the consequent scenarios with a clear objective, for example, the evaluation of the effectiveness of ESI, as demonstrated later in Chapter 7. Otherwise, the number of scenarios have to be reduced logically by omitting the infeasible scenarios depending on the context or mathematically by filtering the worst performing scenarios, for instance. Thus, only the most relevant scenarios are considered.

This case study faces the same challenges related to the nature of the quantitative model used, as discussed in Section 5.1.4. However, at this point of the project the communication with the modellers was initiated on what data is required from the model and what information is needed for the model to be able to deliver. This communication continued until the interaction between the conceptual system model and the quantitative model became clear, as currently described in Section 4.2 and implemented in Chapter 7.

Along with the heat case study configurations, the various configurations of this storage case study are used to develop a generalised RSAM in Chapter 6. This model resembles the conceptual system model of a combined variety of ESI configurations, which can be used as a standard, modular approach for stage 1 of the evaluation framework in different contexts.

5.4. Framework Validation

After testing the evaluation framework on the Findhorn heat and storage case studies, the developed framework was presented to experts, for validation in terms of its design, implementation procedure and case study application. The ultimate purpose of this exercise was to receive feedback from experts on the strengths of the framework and the opportunities for improvement.

This section explains the definition and method for validation adopted, discusses the ethical consideration associated with this exercise, and outlines the feedback received from experts along with improvements and clarifications subsequently made to the evaluation framework. Appendix D accompanies this section with relevant material including the participant consent form, pre-workshop briefing document, post-workshop questionnaire, and the workshop presentation slides.

5.4.1. Validity

Validity of the proposed framework is important to ensure its quality, utility and credibility (Cloquell-Ballester et al., 2006). It can be thought of as an evaluation of an evaluation, or a meta-evaluation, to assess the strengths and weaknesses of the framework, the appropriateness of indicators, and the quality of implementation (Ramos and Caeiro, 2010). Generally, the validation process can be applied at the level of indicators making up the assessment or at the level of the framework as a whole (Meul et al., 2009). However, it is said that the validity of indicators largely follows from the validity of the framework behind it (De Neufville, 1978).

Based on the definition suggested by Bockstaller and Girardin (2003), three types of validity can be realised: design, output and end-use validity. Design validity relates to the scientific foundation of the framework, while output validity relates to the reliability and credibility of the framework output, and end-use validity looks at the usefulness of the framework in serving its designated purposes (Bockstaller and Girardin, 2003). This definition has been adopted in this research as it maps well to the framework development stages (see Figure 5.28) and relates partly to the WES principles used to develop the framework such as the applicability principle. Similar distinctions have been also proposed by other studies using slightly different terminology, for instance:

- Theoretical, operational, experiential validity (De Neufville, 1978)
- Conceptual relevance, feasibility of implementation, interpretation and utility (Fisher, 1998)
- Conceptual coherence, operational coherence, utility (Cloquell-Ballester et al., 2006)
- Validity of the conceptual model, implementation, and model output (Augusiak et al., 2014)

5.4.2. Validation Method

The validation of the evaluation framework developed in this research followed the method for scientific validation using experts' judgements. The scientific validation method provides rigour and objectivity to the developed framework by integrating the independent experts' judgements (Cloquell-Ballester et al., 2006). A collaborative process as such is considered a good practice for validation to ensure the credibility, transparency and robustness of the framework (Ramos and Caeiro, 2010). This method for validation involves three steps.

The first step is reporting the framework design and its underlying concepts, methods, assumptions, and purpose, in addition to the validation process to the experts (Cloquell-Ballester et al., 2006). The developed evaluation framework was described to the invited experts in two stages. First, a briefing document was sent to the experts beforehand for familiarity, which is shown in Appendix D.2. The briefing document provided an overview of the workshop objectives and format, and a summary of the framework design, implementation procedure and case study application. Second, the framework was explained to the participants with further elaboration through a presentation in the live session, as described in Section 5.4.3 below, the slides of which are provided in Appendix D.4.

The second step is identifying the validation criteria. The validation criteria are identified in line with the validity definition adopted in this research and the framework stages. The criteria are based on the conceptual coherence, operational coherence and utility of the developed framework (Cloquell-Ballester et al., 2006). The experts' elicitation workshop was designed accordingly to receive their judgments on the three criteria, which map to the three framework stages.

The final step is eliciting experts' judgments. Typically, experts must be chosen with adequate level of knowledge on the subject and motivation to participate in the process, in addition to other logistic factors such as cost, proximity and availability (Cloquell-Ballester et al., 2006). Several techniques could be used to elicit the experts' feedback including questionnaires (Borenstein, 1998; Bautista et al., 2016), semi-structured interviews (Bockstaller and Girardin, 2003), and multi-disciplinary discussions (Meul et al., 2009). This step is explained in more detail in the next section.

5.4.3. Experts Elicitation

To elicit the experts' feedback on the developed evaluation framework the three techniques mentioned were combined. A semi-structured group interview with experts was conducted in the form of an online workshop for the purpose of validation, with questions provided to stimulate individual and group responses. A group interview was chosen to disseminate findings and receive feedback, while generating insights from multidisciplinary discussions between the experts (Saunders et al., 2009; Bloor et al., 2012; Bryman, 2016). A questionnaire was also provided afterwards to capture any post-workshop individual reflection (Appendix D.3). The questionnaire was also used to receive feedback from experts who couldn't join the live session, but were provided with a separate video recording of the presentation instead.

The participants were researchers from different institutions within CESI. Six experts were chosen and invited, to span multiple academic disciplines related to energy research including engineering, computing, mathematics and social sciences. Those were chosen from the CESI pool of experts based on a number of factors. First, their familiarity with the concept of ESI, which makes them capable of understanding the context and providing feedback on the framework based on their research experience without the need to introduce basic concepts. Second, for practical reasons of being able to reach them and expecting engagement due to their commitment to the wider CESI project. Finally, a diverse set of experts was picked in terms of academic disciplines to allow for multidisciplinary discussions to take place and generate insights. There was only one exclusion criteria for the academics that have taken part in this research, particularly in the scenario formulation and quantitative modelling of the case studies as mentioned earlier, to avoid a conflict of interest. The number of invited experts was within the typical range recommended for similar workshops (Saunders et al., 2009; Bloor et al., 2012; Bryman, 2016). Eventually, four of the invited experts attended the live session and two other experts were only able to watch the recorded presentation.

The elicitation workshop itself followed a three-fold validation process looking at the design, output and end-use of the proposed framework (Figure 5.28). The workshop was therefore divided into three parts representing different phases involved in the design (presented in Section 4.1), implementation (presented in Section 4.2) and application (demonstrated with examples from the Findhorn heat case study presented in this chapter) of the framework. Each part started with a presentation and was followed by a facilitated discussion. The workshop presentation slides are available in Appendix D.4.

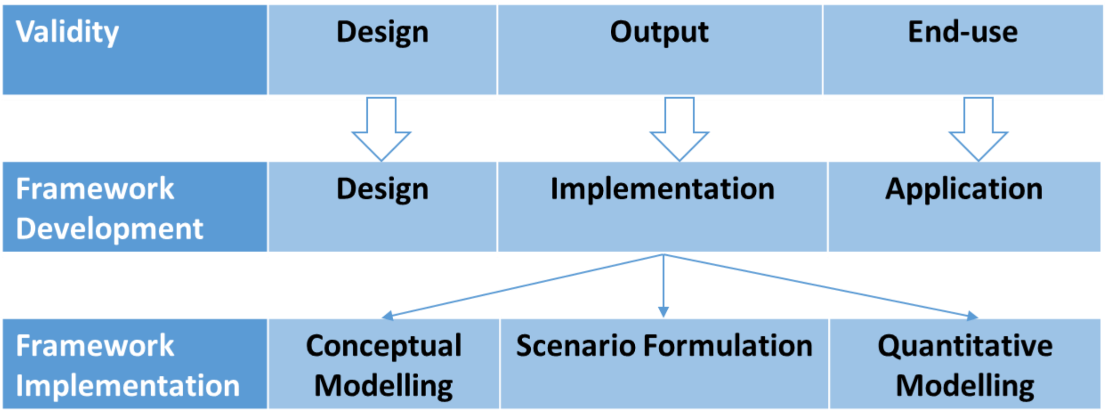


Figure 5.28 Validation process and the evaluation framework structure

5.4.4. Ethical Considerations

The ethical considerations relevant to the framework validation method involving human participants fall under four categories: informed and voluntary consent from participants, participants' privacy and confidentiality, risk minimisation, and conflict of interest (Saunders et al., 2009; Bloor et al., 2012; Bryman, 2016).

First, a consent form was attached with the briefing document sent to the invited experts, which informs them about the workshop purpose, format and intended use of this research as described in the previous sections, in addition to how the data is being recorded and managed. The consent form is provided in Appendix D.1, and allowed participants to indicate that they understand the nature of the research and that they give their permission for the session to be recorded. The consent form also included contact details if the participants have any concerns.

Second, as stated in the consent form, responses from the experts are combined, reported and may be published in anonymised form, and that personal information are not recorded with the responses. Similarly, a data privacy statement was included in the questionnaire (Figure D.6) outlining the purpose of this research and the mentioned measures of anonymity. The statement also indicated that by taking part in the questionnaire, participants agree to those terms. Contact details were included in the statement in case of any concerns. In this regard, original data in the form of written notes from the live session and questionnaire responses have been destroyed/deleted after being copied into an electronic document anonymously. Furthermore, the live session recording has encountered a technical issue with the audio not being recorded. This meant that the recording was not of any use and was subsequently deleted.

Third, with the start of the COVID-19 pandemic in early 2020, a decision was made to move the workshop to an online setting to avoid the associated health risks, even before a lockdown was enforced in the UK. There are risks to holding the workshop virtually rather than in person. The risks were mitigated by have a clear goal, having participants who already knew one another, having common interest in the CESI project, and valuing all contributions in the discussion (White, 2014; Roos et al., 2020).

Finally, while the invited experts are all part of the CESI project, a conflict of interest was not expected as there is no financial gain from this research. There is also no direct professional gain, with the progress of this PhD project being independent from the progress of the research activities carried out by the participants for CESI. As mentioned earlier, academics who have directly contributed to the framework application were excluded to avoid potential conflict of interest. It is worth mentioning here the importance of maintaining the integrity of this research by being truthful and promoting accuracy (Saunders et al., 2009). With this in mind, and given that the purpose of the validation being to receive feedback in order to improve the developed evaluation framework, it was important to accept and report all comments including on both the strengths and weaknesses of the framework, as discussed in the next subsection.

5.4.5. Experts Feedback and Subsequent Improvements

The participants generally showed a positive attitude towards the proposed framework during the discussions. The participants thought the framework provided a good level of accuracy, credibility, coherence and utility, and that they were ‘somewhat likely’ to use the framework. They agreed that it was important that the framework allows for the following:

- Show the relationships between different system components
- Model the system at different levels
- Present the system requirements in relation to multiple stakeholders
- Link the system components and functionalities to deduce evaluation criteria and indicators
- Use to make informative judgements on the performance of different scenarios

The other particular points and suggestions raised in the discussion can be divided into six key areas and are presented in Table 5.4, in line with the validation structure. Subsequent improvements to the framework in response to the feedback are also discussed in Table 5.4.

Based on the experts' feedback, the strengths of the framework can be summarised as: being comprehensive, flexible and transferable; and providing a structured approach with a unified language for ESI understanding and evaluation. On the other hand, the downside of the framework lies in that it needs to be contextualised for each evaluation, and this could take some effort for learning the methods used, such as SysML. Another downside identified is that the framework is still dependent on the quality of the data available. Accordingly, there is room for improvement as suggested by the participants that relates mainly to the consistent, standardised application of the framework.

As discussed in Table 5.4, the key improvements to the evaluation framework based on the experts' feedback include:

- more clarity in describing the conceptual design of the framework (Figure 4.1)
- an acknowledgment of the need for a transparent, participatory approach to the framework application to ensure the representativeness of stakeholders and requirements for a multidimensional and systematic evaluation (Sections 2.3.2, 2.3.6, 4.1.2, 4.1.5, 6.2)
- a detailed description of the framework implementation stages including a clear distinction between the three stages, the interaction and feedback loops between them, and the best types of scenarios and quantitative models suited for the developed framework application (Section 4.2)
- a standard, consistent method to apply the framework using the RSAM as a flexible template, particularly for the first stage of the evaluation framework (conceptual modelling), which enhances the usefulness of the framework (Chapter 6)

Table 5.4 Experts comments on the framework validity and subsequent improvements

Validity	Framework	Experts Comment	Response and Improvement
Design	Conceptual design	1) Show feedback loops where necessary and be clearer in the influence between the different objects in the conceptual framework. This comment refers to the diagrams shown in slides 7 and 10 in the workshop presentation slides in Appendix D.4.	1) Generally, the evaluation of the conceptual design includes assessment of whether the structure, concepts, assumptions and causal relationships are reasonable to form a logically consistent model (Augusiak et al., 2014). Based on the feedback, it was shown that the conceptual design is logical, but its representation in diagrams needs more clarification. Thus, the first diagram that shows the proposed framework design has been updated to the one presented in Figure 4.1 to include a legend of the shapes used for clarity. The second diagram that describes the framework implementation stages was also updated to the one presented in Figure 4.9 to reflect the improvements made to the framework, which include clearer distinction between the three stages and feedback loops between them. Those have been termed as 'Conceptual Modelling', 'Scenario Formulation' and 'Quantitative Modelling' instead of 'Problem Structuring', 'Derivation of Criteria and Indicators' and 'Scenario Formulation'. The inputs and outputs of the framework have been presented separately in Figure 4.10, after being included in the original diagram presented to the experts.

	Stakeholders and requirements	2) Recognise the need for transparency in the choice of stakeholders and prioritization of requirements 3) Ensure requirements are representative by getting an appropriate mix of stakeholders 4) Consider the impact of having different stakeholders in different scenarios on the evaluation	2-3) Discussions around stakeholders and requirements have been improved since the validation exercise, presenting source information and assumptions in Section 6.2, highlighting that a participatory approach is important for the multidimensional and systematic evaluation principles (Sections 2.3.2, 2.3.6), and that this is acknowledged in the framework design (Sections 4.1.2, 4.1.5). Yet, this research didn't aim to reach out directly to stakeholders but rather presents a flexible, modular approach to include stakeholders' objectives for a socio-technical evaluation. 4) To maintain consistency and comparability across scenarios, stakeholder groups are considered without further decomposition. This is highlighted in Section 6.2.1.
	Evaluation principles	5) The systematic principle should account for technical and political transparency in addition to replicability 6) Consider trade-offs between principles, if applicable	5) Transparency is recognised in the systematic principle as well as the recommended participatory approach, as mentioned in comment 2-3. 6) As suggested by the experts, the WES principles discussed in Chapter 2 are not necessarily discrete but actually have some overlaps. In particular, the multivectoral and systemic principle are interrelated in the scope of interactions between the integrated energy systems. However, one focuses on horizontal interactions while the other focuses on vertical interactions. In this case, there is no clear trade-off

			between the two principles, at least at the physical system level. Another example is the relation between the multidimensional and systematic principles in the scope of the participatory approach where multiple stakeholders are involved in the evaluation process. Again, there is no clear trade-off between the two principles in this case.
Output	Conceptual system model	7) Consider the impact of including prosumers on the system architecture and evaluation 8) Clarify the relation between the SysML model and simulation model 9) Consider the impact of uncertainty on the validity of the framework	7) The RSAM presented in Chapter 6 and the full case study application presented in Chapter 7 were updated to include prosumers as one of the stakeholder groups represented, in addition to DERs as a possible associated physical system component. These were not initially considered in the test case studies. 8) The framework implementation description has been significantly adjusted since the validation exercise to what is currently presented in Section 4.2. This is to distinguish between the three methodological stages involved, clarify the interaction and feedback between them, and identify the best types of scenarios and quantitative models suited for the developed framework application. 9) We assume that uncertainty is not generated within the evaluation but is carried from the uncertainty identified in datasets and quantitative models. This is not within the direct scope of this research, but is acknowledged in the discussion of

			the full case study results in Chapter 7 (Section 7.6.2).
	Scenarios and results	10) Reduce the number of scenarios analysed 11) Stick to SysML for results visualization, if applicable 12) Outline what type of scenarios are best suited for the framework	10) A limited number of scenarios has been developed for the analysis in the first place for the full case study presented in Chapter 7 based on contextual factors and according to the updated scenario specification of Section 4.2. 11) An approach for results visualisation from the evaluation framework had not been set at the time of the validation framework. This approach was later chosen, as presented in Section 4.2.4, to be backed up by the SysML graphical representation of the system interlinkages and measures of effectiveness. 12) See comment 8.
End-use	Usefulness	13) Consider a standard, consistent method to use the framework	13) A RSAM that can be used as a standard conceptual system model for the first stage of the evaluation framework was developed, in addition to clarifying the relation between the conceptual model and quantitative models needed for the third stage of the evaluation, as discussed in Section 4.2. The idea of the RSAM was discussed in the workshop. Such a modular and flexible approach to be applied in different contexts was appreciated by participants. It was thought to be a good way to facilitate and structure interactions and conversations around ESI and allows to visualise the system and its various states.

5.5. Summary

In this chapter, the developed evaluation framework is tested in two case studies based on the local energy system in Findhorn village and validated through experts' feedback elicitation. The first case study examines different system configurations to satisfy heat demand in Findhorn and the second investigates the impact of energy storage in an integrated energy network. The two case studies are used for the gradual learning and improvement of the framework without focusing on the soundness of any empirical findings. This is due to a number of limitations. First, the sufficient size of the energy system in Findhorn, which doesn't allow for a complete assessment of the value of ESI. Second, the nature of the quantitative model used being a simulation and operational model without considering optimal energy flow and optimal planning decisions. Finally, the types of data and scenarios available, which are not designed for the purposes of this project but are the resources initially available for testing the framework. However, through the application of different framework stages, the two case studies have served the following objectives:

- demonstrating the framework application to the experts' validation workshop
- creating the RSAM presented in Chapter 6
- clarifying the link between the conceptual system model and the quantitative models
- using the learnings and feedback to improve the framework and apply it to a full case study presented in Chapter 7

Upon testing, the framework was presented to experts for validation and feedback. This was carried out in a semi-structured group interview held virtually with experts from different disciplines around energy research, and a questionnaire to receive the feedback. The ethical considerations for this method are discussed including the informed and voluntary consent from participants, participants' privacy and confidentiality, risk minimisation, and conflict of interest. The validation was based on the conceptual coherence, operational coherence and utility of the developed framework. The feedback received was helpful to improve the framework presentation and application. According to the experts' feedback, the strengths of the framework can be summarised as: being comprehensive, flexible and transferable; and providing a structured approach with a unified language for ESI understanding and evaluation. On the other hand, the main improvements relate to the development of the RSAM as a modular, standardised approach to apply stage 1 of the framework, and the improved description of the framework implementation stages to clarify the interaction and feedback between them. Those improvements and the learnings from the test case studies are implemented in a full case study on the energy system of the North of Tyne region in England, which is presented in Chapter 7.

Chapter 6 Reference System Architecture Model

This chapter presents a high-level Reference System Architecture Model (RSAM) for integrated energy systems. The RSAM was developed as a result of replicating stage 1 of the framework implementation (conceptual modelling) and based on the experts' feedback on the need for a consistent, standardised application of the framework. The RSAM offers a holistic representation of the whole energy system (WES) identifying structural and functional relationships and interactions between its physical components and with its stakeholders. The RSAM is developed based on the ESI-SoS architectural framework and using SysML diagrams, as described in Chapter 4. Accordingly, the RSAM includes diagrams representing the structure, composition, stakeholders, requirements, and measures of effectiveness of the energy system. The architectural framework follows a requirements-based approach that shows requirements in the context of different system stakeholders and constituent systems. Additionally, this architectural framework provides a traceability view that maps requirements with system components, functions, and measures of effectiveness at different levels. The RSAM is modelled as a System-of-Systems (SoS), thus decomposing the WES into its Constituent Systems (CSs) at different levels of abstraction. This includes various energy system components (generation, networks, storage, demand) across multiple energy vectors (electricity, gas, heat).

The RSAM presented can be used as an approach for WES analysis to inform decision making on opportunities for synergies and trade-offs across the whole system. Moreover, the RSAM can be used as a reference for evaluating the system effectiveness in achieving its objectives while capturing emergent behaviour at the whole system level and reducing complexity through abstraction. This is done by using system requirements representing stakeholders' objectives as a benchmark against system performance. Finally, the RSAM describing the physical system architecture serves as a basis for further architectural analysis including the market and ICT architectures to enhance stakeholder roles and investigate interoperability.

Section 6.1 presents an overview of reference system architectures. The system stakeholders and requirements are identified in Section 6.2 through a literature review, followed by presenting the RSAM diagrams in Section 6.3. The usefulness of the RSAM is discussed in Section 6.4. Finally, Section 6.5 summarises this chapter.

6.1. Overview

Developing a RSAM for an increasingly complex and integrated system provides several advantages. First, it offers a common taxonomy, vision and modularisation that facilitate the system understanding and development by multiple stakeholders. Second, it allows for an effective management of synergies across system components, provides guidance on best practice and common patterns, and serves as a basis for future system change. Also, it supports interoperability between the integrated system components describing interfaces and representing system level functions and qualities (Cloutier et al., 2010). Moreover, a RSAM that describes the system structure, behaviour, and requirements for integrated energy systems can support identifying the interdependencies between different systems, as well as informing decision making on the optimal operation and planning of integrated systems (Lubega and Farid, 2016).

This chapter presents a RSAM for integrated energy systems with multiple vectors of electricity, gas and heat. While there has been previous work around system architectures for smart grids and microgrids, these efforts have been limited to the electricity system. For instance, several system architecture models describe smart grids control and management (Lopes et al., 2011; Perez et al., 2015; Worighi et al., 2019), microgrids control and management (Mahmoud et al., 2015; Zhao et al., 2018), energy internet for renewable energy delivery and management (Wang et al., 2018), and virtual power plants for the optimal management of distributed energy resources (Pasetti et al., 2018). Notably, a Smart Grid Architecture Model (SGAM) is developed and has evolved into a standard approach to design, analyse and evaluate smart grids. However, there is a need to expand the SGAM to include the gas and heat systems (Uslar et al., 2019).

As discussed in Section 2.2, the energy system architecture is expected to change upon ESI. This will include new planning and operational paradigms needed to account for the complexity involved and the emerging behaviour (Hosseini et al., 2020), new market structures and governance frameworks developed to take advantage of ESI (Jamasb and Llorca, 2019), and more ICT systems and advanced control methods needed to maintain interoperability between the different integrated components (Farid et al., 2016). Therefore, it is important to identify and understand those relationships and interactions to design, manage and evaluate integrated energy systems.

The energy system architecture can be described in three layers. The first is the physical layer focused on physical interactions, dependencies, and constraints. The second is the market layer focused on policy, regulation, and commercial interactions between actors. The third is the ICT layer focused on arrangements that enable communication within and between actors and components, in addition to interoperability and cyber security (Energy Systems Catapult, 2017). This definition is adopted in this research, although similar distinctions with different terminology can be found, for instance, with five layers: device layer, local control layer, communication, information and computation layer, system control layer, and market layer (Mittal et al., 2015). This is also in line with the five layers defined by the SGAM, being the component, function, business, communication and information layers (Uslar et al., 2019). In this project the focus is on the physical layer, which can serve as a basis for further understanding and analysis of the market and ICT layers. The physical layer comprises the energy infrastructure used to generate, transform, and transport energy. For integrated energy systems, this include networks and storage technologies for different vectors, and energy vector conversion technologies (CHP, P2G, HPs) (Guelpa et al., 2019).

6.2. System Stakeholders and Requirements

In this section, the WES stakeholders and requirements (functional and non-functional) are identified through a literature review of related work and common practice. This technique is chosen for identification, as opposed to others mentioned in Section 4.1.2, due to the project's limited scope and time, and also for the purpose of the RSAM the interest is in generic stakeholder groups. Typical stakeholder groups that directly affect energy system planning and operation are identified first. Then, non-functional requirements are assumed to reflect actual stakeholders' objectives, as per common practice. Finally, use cases for different technologies are identified to represent the functional system requirements. The findings of this section are used to develop the RSAM in Section 6.3, where stakeholders and requirements are linked to each other and to other system components leading up to the evaluation.

6.2.1. Stakeholders

Previous work carried out, particularly by the IET and the Energy Systems Catapult, have examined carefully stakeholders involved with the current and future energy system across all vectors. The stakeholders identified in different reports produced by the IET and the Energy Systems Catapult along with other academic papers are presented in Table 6.1.

Table 6.1 Literature survey of the whole energy system stakeholders

References	**Stakeholders**
(IET, 2017e; IET, 2017c; IET, 2017d; IET, 2017f; IET, 2017a)	• End users (domestic, commercial, industrial) • Operators of (generation, storage, networks) across all vectors • Products supply chains (manufacturers, vendors, developers, installers, maintenance) • Energy services providers (suppliers, aggregators, DSR, virtual power plants, virtual energy communities, Internet of Things, smart meters, energy

	management, heat services (waste recovery, CHP, DHN), transport services (EVs, chargers, agencies)) • Government (energy policy) • Local authorities and planning authorities • Wider society (society needs) • User group representatives • Consultancies and media • Academia and research councils • Regulators • Prosumers
(Energy Systems Catapult, 2017; Energy Systems Catapult, 2019)	• Government (National, Regional, Local) • Citizens, consumers and society • Households and businesses • Manufacturers and product vendors • Investors • System and reserve operators • Providers of (energy services, storage, distribution, production) for each vector • Policy makers • Regulators
(Rojas and Rousan, 2017)	• Consumers, Vendors, service providers (procurement, construction), project (owners, managers, financiers), utilities, operators
(Grünewald et al., 2012)	• Demand side, Network, Generators, Storage, Public sector, Consultants, Academia
(Bale et al., 2015)	• End users (households and businesses) • Energy conversion and supply companies (generators and suppliers) • Economic and environmental regulators • Governments (local and central)

The system stakeholders are identified as stakeholder groups and are included in the RSAM if they are directly involved in the energy system planning and operation. Hence, stakeholders such as developers, vendors, manufacturers, consultancies, and those representing media and research are not considered. Moreover, since the market layer is not directly examined in this project, stakeholders such as the regulator and other market players are not included. The detailed composition of the identified stakeholder groups is also out of the scope of this project. Accordingly, the final list of stakeholder groups considered includes the following:

- the government bodies overseeing the energy policy at various levels of governance (national, regional, local)
- the operators managing the CSs or elements thereof (generation, networks, storage)

- the local community (citizens, society) that takes part in the planning process and shows environmental, social, or other values
- the end-users demanding and consuming energy (domestic, commercial, industrial)
- the prosumers with embedded energy generation capacity (domestic, commercial, industrial)

However, it is important to be careful with assumptions around the inclusion and exclusion of stakeholders and what impact this could have on the evaluation and any actions that could be based on it. Therefore, it is worth considering a transparent, participatory approach for involving a wide range of stakeholders into such conversations in real life applications.

6.2.2. Non-functional Requirements

Non-functional requirements refer to what the system features must be and set limits to how well the system performs its functions. These include constraints, criteria, behaviours, performance targets, and what is known as '-ilities' (quality, reliability, scalability, compatibility, etc.) (EPRI, 2008). A literature review around current and future energy system requirements is carried out to identify objectives set by different stakeholder groups, which is summarised and presented in Table 6.2.

Table 6.2 Literature survey of the whole energy system non-functional requirements

References	**Requirements**
Smart Local Energy Systems (Gooding et al., 2020; Ford et al., 2021)	• Flexibility in planning and operation (Flexibility across vectors; Network efficiency; Reducing limitations to RES integration; Removal of network constraints; opportunities for higher energy use activities) • Technology enabled CO_2 reduction (electric heating, EVs take up) • Supporting and empowering communities (reduction in fuel poverty, community empowerment, increased self-sufficiency) • Place based prosperity (job creation) • Improving visibility and control (demand-side management, informed decision making, tailoring energy assets to local conditions) • Increased energy efficiency, better service offering
Whole Energy Systems (Energy Systems Catapult, 2019)	Consumer centric, societal, physically constrained, commercially aligned, secure and resilience
Microgrids (Rojas and Rousan, 2017)	Reliability, lower costs, lower emissions, resilience, cyber security
Distributed systems (Grünewald et al., 2012)	• System operation, balancing, flexibility, volatility, EV integration • Generation capacity, network reinforcement, infrastructure cost • Consumer engagement, consumer cost • Security, Resilience • RES integration, Use excess electricity, CO_2 reduction, Jobs

Demand side (Kubli et al., 2018; Döbelt and Kreußlein, 2020)	• Consumers: secure energy supply, legal matters of the contract, grid stability • Prosumers: control of their energy production, installation and maintenance costs, regulatory and administrative difficulties, connectedness, independence, self-consumption, power composition, taxation, grid stability, data protection, clear information on pricing • Prosumers willingness for providing flexibility: Comfort/convenience, compensation/incentives
Future energy system requirements (IET, 2017b; IET, 2017d; IET, 2017e)	• Cross vector opportunities for (flexible demand, storage, generation, arbitrage) • Manage interfaces with connected energy systems and collaborate to optimise planning and operation • Ability for vector conversion and transport • Achieve policy objectives (deliver the energy trilemma, decarbonisation, affordability, cost-effectiveness, innovation) • Deliver high quality service • Respond to changes (resilience, restoration, response to extreme events) • Active network management (frequency response, balancing and reserves (ancillary services), constraint management, demand response) • Security of supply (cold start, emergency procedures for speed restoration, black start capability, islandability, availability, reliability, stability, emergency recovery, diversity, flexibility) • more control, access to data (relating to energy consumption, generation, capacity and associated price signals), cyber security • customer needs (flexibility, comfort, cost, efficiency, control, monitoring, affordability) • off-grid services (power island, community services (Peer-to-Peer)) • Local energy independence (self-sufficiency) • New commercial arrangements (market mechanisms) for exchanging services between customers, communities and other system players • Facilitate active engagement of customers • Aligned financial incentives across the sector

Some of the requirements identified in the literature review are discarded due to the scope of the project, although remain important for future work. For instance, job creation is not considered since macroeconomic modelling is not carried out. Other examples are cyber security, data protection and interoperability, which relate mainly to the ICT system layer. Similarly, requirements related to the market structure, business models, and financial incentives are not included. On the other hand, non-technological matters that cause concern for prosumers, such as regulatory and administrative burden and installation and maintenance costs are not considered here as requirements. However, those aspects would still be useful for the evaluation if considering behavioural factors and technology adoption. It is also assumed that basic operability (normal execution, forecasting, monitoring, control, maintenance, settlements) of the energy systems is maintained.

The key requirements are thematically grouped into the following:

- Deliver energy services
- Achieve the trilemma policy objectives: Decarbonisation, Affordability, Security
- Achieve decarbonisation: Reduce carbon emissions, Integrate RES, Improve efficiency, HPs and EVs uptake
- Affordability: reduce/optimise costs
- Security of supply: Reliability, Resilience, Flexibility (across vectors)
- Provide access to the grid and maintain comfort/convenience

The identified requirements are assigned to corresponding stakeholders in Section 6.3.2.

6.2.3. Functional Requirements

Function requirements typically refer to what the system must do or deliver (EPRI, 2008). In the context of this project, functional requirements refer to the functions performed by CSs. In particular, we are interested in use cases of technologies that make up the coupling system, i.e. CHP, P2X, and HPs, in addition to the role of energy storage in the whole system. Use cases provide context to requirements by showing how the systems can be used. Use cases for each technology are identified from the relevant literature as shown in Table 6.3.

Table 6.3 Literature survey of energy technologies use cases

Technology	**Requirements**	**References**
Energy Storage	• Peak shaving • Provide network services and defer upgrade (voltage control, reliability, black start, power flow management, mitigate losses) • Avoid RES curtailment • System balancing • Arbitraging prices	(DNV GL, 2016; Santos et al., 2017)
Power-to-X	• Vector shifting • Avoid RES curtailment • Integrate energy systems (interconnection between energy markets, synergy with other networks, produce renewable gas for heating, produce fuel for mobility) • Provide ancillary services (voltage and frequency regulation) • Bulk storage and RES integration • System management (congestion)	(Brunner et al., 2015; Mazza et al., 2018; Lewandowska-Bernat and Desideri, 2018)

	• Network upgrade deferral • Reduce energy losses • Balance intermittent RES surplus	
Combined Heat & Power	• Efficient use of energy • Low transmission losses • Cleaner technology	(Andersen et al., 2008)
Heat Pumps	• Transform electricity to heat • Increase performance • Cost efficiency • Grid stability • Use excess RES • Thermal storage	(Guelpa and Verda, 2019)

It is clear that ESI technologies have similar requirements to deliver to the energy system. This validates the assumption of grouping those technologies under one CS, which is the coupling system. Accordingly, requirements for the coupling system are unified as follows:

- Shift energy vector/integrate energy systems
- Reduce energy use and losses/Improve efficiency
- Provide network services
- Use excess RES/Avoid RES curtailment

On the other hand, while energy storage technologies share similar functions with ESI technologies, they are considered separately because their functions are restricted to one energy vector. Thus, they are contained within the electricity, gas or heat CSs, respectively, and their functions are summarised by one requirement of providing storage services.

6.3. System Model

The RSAM is presented in this section according to the system levels and views of the ESI-SoS architectural framework presented in Table 4.2. The model represents a high-level system architecture for an integrated energy system consisting of the electricity, gas and heat systems, in addition to the coupling system. The scale of integration is considered at the distribution network level, and accordingly the system boundaries are determined to be the local energy system.

6.3.1. Context Level

At the context level, the system is defined in terms of its CSs and stakeholders using block definition diagrams. Figure 6.1 shows the CSs, namely the electricity, gas, and heat systems, as well as the coupling system that represents ESI technologies.

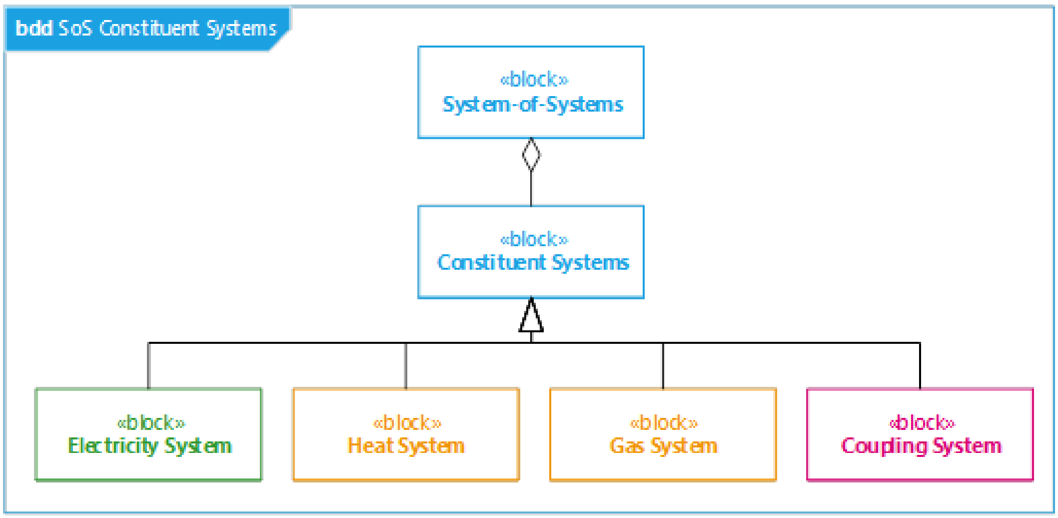


Figure 6.1 Context level: Constituent systems

Figure 6.2 shows the system stakeholder groups identified in Section 6.2 including:

- the government overseeing the energy policy (at various levels of governance)
- the system operators managing the CSs or parts of it
- the local community that takes part in planning and might show eco-friendly values
- the end-users demanding and consuming energy
- the prosumers with embedded energy generation capacity

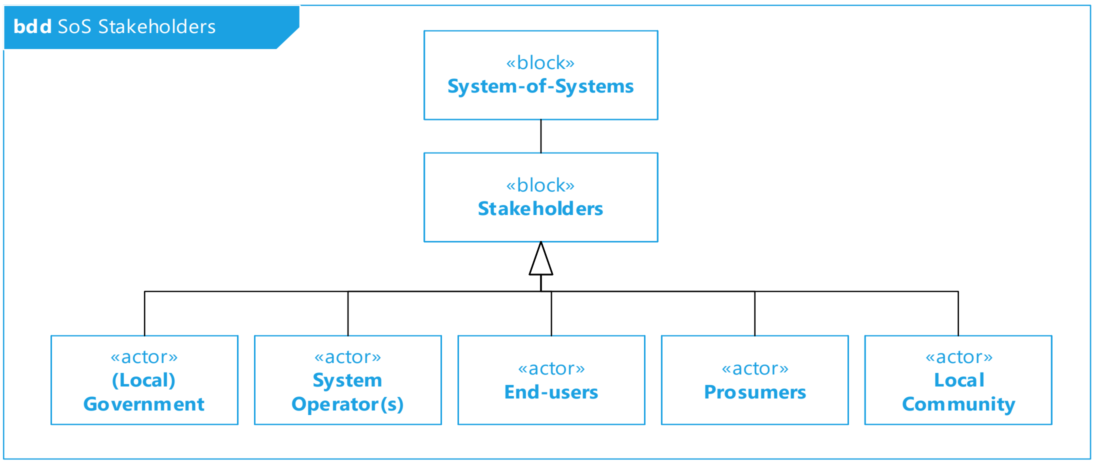


Figure 6.2 Context level: Stakeholder groups

As mentioned earlier, the detailed composition of those groups is out of the scope of this project. The stakeholder groups included here are those that directly influence the energy system planning and operations. Accordingly, stakeholders such as developers, vendors, manufacturers, and those from media and research are not considered. Moreover, since the market layer is not directly examined in this research, stakeholders such as the regulator and other market players are not included.

6.3.2. System-of-Systems Level

The second level in the ESI-SoS architecture framework is the SoS level. At this level, the structure of the system is first defined. Figure 6.3 is an internal block diagram that shows the structural relationship between CSs at the highest level of abstraction.

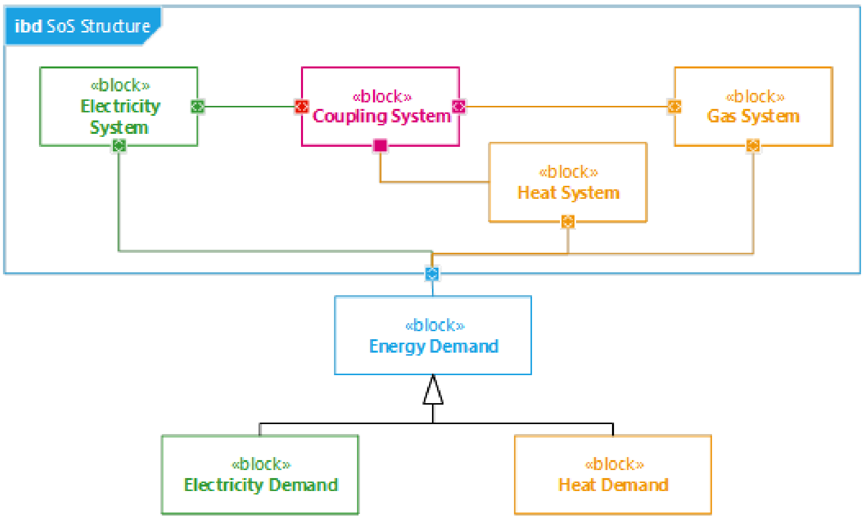


Figure 6.3 SoS Level: Structure

As mentioned previously, system requirements sit at the heart of the conceptual system model development process, as per the SoS-ACRE architectural framework. Therefore, it is important to define the requirements at the SoS level before putting them in context with the system stakeholders. Figure 6.4 shows a requirements description diagram. The requirements at this level are related to the stakeholders' objectives that the SoS should deliver.

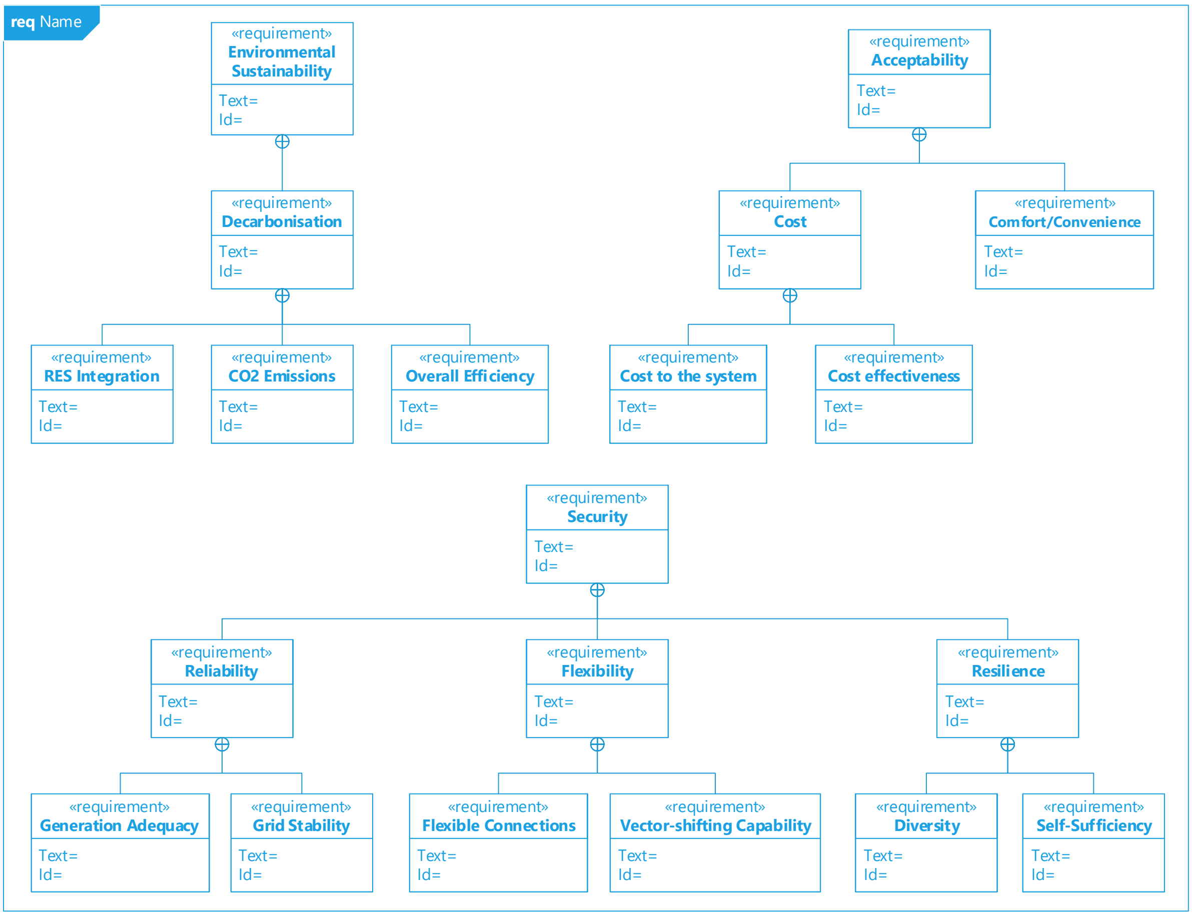


Figure 6.4 SoS Level: Requirements description

The starting point is that there is a requirement to achieve the energy trilemma policy objectives while delivering the required energy demand to end-users. The energy trilemma refers to the three dimensions of environmental sustainability, social and economic acceptability, and the technical energy security. These dimensions therefore correspond to objectives for decarbonising the energy sector, optimising costs, and maintaining a reliable, resilient, and flexible energy system. Additionally, prosumers require access to the grid and a requirement to retain their comfort and convenience.

The defined requirements are attributed to stakeholders and are also linked to each other in the requirements context view through a use case diagram, shown in Figure 6.5. The trilemma requirements constrain the requirement of delivering energy. They also extend to more detailed requirements or more specific targets. For instance, decarbonisation includes requirements such as reducing carbon emissions, integrating more RES, and improving overall efficiency.

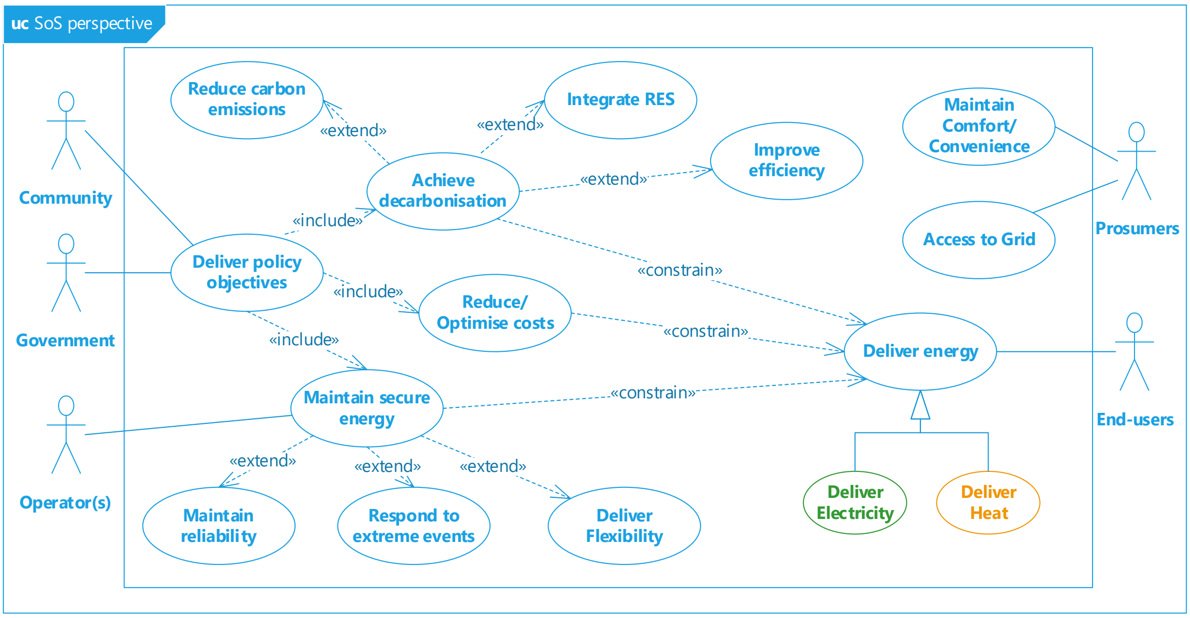


Figure 6.5 SoS level: Requirements Context

6.3.3. Constituent Systems Level

At this level, the CSs are first defined in terms of their composition. The block definition diagrams in Figure 6.6 show the composition of each CS. Upstream components relate to the national transmission networks of the electricity and gas systems, respectively.

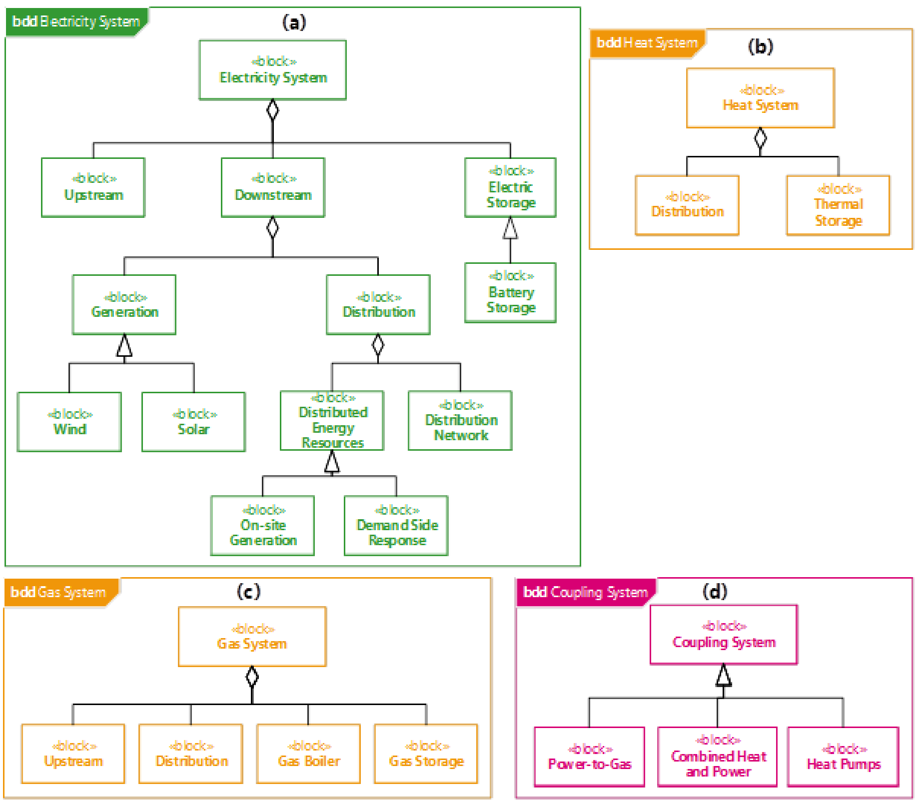


Figure 6.6 CSs level: Composition of (a) Electricity system; (b) Heat system; (c) Gas system; (d) Coupling system

The next view shows the system structure at the CSs level. This is shown by the internal block diagram in Figure 6.7, where the relations between the system elements making up the CSs are visualised.

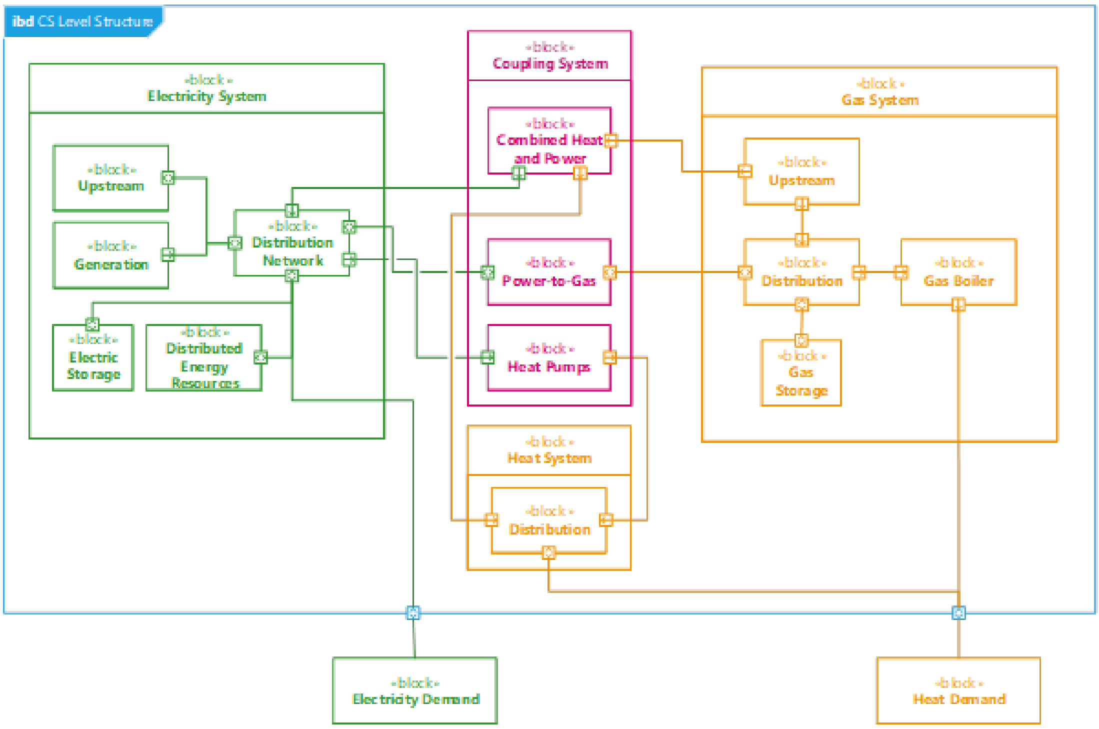


Figure 6.7 CSs level: Structure

Figure 6.8 shows the requirements context interaction view in the form of a use case diagram. Requirements at this level show the functionalities that each CS delivers. However, these are shown in relation to other CSs and to the SoS. The latter shows how CSs contribute to achieving the higher-level requirements. Those contributions mainly emerge from the interaction between the different CSs. For instance, the coupling system can deliver flexibility to the SoS through shifting energy vector between the different CSs. Moreover, using CHP and HPs is expected to reduce the overall energy use. The coupling system can also provide grid services by relieving network constraints across vectors, and thus could delay network upgrades and reduce costs and losses.

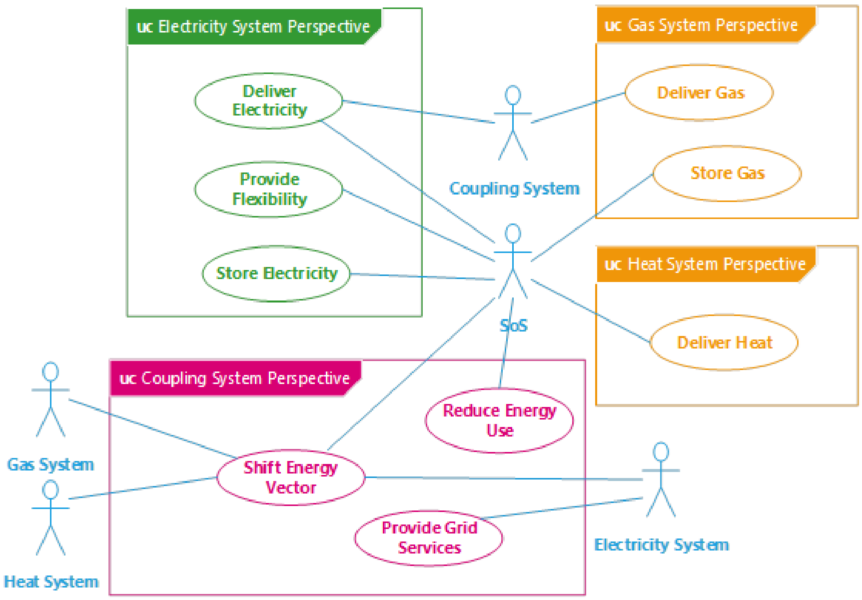


Figure 6.8 CSs level: Requirements context interaction

6.3.4. Whole System Level

Finally, the traceability and measures of effectiveness views are presented at the cross-cutting whole system level. The traceability view, presented in Figure 6.9, shows the relations between different system components at different levels. This includes CSs, system elements, and requirements at both the SoS and CSs levels. In particular, the system requirements are traced to the functionalities that satisfy it and the system elements from where its level of satisfaction can be measured. The traceability view can therefore support the realisation of possible trade-offs and synergies between the different system components.

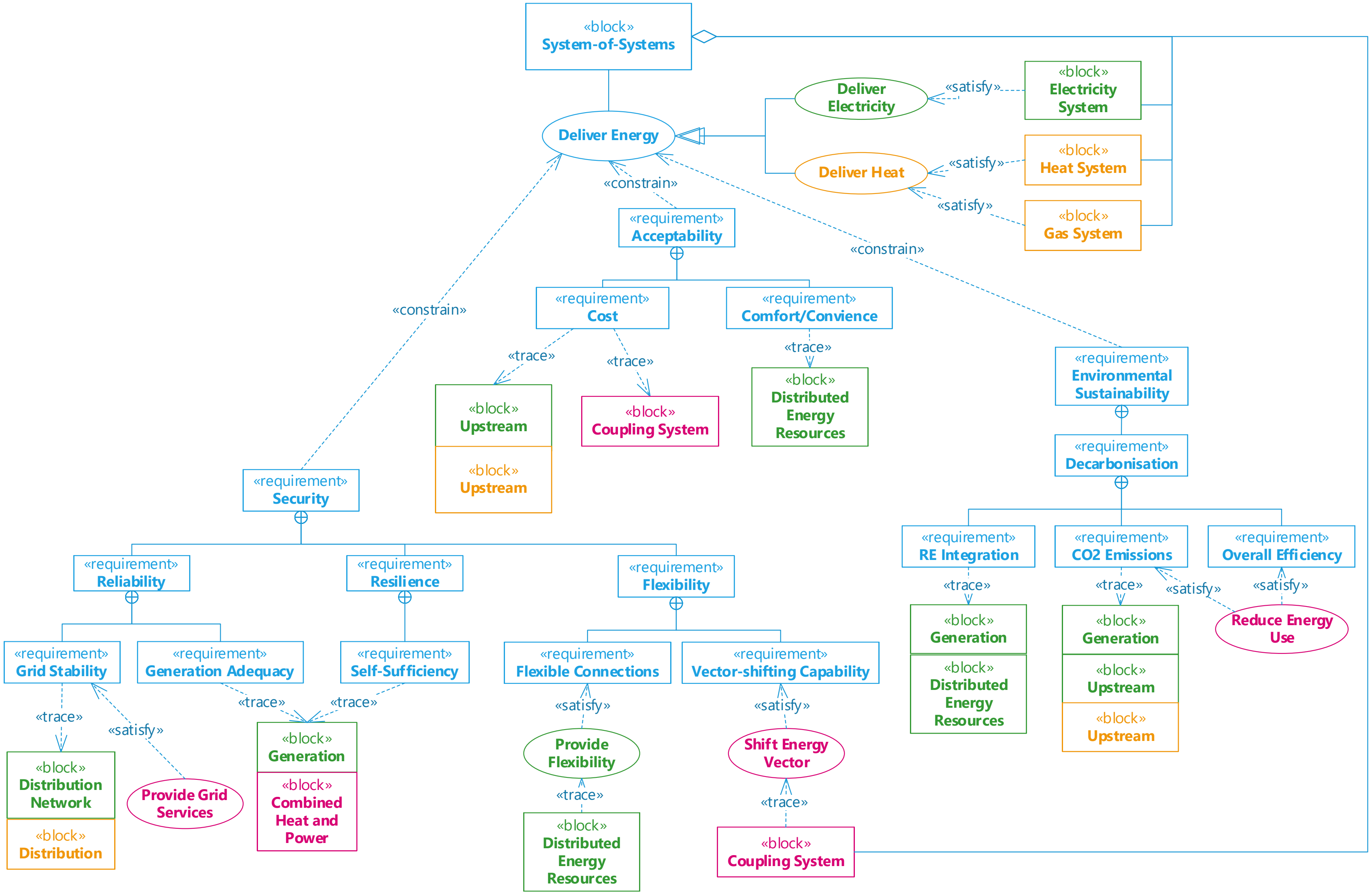


Figure 6.9 Whole system level: Traceability

Accordingly, measures of effectiveness are defined to evaluate the system performance against its requirements. Figure 6.10 shows the measures of effectiveness in a parametric diagram. For instance, decarbonisation is evaluated by three criteria: CO_2 emissions, RES integration and the overall energy efficiency. To measure the state of those criteria, each one is assigned a quantitative parameter, i.e., an indicator. CO_2 emissions can be directly measured as the amount of emissions related to energy supply; RES integration is measured by the share of RES from the total energy supply; and the overall efficiency is measured as the energy saving ratio, which indicates the difference in the amount of primary energy input to the system for different scenarios. In this case, the three indicators relate to energy generation assets or energy imports from upstream as shown in Figure 6.9. In addition, the overall efficiency requirement is supported by the 'reduce energy use' requirement of the coupling system.

The cost criterion is evaluated by two aspects, cost to the system and cost effectiveness. The cost to the system is measured as the sum of the cost of energy import from upstream components and the cost of integration from the coupling components. Cost effectiveness can be measured by the abatement cost of CO_2, which is the ratio of total costs to the amount of CO_2 emissions reduced. Furthermore, the comfort and convenience requirement can be measured qualitatively as the willingness of prosumers to shift their energy behaviour.

Energy security is evaluated by three technical criteria: reliability, resilience, and flexibility. Reliability has two aspects: generation adequacy measured through the capacity margin of generation assets, and the grid stability measured by when the voltages in the power and pressures in the gas distribution networks are within acceptable ranges. The latter is supported by the 'provide grid services' requirement of the coupling system. Resilience also has two aspects: diversity of primary energy resources and self-sufficiency in terms of local energy generation. Finally, flexibility is measured by the availability of the components that provide flexibility, namely the coupling system technologies, DER, electric storage, and gas storage as shown in Figure 6.10.

As discussed previously, the specific choice of indicators also depends on the data availability. The indicators in Figure 6.10 are presented to provide guidance and are not definitive or exhaustive. Indicators can be changed depending on the application, and are thus not individually discussed in further detail here.

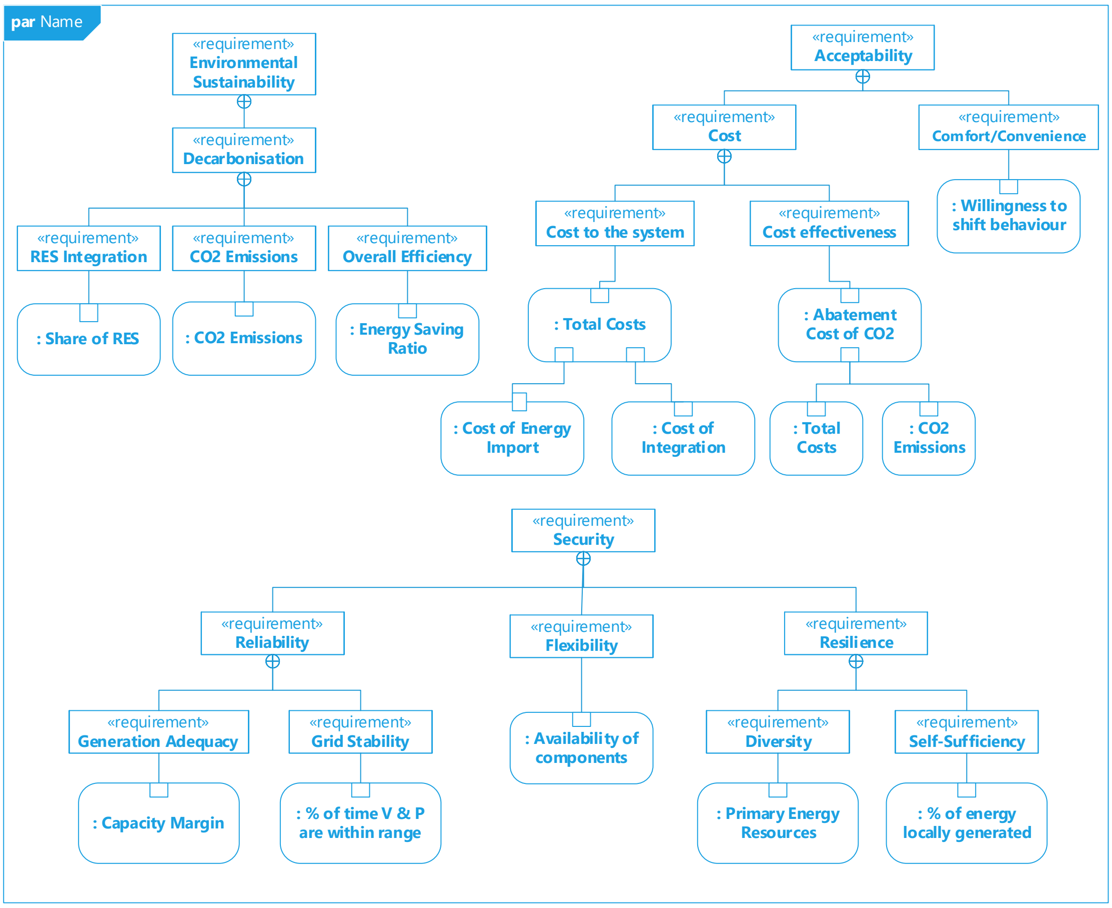


Figure 6.10 Whole system level: Measures of effectiveness

6.4. Discussion

The RSAM presented in this chapter can be shown to fulfil multiple objectives, as demonstrated later in Chapter 7. First, it allows for a WES analysis of the integrated energy systems. This includes looking at the system in the context of multiple perspectives related to different stakeholders. Thus, the energy system is considered within a broader environmental, economic, and social context (Bale et al., 2015). Moreover, it considers the multiple energy vectors involved and identifies the interactions between the different energy systems at different levels. The RSAM provides this by portraying the system as a SoS and thus decomposing it into different levels and different CSs. Additionally, the system model defines the interactions within the WES and with the system environment through the requirements-based approach. Whole systems analysis can inform planning and decision making on opportunities for cost savings and efficiency gains through synergies and for avoiding unintended impacts across the system (Energy Systems Catapult, 2019; Cambini et al., 2020).

Second, the RSAM serves as a reference for evaluating the system effectiveness in achieving its objectives. In particular, it can be used as a standard conceptual model for stage 1 of the evaluation framework developed in Chapter 4. The requirements-based approach sets a benchmark whereby the system performance is evaluated against the stakeholders' goals and needs. The level of satisfaction of the requirements is then a measure of how good the system is in delivering the expected functions to achieve set objectives. The system model provides this by mapping the requirements:

- in relation to each stakeholder at the SoS level, e.g., maintaining energy security, including delivering flexibility, associated with the operators (Figure 6.5)
- of each CS in relation to other CSs and to the SoS, e.g., shifting energy vector being provided by the coupling system and benefiting the gas and heat systems, in addition to contributing to the SoS requirements such as delivering flexibility (Figure 6.8)
- with the relevant system components and functions at different levels, e.g., the flexibility requirement being traced to the shifting energy vector functionality provided by the coupling system, storing energy functionality provided by electric and gas storage, and to providing flexibility by the DER components (Figure 6.9)
- with the indicators used for measurement and evaluation, e.g., the flexibility requirement measured by the availability of components providing the relevant functionalities as identified in the previous point (Figure 6.10)

As a RSAM, the approach lends itself to be used as an adaptable, modular approach for evaluation. Stakeholders, requirements, CSs, system components, and accordingly measures of effectiveness can be added or removed depending on the specific application. Another advantage for using this approach for evaluation is the ability to capture emergent behaviour resulting from interactions between CSs through traceability, while also reducing the complexity involved through system abstraction. This enables better understanding of systemic properties such as resilience and flexibility (Bale et al., 2015).

Take the example of two system configurations, one with separate CSs and single vector energy storage and another with integrated CSs and cross vector storage. Comparing the performance of the two systems under the same supply and demand conditions, the integrated system is expected to exhibit emergent flexibility at the SoS level, in addition to the flexibility provided separately by each CS. In this case, the emergent flexibility is traced to the coupling system and it can be evaluated by comparison using the measures of effectiveness presented in Figure 6.10.

Scenario analysis and comparison as such is enabled when combining the RSAM with the scenario formulation and quantitative modelling stages as described in Section 4.2. This can aid decision making by:

- using the system architecture approach to explore future potential pathways of the energy system
- testing and evaluating the impacts of implementing changes such as integration through simulation and quantification
- realising potential synergies and trade-offs upon integration
- representing different actors and components at different levels for a socio-technical analysis

Finally, the RSAM presented in this chapter provides a basis for further architectural analysis. This is supported by the use of MBSE in the development of the RSAM, which makes the model reusable, repeatable, and extendable for future studies (Topper and Horner, 2013). For instance, the physical system layer described in this chapter can serve as a building block for developing the full energy system architecture with the market and ICT layers. For the market layer, the roles of the different stakeholders can be enhanced based on their requirements and the contractual relationship between stakeholders defined in terms of their physical interactions. For the ICT layer, cyber-physical interfaces and interoperability within the whole energy system layers and components upon integration can be further investigated. Data and information exchanges are essential for proper integration and coordination (Cambini et al., 2020), while interoperability is necessary to ensure system resilience and flexibility (Energy Systems Catapult, 2019). This is in line with the co-evolutionary analysis of different architectural layers proposed in Section 3.3.3.

6.5. Summary

This chapter presents a high-level reference system architecture model (RSAM) for integrated energy systems with the multiple vectors of electricity, gas and heat. The RSAM describes the system architecture using multiple views representing the system structure, composition, requirements, and measures of effectiveness. System stakeholders and requirements are first identified through a literature review. The system model is then developed using the architectural views and SysML diagrams identified by the ESI-SoS architectural framework. This framework depicts the integrated energy system as a SoS with different CSs interacting at multiple levels. The requirements-based approach followed supports the identification of system interactions and provides a benchmark for evaluating the system effectiveness in achieving its stakeholders’ objectives. Therefore, the RSAM is useful for whole energy system analysis and evaluation.

The RSAM resembles a standard conceptual system model that represents an integrated configuration of energy systems and includes a wide range of energy technologies. This provides a flexible, modular approach to the implementation of stage 1 of the developed evaluation framework. The RSAM still has to be coupled with scenario formulation and quantitative modelling for the full application of the framework.

The RSAM presented here is limited to the physical system layer of the integrated energy system, which focuses on physical interactions and interdependencies. Therefore, future work includes building on the physical layer for further analysis of the market and ICT layers to develop a comprehensive energy system architecture. Furthermore, the transport sector should also be incorporated into the integrated system model with the increased adoption of electric vehicles and the effect this has on the whole energy system. MBSE techniques and a generic architectural framework provide a useful means for reusing and extending the system architecture presented in this chapter for future work.

Chapter 7 Case Study: North of Tyne Region

This chapter presents a demonstration of the evaluation framework developed in Chapter 4, using the RSAM approach presented in Chapter 6 and through scenarios based on the case study of the North of Tyne (NoT) region in England. The case study aims mainly to explore the value of ESI as a future pathway for the energy transition in the region. The scenario analysis is carried out with different network configurations (electricity, heat, gas) and coupling technologies (CHP, P2G, HPs), and under varying conditions of energy supply and demand. The analysis is supported by an optimisation model for integrated energy networks operation developed by colleagues at CESI and populated by actual data of the energy system in the region (Appendix E and F).

This chapter has several objectives:

- Demonstrate the applicability and usefulness of the evaluation framework on a larger scale and more complex energy system
- Implement improvements on the framework based on the learnings from the test case studies and feedback from experts
- Provide empirical evidence on the effectiveness of energy systems integration as a pathway to achieve the energy transition targets at a regional level using the framework

The NoT region presents an interesting case study area as it combines urban and rural settings, includes residential, commercial and industrial demands, has ambitions at the local level to reach net-zero targets, and has seen an increase in RES capacity in recent years. This makes the energy system in the region more complex to study than the case study of the Findhorn village for demonstrating the evaluation framework. The region also houses a number of research facilities and initiatives that make the case study data accessible.

The rest of the chapter is outlined as follows:

- Case study area description (Section 7.1)
- Scenario formulation (Section 7.2)
- Conceptual modelling (Section 7.3)
- Quantitative modelling and data (Section 7.4)
- Case study results (Section 7.5)
- Discussion (Section 7.6)
- Summary (Section 7.7)

7.1. Case Study Area Description

The NoT region is a recently established combined authority that covers the local authority areas of Newcastle upon Tyne, North Tyneside, and Northumberland in the North East of England. The region covers an area adding up to around 5,277 km^2 and has an estimated population of 833,000 with more than 360,000 households (BEIS, 2020e; BEIS, 2020f). An overview of energy consumption and emissions figures from the region, in addition to an outline of the local net zero plans are presented in the following sections, for context.

7.1.1. Energy Consumption and Emissions

The region has a variety of features in terms of energy such as a legacy of high rates of fuel poverty, high proportion of off-gas properties, above average domestic gas consumption per meter, a number of existing district heating schemes, and a significant RES capacity expansion. Moreover, the region houses a number of energy research and demonstration facilities including Newcastle University, CESI, InTEGReL[7], Helix site and others (North East LEP, 2019).

In 2016, fuel poverty rates were estimated to be around 14.4%, 11.2% and 12.8% of households in Newcastle upon Tyne, North Tyneside and Northumberland, respectively. In fact, data show that rates have improved to 10.6%, 7.6% and 9.8%, respectively in 2018, while the national average stands at 10.2% (BEIS, 2020e). The percentage of properties not connected to the gas grid is 11% for Newcastle, 4% for North Tyneside, and 18% for Northumberland, compared to a national average of 14% (North East LEP, 2019). Furthermore, the wider North East region has around 9% of the overall UK heat networks and has a significant potential for deployment of geothermal heating schemes (North East LEP, 2019).

The total energy consumption in the region for domestic, commercial, industrial and transport sectors was estimated to be 1486.4 ktoe in 2018, which is around 17.3 TWh. This is around 1% of the UK total energy consumption in 2018. The commercial and industrial demand makes up around 37% of the total consumption, the domestic sector consumes 35%, while the transport demand stands at 28% (Figure 7.1) (BEIS, 2020d).

[7] Integrated Transport Gas Electric Research Laboratory

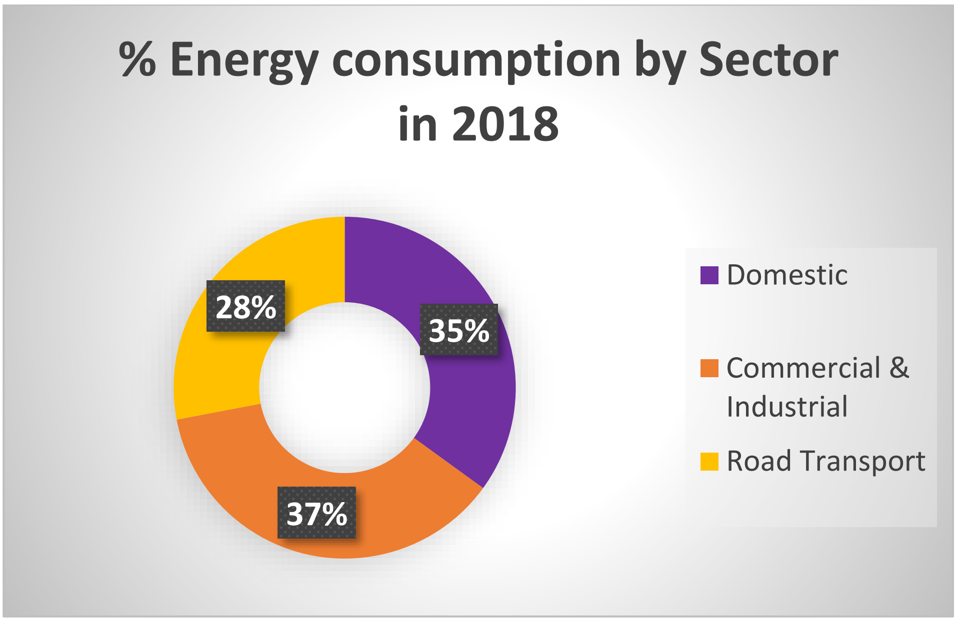


Figure 7.1 North of Tyne energy consumption breakdown by sector Produced from data available in (BEIS, 2020d)

The domestic consumption is mainly supplied by gas (75%) followed by electricity (20%) and other fuels (5%). Similarly, the commercial and industrial sectors are mainly supplied by gas (43%) followed by electricity (35%) and other fuels (22%) (Figure 7.2). Looking at the gas and electricity consumption, it is noted that gas consumption is mainly for domestic purposes with around 62% while around 38% goes to the industrial and commercial sectors. On the contrary, the electricity consumption is dominated by the industrial and commercial sectors with around 65%, while the domestic consumption is around 35% (BEIS, 2020d).

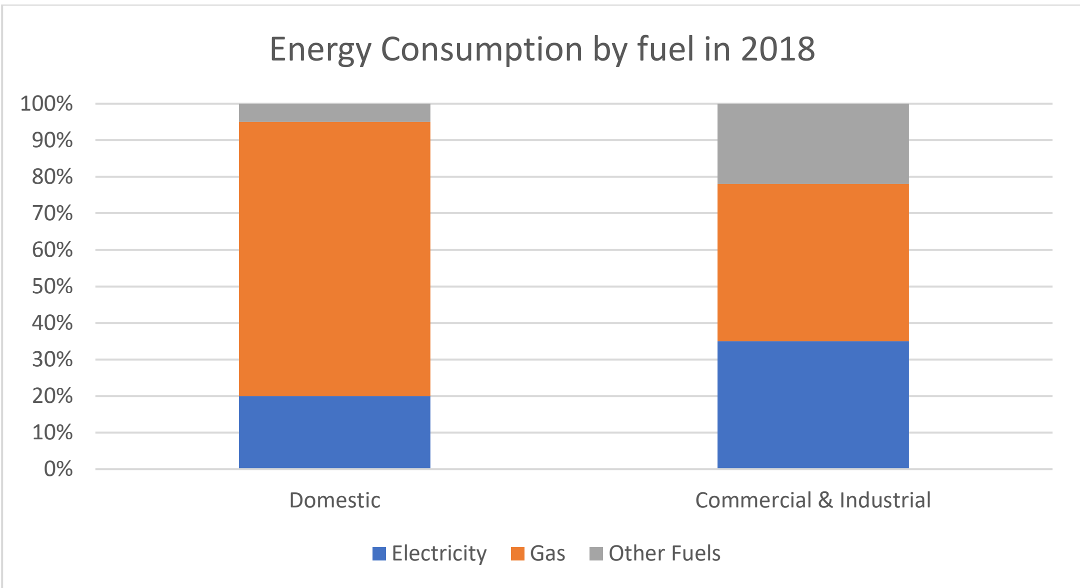


Figure 7.2 North of Tyne energy consumption breakdown by fuel Produced from data available in (BEIS, 2020d)

The renewable energy capacity has increased in the region by around 240% from 244.9 MW in 2014 to 837.6 MW in 2019, while generation from RES has increased by around 121% from around 517.5 GWh in 2014 to around 1146.4 GWh in 2019. The increase in both RES capacity and generation has been dominated by the expansion of solar PV, onshore wind and offshore wind in Northumberland (BEIS, 2020c).

Table 7.1 Renewable energy expansion in the NoT region between 2014 and 2019

	2014	**2019**	**Growth (%)**
Renewable energy total installed capacity (MW)	244.9	837.6	242
Renewable energy total generation (MWh)	517,531	1,146,397	121

Accordingly, carbon emissions in the region have seen a decrease between the years 2014 and 2018 as shown in Table 7.2. The wider North East region experienced the largest percentage reduction in CO_2 emissions in the UK from 2005 to 2018, in part due to industrial closures (BEIS, 2020f).

Table 7.2 Carbon emissions in the NoT region between 2005 and 2018

	2005	**2014**	**2018**	**2005-2018 change (%)**	**2014-2018 change (%)**
Total Carbon Emissions ($ktCO_2$)	7,243.7	3,313.2	2,837.0	−60.83	−14.37
Per capita Emissions	27.0	12.6	10.6	−60.83	−16.23
Emissions per km^2	34.7	24.5	21.2	−38.85	−13.38

In 2005, the industrial and commercial sectors were responsible for the majority of carbon emissions in the region with 58.2% compared to 23.9% by the domestic sector and 17.9% from transport. In 2018, the transport sector takes the lead by 34.7% while the industrial and commercial sectors come next with 33.5% followed by the domestic sector with 31.9% of emissions (BEIS, 2020f).

Net carbon emissions by sector are shown in Figure 7.3 (BEIS, 2020f), including emissions from Land use, Land use change and forestry (LULUCF). This includes removals of carbon dioxide from the atmosphere, and so its value is negative in this case. It is worth noting that the North East has the second largest sink of LULUCF CO_2 per capita emissions (−0.5 tCO_2 per person) in the UK due to its large area of forest land, partly offsetting its higher level of emissions from the industrial and commercial sector than most regions (BEIS, 2020f).

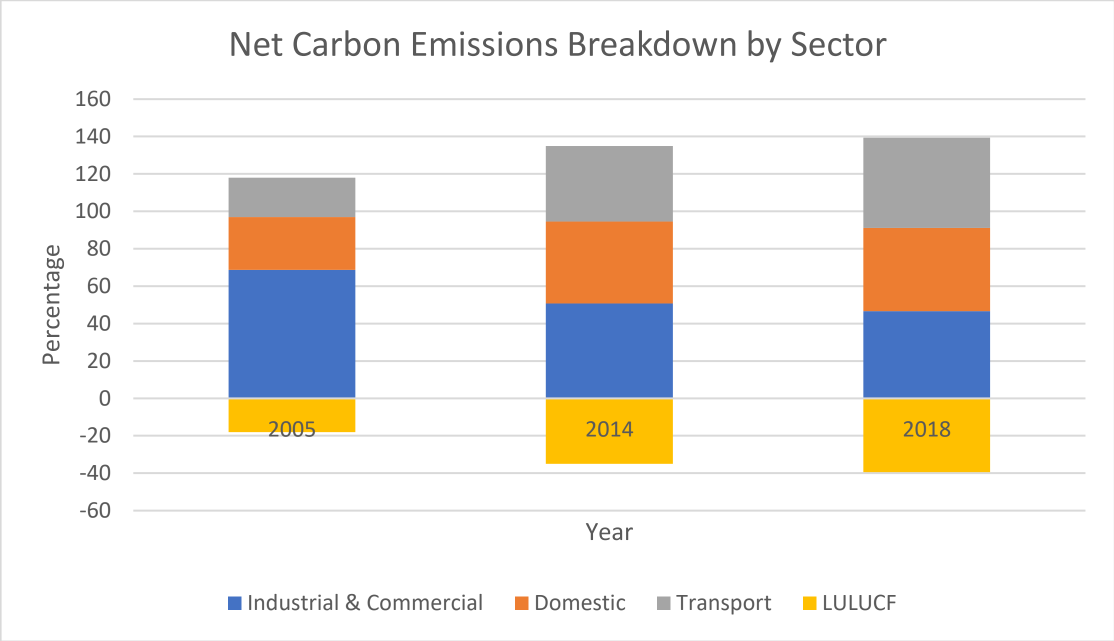


Figure 7.3 Net carbon emissions breakdown by sector in the NoT
Produced from data available in (BEIS, 2020f)

This overview of energy figures shows that the energy consumption in the region is dominated by gas, which is typically used for heating purposes in the domestic and commercial & industrial sectors. This reiterates the need to decarbonise heating. This could benefit from the potential for RES expansion in the region as well as for district heating. Again, this raises the prospects of ESI as a pathway to achieve net-zero carbon emissions targets through coupling the multiple vectors of electricity, gas and heat present in the region. It is worth noting that the transport sector is another priority for decarbonisation as evident by the carbon emissions figures, which can be boosted by ESI as well but this is outside the scope of this research.

7.1.2. Net Zero Plans

The decarbonisation plans for the region are, at least, in line with the national targets for net-zero carbon emissions by 2050, with some more ambitious targets to achieve decarbonisation by 2030. The plans typically include more RES expansion, increasing electrification of heat and transport, and wider district heating schemes (Newcastle City Council, 2020; North Tyneside Council, 2020; Northumberland County Council, 2020). Thus, this case study aims to explore the prospects of ESI in the region with the expected increase in deployment of RES and electric heating technologies.

The NoT combined authority has announced a climate emergency in 2019, but while it doesn't have its own roadmap, the NoT combined authority supports the plans of its three member local councils, each of which outline their own plan for net-zero as follows:

- Newcastle City Council committed to be carbon neutral by 2030 and to power the city with 100% clean energy by 2050 (Newcastle City Council, 2020)
- North Tyneside Council committed to be carbon neutral by 2050 and to achieve 50% reduction in emissions by 2027 from a 2010 baseline (North Tyneside Council, 2020)
- Northumberland County Council committed to be carbon neutral by 2030 (Northumberland County Council, 2020)

The three local authorities have set plans considering similar priority areas of action to achieve net-zero by decarbonising electricity, heat and transport. These are mainly related to:

- Improving energy efficiency measures in buildings
- Increasing rooftop solar PV installations
- Installing heat pumps
- Establishing low carbon district heating networks
- Blending hydrogen with gas
- Using renewable biofuels and biogas
- Transitioning to electric vehicles

Other areas of action include improving education, tackling fuel poverty, limiting commute to walking and cycling options, reducing waste emissions and capturing emissions.

The plan by Newcastle is the only one that sets specific targets, although provisional. For instance, targets are observed to install heat pumps in 57% of homes and 60% of non-domestic properties, supply 20% of homes and 74% of non-domestic properties from low carbon district energy networks, and reach a 20% of hydrogen mix with gas for all properties. The plan claims that even if all those targets are achieved, only 79% of the net-zero target would be achieved and that the remaining emissions will need to be offset or inset[8]. Reaching net-zero will also still depend on the upstream electricity grid emissions reduction, which might reach just 82% by 2050 (Newcastle City Council, 2020). On the other hand, the North Tyneside action plan does not include specific targets for different sectors but rather presents different scenarios on how the net-zero target could be reached. It is, however, anticipated that 100% roll out of electric heating to viable homes is required by 2050 (North Tyneside Council, 2020).

[8] Carbon inset is similar to offset but takes places within the organisation's value chain

In this context, scenarios are designed for this case study and described in Section 7.2, before the framework application is demonstrated in Section 7.3, while the relevant model and data are presented in Section 7.4.

7.2. Scenario Formulation

The case study scenarios are designed to capture the value of integration under extreme conditions of change and constrain to the whole energy system, assuming no major network upgrade is made. Therefore, the baseline is chosen to be the coldest day recorded in November 2019, where the total energy demand is at its annual peak. Other scenarios consider higher RES supply and higher daily electric load peak due to the penetration of HPs.

The scenario analysis here doesn't aim to make projections based on the local authorities' plans or to critique them, but rather is explorative to consider the possible impact of ESI as a direction for the energy transition to decarbonisation, due to the following limitations. While we aim for a whole systems approach to the evaluation, it is still not possible to model the whole economy in this case. The scenarios and modelling are not designed to consider the temporal dynamics of the energy transition over the years up to 2030 or 2050, but as a steady state snapshot of the energy system at one point of time. As mentioned before, this study is focused on the physical system architecture, and thus the scenario analysis reflects technical changes without considering different aspects related to governance and markets that may be necessary for the transition.

The case study is designed to investigate the impacts of integration between the electricity and gas systems through CHP and P2G and the increased electrification of heat through HPs on the whole energy system. Six scenarios are formulated as a combination of different configurations and supply and demand conditions. The different system configurations are:

- Unidirectional integration via CHP
- Unidirectional integration via CHP + HPs
- Bidirectional integration via CHP and P2G
- Bidirectional integration via CHP and P2G + HPs

Note that unidirectional integration refers to the vector shifting capability from one network to another, in this case from the gas network to the electricity network through CHP. On the other hand, bidirectional integration indicates the capability of the system to shift the energy vector in both directions, i.e. from the gas network to the electricity network and vice versa, as in the case with both CHP and P2G.

For each configuration, different cases of supply and demand conditions are explored:

- Baseline RES: current supply conditions in the area, based on the data available from the local electricity and gas networks operators, as described in Section 7.4.2
- High RES: increase in available wind generation output, 700% increase
- Baseline Load: current demand conditions in the area, based on the data available from local electricity and gas networks operators, as described in Section 7.4.2
- High Load: increase of total electric load (15%) and peak electric load (20%) due to the penetration of HPs
- High P2G: wide expansion of P2G capacity

Table 7.3 below summarises the six scenarios.

Table 7.3 North of Tyne scenario formulation

Scenario	**Configuration**	**Supply and Demand Conditions**
1	Unidirectional integration	Baseline RES, Baseline Load
2	Unidirectional integration + HPs	Baseline RES, High Load
3	Bidirectional integration	Baseline RES, Baseline Load
4	Bidirectional integration + HPs	Baseline RES, High Load
5	Bidirectional integration	High RES, Baseline Load, High P2G
6	Bidirectional integration + HPs	High RES, High Load, High P2G

A number of assumptions have been considered as follows:

- The change in the High Load scenarios is assumed to reflect a 20% increase in HPs use in the domestic sector (Love et al., 2017).
- The 700% increase in the High RES scenarios is assumed given the huge potential for offshore RES in the region, the increase the region has seen in RES capacity in recent years (240%), and the region's decarbonisation ambitions.
- The changes in supply and demand conditions are assumed to apply uniformly to the region's local authorities.
- The actual NoT system has 3 gas-fired generators with total capacity of 110 MW. In our scenarios, those are replaced by 3 CHP plants with the same capacity increasing the total capacity of CHP in the region to 120 MW.
- Getting higher rates of RES generation into the system was not possible without much higher P2G capacity due to local network constraints, thus scenarios 5 and 6.
- The additional P2G assets in scenarios 5 and 6 are placed next to the wind farms which are added into the model to increase the penetration level of the renewable energy.

- Single vector storage technologies are not included in this analysis.

7.3. Conceptual Modelling

The evaluation framework is applied to this case study to evaluate the effectiveness of ESI towards achieving the energy transition objectives in the NoT energy system. The framework is implemented according to the three stages in Figure 4.10: conceptual modelling, scenario formulation and quantitative modelling. For the conceptual modelling stage, the RSAM presented in Chapter 6 is employed, given that the same inputs (architectural framework and system requirements) apply. In this case, the RSAM is used as the template whilst omitting or keeping the relevant components where necessary. The conceptual model is coupled with scenario formulation and quantitative modelling for the full application of the framework. The quantitative modelling stage is described in Section 7.4, while the scenario formulation stage that has been described in Section 7.2 is used to inform the two other stages.

As discussed in Chapter 4, the core of the evaluation framework is in developing the conceptual system model for the different scenarios formulated leading up to a set of indicators for evaluation. Eventually, the conceptual system model provides a set of indicators along with a traceability diagram that reflects the structural and functional interactions between different system components at different levels. This helps reduce the complexity of the WES for the purposes of the evaluation and allows for a socio-technical evaluation of the system against stakeholders' requirements.

In this case study, four configurations are considered with combinations of coupling technologies. Accordingly, four system models are required to carry out the analysis. All four have the same CSs (electricity, gas, heat, coupling system) but have different coupling system components. This would mainly affect the structure, composition and traceability views of the ESI-SoS architectural framework described in Table 4.2. Otherwise, the context definition, requirements, and measures of effectiveness diagrams are similar across all configurations and scenarios. The scale of integration is considered at the distribution network level, and accordingly the system boundaries are determined to be the local energy system. The conceptual system model is developed using SysML stencils on Microsoft Visio and colour coding is used for facilitating traceability.

7.3.1. Context Level

The first level of the ESI-SoS architectural framework is the context level. At this level, the system CSs and stakeholders are specified. In this case, this is the same as those of the RSAM shown in Figures 6.1 and 6.2 for all scenarios, provided again in Figures 7.4 and 7.5.

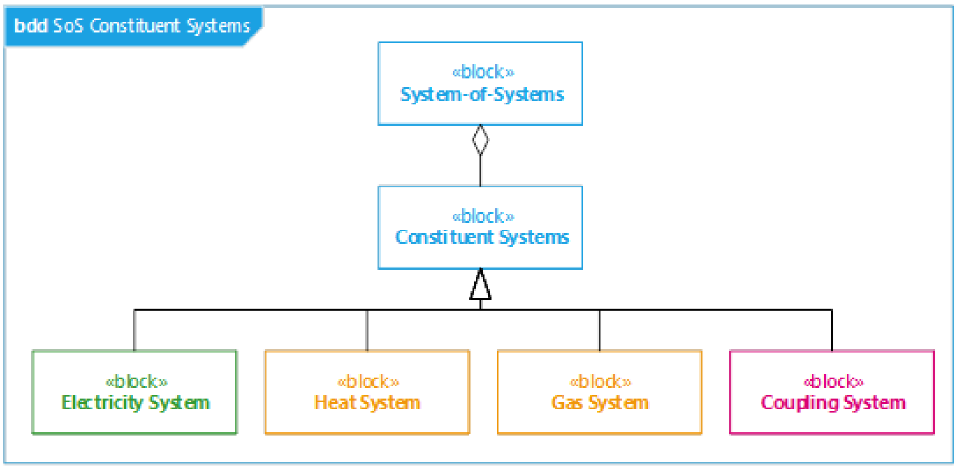


Figure 7.4 North of Tyne Context level: Constituent systems

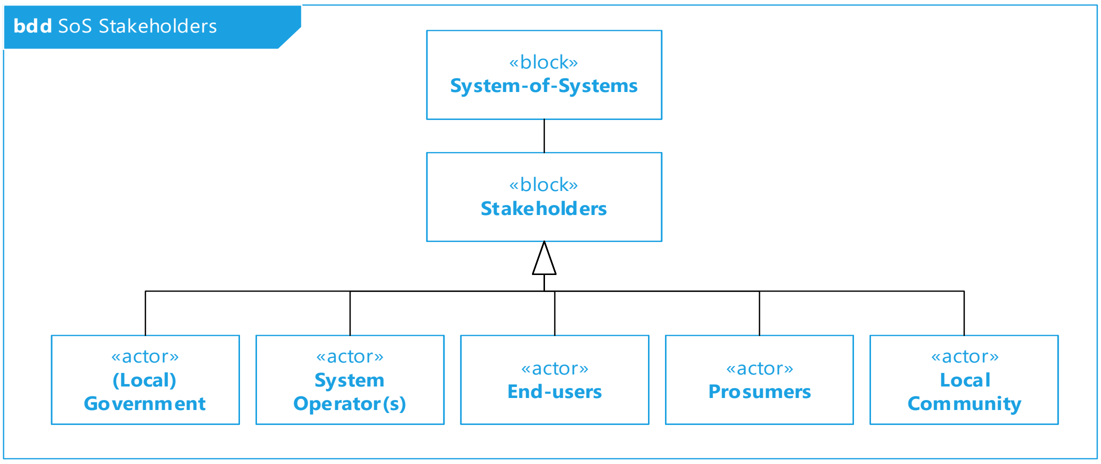


Figure 7.5 North of Tyne Context level: Stakeholder groups

7.3.2. System-of-Systems Level

Given that CSs and stakeholders are the same as for the RSAM, views at this level are again similar to those presented in Section 6.3.2 (Figures 6.3-6.5), provided in Figures 7.6-7.8.

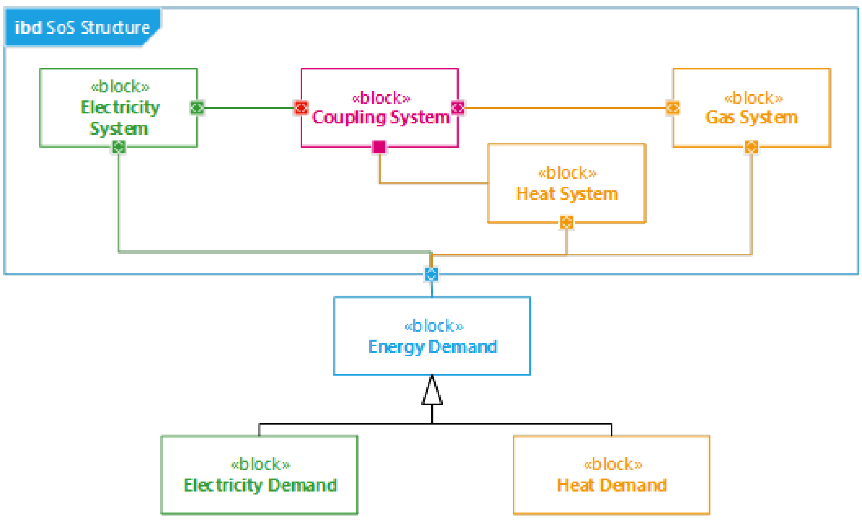


Figure 7.6 North of Tyne SoS level: Structure

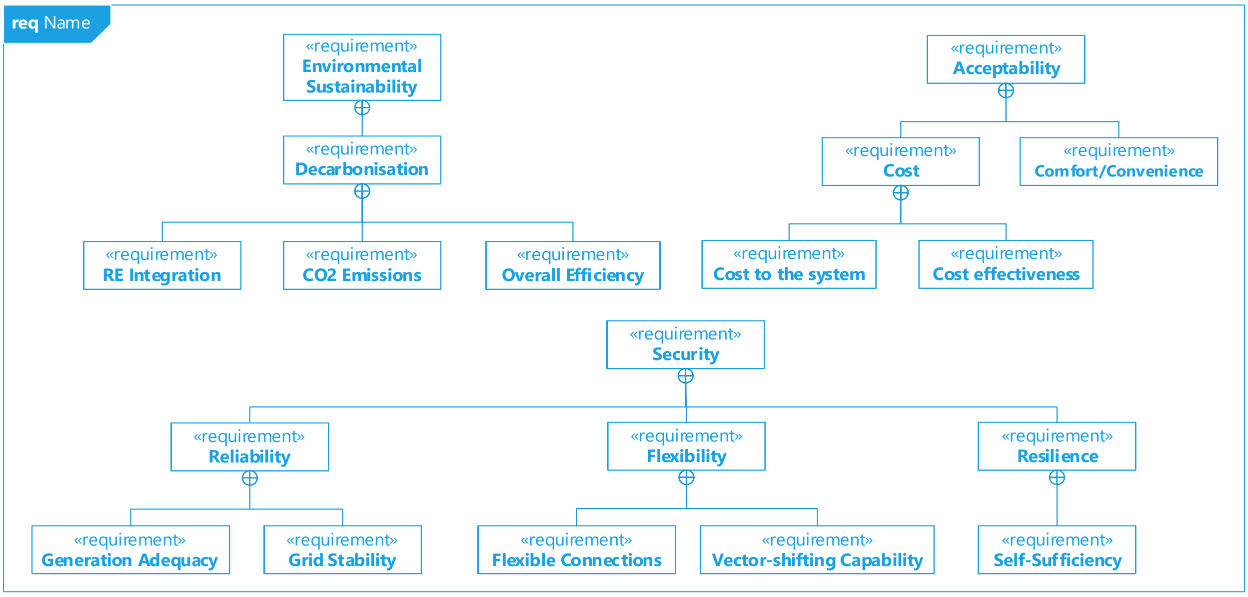


Figure 7.7 North of Tyne SoS level: Requirement desrcription

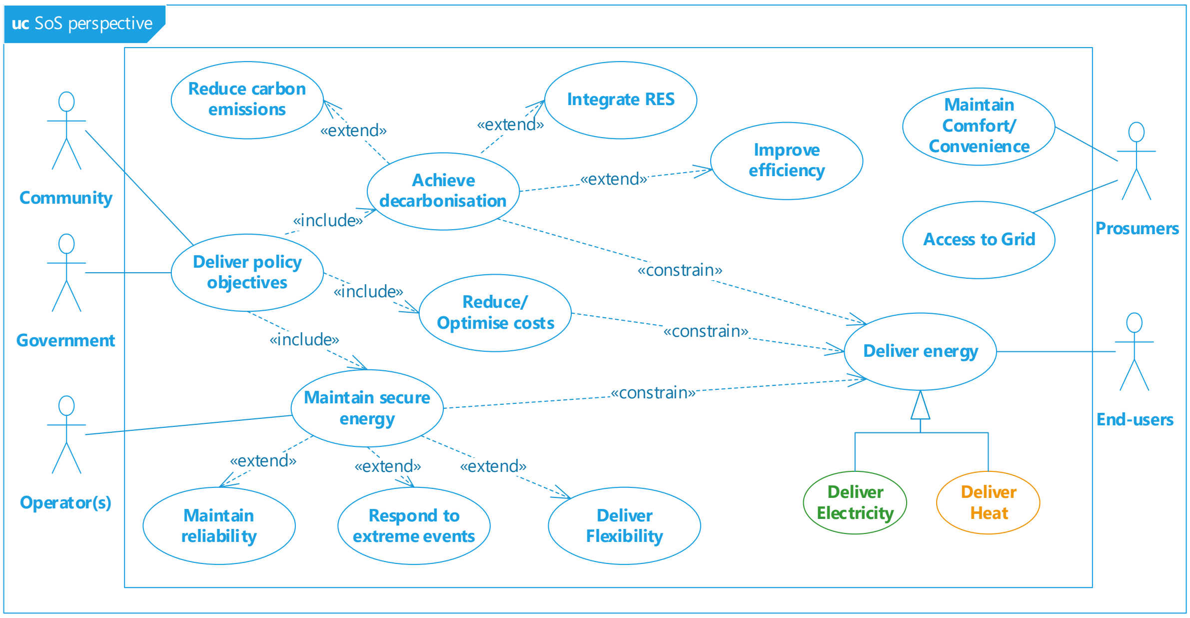


Figure 7.8 North of Tyne SoS level: Requirement context

7.3.3. Constituent Systems Level

The differences between scenarios are realised at this level, where the coupling system composition is different across the given scenarios. The composition of the electricity, gas and heat systems shown in Figure 7.9 is similar to that presented in Figure 6.6 (a,b,c), however excluding storage components from the three CSs, respectively, and is the same across all scenarios. The upstream component in the electricity and gas system relates to the respective national transmission networks.

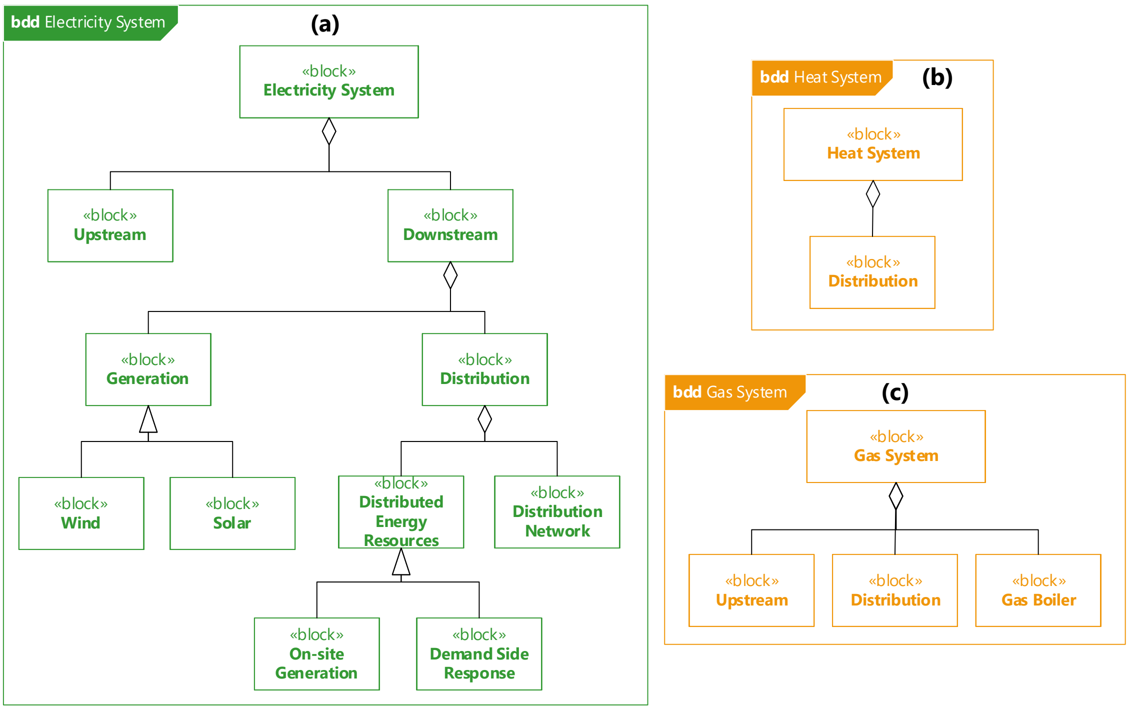


Figure 7.9 North of Tyne CS level: Composition of (a) Electricity system; (b) Heat system; (c) Gas system

For the coupling system composition (Figure 6.6-d), the relevant technologies are maintained where applicable for different scenarios:

- Scenario 1: only CHP is included (Figure 7.10-a)
- Scenario 2: CHP and HPs (Figure 7.10-b)
- Scenarios 3 & 5: CHP and P2G (Figure 7.10-c)
- Scenarios 4 & 6: CHP, P2G, and HPs (Figure 7.10-d)

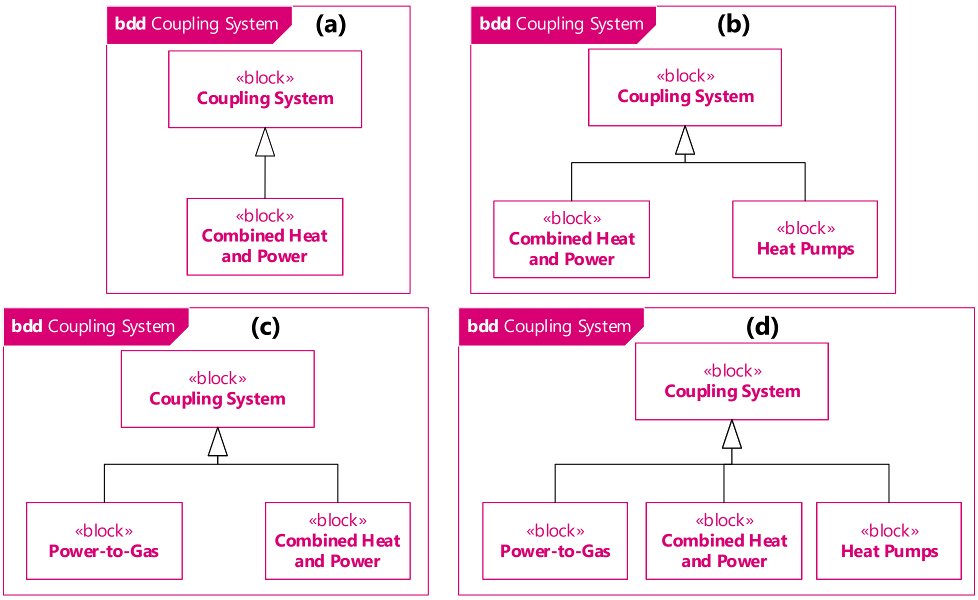


Figure 7.10 North of Tyne CS level: Composition of the Coupling system for scenario (a) 1; (b) 2; (c) 3 & 5; (d) 4&6

Accordingly, the system structure at this level is changed from Figure 6.7 based on what technologies are considered for the coupling system in different scenarios as shown in Figures 7.11-7.14. The main difference between the four diagrams is the connection between the energy CSs through the different available coupling technologies.

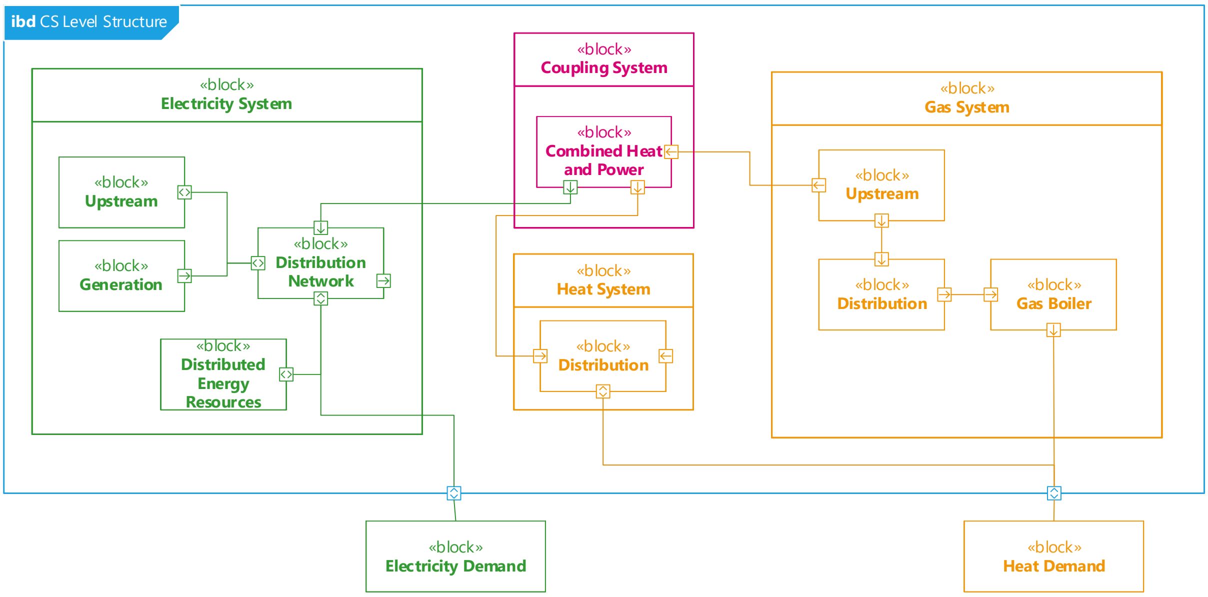


Figure 7.11 North of Tyne CS level: Structure for scenario 1

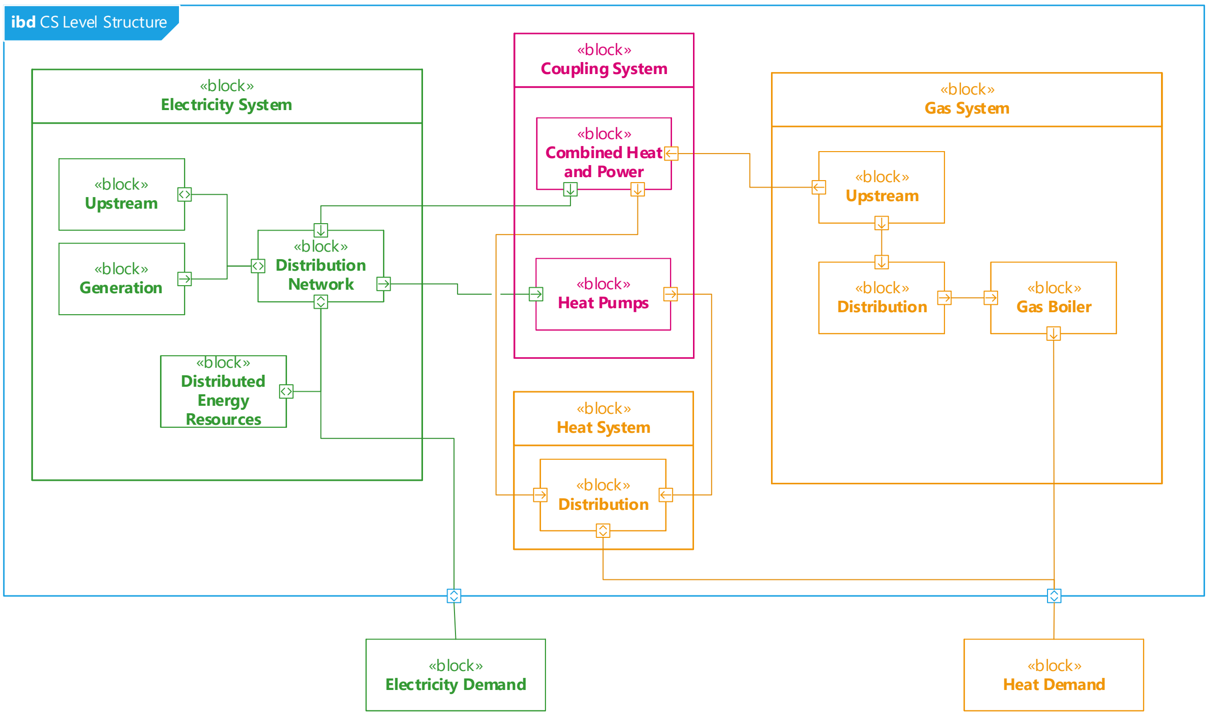


Figure 7.12 North of Tyne CS level: Structure for scenario 2

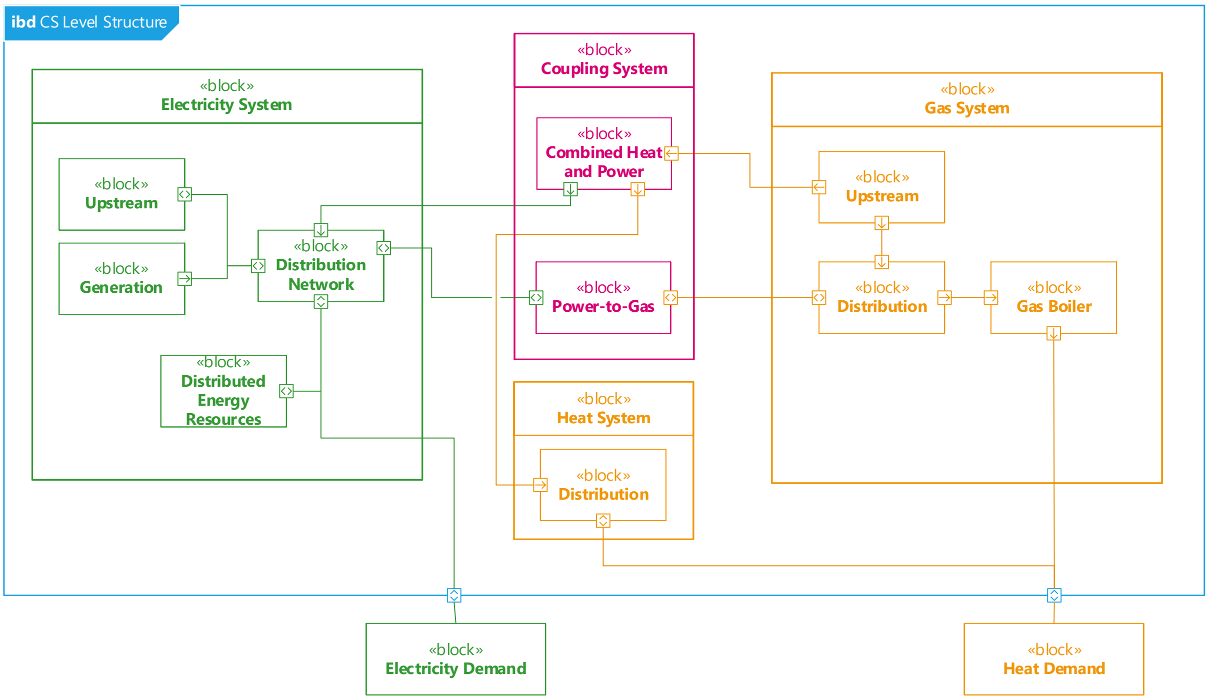


Figure 7.13 North of Tyne CS level: Structure for scenarios 3 & 5

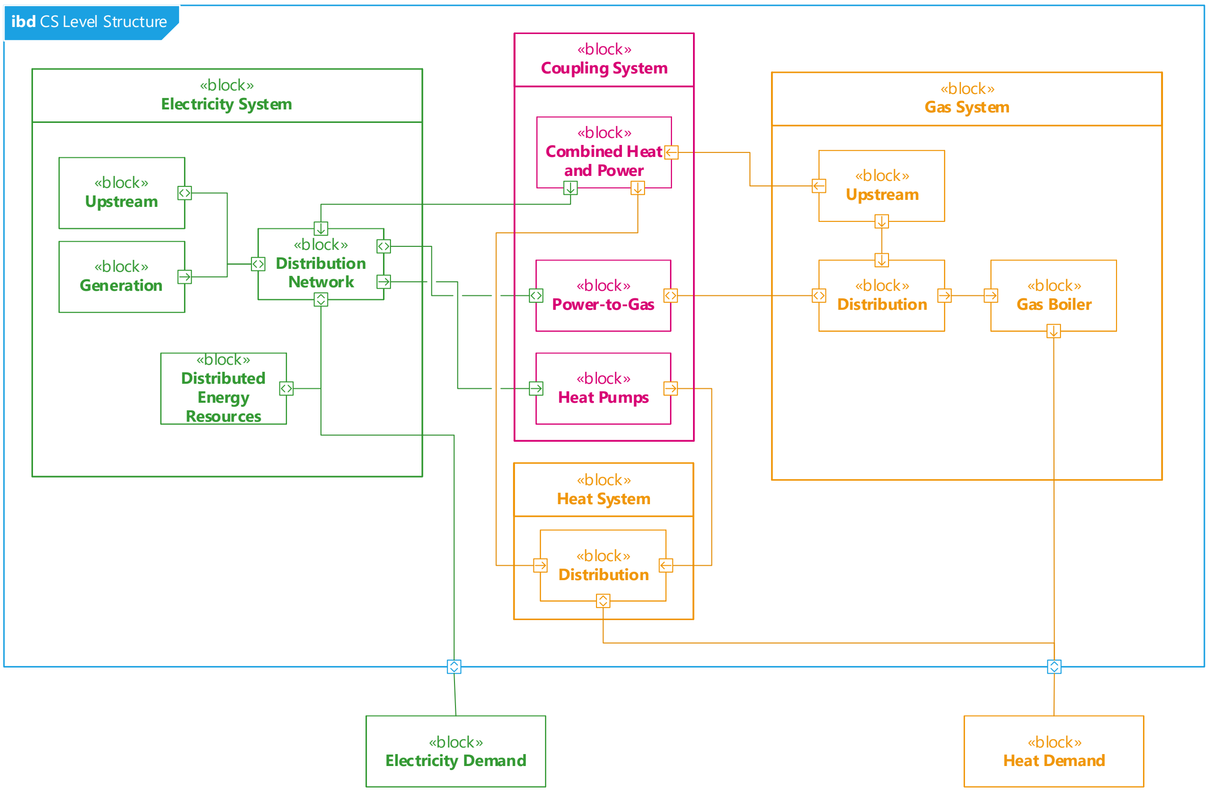


Figure 7.14 North of Tyne CS level: Structure for scenarios 4&6

Finally, requirements at this level are slightly changed from Figure 6.8 of the RSAM and are shown again in Figure 7.15. The change relates to functions provided by single vector energy storage, not available in this case study. As mentioned previously, ESI technologies are grouped into the coupling system given that they all share similar functionalities in this respect, and are therefore unchanged for different scenarios.

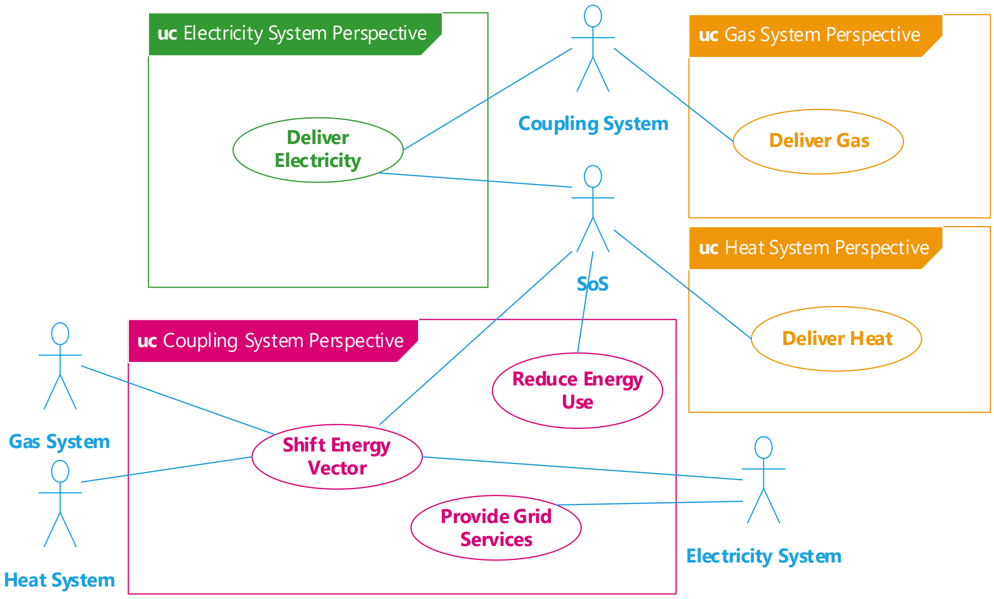


Figure 7.15 North of Tyne CS level: Requirements context interaction

7.3.4. Whole System Level

The modular nature of the RSAM is evidently useful here. The traceability view in Figure 6.9 need only to be slightly modified to accommodate the various coupling components involved. Also, components and functions related to energy storage are removed as shown in Figure 7.16 for all scenarios.

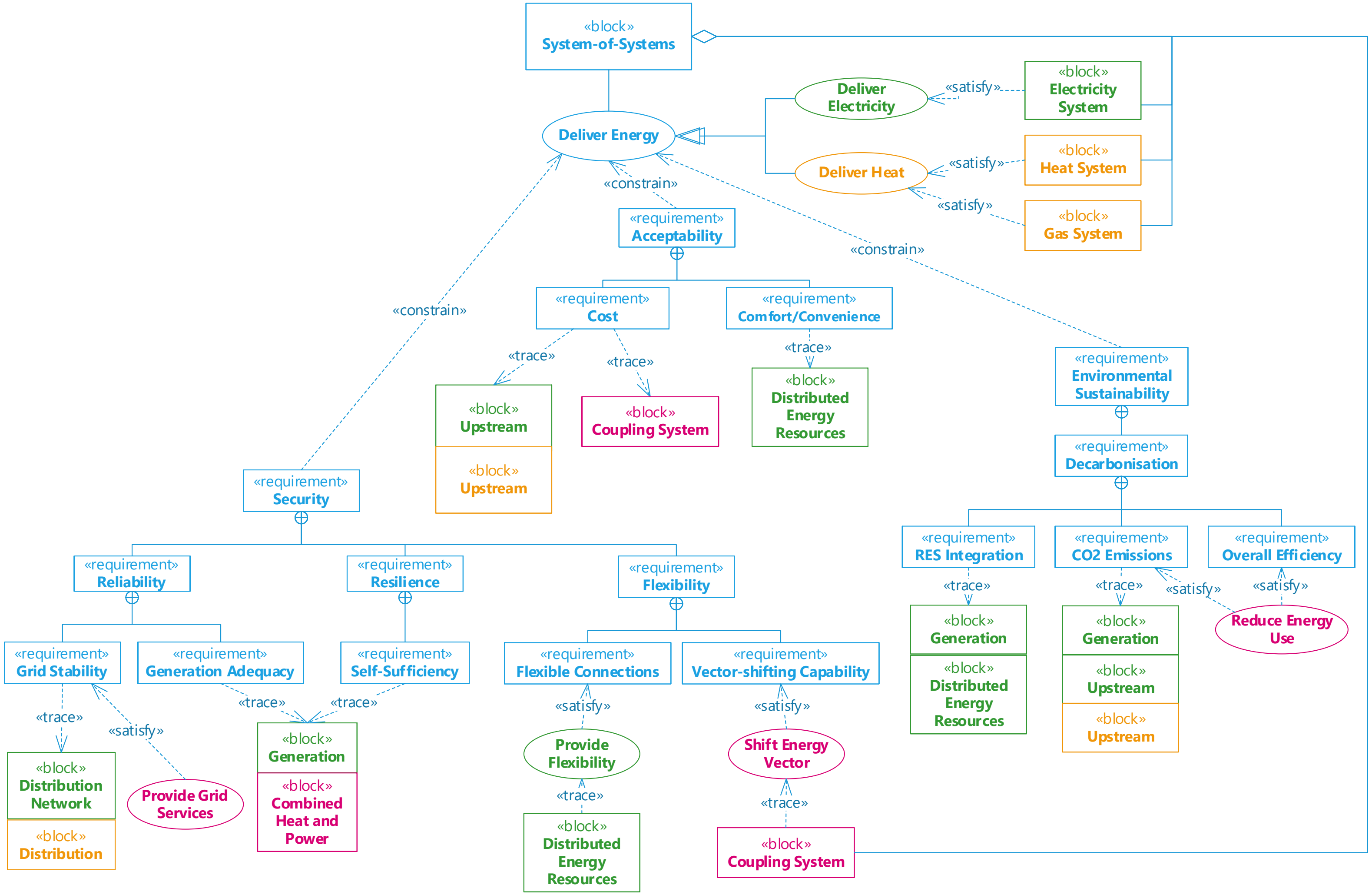


Figure 7.16 North of Tyne Whole System level: Traceability

On the other hand, the measures of effectiveness view in Figure 6.10 is unchanged. This is important for comparability across the different scenarios. However, note that the diversity indicator is omitted since it is not applicable to the scenarios under study as there is no change in the components of the energy supply mix.

Moving from the traceability diagram to assigning the measures of effectiveness is not an automatic step. It involves looking at suitable indicators that are used to measure the state of the evaluation criteria guided by the traceability view, and considering the data availability required to calculate those indicators supported by the quantitative model. Accordingly, indicators presented in the measures of effectiveness view in Figure 7.17 are believed to be suitable for the evaluation in this case, although they do not present an exhaustive or restricted list. The indicators and relevant output parameters are discussed further in Tables 7.4 and 7.6.

As mentioned previously, the evaluation criteria reflect multiple stakeholders' requirements and functional requirements at different levels, allowing for a socio-technical evaluation of the WES. This also provides a flexible, modular approach for the evaluation where if new stakeholders or different requirements are realised, this is reflected throughout the conceptual model diagrams. In this context, note that some elements included in earlier views are omitted from the analysis presented later, such as distributed energy resources, due to the lack of data around it in this case.

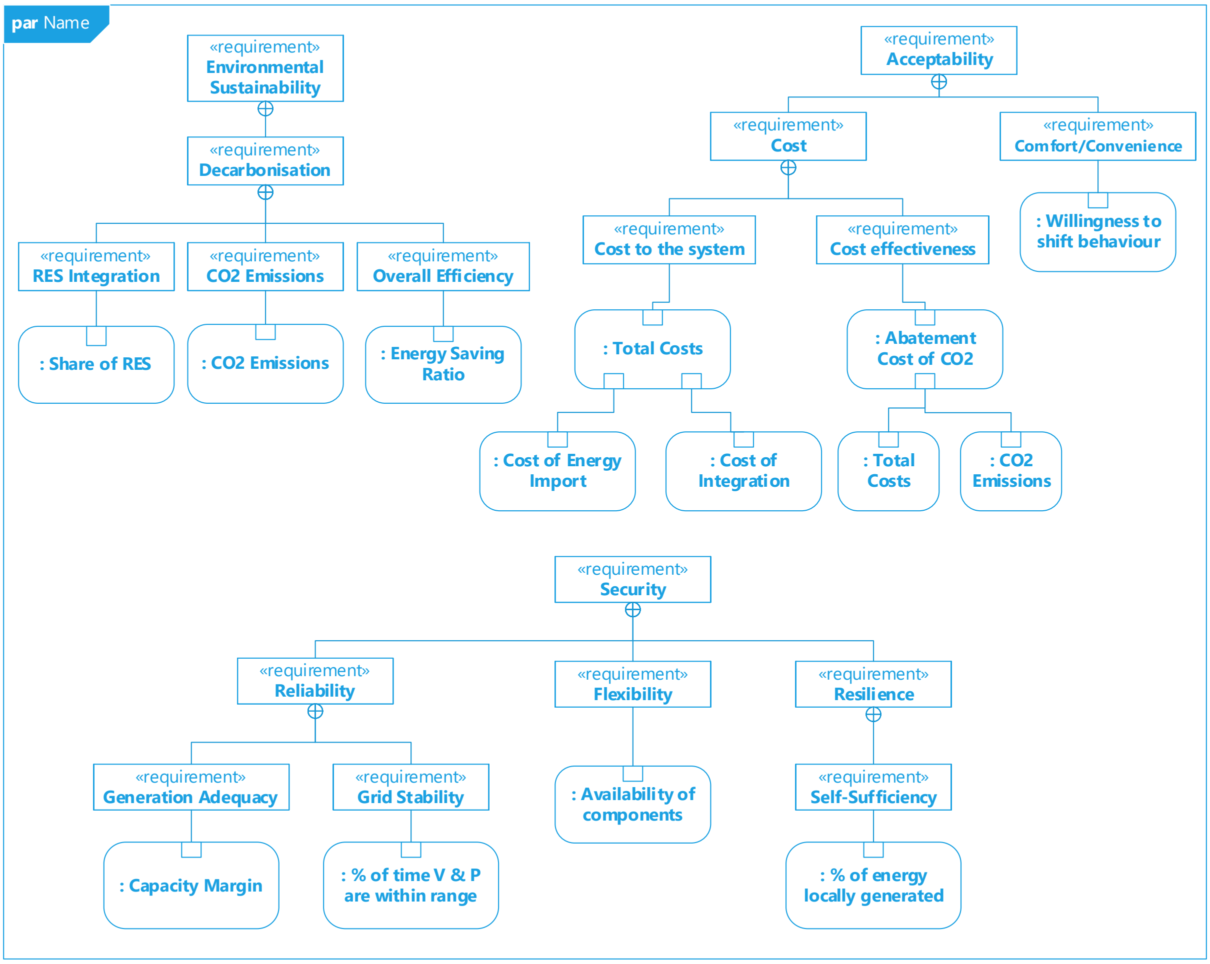


Figure 7.17 North of Tyne Whole System level: Measure of effectiveness

7.4. Quantitative Modelling and Data

7.4.1. Network Model

The analysis is supported by an optimal power and gas flow simulation model for the operation of the integrated electricity and gas networks with different coupling components at the transmission and distribution levels. This model is an updated version of the models used for the Findhorn case studies, in that it considers the optimal operation of the integrated networks. This model also facilitates the consideration of all the parameters affecting the optimal operation of integrated energy systems, such as different gas mixtures, gas temperature, pipeline characteristics and the electricity network topology. The model is developed in MATLAB and includes a set of nonlinear equations constrained by voltage and pressure balances for electric and gas network nodes, respectively. The optimisation is based on a cost minimisation objective function subject to physical constraints. The cost function includes the cost of electricity generation from different sources and the cost of gas supply from upstream networks. The inputs, outputs, and mathematical formulations of the model are described in Appendix E.

The model represents the same energy system topology abstracted for the conceptual system model. Note, however, that the jurisdictional boundaries of the combined authority district may not be the same as the area covered by the energy networks. For instance, the network extends into parts of Gateshead and County Durham, which are not officially within the jurisdiction of the NoT combined authority. Appendix E.3 provides the integrated energy network map and schematic.

The coupling components considered in the model are CHP and P2G, while HPs are considered as additional electric load without considering the provision of demand-side response (DSR). District heating networks are not explicitly modelled in the system, but heat output from CHP is assumed to feed into those. Furthermore, energy storage technologies are not considered in the model as it requires a computational effort that was not available to run the model. In fact, the region currently lacks significant energy storage assets.

7.4.2. Network Data

The model is populated by actual data of the NoT energy system for energy supply and load profiles and network flows (Wardle et al., 2020). For the gas network, Northern Gas Networks, the gas distribution network operator in the region, has provided data of the hourly demand at each network node for a set of typical days. For this study, the demand data for a cold winter day is interpolated to get the half-hourly demand data set. For the electricity network, Northern Powergrid, the electricity distribution network operator in the region, has provided datasets of half-hourly metered data for the primary substations on the network. The data provided covered the period from January 2016 to June 2020, of which the 15^{th} of November 2019 was chosen for this study showing the peak demand. Along with the gas network data on the typical cold winter day, this day is expected to be a time of system stress.

Figures 7.18 and 7.19 show the load profiles for the total electric and gas demands in the region for the baseline and high load scenarios. The electric demand is aggregated to the electric substation level. That is considering the effect of the increased electric demand for heating through HPs on the electric substation rather than individual households. The change in the electricity load profile for the High Load scenarios represents a 20% increase in the peak load and involves a shift in the morning peak hours as estimated in (Love et al., 2017).

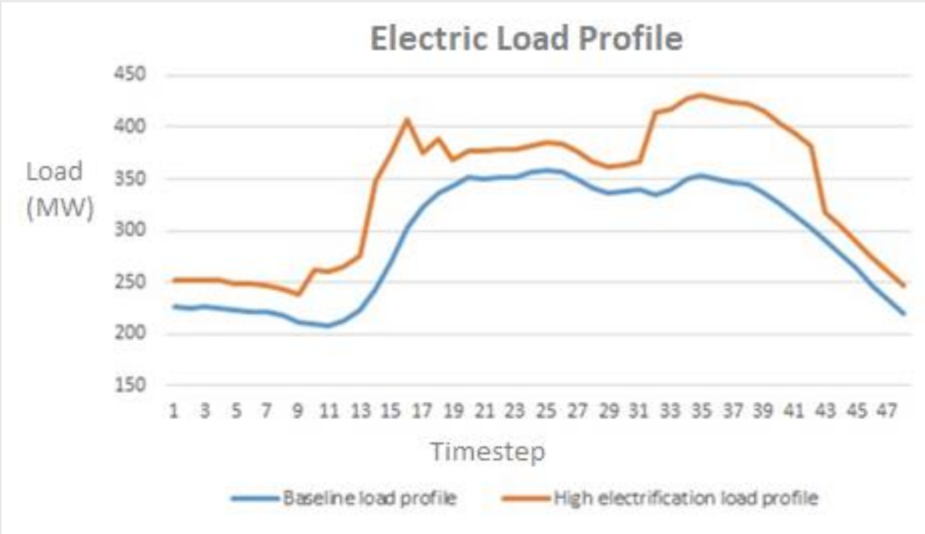


Figure 7.18 Electricity load profiles for the baseline and high load scenarios

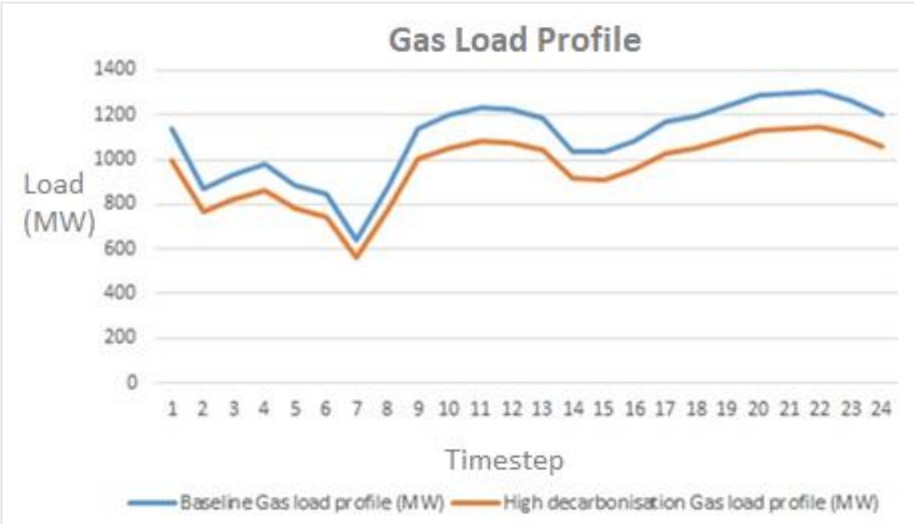


Figure 7.19 Gas load profiles for the baseline and high load scenarios

Figure 7.20 shows the profiles of the total wind generation for the baseline RES and high RES scenarios in the region, while Figure 7.21 shows the profile of the total PV generation for all scenarios in the region. Baseline data were provided by Northern Powergrid.

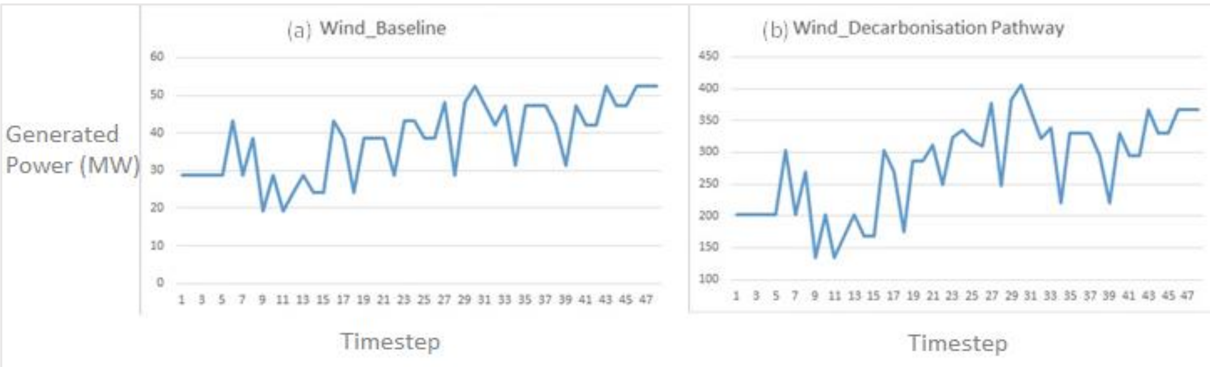


Figure 7.20 Wind generation profile for (a) baseline and (b) High RES scenarios

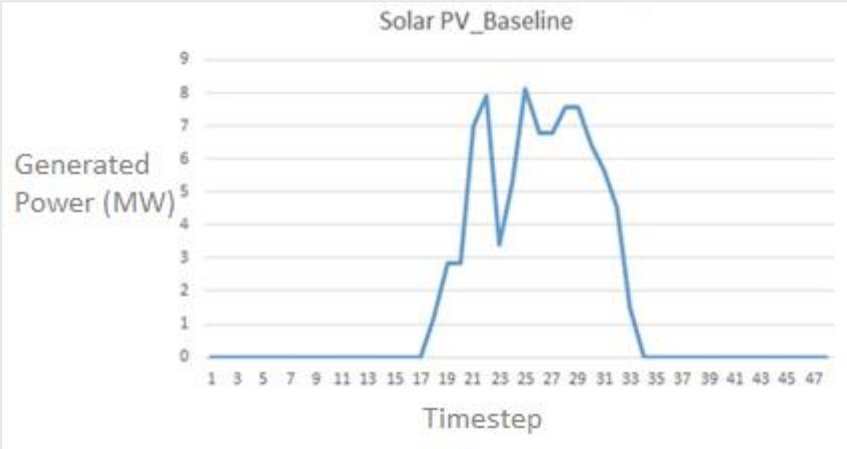


Figure 7.21 Solar PV generation profile for all scenarios

7.4.3. Model Parameters

After running the simulations for each scenario, parameters related to the heat and electric loads, renewable energy generation, coupling components outputs and capacity, electricity and gas upstream imports are obtained (Table 7.4). Those are the output parameters required to calculate the identified indicators described in detail in Table 7.6. The numerical values of the model output parameters for all scenarios are provided in Appendix F.

Table 7.4 Simulation model output parameters

Load (MWh/MW)	Total Final Heat Load
	Total Final Electric Load
	Total Final Energy Load
	Peak Heat Load
	Peak Electric Load
	Peak Total Load
Renewable Energy Generation (MWh)	Total Wind generation
	Total Wind wasted
	Maximum Wind available
	Total Solar generation
	Total Solar wasted
	Maximum Solar available
CHP (MWh/MW)	Total Heat production
	Total Electricity produced
	Maximum Capacity
P2G (MWh/MW)	Total input
	Total output
	Total waste
	Maximum Capacity
Upstream Energy	Energy imported from upstream (MWh)
	CO_2 emissions from upstream (tCO_2)

(Gas network, Electricity Network, Total)	Cost of import from upstream (£)

In addition to those parameters, the following factors for cost and carbon emissions are considered (Table 7.5).

Table 7.5 Cost and emission factors

Cost of upstream import (£/MWh)	Electricity Network	28.06	(OFGEM, 2021)
	Gas Network	9.42	
Carbon emissions of upstream import (kgCO_2eq/MWh)	Electricity Network	253	(BEIS, 2020b)
	Gas Network	203	
Cost of coupling components (£/MWh)	CHP	25	(BEIS, 2020a)
	P2G	55	(McDonagh et al., 2018)
	HP (air-sourced)	36	(Hansen, 2019)

The cost of energy import from upstream reflects an annual average of the sum of network charges on the customer for the electricity and gas transmission networks (OFGEM, 2021). This is the cost accounted for in the optimisation as operational cost for electricity generation and gas supply, while capital and carbon costs are not included. The carbon emission factors are published average values for the UK supply of electricity (including T&D losses) and natural gas (including limited amount of biogas) (BEIS, 2020b). The cost of coupling components reflects the levelised cost of energy for those technologies excluding the fuel cost (electricity or gas), which is already accounted for in upstream costs and is taken to be minimal for local RES generation. The levelised cost is used here to represent a unit cost (£/kWh) in line with the operational costs accounted for in the model as the costs of upstream energy import.

7.5. Case Study Results

After running the simulations for each scenario, indicators are quantified as described in Table 7.6 below. Note that reliability indicators are not included in this case as this is a condition for convergence in the quantitative model used in the analysis.

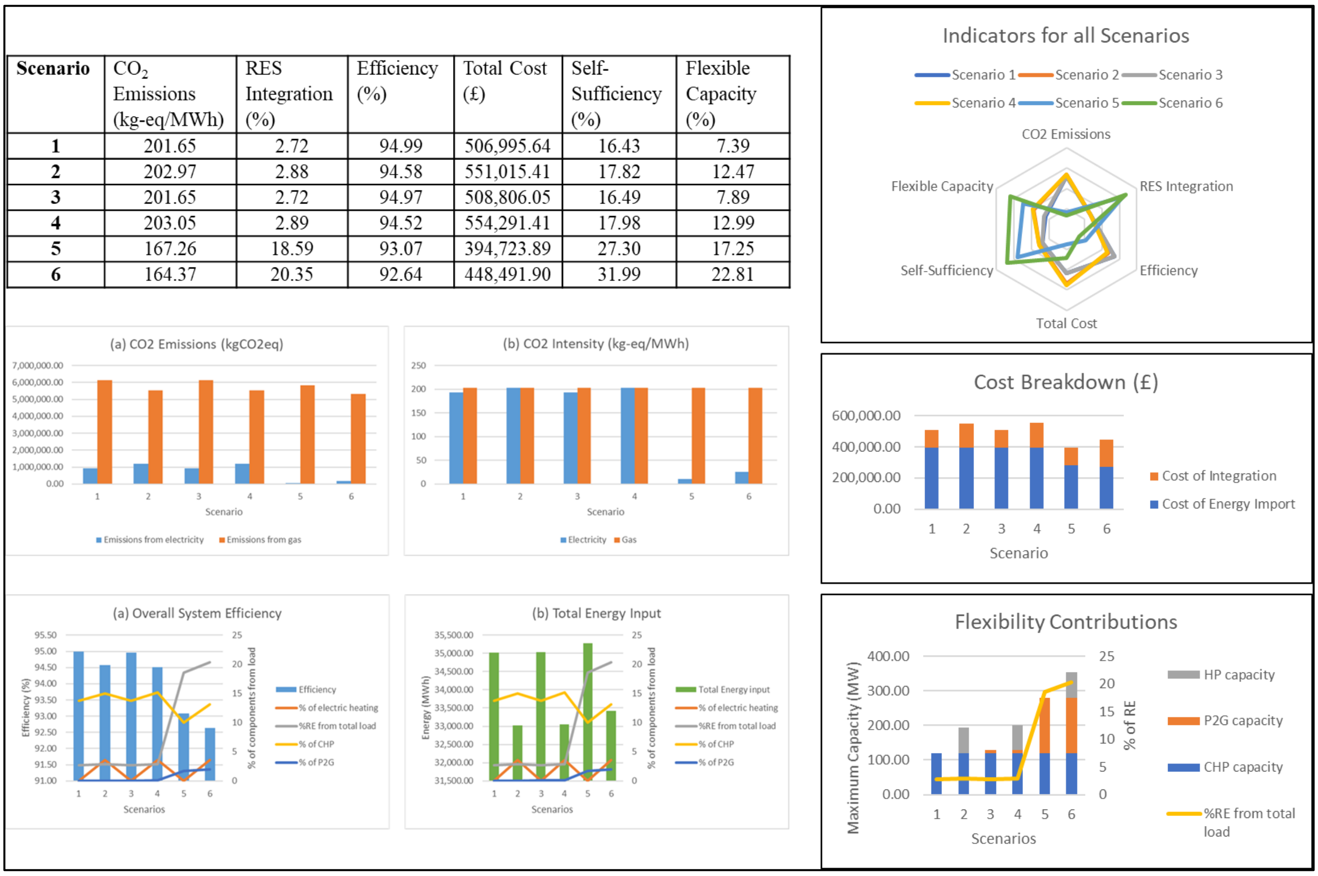
Table 7.6 Indicators description

Dimension	**Indicator**	**Description**	**Model Parameters**
Environmental	CO_2 Emissions Intensity	Amount of CO_2 Emissions per energy supplied (kg-eq/MWh)	Total CO_2 Emission/ Total Energy Input
	RES Integration	% of RES supply from total final energy load	Total used RES / Total Final energy load
	Overall Efficiency	% of total final energy load to total energy input (100 – losses)	Total final energy load / Total energy input and waste (curtailed) RES

Economic	Total Cost	Cost of energy import and integration assets (CHP and P2G)	Total cost of energy imported from upstream + Cost of CHP and P2G
Resilience	Self-Sufficiency	% of local energy generation from total energy supply	Local energy generation / Total energy input
Flexibility	Flexible capacity	% of maximum available capacity of flexible assets (CHP and P2G) from total peak load	(Maximum CHP capacity + Maximum P2G capacity) / Peak Total Load

7.5.1. Dashboard

Based on the approach described in Section 4.2.4, the indicators are not aggregated but are presented in a dashboard. Figure 7.22 presents a snapshot of the dashboard before presenting and describing each graph in more detail.



Scenario	CO_2 Emissions (kg-eq/MWh)	RES Integration (%)	Efficiency (%)	Total Cost (£)	Self-Sufficiency (%)	Flexible Capacity (%)
1	201.65	2.72	94.99	506,995.64	16.43	7.39
2	202.97	2.88	94.58	551,015.41	17.82	12.47
3	201.65	2.72	94.97	508,806.05	16.49	7.89
4	203.05	2.89	94.52	554,291.41	17.98	12.99
5	167.26	18.59	93.07	394,723.89	27.30	17.25
6	164.37	20.35	92.64	448,491.90	31.99	22.81

Figure 7.22 NoT case study results dashboard

First, the values of all indicators for all scenarios are presented in Table 7.7.

Table 7.7 Indicators values for all scenarios

Scenario	CO_2 Emissions (kg-eq/MWh)	RES Integration (%)	Efficiency (%)	Total Cost (£)	Self-Sufficiency (%)	Flexible Capacity (%)
1	201.65	2.72	94.99	506,996	16.43	7.39
2	202.97	2.88	94.58	551,015	17.82	12.47
3	201.65	2.72	94.97	508,806	16.49	7.89
4	203.05	2.89	94.52	554,291	17.98	12.99
5	167.26	18.59	93.07	394,724	27.30	17.25
6	164.37	20.35	92.64	448,492	31.99	22.81

Second, a radar chart is produced to compare the different scenarios with respect to the six indicators (Figure 7.23). To do this, the indicators values are normalised to fit into the uniform scale of the radar chart. This is based on the mean normalisation method given as: $x' = \frac{x - \text{average}\,(x)}{\max(x) - \min\,(x)}$. Normalised values are provided in Appendix F.

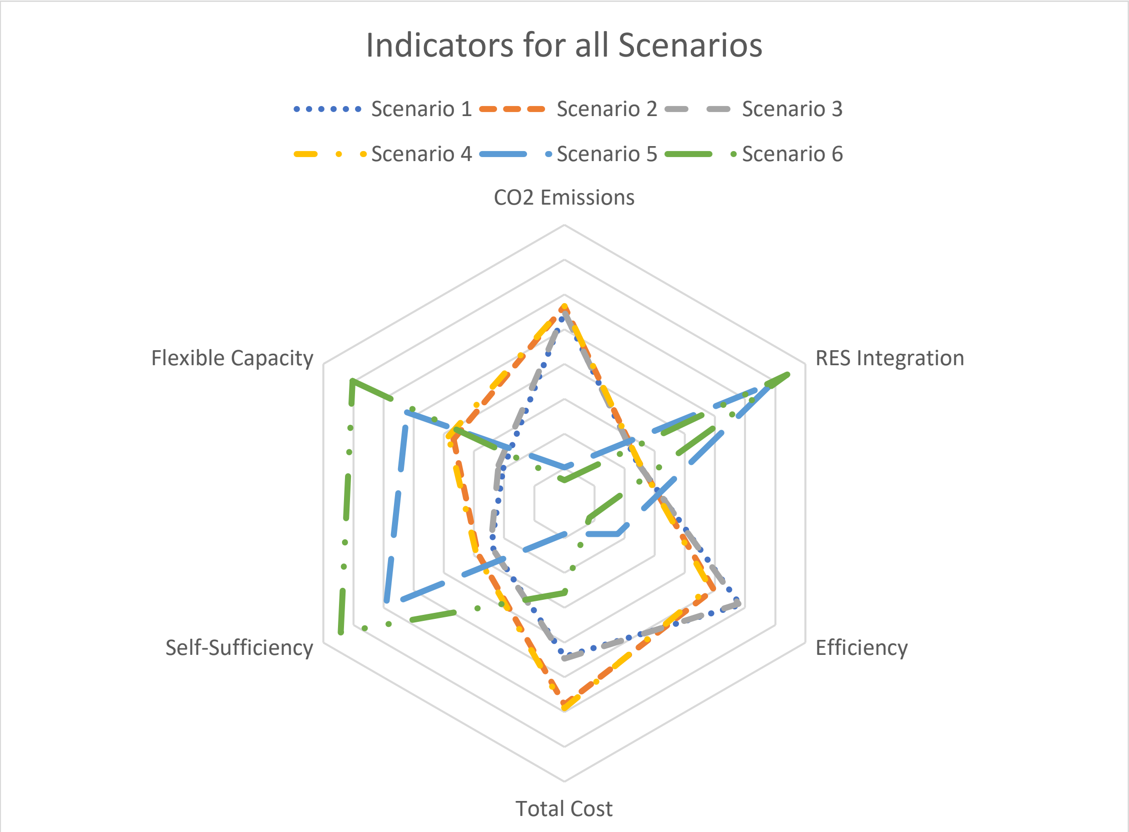


Figure 7.23 Radar chart of indicators for all scenarios

It can be noticed from Table 7.7 and Figure 7.23 that scenarios 1 and 3 and scenarios 2 and 4 show very similar values. This means that adding P2G to the system with small capacity has a very minimal impact in all terms including RES integration. This conclusion has been reached earlier in the analysis and as mentioned earlier it is due to local network constraints that prevent getting more RES into the system. Conversely, scenarios 5 and 6 with major increase in P2G capacity and consequently in flexible capacity, have shown an increase in RES integration that affect other indicators such as carbon emissions and self-sufficiency. This can be explained by the fact that electricity is more expensive than gas, thus drawing electricity to convert into gas is not economic. However, in the case where RES is abundant, using the surplus low cost electricity becomes competitive.

To realise the impact of HPs, scenarios 1 and 2, 3 and 4, and 5 and 6 are compared. For scenarios 1 & 2 and scenarios 3 & 4, similar trends are noticed with HPs increasing the total system cost and reducing the overall system efficiency. At the same time, those scenarios do not show major improvements in terms of RES integration, self-sufficiency, and CO_2 emissions despite the increase in flexible capacity. On the other hand, comparing scenarios 5 & 6 shows improvements in most indicators including RES integration, but with higher costs and lower efficiency.

To draw a better picture on the relations between indicators and the different system components, some indicators are further broken down and shown relative to other indicators following from the relations in the traceability view in Figure 7.16.

7.5.2. Environmental Indicators

The first indicator is the intensity of carbon emissions that is calculated as the ratio of the total CO_2 emissions over the total energy input to the system. The latter in this case includes generation from RES (solar and wind), generation from CHP plants, and imported energy from upstream. In addition to the carbon intensity value, we are interested in tracing the contribution of different vectors and thus the carbon emissions and intensity of electricity and that coming from gas are compared (Figure 7.24).

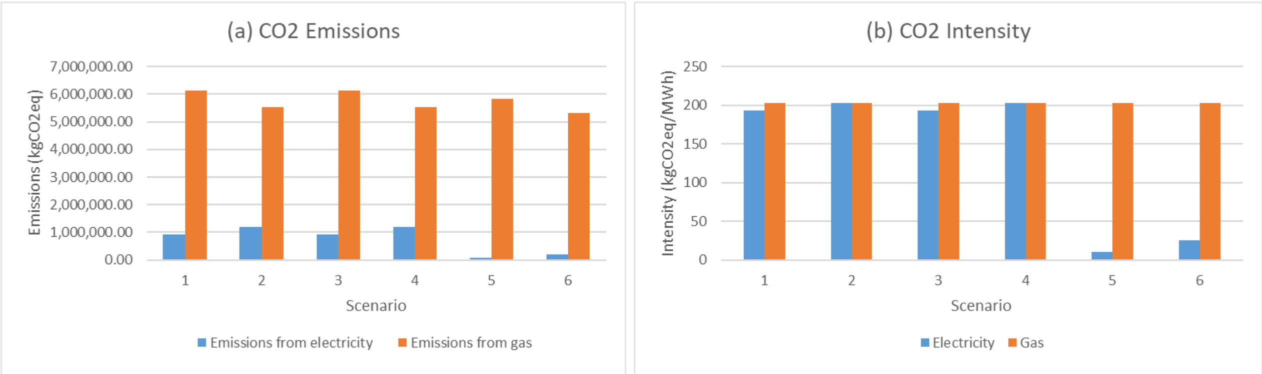


Figure 7.24 Electricity and gas (a) CO_2 emissions and (b) CO_2 intensity for all scenarios

For electricity, scenarios 1-4 show slight variations for the amount of emissions and the carbon intensity, while for scenario 5 and 6 the amount of emissions becomes negligible (Figure 7.24-a) and the intensity sees a steep decrease (Figure 7.24-b). This is clearly due to the major increase in RES supply. On the contrary, the amount of emissions from gas encounters a decrease for scenarios with HPs (2,4,6) but the intensity stays the same across all scenarios. The absolute decrease in emissions is mainly due to a fraction of heating being satisfied by electric heating (around 12%), which means that the amount of gas imported from upstream is decreased. Note that the decrease in scenario 5 emissions is due to the lower CHP generation with more electricity demand being met by RES. However, the intensity stays the same across all scenarios because the amount of renewable gas produced via P2G is still minimal (around 2%) compared to the amount of upstream gas used for heating or for generation through CHP plants. Note that the combined CO_2 intensity for electricity sources becomes lower than that of gas when combined with local RES generation, again highlighting the prospects of heat decarbonisation through ESI.

The second key indicator is RES integration, which is calculated as the % of energy supply from RES over the total final energy load. The total final energy load is defined by the load profiles described earlier. This indicator is presented on its own, but is also shown in correlation with other indicators including efficiency and flexibility (Figures 7.25 and 7.27).

The third environmental indicator is the overall efficiency, which represents the system losses due to RES curtailment, network losses, and technology efficiencies. To understand the sources of losses to which it could be traced to, this indicator is shown in relation with the percentages of RES, CHP, P2G, and HPs from the total final energy load (Figure 7.25).

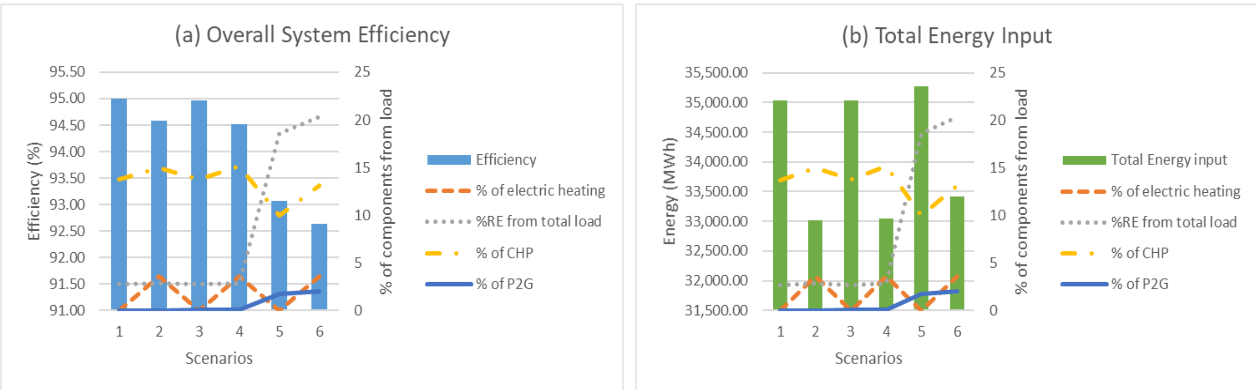


Figure 7.25 (a) Overall system efficiency values and (b) Total energy input compared with system components for all scenarios

From Figure 7.25-a, it could be said that system losses increase with the expansion of HPs, RES, CHP, and P2G. However, this is not to be confused with the expected requirement of HPs and CHP to reduce the overall energy use as evident in Figure 7.25-b, while delivering the same energy service, which in this case is heat. Thus, the system losses can be attributed to the electricity network losses driven by more flow from the increased RES supply and the increased HPs demand, in addition to losses from RES curtailment and P2G efficiency losses.

7.5.3. Acceptability Indicators

The cost to the system is calculated as the sum of energy imported from upstream (electricity and gas) and the cost incurred by the coupling components (CHP, P2G, HPs). The cost breakdown is shown in Figure 7.26. Note that the cost is limited to the operational costs, since the analysis is based on an operational model that doesn't account for capital and carbon costs. Thus, the total cost is dominated by the cost of energy imported from upstream.

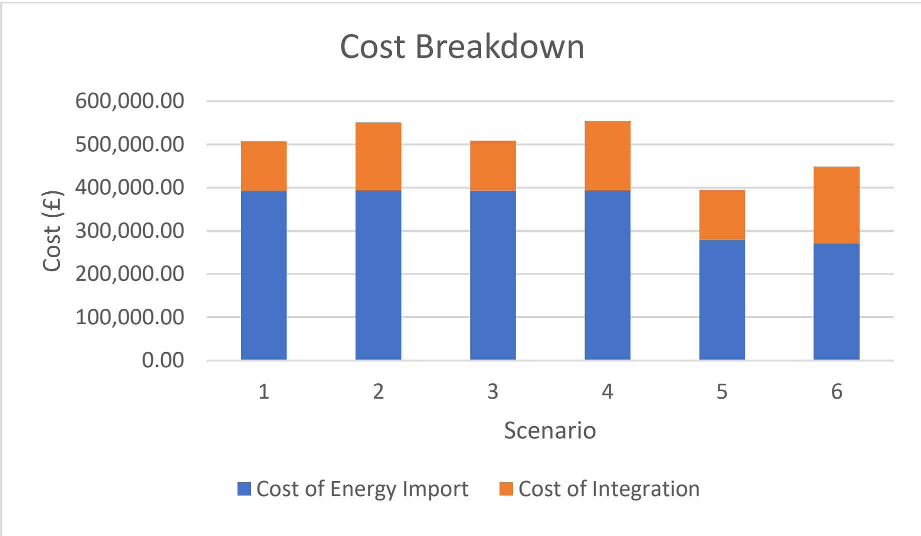


Figure 7.26 Cost breakdown for all scenarios

Another indicator of cost is the abatement cost of CO_2, which relates economic and environmental aspects and represents cost-effectiveness, which is typically important for decision-making. It is calculated as the ratio of additional costs incurred to the amount of CO_2 reduced in a scenario compared to the baseline scenario. However, this indicator faces two limitations in this case. First, the cost calculated includes only the operational costs and doesn't include the capital costs, which are significant when considering the implementation of P2G for example. Although cost unit factors used for coupling components take into account the levelised cost of those technologies, this cost even though indicative would still not be sufficiently representative in this analysis for decision-making on cost-effectiveness. Second, some scenarios show an increase in emissions from the baseline scenario or at least no change. Thus, it is not sensible to compare the cost effectiveness of reducing emissions between scenarios heading in different directions.

Note also that an indicator for comfort and convenience, such as the willingness to shift behaviour, is not realised in this analysis. This is important to evaluate the quality of the energy service, such as heat, when it is being delivered in different forms. However, such indicators are typically qualitative and require direct involvement with consumers and prosumers on the ground through surveys or interviews in the region, which is outside the scope of this project.

7.5.4. Security Indicators

Reliability indicators, such as generation capacity margin and networks capacity, are not applicable in this case given that reliability constraints are a condition for the model convergence. The requirement of providing grid services is therefore not evaluated since DSR is not considered in the model.

Self-sufficiency is calculated as the % of local generation to the total energy input and is considered an indicator of resilience to supply disruptions.

The system flexibility is considered as the ratio of the maximum available capacity of flexibility assets to the peak energy load. In this case, flexibility assets are limited to the coupling components since there is no electric or gas storage and no DSR. To trace the contribution of the different coupling components, the capacities are broken down and shown in relation to the RES integration indicator (Figure 7.27).

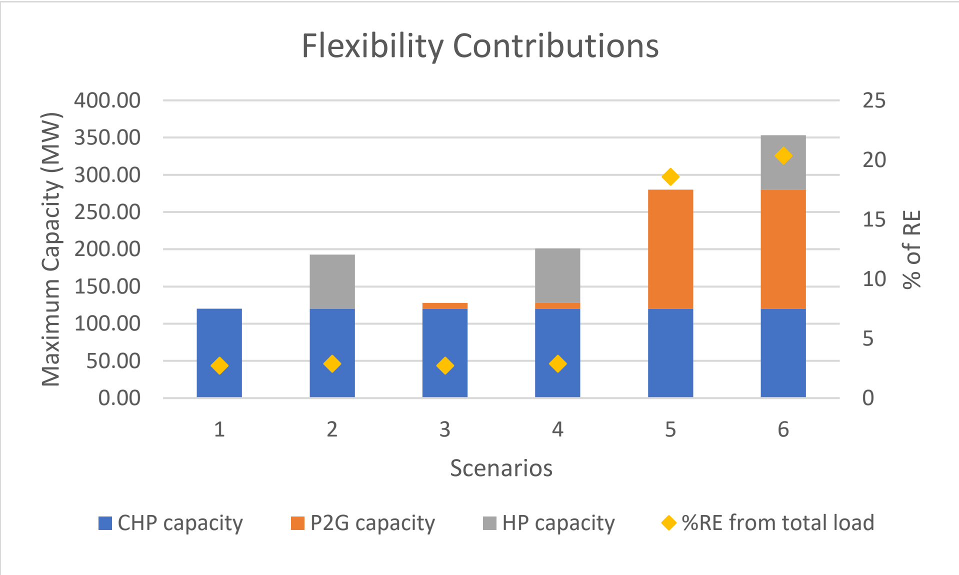


Figure 7.27 Flexibility contributions by coupling components for all scenarios

As mentioned previously, P2G is the main contributor to flexibility and RES integration as evident in Figure 7.27. A major expansion in P2G capacity is necessary to realise the impact. On the other hand, HPs on their own seem to have a limited impact on RES integration. This is due to how the technology is accounted for in the model as a load component without the provision of DSR. However, when HPs are used in combination with high P2G capacity as in scenario 6, HPs are able to absorb more of the RES into the system and to reduce curtailment.

Finally, an indicator that is not included in this analysis is the % of heat electrification (uptake of HPs) since it is an exogenous variable to the model. However, given that net-zero plans typically set objectives for electrification of heat (and transport) then this is an indicator to consider in other cases where technology diffusion and adoption is considered dynamically.

7.6. Discussion

The objectives of this case study outlined earlier are to demonstrate the applicability and usefulness of the framework on a more complex energy system, implement the improvements on the framework based on the previous learnings, and provide empirical evidence on the effectiveness of ESI as a pathway for the energy transition. In the scope of those objectives, this section first discusses, the empirical findings of the case study followed by an acknowledgment of uncertainty around the results. Secondly, the framework application is discussed in terms of addressing the increased complexity of the case study and the improvements made to the framework compared to the test case studies presented in Chapter 5. Finally, the limitations of this case study are discussed.

7.6.1. Findings

The results of the case study presented in Section 7.5 show that ESI provides a direction towards achieving the energy transition objectives. The results are evaluated in line with the traceability view presented in Figure 7.16, which includes the system requirements at both the SoS and CSs levels. Thus, the level of satisfaction of the identified system requirements at different levels indicates the level of ESI effectiveness. This is only relative in this case comparing between scenarios rather than with respect to an absolute target.

Overall, the scenario analysis has shown that integration through coupling components, particularly P2G, is an effective measure to enable more RES into the system while providing means for a viable network management. Scenarios 5 and 6 with high P2G capacity have seen improvements in all indicators to achieve the set objectives, except for overall efficiency. This is still an acceptable reduction of around 2% and is to be expected with the increased electrification, given that losses from the electricity network are naturally greater than those associated with the gas network.

In terms of system requirements and starting with the requirement to deliver energy in different forms to end-users, this requirement is physically satisfied within the quantitative model. In terms of the requirements to achieve the energy trilemma policy objectives, with regards to environmental sustainability, the requirement to integrate RES into the system is delivered with increased system integration, particularly with high capacity of P2G. In terms of overall efficiency, the overall energy use of the system is lower due to CHP and HPs despite increasing the system losses relative to the total energy input to the system. This is reflected numerically with the CO_2 emissions reduction in scenario 5 with bidirectional integration and even lower in scenario 6 with the addition of HPs.

Getting more RES generation to cover the electric load including for heating also reduces the cost to the system, being dominated by upstream energy imports. This is allowed by the flexible capacity to shift energy vectors provided by the coupling components, mainly P2G. While the reliability and resilience of the system are not examined in response to sudden, extreme events, those criteria are physically satisfied in the simulation model under conditions of system stress.

As mentioned earlier, prospects of DSR are not included in the simulation model, thus the requirements of prosumers in relation to comfort and convenience and access to the grid can't be evaluated.

7.6.2. Uncertainty

The uncertainty of results, and consequently the evaluation, is expected to propagate from the uncertainty identified for the simulation model. The sources of uncertainty can be summarised as follows:

- System parameters, such as the performance factors and efficiency values of CHP and P2G, electricity and gas networks properties (cables, pipes, valves, transformers, etc.), and gas properties (e.g. calorific value)
- Load and generation data, with uncertainty related to the measurement techniques and accuracy of the actual values in the data provided by the network operators
- Environmental effects, such as ambient temperature and availability of RES

Those sources of uncertainty related to the data inputs to the simulation model are outside the scope of this project, and are therefore only acknowledged but not analysed.

Another source of uncertainty can be identified in relation to the unit factors presented in Table 7.5, including the cost factor of upstream energy import, carbon emission factor of upstream energy networks, and the cost of coupling components. Those can be addressed by conducting a sensitivity analysis. This is not only important to account for the uncertainties related to the accuracy of the measurement and reporting of those factors, but also to consider the impact of future changes to those values. The cost factors can change rapidly with technology improvements. Similarly, the network carbon emissions factors are expected to reduce with the increasing RES at national level and the prospects of blending natural gas with hydrogen or other forms of renewable gases, if the UK is to meet its set carbon budgets up until reaching net-zero emissions by 2050 (CCC, 2020). However, since the analysis in this case is based on relative comparison between scenarios, the change in cost and carbon factors is reflected as a relative change among all scenarios, which won't affect the radar chart shape or the intensity indicators, for instance. Nevertheless, this could be different if indicators are given different weights, thus the relative impact of change in those factors could be different on the overall analysis of results.

On the other hand, it is expected that the main change would be caused by the change in the cost factors of energy import from the electricity and gas networks, since it is what goes into the optimisation algorithm. Accordingly, this sensitivity analysis requires a new iteration of running the simulation model.

A detailed uncertainty analysis for integrated energy networks is presented in (Hosseini, Allahham, Walker, et al., 2021), looking at the uncertainty from electricity and heat loads, wind and solar PV generations, and carbon and cost unit factors. The analysis considers the impact of uncertainty on the system performance and is based on the Findhorn case study.

7.6.3. Complexity

The developed framework, particularly the conceptual system modelling stage, aims to facilitate the understanding of the integrated energy system and the deduction of criteria and indicators leading up to the evaluation. In this regard, the framework delivers on this objective even in a larger, more complex energy system like in the NoT region. This is done through the abstraction and decomposition of this system into its different levels and components and focusing on the interaction across the different levels and components. While more effort is needed for such analysis in a larger, more complex case study, this is still achieved and made easier with the modular, standardised approach provided by the RSAM.

During the framework implementation and while dealing with the scenarios and quantitative modelling, it was clear the higher level of detail involved in the NoT case study compared to the Findhorn case study. The framework aims to reduce complexity by abstracting the system at high levels, but in practice lower level challenges should still be considered. For instance, with increasing RES, local network constrains are realised and have to be dealt with in the quantitative model by adding P2G close to the point of wind generation. This highlights the importance of communication and feedback between the conceptual system model and the quantitative model to manage technical complexities.

In terms of results, the dashboard approach for presenting results is supported by the traceability view to realise the contribution of different system components to different system requirements. The traceability view is a condensed representation of the interactions within the system, and a reference point to the other system diagrams that show the structural and functional relationships in more detail. Having the traceability view and the complete conceptual system model behind the indicators set also reduces the system complexity that would otherwise be reflected in the results.

7.6.4. Improvements

Improvements to the framework discussed in Chapter 5 based on learnings from the Findhorn case study and the experts feedback are implemented in this case study. In relation to the limitations discussed for the test case studies in Chapter 5, the scale of the case study, the nature of the quantitative mode, and the types of data and scenarios are addressed.

The scale of the case study is significant to test the framework in dealing with increased complexity as discussed earlier, but also to better investigate the value of ESI. In the NoT case study, the value of ESI is exploited through the scale of RES integration to the system, which is limited in the Findhorn, in addition to the reasonable scale of coupling components relative to the overall energy supply and demand.

The quantitative model used in the NoT case study is still an operational model, so it does pose similar limitations to the case study in terms of optimal sizing, costing and localisation of energy assets. However, the analysis in this case study is based on optimal gas and power flow, where decisions for energy dispatch are made optimally based on operational costs, thus, reducing exogenous variables to the model.

The scenario analysis in the NoT case study is based on scenarios formulated specifically for the purpose of the evaluation targeted in this project. The scenarios are formulated to realise the value of coupling components and evaluate the effectiveness of ESI towards achieving the energy transition objectives. Additionally, the scenario analysis is designed with a sufficient, yet manageable, number of scenarios that encompass different combinations of system configurations and conditions of supply and demand that serve the purpose of the evaluation.

Overall, the full evaluation framework is implemented on this case study after clarifying the interaction and feedback between the framework stages and the communication with the modellers. For stage 1 of the evaluation framework, the use of the RSAM as a standard, modular approach is illustrated. The usefulness of this approach as a reference for WES analysis and a template for stage 1 of the evaluation framework has been demonstrated in this case study. For stage 3 of the framework, the following can be concluded about the typology of quantitative models introduced in Chapter 4:

- In terms of operational models, simulation models are not particularly fit for the purpose due to the limitations discussed in Chapter 5, while optimisation models such as the optimal dispatch model used in this chapter is better fit for the evaluation.
- Generally, optimisation models are expected to be fit for the purpose given that decisions, for both planning and operation, are optimally taken and are typically based on cost minimisation which is important for decision making.
- Hybrid models with both planning and operational aspects are expected to be fit for the purpose given that the technical criteria, such as the flexibility provided by ESI, range in timescale between the short term operation and long term planning.

7.6.5. Limitations

A number of limitations to this case study are identified. First, the type of the quantitative model used in this analysis is an operational model. This type of modelling is valuable for ensuring the system operation on the short term, but planning features are also needed to realise the optimal sizing, costing and localisation of assets for energy generation as well as the coupling components. Furthermore, the use of a steady-state operational model means that system reliability cannot be evaluated dynamically. Second, the model doesn't account for carbon costs, which is a significant factor going forward. In particular, this is expected to have an impact on the interaction between local energy systems and the national energy system, depending on the electricity and gas networks emission factors. Third, energy storage and DSR are not considered in this analysis as other forms of flexibility provision to the system, which are expected to be part of future energy systems, integrated or otherwise. This is due to the lack of data available for those technologies in this particular case study. Finally, this work was started before the COVID-19 pandemic and the data involved are precedent to the times of COVID, which has caused disruption to the energy supply and demand patterns. It is yet to be seen if the energy system goes back to the normal pre-covid patterns or if the pandemic will have a lasting impact on the energy system.

Due to the aforementioned limitations and the number of assumptions involved in the analysis, the findings discussed are deemed applicable to the case study under the stated conditions and assumptions and might not be necessarily generalisable. However, in relation to the developed evaluation framework, the case study demonstrates its applicability and usefulness to a larger, more complex energy system given its generic nature and the modular approach it provides.

7.7. Summary

In this chapter, the developed evaluation framework is applied to a full case study of the local energy system in the North of Tyne (NoT) region in England. The objectives of this case study are summarised as follows:

- demonstrate the applicability and usefulness of the developed framework, including the RSAM, on a larger, more complex energy system
- implement improvements to the framework acquired from the learnings of the test case studies and the experts' feedback
- provide empirical evidence on the effectiveness of ESI towards achieving the energy transition objectives using the framework

Those objectives are fulfilled throughout this chapter in the improved framework application to the case study, while reducing the complexity of the NoT regional energy system, and reaching a set of quantified indicators. The findings show that ESI provides a direction towards achieving the energy transition objectives with more highly integrated scenarios showing improvements in most indicators compared to the other scenarios.

While this case study aims to address the limitations identified previously for the test case studies, a number of limitations still need to be addressed in future work. Those are related to the use of an operational model rather than a planning model, accounting for investment and carbon costs. This is to account for energy systems planning features and the future interaction between the local and the national energy systems, which would partly depend on the electricity and gas networks emission factors and decarbonisation efforts at the national level. Additionally, energy storage and DSR provision should be included as other forms of flexibility to the system, while the transport sector should also be examined as part of the integrated energy system. Finally, in relation to the overall framework, a participatory approach for involving stakeholders with the evaluation in practice by directly eliciting their requirements and getting their feedback as part of the iteration between the framework stages should be considered in practice.

Chapter 8 Conclusion

This final chapter provides a summary of the work presented in the thesis in the scope of the research questions and objectives outlined in Chapter 1. This chapter also reflects on the contributions to knowledge and the limitations of this work in relation to previous work. Accordingly, future work is suggested.

8.1. Research Summary

The overarching aim of this project has been to develop a methodological framework to evaluate the effectiveness of Energy Systems Integration (ESI) as a pathway to achieve the energy transition objectives, set out by the following research question:

- **RQ1:** What is the value of Energy Systems Integration for a sustainable energy transition?

The first research question is broken down to understand the concepts involved and specify the research gaps. Three research questions are thus posed to tackle the main research objective and address the first research question:

- **RQ2:** What is a Whole Energy Systems approach for evaluation?
- **RQ3:** How does Energy Systems Integration drive the energy sustainability transition?
- **RQ4:** How to identify and analyse future structural and functional interactions across integrated energy systems?

Hence, this thesis examines the Whole Energy Systems (WES) approach from which the concept of ESI originates and applies it to evaluation. The WES evaluation principles developed in this research are used to examine the fitness of existing energy sustainability assessment frameworks for evaluating integrated energy systems. ESI is also conceptualised as a transition pathway using a socio-technical sustainability transitions approach. This understanding of ESI provides the theoretical ground to develop the evaluation framework using concepts and methods from systems engineering in a System-of-Systems (SoS) Architecture Methodology. The SoS architecture methodology allows the future structural and functional interactions across integrated energy systems to be conceptually identified and analysed. This conceptual modelling of the integrated energy system is linked with scenario formulation and quantitative modelling in a methodological framework for quantification and assessment. The evaluation framework is tested, validated, and finally applied to a case study to demonstrate its applicability and usefulness to provide evidence around the effectiveness of ESI in achieving a sustainable energy transition.

The specific research objectives achieved in each chapter are discussed below.

Chapter 2 addresses the second research question (RQ2) by defining the principles for the sustainability assessment of integrated energy systems based on the WES approach. Those are termed as the WES principles for evaluation and are:

- Multivectoral, accounting for the interactions between multiple energy vectors and interdependencies between coupled energy systems
- Systemic, reflecting whole system properties emerging from system interactions at different levels
- Multidimensional, considering multiple perspectives and objectives and potential trade-offs or synergies among them
- Futuristic, adapting to major future changes to the energy system structure and function
- Systematic, being flexible to be replicated and adopted in different contexts
- Applicable, proving its usefulness in supporting decision making

The WES principles are derived based on the definition of the WES approach, the impact of ESI on the energy system architecture, and a review of the literature around energy sustainability assessment frameworks. The evaluation principles are utilised to qualitatively appraise existing frameworks and identify their gaps in the evaluation of integrated energy systems. While no existing framework demonstrated all six principles of WES, the evaluation framework developed in this research has been designed to exhibit the six principles.

Chapter 3 addresses the third research question (RQ3) by providing a conceptualisation of ESI from a socio-technical sustainability transitions perspective. Looking at the Multi-System Perspective (MSP) theory in particular, ESI is considered a transition pathway that involves a whole system reconfiguration due to multi-regime interactions across energy systems. This reconfiguration is triggered by the technical coupling between energy systems enabled by ESI technologies (physical system architecture). The reconfiguration is expected to propagate to the institutional level (market system architecture) for co-evolutionary change.

In line with the MSP understanding, integrated energy systems are conceptualised as SoS. The integrated energy system is decomposed into its Constituent Systems (CSs), the electricity, gas and heat energy systems, in addition to the coupling system incorporating ESI technologies. Accordingly, a SoS architecture methodology is proposed to operationalise the MSP and the SoS conceptualisation of ESI. This approach highlights the structural and functional interactions within and across CSs and allows for the analysis of future changes to the energy system architecture at different levels. The SoS architecture methodology makes up the core of the evaluation framework developed in this research.

Chapter 4 addresses the fourth research question (RQ4) and provides the means to address the first research question (RQ1) by developing a methodological framework for the evaluation of ESI. The developed framework exhibits the defined WES principles and operationalises the sustainability transitions approach for ESI. The methodological framework consists of three stages for implementation: conceptual modelling, scenario formulation and quantitative modelling. The key novelty of the framework is in the first stage, which is the conceptual modelling, and in linking this stage with the two other stages. The first stage is based on the SoS architecture methodology to develop a conceptual system model using systems engineering methods. The conceptual model combines stakeholders' requirements with the system structure and function in a system architecture description to provide a socio-technical evaluation. The conceptual model facilitates evaluation by abstracting and decomposing the system into its different CSs at different levels, highlighting structural and functional interactions within and across CSs, and tracing different system components to system requirements. Evaluation criteria are deduced based on this system analysis and as a reflection of the system requirements, while indicators are assigned according to the relationships identified in the conceptual model to measure the level of satisfaction of the system requirements.

The second stage of the framework implementation is the scenario formulation, while the third stage involves quantitative modelling. This is to compare and quantify indicators for different system configurations and under different conditions. Suitable types of scenarios and quantitative models for the scope of the framework are discussed. Those include hybrid scenarios with both explorative and normative features to explore different pathways (such as ESI configurations) towards achieving normative targets (such as net-zero carbon emissions). Similarly, a hybrid type of quantitative models is deemed suitable with both planning and operational features to consider short-term and long-term techno-economic aspects. The framework implementation involves feedback and iteration within and between the three stages. Applying the developed evaluation framework should provide an answer to the first research question.

Prior to that, the framework is tested and validated in **Chapter 5**. The framework testing is conducted through two case studies on the local energy system in Findhorn village, Scotland, with different heating and energy storage technologies. Challenges to the framework implementation are identified such as the communication and interaction between the different stages of the framework. Preliminary findings from the test case studies are presented to academic experts in energy research from multiple disciplines in an online group interview to elicit their feedback for validation and improvement of the framework. The key issue discussed is the need to present a standardised way for the framework implementation. For this, an improved description of the framework implementation and the interaction between its stages has been updated. Moreover, a Reference System Architectural Model (RSAM) is developed to use as a standard, modular approach to implement the first stage of the framework implementation.

Hence, **Chapter 6** supplements the developed framework by a RSAM that is used as a standard conceptual system model for the first stage of the framework implementation. The RSAM is a conceptual system model that describes a comprehensive configuration of the integrated energy system including the electricity, gas and heat systems, coupled by a range of ESI technologies. The RSAM can be used as a flexible, modular approach whereby relevant elements are added or omitted for different applications. The RSAM presented in this thesis is limited to the physical system layer. Therefore, it serves as a basis for further architectural analysis of the market and ICT system layers of the integrated energy system, in addition to supporting the WES analysis and evaluation.

Chapter 7 finally implements the improvements to the framework based on the testing and validation with a full case study application to demonstrate the applicability and usefulness of the developed framework and the RSAM approach. This chapter addresses the first research question (RQ1) by providing evidence on the effectiveness of ESI adopted at the regional level to achieve the energy transition objectives. The case study is based on the local energy system of the North of Tyne region in England and involves comparing different integrated system configurations (combinations of networks and technologies including CHP, P2G and HPs), under different conditions of supply and demand. Thus, the evaluation is conducted relatively between scenarios. It is concluded that P2G is the main contributor to the system flexibility that allows more RES integration into the system, however, only with high capacity of P2G. A limited P2G capacity shows minimal impact in this regard. Moreover, it is shown that scenarios with high P2G capacity see improvements in all indicators to achieve the set objectives, except for overall efficiency where system losses increase. This is only a marginal reduction and is to be expected with the increased electrification, given that losses from the electricity network are naturally greater than those associated with the gas network.

The results are analysed and presented using a dashboard approach, i.e. without the aggregation of indicators. A radar chart is produced to visualise the indicators for all scenarios and other graphs are used to show indicators individually or in relation to each other. The dashboard approach is informed by the traceability view of the conceptual model, which highlights the relationships between different system components, requirements and measures of effectiveness to realise trade-offs and synergies. The limitations to the framework application in the scope of the particular case study are articulated. These are discussed further in Section 8.3.

8.2. Contributions to Knowledge

The research presented in this thesis provides contributions to the knowledge at three levels: conceptual, methodological and empirical (Table 8.1).

Table 8.1 Summary of reseach contributions

Conceptual	**Methodological**	**Empirical**
• Principles for a whole energy systems approach to evaluation • Multi-System Perspective (MSP) for ESI • System-of-Systems conceptualisation of ESI	• Multi-stage evaluation framework • Reference System Architecture Model and ESI-SoS Architectural Framework • MSP operationalisation for tackling sustainability transition research challenges	• Evidence on the effectiveness of ESI for the energy transition

8.2.1. Conceptual Contribution

8.2.1.1. Whole Energy Systems Evaluation Principles

The first conceptual contribution this research makes is the definition of principles for a WES approach to evaluation, where the evaluation should be multidimensional, multivectoral, systemic, systematic, futuristic and applicable. This combination of principles and the description of the WES approach to evaluation is novel. Such an approach is not explicitly defined in the literature. Therefore, an inductive research approach is used to derive those principles by exploring the drivers of change for the energy transition and the expected impacts of ESI on the WES architecture, which would affect the evaluation. The defined principles are not to be seen in tension with other principles relevant to sustainability assessments such as the Bellagio STAMP principles (Gunnarsdottir et al., 2020), but rather to be complimentary. The WES principles are specific to the case of integrated energy systems, whereas the Bellagio STAMP principles apply broadly to any sustainability assessment, with some overlaps between the two. After defining the WES principles, they have been used to qualitatively appraise existing energy sustainability assessment frameworks and identify the research gap for ESI evaluation. Most importantly, the defined principles have also informed the design of the evaluation framework developed in this thesis. Such a framework is required to capture the whole system interactions, quantify interdependencies, and identify the benefits particularly attributed to integration, while considering any trade-offs between the various aspects.

A review of the literature around ESI firstly shows that there is a gap in comprehensive assessment methods and indicators targeting the performance of integrated energy systems (Mancarella, 2014; Abeysekera et al., 2016; Hanna et al., 2018). While there has been progress since the gap was initially identified in developing specific indicators for integrated systems (Mancarella et al., 2018; Moslehi and Reddy, 2018) or focusing on particular technologies (Leitner et al., 2019; Hosseini, Allahham and Adams, 2021), the gap is still applicable when considering holistic sustainability assessment frameworks for those systems. This is verified in this thesis by considering existing frameworks against the WES principles, where none of the reviewed frameworks simultaneously exhibit the six principles required for the evaluation of ESI, making them inappropriate for holistically evaluating future integrated energy systems. While it is common to find multidimensional, systematic and applicable evaluation frameworks, existing frameworks mainly fail in reflecting systemic attributes emerging at the whole system level particularly those related to multivectoral interactions and interdependencies across energy systems. Moreover, existing frameworks generally neglect major structural and functional changes to the energy system in a futuristic evaluation.

8.2.1.2. Multi-System Perspective for ESI

The second contribution relates to the conceptualisation of ESI from a sustainability transitions perspective. First, the MSP theory is applied to the case of ESI as a transition pathway driven by multi-regime interactions across systems leading to a whole system reconfiguration. This is the first attempt to investigate ESI as a pathway in the sustainability transitions literature. An inductive approach is used again to explore concepts from the sustainability transitions research literature relevant to the case of ESI. Some examples involving ESI technologies that create multi-regime interactions have been previously considered (Raven and Verbong, 2007; Haley, 2015; Mazur et al., 2015; Rosenbloom, 2019). However, those case studies focus on institutional interactions (governance, organisational arrangements, political relationships) between the different systems, which is important from an innovation studies point of view to understand the roles of different actors. In contrast, this thesis presents a different approach that starts from a technical standpoint with the technical regimes as an entry point to discuss the transition. In this case, the technical configuration is considered the trigger for the transition driven by a whole system reconfiguration, where the focus is on the new structural and functional couplings created by ESI technologies. The technological reconfiguration would then be resulting in and evolving with new market structures and regulatory frameworks, affecting and being affected by the relationships between actors. Therefore, by developing a better understanding of the physical system layer, this provides the starting point for a co-evolutionary analysis that involves the market system layer, as discussed in Section 8.3 for future work.

8.2.1.3. System-of-Systems Conceptualisation of ESI

Based on the MSP understanding, a SoS conceptualisation for integrated energy systems is proposed, which is an integration of independent systems that act jointly towards a common goal, through synergies, to collectively offer emergent functionality that cannot be provided by CSs alone. Therefore, the integrated energy system is defined as a SoS composed of the electricity, gas and heat CSs, in addition to the coupling system that incorporates ESI technologies. A SoS conceptualisation fits integrated energy systems being characterised by operational and managerial independence, geographical distribution and evolutionary development of its CSs, in addition to emergent functionalities. The SoS conceptualisation for ESI is not totally new, as it has been defined previously based on the SoS characteristics (Mittal et al., 2015) and used to analyse different market designs for future integrated energy systems (Energy Systems Catapult, 2017). However, its novelty in this research is in utilising it to bridge between the qualitative approach of the sustainability transitions frameworks and the quantitative approach of the sustainability assessment frameworks. This conceptualisation enables the use of concepts and methods from systems engineering used for analysing SoS to develop a systems-based evaluation framework that addresses the WES principles and delivers the methodological contributions discussed below.

8.2.2. Methodological Contribution

8.2.2.1. Multi-stage Evaluation Framework

The methodological contribution of this research mainly consists of the methodological framework developed to evaluate ESI and address the gaps in the sustainability assessments for integrated energy systems. The framework is designed based on concepts and methods from systems engineering enabled by the SoS conceptualisation of ESI. Those are combined for a methodological framework that addresses the six WES evaluation principles.

First, the system architecture description of the technical components and future conditions of the energy system, and the system requirements representation of stakeholders' perspectives deliver on the principles for being *multidimensional* and *futuristic*. Second, the SoS modelling approach decomposing the system into its different levels and components allows the evaluation to be *multivectoral* and *systemic*. Finally, the use of MBSE techniques including an architectural framework provides a *systematic* means for conceptual modelling, while *applicability* relies mainly on the data availability and quantitative models suitability for measuring indicators.

In terms of implementation, the developed framework requires iteration and feedback between three stages: conceptual modelling, scenario formulation and quantitative modelling. The novelty of this framework lies mainly in its first stage, which is based on the SoS architecture methodology to develop a conceptual system model. The conceptual model describes the structural and functional interactions across and within the integrated energy systems and traces them to the system stakeholders' requirements and measures of effectiveness. This supports the deduction of the criteria and indicators for evaluation along with a reduced representation of the complex system architecture. This is a largely untapped area of application for such a methodological approach.

This methodology has not been widely adopted outside its origin in systems engineering where it is used, for instance, in applications related to software engineering, enterprise information systems and military defence systems (Davis et al., 2013). Nevertheless, similar approaches related to the concept of system architecture are receiving increased attention in the energy research community. For instance, a system architecture based methodology has been used to represent the interdependencies in water-energy nexus systems to inform operations and planning decisions (Lubega and Farid, 2016); analyse different market designs for future integrated energy systems (Energy Systems Catapult, 2017); understand the interactions between actors in future electricity market configurations (ENA, 2018); standardise smart grid systems design (Uslar et al., 2019); and qualitatively evaluate WES modelling approaches through desirable architecture properties (Scamman et al., 2020; Lowe et al., 2021).

In comparison with other methods, the proposed SoS architecture methodology combines multiple merits as it allows:

- describing functional relations (behavioural influences) between different system components, similar to the System Dynamics method (Bautista et al., 2019; Papachristos, 2019)
- representing structural relations and flows between different system components, similar to system visualisation methods such as the Sankey Diagram (Liu and Mancarella, 2016)

- tracing the relations between high-level goals and lower level requirements, similar to the Strategy Map used in strategic management (Lea et al., 2018)
- facilitating participatory modelling involving stakeholders, similar to the Collaborative Conceptual Modelling method (Neely et al., 2021)

A unique feature that distinguishes the SoS architecture methodology is the ability to represent and analyse SoS specifically, which is the entry point to choose this approach. Another important feature of this methodology is the ability to include measures of effectiveness, or in other words the evaluation criteria and indicators, as part of the conceptual system model. While other methods show the above merits, they do not necessarily link to the evaluation, which is the main objective of this research.

For the second and third stages of the framework, discussions around the suitable types of scenarios and quantitative models for the framework have been presented as mentioned earlier. The framework is developed to be flexibly used in different contexts and is thus theoretically compatible to any type of scenario, given that scenarios are consistent and comparable. However, the type of scenarios formulated can dictate the choice of evaluation criteria and indicators. For instance, criteria can typically be objective focused (translation of objectives into criteria) or alternative focused (highlighting strengths and weaknesses of each alternative) (Trutnevyte et al., 2012). In this framework, criteria highlight both approaches by reflecting the transition objectives and system requirements identified in the first stage at the different system levels, and the variation between alternative system configurations through the scenario formulation. Thus, the system is evaluated against both: (i) the contextual objectives manifested as non-functional requirements at the SoS level and (ii) the functional requirements identified in the first stage at the CS level. This shows the performance of the integrated energy systems in delivering capabilities independently and as a whole. In line with this, indicators are grouped thematically into broader dimensions (e.g. the energy trilemma) to link them with objectives and monitor progress (Narula and Reddy, 2016).

Similarly, the suitability of quantitative models depends on the purpose sought from the use of the evaluation framework. Different energy models serve different purposes and timescales, and eventually provide information to different decision makers (Hughes and Strachan, 2010). In the context of this research, it is concluded through case studies that hybrid models with both planning and operational aspects are expected to be fit for the purpose given that the technical criteria, such as the flexibility provided by ESI, range in timescale between the short term operation and long term planning. Moreover, optimisation models are expected to be fit for the purpose given that decisions, for both planning and operation, are optimally taken and are typically based on cost minimisation which is important for decision making.

Taking a wider look, this integrated methodological framework fits the three requirements for socio-technical energy models (Li et al., 2015). The first requirement is incorporating techno-economic detail including technology cost and performance bounded with operational or resource constraints. This is fulfilled mostly by the quantitative modelling. The second is being explicit about actor heterogeneity with differentiated preferences and behaviours and involving actors that possess agency to shape transitions. This is fulfilled mostly by the conceptual modelling which is based on stakeholders' requirements. Thirdly, there is a requirement to reflect the transition pathway dynamics that include the assessment of normative goals, sufficient time horizons, and radical alternative reconfigurations. This is fulfilled by the overall approach of this research starting with the sustainability transitions conceptualisation leading to the sustainability assessment of integrated energy systems.

The framework's design and implementation is tested and validated in this research through case studies and experts' feedback. To elicit experts' feedback, a virtual semi-structured group interview was conducted with energy researchers from different academic backgrounds followed by a questionnaire. Such a participatory approach has not been previously used to validate energy sustainability assessment frameworks. This exercise was useful to highlight the strengths of the developed framework and the opportunities for improvement. In particular, the need for a consistent procedure to apply the framework was highlighted.

8.2.2.2. RSAM and ESI-SoS Architectural Framework

Through replication and due to the feedback received on the need to standardise the framework application, a RSAM is developed as a standard conceptual system model to be used for the first stage of the evaluation framework. The RSAM can fulfil multiple objectives. First, it allows for a WES analysis that considers the broader environmental, economic and social context, to inform planning and decision making on opportunities for cost savings and efficiency gains through synergies and for avoiding unintended impacts across the system (Bale et al., 2015; Energy Systems Catapult, 2019; Cambini et al., 2020). Second, the RSAM serves as a reference for evaluating the system effectiveness in achieving its objectives. This approach lends itself to be used as an adaptable, modular approach for evaluation. System elements can be added or removed depending on the specific application. Another advantage for using this approach for evaluation is the ability to capture emergent behaviour resulting from interactions between CSs through traceability, while also reducing the complexity involved through system abstraction. This enables better understanding of systemic properties such as resilience and flexibility (Bale et al., 2015), where it has been mathematically verified that ESI offers additional flexibility compared to the separate operation of energy systems (Chicco et al., 2020). Finally, the RSAM can aid decision making when combined with scenario formulation and quantitative modelling by exploring future potential pathways of the energy system, testing and evaluating the impacts of implementing changes through simulation and quantification, and representing different actors and components at different levels for a socio-technical analysis.

In addition to the RSAM, the ESI-SoS architectural framework tailored for the purposes of this project has been established to guide the conceptual modelling stage. The ESI-SoS is a modified version of the SoS-ACRE architectural framework (Holt, S. Perry, et al., 2012), which is adapted to the case of ESI with additional views to clearly show the physical relationships between CS and system components and support the traceability and evaluation of the system effectiveness in relation to system components as well as to requirements. The RSAM and ESI-SoS architectural framework are generic analytical tools that can be used for future research work around integrated energy systems and SoS, as discussed in Section 8.3. For instance, the RSAM provides a basis for further architectural analysis supported by the use of MBSE techniques, which makes it reusable, repeatable and extendable for future studies (Topper and Horner, 2013).

8.2.2.3. Multi-System Perspective Operationalisation

The framework also contributes broadly to the sustainability transitions research area by operationalising the MSP for ESI. It has been suggested that systems engineering offers multiple benefits in understanding socio-technical systems and transitions in a systemic, traceable, and consistent way. However, an adapted systems engineering approach may be needed to consider the particular challenges associated with studying socio-technical integration and socio-technical transitions (Rajabalinejad et al., 2020). The specific methodological contributions to this area are based on the identified methodological challenges in this research field (Holtz et al., 2015; McDowall and Geels, 2017; Köhler et al., 2019; Zolfagharian et al., 2019). Those contributions include utilising a WES approach to the MSP, utilising conceptual level abstraction for system boundary considerations, considering a technical standpoint for studying whole system reconfigurations, facilitating a future-oriented analysis of sustainability transitions and the evaluation of system architectural change, and providing a bridging method between qualitative and quantitative approaches.

To the best of my knowledge, only one effort to directly use such a method from systems engineering for studying socio-technical transitions is found in the literature. The study develops an architectural framework in line with transition frameworks, such as the MLP, to support the planning and execution of sustainable technology projects (Davis et al., 2013). However, the architectural framework developed is restricted to the classical MLP approach, and thus doesn't consider multi-regime interactions as in the case of the MSP, which is relevant to ESI. Furthermore, the architectural framework developed by Davis et al. (2013) is limited to a textual description of the system architecture as opposed to the approach developed in this research where a graphical representation is produced using SysML. This is important to illustrate the structural and functional interactions between the different system components.

8.2.3. Empirical Contribution

This research makes an empirical contribution by showing that ESI provides a direction to achieve the energy transition objectives. The evidence is provided through applying the evaluation framework to a case study of the local energy system of the NoT region in England. The case study involves a number of scenarios with different configurations for the integrated energy system and varying conditions of energy supply and demand. The analysis is supported by a quantitative energy model for quantification. Results for different scenarios are finally presented in a dashboard to realise trade-offs. Such evidence can inform decision making on supporting ESI as a pathway for the energy transition, with an acknowledgement of the assumptions and limitations present.

The results from the case study show that integration through coupling components, particularly P2G, is an effective measure to enable more RES into the system while providing means for a viable network management. Scenarios with high P2G capacity have seen improvements in all indicators to achieve the set objectives including reducing CO_2 emissions and integrating more RES, which was allowed by the flexible capacity to shift energy vectors provided by P2G. Integrating more RES generation to cover the electric load including for heating also reduces the cost to the system, being dominated by upstream energy imports. The only exception is for the overall system efficiency, although with a minimal reduction that is to be expected with the increased electrification, given that losses from the electricity network are naturally greater than those associated with the gas network. Moreover, the system reliability is physically satisfied in the simulation model under conditions of system stress.

The results are in line with concept and review studies that outline the potential benefits of ESI, which include reducing carbon emissions and costs, reducing the use of primary energy, and improving system security with greater flexibility (Kroposki et al., 2012; Mancarella, 2014; Abeysekera et al., 2016; Hanna et al., 2018). This is evident from the evaluation of different scenarios conducted for the NoT case study based on the stakeholders' requirements from one side and the relationships between the assigned indicators on another side.

This research provides a holistic evaluation based on the WES approach that flexibly considers a range of technologies and indicators based on the actual system context. On the other hand, previous studies with empirical findings around ESI evaluation have been limited in scope focusing on either specific technologies or specific indicators. As discussed previously, existing assessment framework do not simultaneously exhibit the WES principles for evaluation. Considering only evaluations of multivectoral energy systems, the results from different studies are still not directly comparable given the different evaluation scope (multidimensional principle), scale (technology, building, network, national; systemic principle), time horizons (from hours to years), methods (indicators, modelling approaches), and applications (case study or standard network). However, like this research, all results generally point towards the direction of the advantages of integrated energy systems over non-integrated system and conclude on the benefits of incorporating different ESI technologies.

For instance, electric heating technologies have been examined to evaluate their impact on the system efficiency and reliability (Leitner et al., 2019), demand-side flexibility (load shifting and consumer comfort) (Zhang et al., 2019), supply-side flexibility (RES integration) (Teng et al., 2016; Bernath et al., 2019), and across techno-economic-environmental parameters (upstream energy import, operational costs, CO_2 emissions) (Hosseini, Allahham and Adams, 2021). Similarly, P2G technologies have been examined to evaluate their technical, economic and environmental impacts looking at a range of indicators such as reducing RES curtailment, networks congestion, upstream energy import, operational costs and carbon emissions (Clegg and Mancarella, 2015; Qadrdan et al., 2015; Parra et al., 2017; Hosseini, Allahham, Vahidinasab, et al., 2021). Additionally, CHP technology has been considered to analyse its technical, economic and environmental impacts in cost value terms (Moslehi and Reddy, 2019). On the other hand, some indicators have been the focus of whole system studies, such as cost and emissions reduction (Liu and Mancarella, 2016), resilience (Moslehi and Reddy, 2018), flexibility (Ameli et al., 2017; Mancarella et al., 2018), and reliability (Li et al., 2016; Lei et al., 2018; Juanwei et al., 2019).

The case study also demonstrates the applicability of the developed framework and its usefulness in reducing the complexity for the holistic evaluation in a regional energy system such as in the NoT. While more effort is needed for such analysis in a larger, more complex case study, this is still achieved and made easier with the modular, standardised approach provided by the RSAM. During the framework implementation and while dealing with the scenarios and quantitative modelling, it was clear the higher level of detail involved in the NoT case study relative to the Findhorn test case study. The framework aims to reduce complexity by abstracting the system at high levels, but in practice lower level challenges should still be considered for feasibility. For instance, with increasing RES, local network constrains are realised and have to be dealt with in the quantitative model by adding P2G close to the point of wind generation. This highlights the importance of communication and feedback between modellers, in this case the conceptual system model and the quantitative model, to manage technical complexities (McDowall and Geels, 2017).

Furthermore, the dashboard approach for presenting results is supported by the traceability view to realise the contribution of different system components to different system requirements. The traceability view is a condensed representation of the interactions within the system, and a reference point to the other system diagrams that show the structural and functional relationships in more detail. Having the traceability view and the complete conceptual system model behind the indicators set also reduces the system complexity that would otherwise be reflected in the results, which is particularly important if they are to be used as input for decision support (Holtz et al., 2015).

8.3. Limitations and Future Work

Despite the contributions the work presented in this thesis make and due to the broad range of issues tackled, a number of limitations are identified raising opportunities for future research work. Three categories of limitations are identified in relation to the research scope, modelling and context. These limitations, summarised in Table 8.2, can be considered for future work accordingly.

Table 8.2 Categories of limitations and headlines for future work

Scope	Modelling	Context
• Architectural layers • Transport system • Flexibility provision	• Planning model • Impact of uncertainty • Participatory approach	• Post-COVID patterns • Whole economy scale • Generalisability

8.3.1. Research Scope

The first limitation is around the overall scope of this research that is limited to the physical layer of the energy system architecture. Thus, the analysis excludes aspects of the market and ICT layers of the energy system architectures. The energy transition is expected to involve co-evolutionary changes between the three layers, with the whole system reconfiguration being triggered by the technical couplings of ESI but propagating to the market structure. Therefore, it is important to investigate this co-evolutionary dynamic going forward in the transition and design appropriate market and governance structures accordingly, to exploit the value of ESI.

Similarly, existing institutional couplings, or the lack thereof, should be examined to facilitate the transition to an integrated energy system rather than being a barrier to this transition. This analysis can be initiated by expanding the RSAM to include descriptions of the market and ICT layers using the SoS architecture methodology used to develop the representation of the physical layer, before having a deeper analysis for each layer.

Examples of considerations for a new market design based on the technical reconfiguration can include the regulatory and economic aspects. Before looking at those considerations, analysis of the physical system layer should demonstrate technical feasibility of the reconfiguration to feed into the discussion of the market layer. The analysis of the market system layer is then carried out to define actors' roles in an integrated energy system and design favourable economic conditions for integrated energy services. This analysis can be done using the same SoS architecture methodology focusing on the structural and functional interactions between stakeholders. This co-evolutionary dynamic between the two layers is the driver towards the socio-technical transition.

First, on the regulatory level, the role of coupling components in providing ancillary services and how they fit with existing market arrangements should be examined. These include flexibility, storage and balancing services for instance. In terms of flexibility, multi-vector shifting needs to be rewarded like other forms of flexibility, while in the case of storage ownership needs to be defined and cross-vector storage should be incorporated within a portfolio of other technologies. For balancing, coupling components such as P2G technologies can provide a quick response to ramp up or down its electricity demand to support network management. Similarly, aggregated demand-side response for electric heating through HPs can support the network at time of constraint by increasing or decreasing consumption while maintaining consumer comfort (Zhang et al., 2019). However, a regulatory framework should be in place to foster and reward these roles within an integrated energy system.

The second consideration is economic in terms of the cost of integration and the price of converted energy. In the case of P2G technologies, the cost of converting electricity into hydrogen or methane gas is higher than the selling price of natural gas. Although technically feasible, economic improvements need to take place. For instance, this could be by improving the technical efficiency of electrolysis units, and thus more investment in research and development can be allocated. Similarly, electric heating provided by HPs could be more expensive to end-users on the short term but more rewarding on the longer term. So, a cost-benefit analysis needs to be accompanied by policy and financing support to drive this transition in favourable market conditions. A co-evolutionary analysis of the physical and market system layers supported by the SoS architecture methodology can highlight the target areas for regulatory changes and policy support for an ESI transition pathway.

In terms of scope, the transport system is also not considered in this analysis although it is expected to be part of the future integrated energy system and play a role in flexibility with the increased electrification and technologies such as Vehicle-to-Grid. The RSAM should therefore be expanded to incorporate the transport system. It is also important to expand the scope in future work to include other forms of flexibility provision such as DSR and single-vector energy storage. The value of ESI in delivering flexibility at scale can be thus investigated in a comparative analysis with other prominent forms of flexibility to realise the most technically feasible and cost-effective options.

8.3.2. Modelling Approach

The second category of limitation and future work concerns the modelling approach. First, the quantitative model used in the case studies to support the evaluation is an operational model. This type of modelling is valuable for ensuring the system operation on the short term, but planning features are also needed to realise the optimal sizing, costing, and localisation of assets for energy generation as well as the coupling technologies. It is therefore worth combining the evaluation framework with a planning model that accounts for investment costs in addition to carbon costs, which is significant going forward. Carbon costs are expected to have an impact on the interaction between local energy systems and the national energy system, depending on the electricity and gas networks emission factors.

Second, the sources of uncertainty have been acknowledged in this study with respect to the system performance parameters, load and generation data, environmental effects, and cost and carbon unit factors. However, the analysis does not directly consider the impact of uncertainty on the evaluation. It is important to be clear about assumptions around the analysis when communicating the findings of the evaluation (Holtz et al., 2015). Therefore, future work can conduct uncertainty analysis to demonstrate the impact of uncertainty on the supporting evidence produced by the evaluation framework.

Finally in relation to the modelling, a participatory modelling approach is recommended when implementing the evaluation framework in practice. This is important to have a transparent process of involving relevant stakeholders and elicit their requirements that the evaluation is based on. Due to the limited scope of this project, requirements have been collected from the literature and assumed to reflect those of key stakeholder groups. It is also important to maintain the participatory approach to disseminate back findings to the stakeholders and receive feedback from them. Therefore, future work could use the developed framework for conceptual participatory modelling and incorporate feedback loops with stakeholders at different stages. This includes, for instance, informing policy of the outcome of the evaluation and exploring changes accordingly needed to support the energy sustainability transition. Future research can also examine the timing and nature of this feedback, in terms of when feedback loops should be incorporated and how will feedback be requested and analysed. This work is currently being implemented extending the NoT case study to involve stakeholders from the region. The plan is to conduct a workshop or a survey with the identified stakeholders to understand their requirements in the context of the energy transition, translate those into quantifiable variables, and use them as inputs for the evaluation framework including for the quantitative modelling and scenario formulation. The novel, intended outcome of this research is particularly at the final stage when findings of the evaluation are reported back to understand how this feedback would affect the stakeholders and decision makers.

8.3.3. Research Context

The third category of limitations and future work is around the general context of the research. This research was initiated before the COVID pandemic and most of the progress was made prior to it. In the context of the energy system, the pandemic has led to changes in the patterns of energy supply and demand including for transport, but it is not clear yet whether it would have a lasting impact on the energy system. The impact might be positive by accelerating the energy transition to achieve net zero carbon emissions, but might also drive the transition in different direction. For instance, it might be that the urgency of ESI is lessened due to the decrease in energy demand, or that ESI becomes a highly localised solution to localised problems. Therefore, the trends going forward with the energy system in the post-pandemic era should be monitored. While it might be outside the direct scope of this thesis, such major events are examined within the MLP landscape level to understand the impact of external shocks on the socio-technical regimes and how they might catalyse or hinder niche-innovation breakthrough. The pandemic has brought forward the significance of landscape changes, the opportunities for change it may bring, and the risk of a rather chaotic transition in a time of crisis as opposed to a managed one (Kanda and Kivimaa, 2020; Sovacool et al., 2020; Wells et al., 2020; Markard and Rosenbloom, 2020).

In terms of trends, a general assumption has been followed in this research around decentralisation and localisation of energy systems (Ford et al., 2021). Case studies have been accordingly designed to investigate the impact of ESI on local energy systems. However, it is worth studying the impact of ESI on a national level and comparing the benefits of both approaches. This has to be accompanied by macroeconomic modelling to realise the impact on the whole economy at both levels, such as with energy prices, economic growth and job creation. The whole research can evolve to develop a comprehensive transition pathway involving ESI and study its implementation across the socio-technical spectrum.

Finally, future work could investigate the generalisability of the research findings presented in this thesis at different levels. The first level is spatial moving up from a local scale to a national scale, in terms of the framework applicability and the value of ESI. The second level is related to whether the approaches taken in this research are transferrable to other socio-technical systems undergoing similar transitions. Future work can therefore investigate the generalisability of the conceptual, methodological, and empirical contributions presented in this thesis.

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Appendix A: Survey of Energy Indicators

Table A.1 Survey of energy indicators

Reference	Dimensions and Indicators			
Energy Matrix (Kisel, 2017)	**Sustainability**	**Affordability**	**Security**	
	Air emissions, nuclear waste, water use, energy efficiency	Households, Competiveness, access	Operational Resilience (flexibility), Technical Resilience (Capacity), Vulnerability, Economic Dependence, Political Affectability	
Sustainable Energy Security (Narula and Reddy, 2016)	**Acceptability**	**Affordability**	**Availability**	**Efficiency**
	Water use, land use, air emissions (GHG)	Cost, volatility, macroeconomic (GDP)	Geological availability, production, supply capability, risk of energy import disruption, resilience to supply disruption, port capacity	Extraction, conversion, imports
IES Life cycle sustainability assessment (Moslehi and Reddy, 2018)	**Environment**	**Economic**	**Technical**	
	Environmental and Health Impacts	Capital Costs & Incentives, Consumption Costs, O&M Costs	Functionality Losses, Penalty Factors	
Energy-chemical systems (He and Feng, 2012)	**Environmental**	**Economic**	**Thermodynamic**	
	waste emission avoidance ratio, CO_2 avoidance cost	primary installed capital cost saving ratio, primary cost saving ratio	Primary energy saving ratio	
Hybrid energy systems (Afgan and Carvalho, 2008)	**Environmental**	**Economic**	**Social**	
	CO_2 emissions	Efficiency, electricity cost, investment cost	NOx emissions	
Renewable heat & Power generation (Dombi et al., 2014)	**Environmental:** GHG emissions, Land demand, energy efficiency, ecological impact	**Socio-economic:** Increase in costs, new jobs, local income		
Biofuel systems (Mangoyana et al., 2013)	**Environmental**	**Economic**	**Social**	
	GHG emissions, Improved land use productivity, Human intoxication, Land use change	investment costs, costs of production, prices of biofuels, other agricultural commodities, investment	Water use, Energy access by local people, Networks, shared norms, values and understanding	

		returns, profitability and employment		
MCA energy scenarios (Witt et al., 2020)	**Environmental**	**Economic**	**Technical**	**Social**
	Metal depletion, Fossil depleting, Global warming potential, Terrestrial acidification, Freshwater eutrophication, Terrestrial exotoxicity	Real gross domestic product, Costs of electricity production and grid expansion	Percentage of plants utilizing RE, Grid efficiency	Import quota for energy sources used, Ratio of wage to capital income, Share of expenditure on electricity of total consumption expenditure, Behavioural adaption costs, PM formation, Photochemical oxidant formation, Human Toxicity
Security interdependencies (Osorio et al., 2017)	**Security:** Generation adequacy (de-rated capacity margin), Resilience (HHI), Reliability (SAIDI), Supply Flexibility, Grid (Capacity adequacy, Ageing), Demand management (Conservation, Efficiency, Demand flexibility), Regulation efficiency (Market performance, Incentives for conventional generation), Sustainability (Affordability, Profitability, Environmental, Fossil fuel dependency), Geopolitics (Import dependency, Vulnerability), Sociocultural factors, Terrorism, Access			
Sustainability evaluation of	**Environmental/Health protection**	**Economic aspects**	**Security of supply**	**Social aspects**

decentralised energy (Karger and Hennings, 2009)	CO_2 emissions, conservation of resources	Number of jobs, Efficiency, Investment, Innovation, Flexibility (market), Income development	Availability, Diversification, Dependency, Security (grid, plants), Reversibility, Fault tolerance	
Energy transitions index (Singh et al., 2019)	**Environmental Sustainability**	**Economic development and growth**	**Security and Access**	**Transition Readiness**
	Air pollution, Energy intensity, Carbon intensity, Carbon per capita	Affordability, Industry competitiveness, Fossil fuel subsidies, Cost of externalities, GDP contribution	Energy access, Quality of supply, Security of supply	Ability to invest, Access to capital, Recent investment in RE/EE, Commitment to Intl agreements, Stable policy, Regulation to support RE/EE/Access, Transparency & political stability, Availability of technology, Innovative business environment, Quality of education, Jobs in RE sector, Energy demand growth, Electricity energy mix, Fossil fuel dependency
UK Energy Security (Watson et al., 2018)	**Availability:** Public opposition, Diversity, Imports and consumption	**Reliability:** Electricity system, Gas system, Electricity interconnector capacity, Demand side flexibility (no of HPs and EVs)		
Irish energy system (Glynn et al., 2017)	**Sovereignty**	**Robustness**	**Resilience**	
	Import share, Non EU share, Share of TPER	Efficiency, Capacity adequacy, Reliability, Congestion, Import capacity	Energy intensity, Sector share of TFC,	
Integrated energy security assessment (Augutis et al., 2017)	**Technical**	**Economic**	**Socio-political**	

Energy Security (Gracceva and Zeniewski, 2014)	**Security:** Stability, Flexibility, Resilience, Adequacy, Robustness			
SoS Environmental Sustainability (Hadian and Madani, 2015)	**Environmental:** Relative aggregate footprint (Land, water, carbon, cost of energy production)			
AESPI (Martchamadol and Kumar, 2013)	**Environmental**	**Economic**	**Social**	**Institutional**
	CO_2 emissions per capita/per GDP	Total primary energy, Final energy consumption, Electricity per capita, Total primary/Final energy intensity, Loss in transmission/ transformation, Reserve production ratio crude oil/natural gas/coal, Industrial, agriculture, commercial, transportation energy intensity, Household energy, electricity per capita, Share of RE/non-carbon, Net import dependency	Household access to electricity, Share of income spent on electricity, Residential energy per household	Ease of business, Effectiveness of government, Financial markets, Goods markets, Labour markets, Level of corruption, Political stability, Private institutions, Protection of property rights, Regulatory quality, Rule of law
Energy security performance (Sovacool et al., 2011)	**Sustainability**	**Affordability**	**Technology development**	**Availability**
	Land use (Forest cover), Water (Water availability), Climate Change (CO_2/capita), Pollution (SO2/capita)	Stability (of electricity prices), Access, Equity, Affordability	Innovation and research (Research intensity), Energy efficiency (Energy intensity), Safety and reliability (Grid efficiency), Resilience (Energy resources and stockpiles)	Security of supply (TPES/capita), Production (Average reserve-to-production for PES), Dependency (Self-sufficiency), Diversification (Share of RE in TPES)
Swiss energy pathways (Volkart et al., 2017)	**Environment**	**Economy**	**Security of Supply**	**Society**
	Metal depletion, Fossil depletion, Ecosystem	Investment costs, O&M costs	Resource autonomy of the supply chain, Resource variability	Human health damages, Expected

	damages, GHG emissions			mortality in severe accidents, Chemical waste, Conflict potential
UK Energy Security (Cox, 2016)	**Sustainability**	**Affordability**	**Reliability**	**Availability**
	GHG emissions and intensity, Primary fuels depletion, Secondary materials depletion, Water usage from cooling and biofuels feedstock production	Cost to the system (Generation cost, Cost of transmission upgrades, Cost of distribution upgrades), Cost to the consumer (Annual retail electricity bills, Impact on levels of fuel poverty)	System Adequacy (De-rated capacity margins, Capacity factors and oversupply, Electricity storage and interconnection), Resilience to sudden changes (Frequency response capability, Short-term Operating Reserve and blackstart capability, Response and reserve requirements, Flexible demand)	Likelihood of domestic disruption to electricity availability (Public approval ratings, Land requirements, Public participation in decisions), Likelihood of nondomestic disruption to electricity availability (Diversity of fuel types in generation mix, Dependence on fuel imports, Diversity and stability of fuel mix)
Energy Justice Metric (Heffron et al., 2015)	Cost benefit analysis (Economics, Politics, Environment)			
Sustainability assessment (Santoyo-Castelazo and Azapagic, 2014)	**Environment**	**Economic**	**Social**	
	Global warming, Resource depletion, Acidification, Eutrophication, Freshwater/Marine aquatic ecotoxicity, Human toxicity, Ozone depletion, Photochemical ozone creation, Summer smog, Terrestrial ecotoxicitiy	Capital costs, Annualised costs, Levelised costs	Security and diversity of supply, Public acceptability, Health and safety, Intergenerational issues	
WEC ETI (WEC, 2019)	**Environmental Sustainability**	**Energy Equity**	**Energy Security**	**Country Context**
	Energy resource productivity (Final energy intensity, Efficiency of power generation and T&D),	Energy Access (Access to electricity/clean cooking), Quality energy access (Access	Security of supply and demand (Diversity of primary energy supply, Import dependency),	Macroeconomic stability, Governance (Effectiveness, Political stability, Rule of law,

	Decarbonisation (Low carbon electricity generation, GHG emissions trend), Emissions and poluution (CO_2 intensity, CO_2/CH_4 emissions/capita, PM2.5/10)	to modern energy), Affordability (Electricity/Gasoline and diesel/Natural gas prices, Affordability for residents)	Resilience (Diversity of electricity generation, Energy storage, System stability and recovery capacity),	Regulatory quality), Stability for investment and innovation (Foreign direct investment net inflows, Ease of doing business, Perception of corruption, Efficiency of legal framework in challenging regulation, Intellectual property protection, Innovation capability)
WEF EAPI (WEF, 2017)	**Environmental Sustainability**	**Economic growth and development**	**Energy access and security**	
	Average fuel economy for passenger cars, PM2.5/CH4/NO2/CO_2, Alternative and nuclear energy	Energy intensity/GDP, Fuel imports/exports, Electricity prices for industry, Diesel/gasoline subsidies	Self-sufficiency (Diversification of import counterparts, Energy imports), Diversity of TPES, Level and quality of access (Electrification rate, Quality of electricity supply, Population using solid fuels for cooking),	
Sustainable development energy (Shaaban and Scheffran, 2017)	**Environmental**	**Economic**	**Technical**	**Social**
	CO_2/NO_x/SO_2 emissions	Investment cost, Job creation, Cost of electricity, O&M cost	Efficiency of energy generation, Resource potential, Reliability of supply, Water consumption	Safety, Social Acceptability

Appendix B: Findhorn Integrated Networks Model

This appendix presents the mathematical formulation and algorithms included in the integrated networks simulation model used for the Findhorn case studies presented in Chapter 5, based on the work developed in (Hosseini, Allahham and Adams, 2021; Hosseini, Allahham, Vahidinasab, et al., 2021).

B.1. Heat Case Study

B.1.1. Model Algorithms

The algorithm of the model implemented and developed in MATLAB to simulate the operation of the integrated gas and electricity networks at the distribution and transmission levels is shown in Figure B.1.

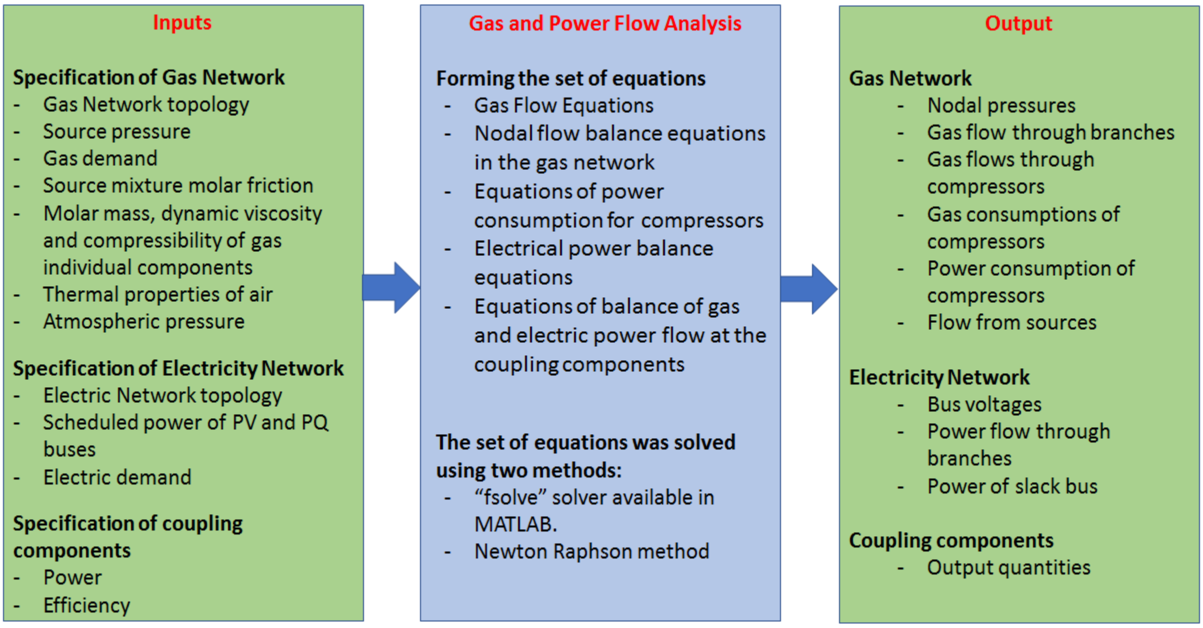

Figure B.1 Overall schematic of the Findhorn model implementation algorithm

Two methods are used to solve the gas and power flow in these integrated networks. The first one is the "fsolve" solver of MATLAB, which is used to solve the set of nonlinear equations and find the values of the unknown variables. Once the values of nodal pressures and the values of bus voltages are obtained, the values of the flows of the gas pipelines and the power flow through electricity branches are calculated using the gas and power flow equations. The second method of calculation is a general approach executing a single gas and power flow analysis in a unified framework based on the Newton–Raphson formulation. The formulation is obtained by combining the stated flow models considering the link between both infrastructures through gas-fired power plants connected to gas pipelines and P2G. The state variables of gas network are the pressures of the nodes and the energy consumption of the compressors. For the electric network, the state variables are the angle (θ) and the magnitude of the bus voltages. In addition, the power generated by the generators driven by gas turbines is also calculated. Then, the set of equality equations F(X) are solved using Newton-Raphson method by forming a Jacobian matrix in the iterations. Here, it is important to mention that the "fsolve" function also solves the same set of equations in a unified method.

B.1.2. Mathematical Formulation

The underlying mathematical formulation for the integrated gas and electricity networks model at the transmission and distribution levels is described by the following equations.

8.4. Matrix representations of the Gas Network

The architecture of a network can be described by the branch-nodal incidence matrix A. This matrix is rectangular, with the number of rows equal to the number of nodes (including reference nodes), and the number of columns equal to the number of pipelines in the network. The element A_{ij} of the matrix A corresponds to node i and branch j, and is defined as: $A_{ij} = 1$, if pipeline branch j enters node i, $A_{ij} = -1$ if pipeline branch j leaves node i, and $A_{ij} = 0$ if pipeline branch j is not connected to node i. Another matrix is introduced later to describe the architecture of gas network when compressors are present in the network.

8.5. The generalised gas flow equation

The generalised gas flow equation used for calculation of flow of the branch based on the pressures of the two ends of the branch, neglecting the elevation difference, is:

$$q = \pi \sqrt{\frac{R_{air}}{8}} \times \frac{T_n}{p_n} \times \sqrt{\frac{(p_1^2 - p_2^2) \times D^5}{f.S_{mix}.L.T.z_{mix}}} \tag{1}$$

where:

q	Gas flow in Standard Temperature and Pressure (STP) conditions,
R_{air}	Air constant
T_n	Standard temperature
p_n	Standard pressure
p_1	Absolute gas pressure at the sending end of the pipe
p_2	Absolute gas pressure at the receiving end of the pipe
D	Pipe diameter
f	Friction factor
S_{mix}	Specific gravity of the gas
L	Length of the pipe

T	Gas temperature
z_{mix}	Compressibility factor

Friction factor (f) is calculated based on the value of the Reynolds number (Re):

$$Re = \frac{D.v.\rho_{mix}}{\mu_{mix}} \tag{2}$$

where the value of the velocity of the gas flow (v) is calculated using the pipe cross sectional area (A) as:

$$v = \frac{q}{A} = \frac{q}{(\pi/4).D^2} \tag{3}$$

and the value of density of the gas mixture (ρ_{mix}) is calculated using:

$$\rho_{mix} = S_{mix} \times \rho_{air} \tag{4}$$

where the specific gravity of the gas mixture (S_{mix}) is as follows:

$$S_{mix} = \frac{z_{air}.\sum_{i=1}^{N_c}(y_i.M_i)}{M_{air}.z_{mix}} \tag{5}$$

and the value of compressibility factor of the gas mixture (z_{mix}) is obtained by:

$$z_{mix} = 1 - \left(\sum_{i=1}^{N_c}(y_i.c_i)\right)^2 \tag{6}$$

Also, the value of dynamic viscosity of the gas mixture (μ_{mix}) is computed as follows:

$$\mu_{mix} = \frac{\sum_{i=1}^{N_c}\left(y_i.\mu_i.M_i^{0.5}\right)}{\sum_{i=1}^{N_c}\left(y_i.M_i^{0.5}\right)} \tag{7}$$

The explanation of the parameters of the above formulations is as follows:

Re	Reynolds number of the gas flow
v	Velocity of the gas flow
ρ_{mix}	density of the gas mixture
μ_{mix}	dynamic viscosity of the gas mixture
A	Cross sectional area of the pipe
ρ_{air}	Density of air in STP condition
z_{air}	Compressibility factor of air in STP condition
N_c	Number of components of the gas mixture
y_i	Molar fraction of the component i in the gas mixture
M_i	Molar mass of the component i in the gas mixture

M_{air} Molar mass of air

c_i Summation factor

μ_i dynamic viscosity of the component i in the gas mixture

Substituting the equations (5) and (6) in (4) and replacing the equations (3), (4) and (7) in (2), the equation for calculation of Reynolds number will be equal to:

$$Re = \frac{\rho_{air}}{(\pi/4)} . \frac{q.S_{mix}}{D} . \frac{\sum_{i=1}^{N_c}(y_i . M_i^{0.5})}{\sum_{i=1}^{N_c}(y_i . \mu_i . M_i^{0.5})} \tag{8}$$

Once the value of the Reynolds number is calculated, the value of the friction factor (f) can be calculated based on the regime of the flow as follows:

- Laminar flow ($Re < 2300$):

$$f = \frac{64}{Re} \tag{9}$$

- Turbulent flow ($Re > 4000$):

In this case, which frequently happens in the gas networks, the friction factor is calculated using the Colebrook's equation, which has empirically been developed based on Moody chart:

$$\frac{1}{\sqrt{f}} = -2 \times log_{10}\left(\frac{\epsilon/D}{3.7} + \frac{2.51}{Re.\sqrt{f}}\right) \tag{10}$$

in which ϵ is the roughness of the internal surface of the pipe.

8.6. Calculation of the flow of the branches

The solution process starts with a guess of the values of the nodal pressures. These values are corrected in each iteration until the amount of correction is small enough and the set of non-linear equations converges to the final solution. In other words, the values of nodal pressures are known in each iteration. Therefore, the next step of the problem is to calculate the values of flows of the branches given the values of the nodal pressures of the two ends of the pipe.

As can be seen from Equation (1) calculation of the value of the flow needs the value of the friction factor of the pipe. However, as was observed from either of the equations (9) or (10) the calculation of the friction factor depends on the value of the Reynolds number, which itself depends on the value of the flow of the branch according to Equation (8). Therefore, the value of the flow needs to be calculated through iterations. In other words, once the value of the nodal pressures of the two ends of the pipe are known, a value for the flow of the branch is guessed. Then, the value of the Reynolds number is calculated using (8). Afterwards, based on the regime of the flow the value of the friction factor (f) is computed from (9) or (10). Subsequently, the new value of the flow of the pipe is calculated using (1). If the difference between the new value and the old (guess) value is acceptable the iteration stops and the solution is found. Otherwise the process is repeated with the new value of the flow until the convergence.

Weymouth Equation

Another flow equation used for high pressure networks, such as transmission networks, is the Weymouth equation. The main assumption in derivation of Weymouth equation is that the friction factor is only dependent on the diameter of the pipe, which is reasonable for the fully turbulent flow regime. Consequently, in the fully-turbulent flow conditions in high pressure transmission networks, the friction factor is calculated using:

$$f = \frac{0.032}{D^{1/3}} \tag{11}$$

Then, the flow equation becomes:

$$q = S_{ij} M_k \sqrt{S_{ij}\left(p_i^2 - p_j^2\right)} \tag{12}$$

$$M_k = \eta_{pk} \; \frac{18.062\, T_n D^{8/3}}{P_n \sqrt{S_g L T Z_g}} \tag{13}$$

where:

S_{ij}	Flow direction, where $S_{ij} = 1$ if $P_i > P_j$, and $S_{ij} = -1$ if $P_i < P_j$,
T_n	Standard temperature
P_n	Standard pressure
D	Pipe diameter
S_g	Gas gravity
T	Average gas temperature
z_g	Average gas compressibility factor
η_{pk}	Pipeline efficiency
p_i	Absolute gas pressure at the sending end of the pipe
p_j	Absolute gas pressure at the receiving end of the pipe
L	Pipeline length

As indicated in equation (12), gas flow can be determined once p_i and p_j are known for given conditions. Equation (12), known as Weymouth flow equation, is most satisfactory for large diameter (≥ 10 inches) lines with high pressures. The developed framework uses this equation to calculate the flow through the branches of transmission networks.

8.7. Pressure regulator modelling

The output pressure of the pressure regulators is regulated by the gas network operator. Therefore, the gas network downstream of a pressure regulator itself has been treated as a gas network with a source pressure equal to the output pressure of the pressure regulator, which is known and kept fixed by the network operator.

8.8. Compressor modelling

A key characteristic of the centrifugal compressor is the horsepower consumption, which is a function of the amount of gas that flows through the compressor and the relative boost ratio between the suction and the discharge pressures. The compressor horsepower (BHP) equation is given as follows:

$$BHP_{ij} = B_k q_k \left[\left(\frac{p_j}{p_i} \right)^{z_{ki}\left(\frac{\alpha-1}{\alpha}\right)} - 1 \right], \qquad B_k = \frac{3554.58\, T_{ki}}{\eta_k} \left(\frac{\alpha}{\alpha - 1} \right) \tag{14}$$

where

q_k	Flow rate through compressor,
p_i	Compressor suction pressure,
p_j	Compressor discharge pressure,
z_{ki}	Gas compressibility factor at compressor inlet,
T_{ki}	Compressor suction temperature,
α	Specific heat ratio,
η	Compressor efficiency.

8.9. Conservation of Mass Flow equation

The mass flow balance equation at each node can be written in matrix form as

$$Aq_p + Uq_C + W - T\tau = 0 \tag{15}$$

where

q_p	Vector of flow rate through pipelines,
q_c	Vector of flow rate through compressor,
A	Branch-nodal incidence matrix,
W	vector of gas supply and demand at each node,

T Matrix represents where gas is withdrawn to power the gas turbine of the compressor,

τ Gas supplied to the gas turbine of the compressor,

U Matrix describes the connection of compressors and nodes.

In addition to the matrix A, which represents the interconnection of pipelines and nodes, we define the matrix U, which describes the connection of compressors and nodes. In this matrix, the item U_{ik} is +1, if the *k*th compressor has its outlet at node i, and -1; if the *k*th compressor has its inlet at node i, 0 otherwise. The vector of gas injections W is obtained by

$$W = W_S - W_L \tag{16}$$

Where

W_S A vector of gas supplies at each node;

W_L A vector of gas demands at each node.

The matrix T and the vector τ represent where gas is withdrawn to power a gas turbine to operate the compressor. In the matrix T, the item T_{ik} is +1; if the kth compressor's turbine gets gas from node i, and 0 otherwise. Analytically, the gas supplied to the gas turbine of the compressor k can be approximated as

$$\tau = \alpha_k + \beta_k BHP_k + \gamma_k^2 BHP_k^2 \tag{17}$$

where $\alpha_k, \beta_k, \gamma_k$ are compressors gas consumption coefficients.

Mathematical Model of the Electricity Network

An AC power flow model is used to represent the electricity network. The steady state operation of a power system is formulated by stipulating that, at each system's bus, the power injected by generators, the power demanded by loads, and powers exchanged through the transmission elements connected to the bus must add up to zero. This applies to both active and reactive powers. Consequently, the real and reactive power injections at bus i need to satisfy the following equations:

$$P_{G_i} - P_{L_i} - P_i(V,\theta) = 0 \tag{18}$$

$$Q_{G_i} - Q_{L_i} - Q_i(V,\theta) = 0 \tag{19}$$

Where

P_{G_i} real power generation at bus i,

P_{L_i} real power load at bus i,

Q_{G_i} reactive power generation at bus i

Q_{L_i}	reactive power load at bus i,
P_i	real power injection at bus i,
Q_i	reactive power injection at bus i,
V	Bus voltage magnitude vector,
θ	Bus voltage angle vector.

Coupling Components

The relationship between the natural gas and electricity networks is provided by Power-to-Gas and the gas-fired turbines' generators i.e. gas turbines or the CHP, which act as energy converters. This coupling is mathematically formulated by Equations (20) and (21).

$$q_{generator} = \frac{3600\ P_{generator}}{\eta_{generator} * 37.26} \tag{20}$$

$$q_{P2G} = \frac{P_{P2G} \times \eta_{P2G}}{11.57} \tag{21}$$

where

$q_{generator}$	gas flow supplied to the gas-fired turbines' generator,
$P_{generator}$	generated real power,
$\eta_{generator}$	Generator efficiency,
q_{P2G}	Gas flow produced by the P2G unit,
P_{P2G}	Real power supplied to the P2G unit,
η_{P2G}	efficiency of P2G unit,

The impact of the coupling components will be considered into Equation (15), (16) and (18), where these components affect the items (W_s), (W_L), (P_L) and (P_G).

Integrated Gas and Power flow solution

The integrated gas and power flow formulation of the natural gas and electricity infrastructures is obtained by combining the stated flow models considering the link between both infrastructures through gas-fired power plants connected to gas pipelines and power-to-gas units using electrical energy. Hence, the set of nonlinear equations that must be solved for the state variables of both infrastructures is given. The proposed solution approach consists of applying Newton-Raphson's method (or using the" fsolve" function in MATLAB) to provide an approximate solution to the total set of equality constraints. The Jacobian matrix used in Newton's solver is given by Equation (22):

$$J = \begin{bmatrix} \frac{\partial \Delta q}{\partial p} & \frac{\partial \Delta q}{\partial BHP} & \frac{\partial \Delta q}{\partial P_G} & 0 & 0 \\ \frac{\partial \Delta BHP}{\partial p} & \frac{\partial \Delta BHP}{\partial BHP} & 0 & 0 & 0 \\ 0 & 0 & \partial \Delta P_G / \partial P_G & 0 & 0 \\ 0 & \partial \Delta P / \partial BHP & \partial \Delta P / \partial P_G & \frac{\partial \Delta P}{\partial \theta} & \frac{\partial \Delta P}{\partial V} \\ 0 & 0 & 0 & \frac{\partial \Delta Q}{\partial \theta} & \frac{\partial \Delta Q}{\partial V} \end{bmatrix} \quad (22)$$

Note that the number of equation which is $NN - NS + NC + N_{coupling} + 2 * nbb$ equations, must equal to the number of unknown decision variables ($NN - NS + NC + N_{coupling} + 2 * nbb$), where:

NN : The number of the nodes of the gas networks,

NS: The number of gas sources,

NC: The number of compressors,

$N_{coupling}$: The number of coupling components, and

nbb : The number of buses in the electrical network.

This is a necessary condition to solve the integrated gas and power flow by using Newton-Raphson or other iterative methods.

B.2. Storage Case Study

The same algorithm and mathematical formulation presented in Section B.1 is used for the storage case study except for additional parameters and equations specific for storage technologies. Those are summarised as follows.

The relevant energy storage parameters are the capacity of electric storage technologies in MWh and the state-of-charge (SoC). The initial and final SoC values for all the storage devices are considered to be equal to zero.

In terms of the mathematical formulation, in addition to the gas and power flow equations mentioned earlier, equations representing energy storage management are included where the SoC of electric storage (SoC_E) is defined as:

$$SoC_e = \frac{E_E^{available}}{C_E} \times 100\ (\%) \quad (23)$$

in which $E_E^{available}$ (MWh) is the amount of available energy and C_E(MWh) is the capacity of the electric storage.

The change in the SoC of the electric storage (ΔSoC_E) during the time step t with the length $\Delta t(h)$ is calculated using:

$$\Delta SoC_E = \frac{E_E^{Charge/Discharge}}{C_E} \tag{24}$$

in which $E_E^{Charge/Discharge}$ (MWh) is the amount of charged or discharged energy from the electric storage technology during the time step t with the length $\Delta t(h)$.

Another form of storage is represented, which is the cross-vector storage (CVS) through P2G technology, where the state of stored energy is defined by:

$$LoG_{CVS} = \frac{V_{CVS}^{Available}}{C_{CVS}} \times 100\ (\%) \tag{25}$$

where LoG is the level-of-gas, $V_{CVS}^{Available}$ is the amount of gas available in the CVS (m^3), and C_{CVS} is the capacity of CVS (m^3).

The change in the LoG of the CVS (ΔLoG_{CVS}) during time step t with the length $\Delta t(h)$ is:

$$\Delta LoG_{CVS} = \frac{q_{i/o}\Delta t}{C_{CVS}} \tag{26}$$

where $q_{i/o}$ (m^3/h) is the input/output gas flow into/out of the CVS during the time period Δt.

Electric storage is usually used to cover the short-term energy shortage, while CVS can be considered as long-term storage. Hence, the charging priority is given to electric storage. Additionally, in every conversion unit, some part of the energy is lost due to conversion inefficiencies. Furthermore, the emission of the electricity network is higher than the emission of the gas network. Therefore, the surplus of RES is first directed to the electricity storage and then to the gas storage after conversion. This is based on an algorithm that first calculates the required energy (E_{RQD}) from the point of common coupling (e.g. slack bus). The E_{RQD}, which is calculated by the model of the electricity network, represents the amount of power required by the slack bus of the electricity network to meet the electric load. The E_{RQD} is compared with the available generation from RES. If generation from RES is smaller than the E_{RQD}, then the RES and the available storage in the electricity side meet all or part of the E_{RQD}. Otherwise, all the generation of RES is supplied to the network and the surplus (E_{SUR}=$E_{RES\text{-}E}$-E_{RQD}) will be stored in the electric storage, provided that it is not full. If the electric storage becomes full, or if it was already full, then the rest or all of the surplus generation of RES is directed to the P2G unit to be converted into natural gas and stored in the CVS technology. If the CVS technology is full, then the output of the P2G is directly injected into the gas network.

Appendix C: Findhorn Storage Case Study Results

Table C.1 Environmental indicators for Findhorn storage case study

Scenario	Environmental		
	Decarbonisation		Efficiency
	CO_2 Emissions (kg-eq/MWh)	RE Integration (%)	Overall Efficiency (%)
Config1_Sc1	174.81	11.79	95.47
Config1_Sc2	175.43	11.29	95.40
Config1_Sc3	178.60	8.85	95.40
Config1_Sc4	171.93	14.02	95.53
Config2_Sc1	169.70	15.72	95.46
Config2_Sc2	170.61	15.00	95.39
Config2_Sc3	175.41	11.30	95.39
Config2_Sc4	168.98	16.26	95.39
Config3_Sc1	146.99	29.05	88.01
Config3_Sc2	154.59	24.21	89.30
Config3_Sc3	174.33	12.10	92.06
Config3_Sc4	89.72	72.63	75.40
Config4_Sc1	148.06	29.05	89.20
Config4_Sc2	155.95	24.21	90.43
Config4_Sc3	175.77	12.10	92.65
Config4_Sc4	89.30	72.63	76.20

Table C.2 Economic indicators for Findhorn storage case study

Scenario	Economic			
	Whole System Cost			Cost-effectiveness
	Cost of Energy Import (£)	Cost of Flexibility (£)	Total Cost (£)	Abatement Cost of CO_2 (£/kgCO2)
Config1_Sc1	1,936	0.00	1,936	
Config1_Sc2	2,364	0.00	2,364	−689.03
Config1_Sc3	2,536	0.00	2,536	−158.34
Config1_Sc4	1,441	0.00	1,441	−171.88
Config2_Sc1	1,706	230	1,936	0.04
Config2_Sc2	2,103	261	2,364	101.89
Config2_Sc3	2,363	173	2,536	−1,001.00
Config2_Sc4	1,343	103	1,446	-83.98
Config3_Sc1	1,736	2,690	4,426	89.47
Config3_Sc2	2,177	2,518	4,695	136.44
Config3_Sc3	2,469	1,208	3,677	3,589.93
Config3_Sc4	960	5,891	6,851	57.75
Config4_Sc1	1,583	2,594	4,177	83.73
Config4_Sc2	1,987	2,379	4,366	128.79
Config4_Sc3	2,324	1,062	3,387	−1,512.48
Config4_Sc4	890	5,903	6,793	56.80

Table C.3 Technical indicators for Findhorn storage case study

Scenario	Technical	
	Resilience	**Flexibility**
	Self-Sufficiency (%)	Flexible Capacity (%)
Config1_Sc1	11.25	0.00
Config1_Sc2	10.77	0.00
Config1_Sc3	8.44	0.00
Config1_Sc4	13.40	0.00
Config2_Sc1	15.01	9.76
Config2_Sc2	14.31	8.13
Config2_Sc3	10.78	8.13
Config2_Sc4	15.51	12.20
Config3_Sc1	31.99	60.98
Config3_Sc2	27.05	50.81
Config3_Sc3	16.74	50.81
Config3_Sc4	61.64	76.22
Config4_Sc1	32.42	95.12
Config4_Sc2	27.39	79.27
Config4_Sc3	16.85	79.27
Config4_Sc4	62.30	118.90

Appendix D: Framework Validation Workshop Material

This appendix includes the framework validation workshop material including the participant consent form (Section D.1), pre-workshop briefing document (Section D.2), post-workshop questionnaire (Section D.3), and the workshop presentation slides (Section D.4).

D.1. Participant Consent Form

The text below was included in the participant consent form sent to the invited experts outlining the workshop objectives and format, and indicating how data is recorded and managed.

Workshop Overview

The aim of this workshop is to get feedback from experts around a proposed evaluation framework developed as part of a PhD project on assessing the sustainability performance of future whole energy systems. The feedback will help validate and improve the conceptual and methodological design and the application of the evaluation framework.

The workshop follows a three-fold validation process of the proposed framework looking at its design, output and usefulness. The workshop is therefore divided into three parts representing different phases involved in the design, implementation and application of the framework. Each part starts with a brief presentation and is followed by a structured discussion.

Your consent

The workshop will be recorded. Your input to the workshop will be combined with the views of others in order to validate and improve the conceptual and methodological design and the application of the evaluation framework. Your personal information will not be recorded. Your name shall not be used to identify your responses, all responses shall be anonymised.

Please complete the following information and return to a.e.h.berjawi2@newcastle.ac.uk

(Tick ☑ the appropriate box)

☑ I understand the nature of the research

☑ I give permission for the workshop I attend to be recorded for use by Ali Berjawi for the purpose explained above

☑ I understand any responses I give during the workshop may be published in an anonymised form

Your name:

Date:

D.2. Pre-Workshop Briefing Document

The text below was included in the document circulated before the workshop to familiarise the experts with the developed evaluation framework and introduce its different stages.

Workshop Overview

The aim of this workshop is to get feedback from experts around a proposed evaluation framework developed as part of a PhD project on assessing the sustainability performance of future whole energy systems. The feedback will help validate and improve the conceptual and methodological design and the application of the evaluation framework.

The workshop follows a three-fold validation process of the proposed framework looking at its design, output and usefulness. The workshop is therefore divided into three parts representing different phases involved in the design, implementation and application of the framework. Each part starts with a brief presentation and is followed by a structured discussion. An online questionnaire is available to provide your feedback.

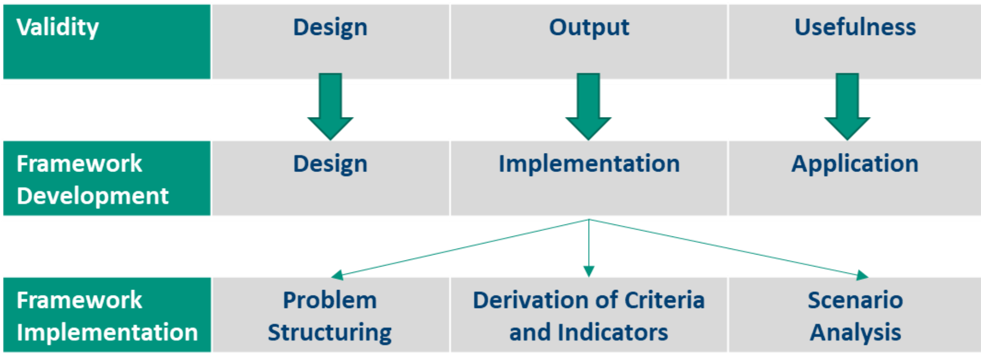

Figure D.1 Validation process and the evaluation framework structure

The following information introduces and defines the concepts and methods used to develop and implement the framework.

Framework Design

A whole energy systems approach to planning and operation of energy systems is a holistic approach that looks at:

- multiple energy vectors: power, gas, heat
- energy supply chain span from generation to end-use, through infrastructure and markets
- the system environment comprising different stakeholders with multiple perspectives and objectives, including the technical, environmental, economic, political and social aspects

Similarly, the rationale behind the proposed framework is the need for a whole energy systems approach to the evaluation of those systems. This approach has been translated into a number of principles that the evaluation framework should exhibit. These are summarised as follows:

- Multivectoral, accounting for the interactions between multiple energy vectors and interdependencies between coupled energy systems
- Systemic, reflecting whole system properties emerging from system interactions at different levels
- Multidimensional, considering multiple perspectives and objectives and potential trade-offs or synergies among them

Three further characteristics are considered useful for the evaluation framework, which are:

- Futuristic, adapting to major future changes to the energy system structure and function
- Systematic, being flexible to be replicated and adopted in different contexts
- Applicable, proving its usefulness in supporting decision making

To address those characteristics and reflect a whole systems perspective, concepts and methods from systems engineering are employed to build up the evaluation framework. These are:

- System architecture, includes principles and guidelines governing the system structure, functions, the relationships between its components and with its environment, and how it will meet its requirements
- System requirements, refer to the functions and capabilities that the system needs to fulfil or acquire, and are mainly related to the needs of stakeholders
- System-of-systems (SoS), defined as integration of independent systems that act jointly towards a common goal, through synergies, to collectively offer emergent functionality that cannot be provided by constituent systems alone
- Model-based systems engineering (MBSE), is the formalised application of modelling to support system design, architecture, analysis and evaluation
- Architectural framework, is a structured practice specifying the system views required to describe a system architecture

The first aim of adopting those concepts and methods is to develop a conceptual model of the energy system, whereby system requirements and the system architecture are identified. This allows for a socio-technical evaluation by assessing the system performance against requirements corresponding to stakeholders' objectives. This is done by matching the requirements to the relevant functionalities delivered by the system and the capabilities it acquires. This will facilitate the derivation of appropriate evaluation criteria and indicators that represent the level of satisfaction of the system requirements. This will deliver on the evaluation principles identified for being multidimensional and futuristic.

Using a SoS approach allows the evaluation to be multivectoral and systemic, where the energy system is modelled at different system levels and decomposed into different constituent systems. This will highlight the interactions, interdependencies and emergent behaviour between different energy vectors and system components. For instance, using this approach intends to better capture the value of flexibility and resilience across the whole system.

MBSE is the process used to develop conceptual models that represent the system architecture, including its structure, functions and requirements. MBSE is supported by the Systems Modelling Language (SysML), which is a graphical modelling language for designing and analysing complex systems. An architectural framework is needed to systematically guide the system modelling and analysis in order to capture different perspectives and viewpoints.

Framework Implementation

To implement the framework, a stepwise procedure is developed comprising of:

- Problem structuring

The first stage of the evaluation framework involves developing a conceptual system model including creating context, structural and functional models of the system. This is done following an architectural framework, applying a SoS approach, and using MBSE techniques.

- Derivation of criteria and indicators

The second stage involves deriving appropriate evaluation criteria and assigning corresponding indicators to the relevant system requirements, components and functions. Evaluation reflects both contextual objectives at the SoS level and the functional requirements at the constituent systems level. This shows the performance of the energy systems in delivering capabilities independently and as a whole. Benchmarking is set based on the scope and purpose of the evaluation. This can be with respect to set objectives or relative to other scenarios.

- Scenario analysis

The final stage of the framework involves applying the steps in stages 1 and 2 for different scenarios and quantifying assigned indicators. Data for scenarios are fed from existing demonstration systems or simulation models of future systems. Indicators are combined in a dashboard to present findings with respect to multiple dimensions without masking trade-offs. Findings of different scenarios are then compared and analysed to examine whether the targets and objectives can be achieved synergistically or whether they require trade-offs.

Framework Application

The framework is applied to a case study to demonstrate its applicability and usefulness. The case study is based on the Findhorn village demonstrator and involves eight scenarios to deliver heat with different networks configurations (electricity, gas, heat) and coupling technologies (Combined Heat and Power and Heat Pumps).

The system structure, behaviour and requirements are modelled for each scenario using MBSE. System modelling is guided by an architectural framework that describes the required system views for the analysis at different system levels. The focus is on the physical system architecture, while the market and cyber/information layers are out of the scope of this study. Appropriate evaluation criteria and indicators are then derived and quantified, and the results obtained are finally compared for different scenarios in a multicriteria assessment.

Reference System Architecture

The above exercise leads to the development of a system architecture that can be employed as a reference for the evaluation of whole energy systems. A high-level architecture that describes the principles governing the structure and composition of the systems, the functionalities required from the system to deliver, the operations needed to deliver them, and the measures of effectiveness. This can be readily used for the purpose of evaluation without the need for going through the evaluation framework procedure described.

The reference system architecture can also serve as a basis to

- design, validation and demonstration of future integrated energy systems
- define and enhance the roles of the different actors involved
- examine cyber-physical interfaces within the whole energy system required for interoperability between the different system components and issue related to cyber security and data sharing

D.3. Post-Workshop Questionnaire

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Meta-Evaluation Workshop

Questions for the workshop participants to engage in the discussion and provide feedback.
The questions below are general to frame your response. Please feel free to elaborate.

1 **Discussion Questions** > 2 Survey Questions

Participant Information

Name *

First Last

Organisation

Email

Part 1

Questions to be answered after the first part of the workshop related to the framework design

1- What do you think about the evaluation principles identified?
Are they necessary in the first place, and how much do they reflect a whole energy systems approach?

2- What do you think about the conceptual design of the framework, in terms of scientific soundness and appropriateness to address the evaluation principles?

Figure D.2 Questionnaire - Part 1

Part 2

Questions to be answered after the second part of the workshop related to the framework implementation

3- Why do you think the framework procedure is, or is not, robust and consistent?

4- How much does the framework output (the system model) achieve the intended purpose of addressing the evaluation principles?

5- What could be the most useful way to visualise and interpret the results for informing decision making?

Figure D.3 Questionnaire - Part 2

Part 3

Questions to be answered after the last part of the workshop related to the framework utility

6- What do you think of using the reference system architecture concept for evaluation?

Would it be more useful to have a readily available system architecture model than to go through the framework process to develop one?

7- Can you think of other applications that a reference system architecture would be useful for?

Closing Question

8- Overall, what do you think are the strengths and weaknesses of the proposed framework?

Figure D.4 Questionnaire - Part 3

1- Do you understand what the framework intends to deliver?

○ Yes ○ No ○ Somehwat

2- How likely are you to use the framework?

○ Not likely ○ Somewhat likely ○ Very Likely

3- How do you evaluate the following attributes of the framework

	Poor	Fair	Good	Very Good
Accuracy	○	○	○	○
Credibility	○	○	○	○
Coherence	○	○	○	○
Utility	○	○	○	○

4- How important is it that the framework allows the following:

	Not Important	Somewhat Important	Importnat	Very Important
Show the relationships between different system components	○	○	○	○
Model the system at different levels	○	○	○	○
Present the system requirements in relation to multiple stakeholders	○	○	○	○
Link the system components and functionalities to derive evaluation criteria and indicators	○	○	○	○
Make informative judgements on the performance of different scenarios	○	○	○	○

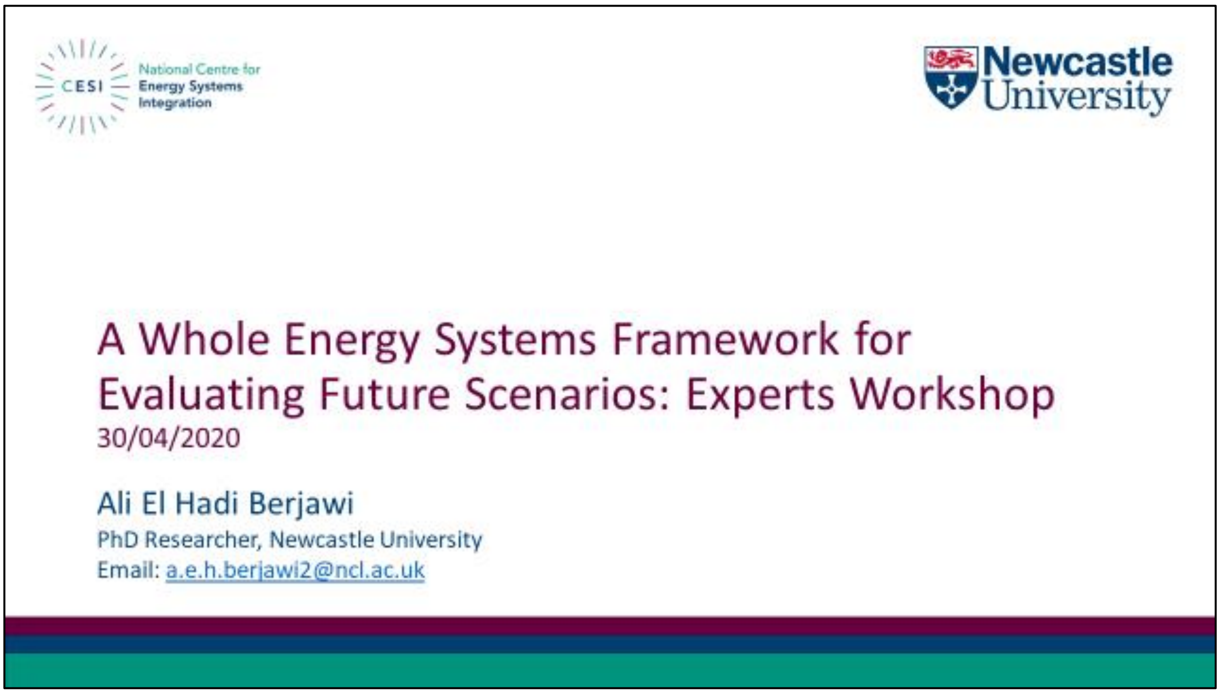
Figure D.5 Questionnaire – Survey questions

Data Protection Statement

The data will be used for a PhD research project by Ali Berjawi. Your input will be combined with the views of others in order to validate and improve the conceptual and methodological design and the application of the proposed evaluation framework. Your personal information will not be recorded. Your name shall not be used to identify your responses, all responses shall be anonymised. By participating in this questionnaire, you are agreeing to the above terms. If you have any concerns please contact a.e.h.berjawi2@ncl.ac.uk

Figure D.6 Questionnaire - Data protection statement

D.4. Workshop Presentation Slides



National Centre for Energy Systems Integration

Workshop Structure

- Introduction
- Framework Design
- Framework Implementation and Application
- Reference System Architecture
- Closing

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National Centre for Energy Systems Integration

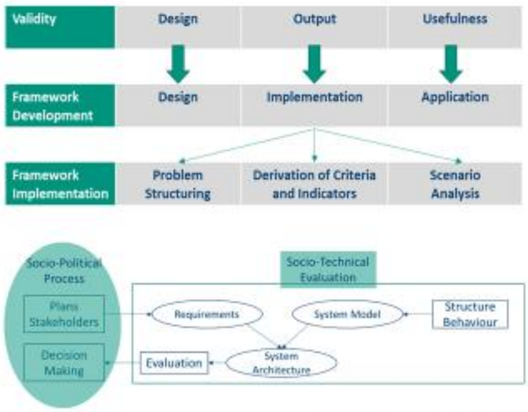
Introduction

Workshop Objective

- Experts feedback
- Validation

Context

- The Energy Transition
- Energy Systems Integration
- The Energy Trilemma



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Session 1: Outline

- Evaluation principles for a whole energy systems approach
  - What do you think about the evaluation principles identified?
  - Are they necessary in the first place, and how much do they reflect a whole energy systems approach?
- Framework conceptual design
  - What do you think about the conceptual design of the framework, in terms of scientific soundness and appropriateness to address the evaluation principles?

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Framework Design

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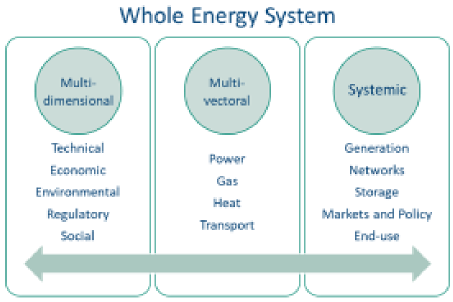
- Whole Energy Systems Approach
- Evaluation Principles
  - Multidimensional
  - Multivectoral
  - Systemic
  - Futuristic
  - Systematic
  - Applicable



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Framework Design

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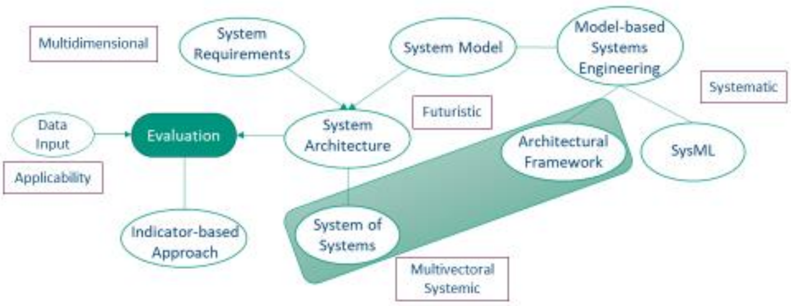
- Concepts and Methods



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Session 1: Discussion

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- What do you think about the evaluation principles identified?
  - Are they necessary in the first place, and how much do they reflect a whole energy systems approach?
- What do you think about the conceptual design of the framework, in terms of scientific soundness and appropriateness to address the evaluation principles?

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Session 2: Outline

- Framework procedure for application
  - Why do you think the framework procedure is, or is not, robust and consistent?
- System architecture model for case study
  - How much does the framework output (the system architecture model) achieve the intended purpose of addressing the evaluation principles?
- Case study results
  - What could be the most useful way to visualise and interpret the results for informing decision making?

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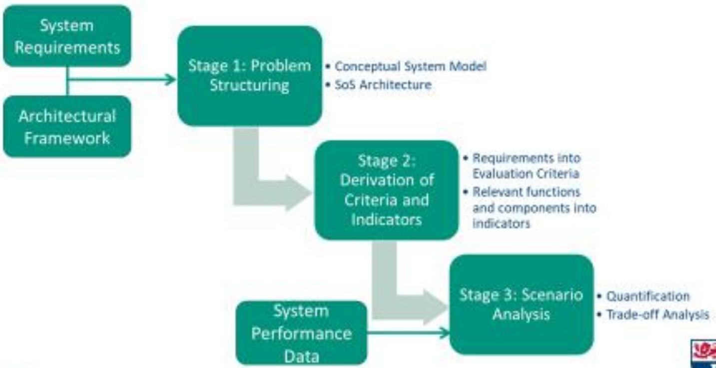
National Centre for Energy Systems Integration (CESI)

Framework Implementation

- Framework Procedure



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Framework Implementation

- Architectural Framework
  - adapted from the SoS-ACRE framework

Level	View		SysML Diagram
Context (System Definition)	System Boundary Constituent Systems	System Environment Stakeholders	Block Definition
System-of-Systems	Structure		Internal Block
		Requirements	Use Case
	Operations		Activity, Sequence
Constituent System	Composition Structure		Block Definition, Internal Block
		Requirements	Use Case,
	Operations		Activity, Sequence
System Element	Composition, Properties		Block Definition
Performance Evaluation	Evaluation Criteria (measures of effectivness) Indicators		Requirements Parametric

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Framework Application

- Findhorn Case Study
- Nine scenarios for integrated systems to deliver heat
- Focus on the physical architecture (Energy supply and infrastructure)
- Overall requirement to achieve the energy trilemma objectives while meeting energy demand

No.	Description	Networks meeting the heat load
1	All electric – Electric Heaters (EH)	Electricity Network (EN)
2	All gas – Gas Boilers (GB)	Gas Network (GN)
3a	Gas & electric – GB and Air-sourced Heat Pump (ASHP)	GN, EN
3b	Gas & electric – GB and ASHP	GN, EN
4a	High Temperature Geothermal with EH at DHN source	District Heating Network (DHN)
4b	Low Temperature Geothermal (LTGR) with EH at DHN source	DHN
5	CHP	DHN
6	LTGR and EH at final load	EN, DHN
7	LTGR and GB at final load	GN, DHN

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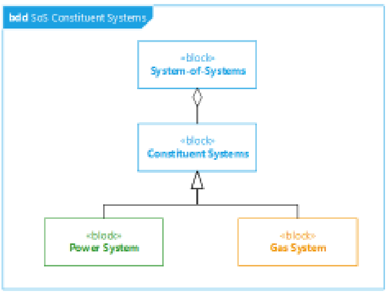
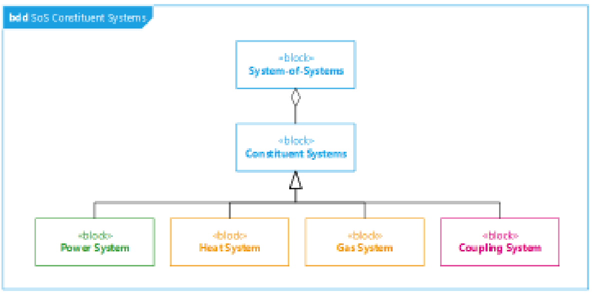
System Model

- Context Level: Constituent Systems

Scenario 2



Scenario 7



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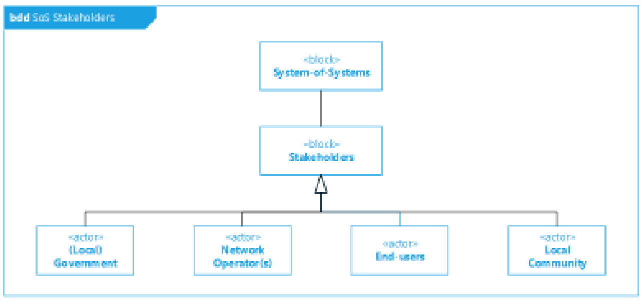
System Model

- Context Level: Stakeholders
  - For all scenarios



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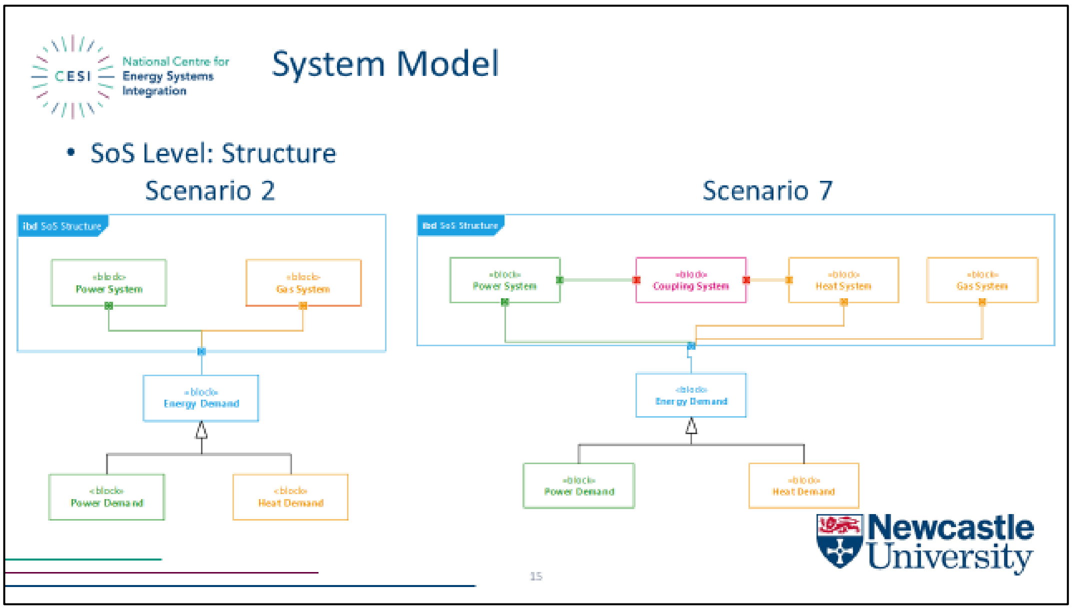
National Centre for Energy Systems Integration
CESI
System Model
SoS Level: Structure
Scenario 2
Scenario 7
ibd SoS Structure
«block» Power System
«block» Gas System
«block» Energy Demand
«block» Power Demand
«block» Heat Demand
«block» Coupling System
«block» Heat System
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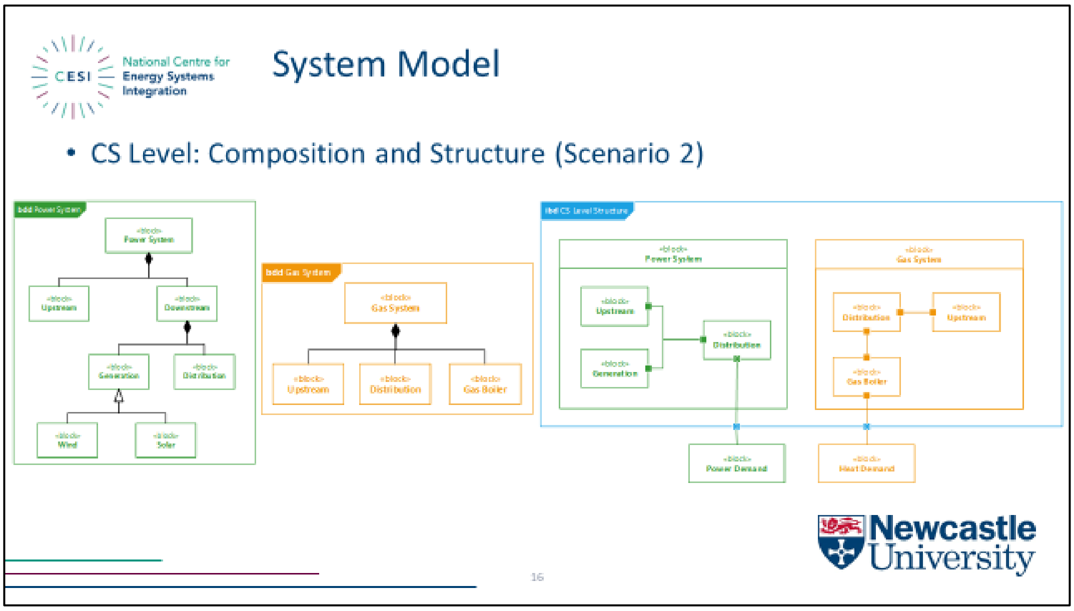
National Centre for Energy Systems Integration
CESI
System Model
CS Level: Composition and Structure (Scenario 2)
bdd Power System
bdd Gas System
ibd CS Level Structure
«block» Power System
«block» Upstream
«block» Downstream
«block» Generation
«block» Distribution
«block» Wind
«block» Solar
«block» Gas System
«block» Gas Boiler
«block» Power Demand
«block» Heat Demand
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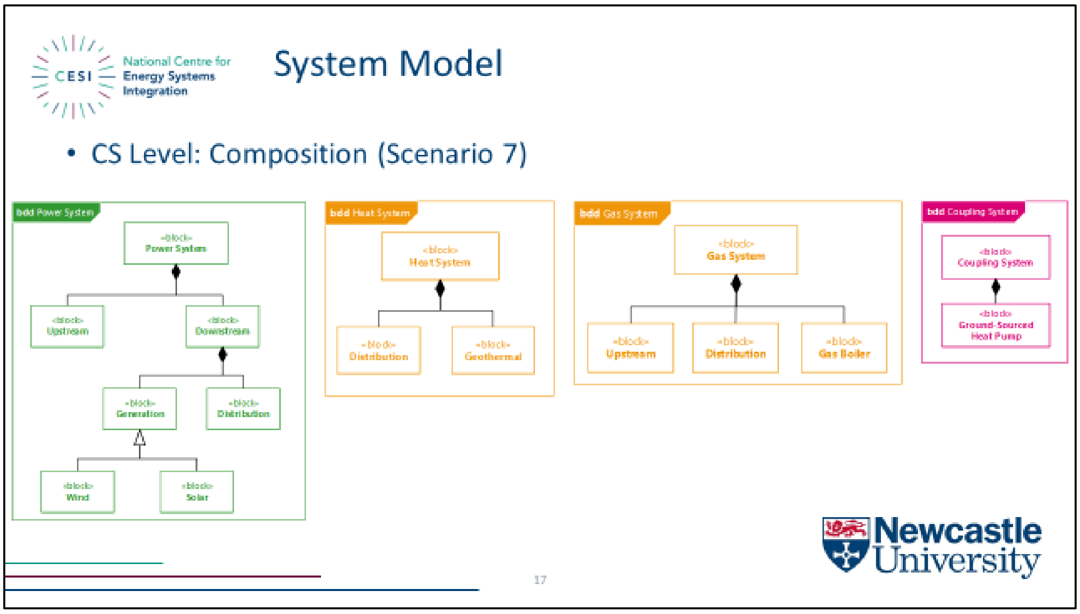
National Centre for Energy Systems Integration
CESI
System Model
CS Level: Composition (Scenario 7)
bdd Power System
bdd Heat System
bdd Gas System
bdd Coupling System
«block» Power System
«block» Upstream
«block» Downstream
«block» Generation
«block» Distribution
«block» Wind
«block» Solar
«block» Heat System
«block» Geothermal
«block» Gas System
«block» Gas Boiler
«block» Coupling System
«block» Ground-Sourced Heat Pump
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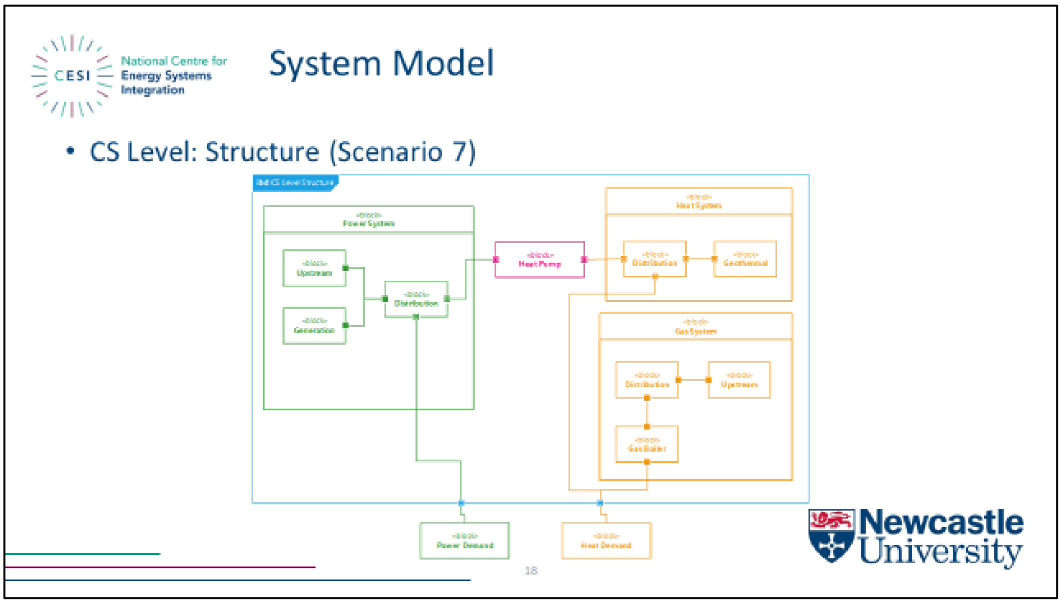

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CESI
System Model
• CS Level: Structure (Scenario 7)
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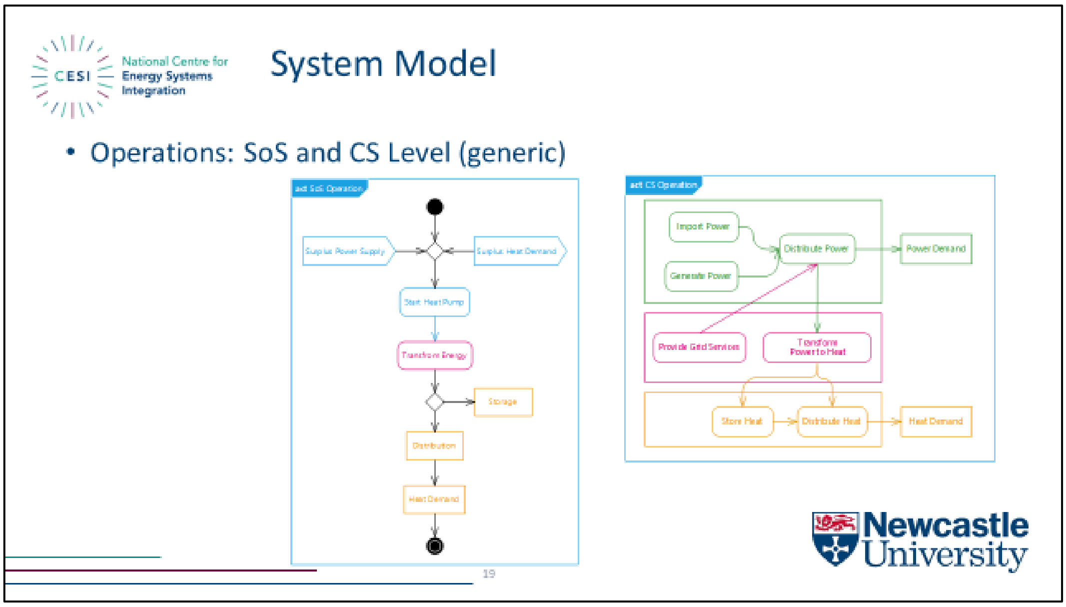

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CESI
System Model
• Operations: SoS and CS Level (generic)
act SoS Operation
Surplus Power Supply
Surplus Heat Demand
Start Heat Pump
Transform Energy
Storage
Distribution
Heat Demand
act CS Operation
Import Power
Generate Power
Distribute Power
Power Demand
Provide Grid Services
Transform Power to Heat
Store Heat
Distribute Heat
Heat Demand
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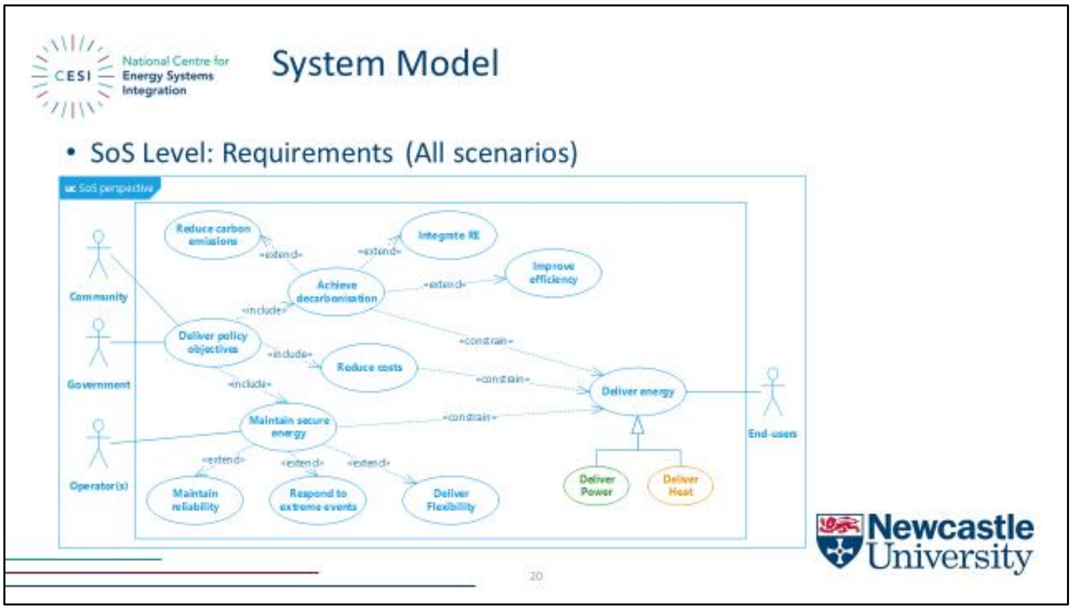

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CESI
System Model
• SoS Level: Requirements (All scenarios)
uc SoS perspective
Community
Government
Operator(s)
End-users
Reduce carbon emissions
Integrate RE
Improve efficiency
Achieve decarbonisation
Deliver policy objectives
Reduce costs
Deliver energy
Maintain secure energy
Maintain reliability
Respond to extreme events
Deliver Flexibility
Deliver Power
Deliver Heat
«extend»
«include»
«constrain»
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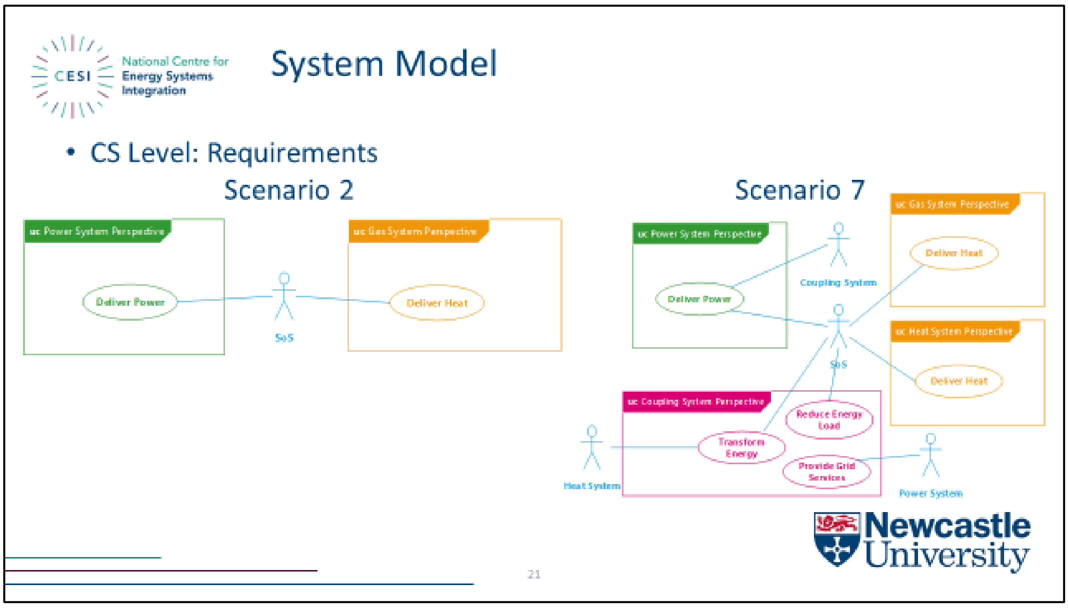
20


National Centre for Energy Systems Integration
CESI
System Model
• CS Level: Requirements
Scenario 2
Scenario 7
uc Power System Perspective
Deliver Power
SoS
uc Gas System Perspective
Deliver Heat
uc Power System Perspective
Deliver Power
Coupling System
uc Gas System Perspective
Deliver Heat
SoS
uc Heat System Perspective
Deliver Heat
uc Coupling System Perspective
Reduce Energy Load
Transform Energy
Provide Grid Services
Heat System
Power System
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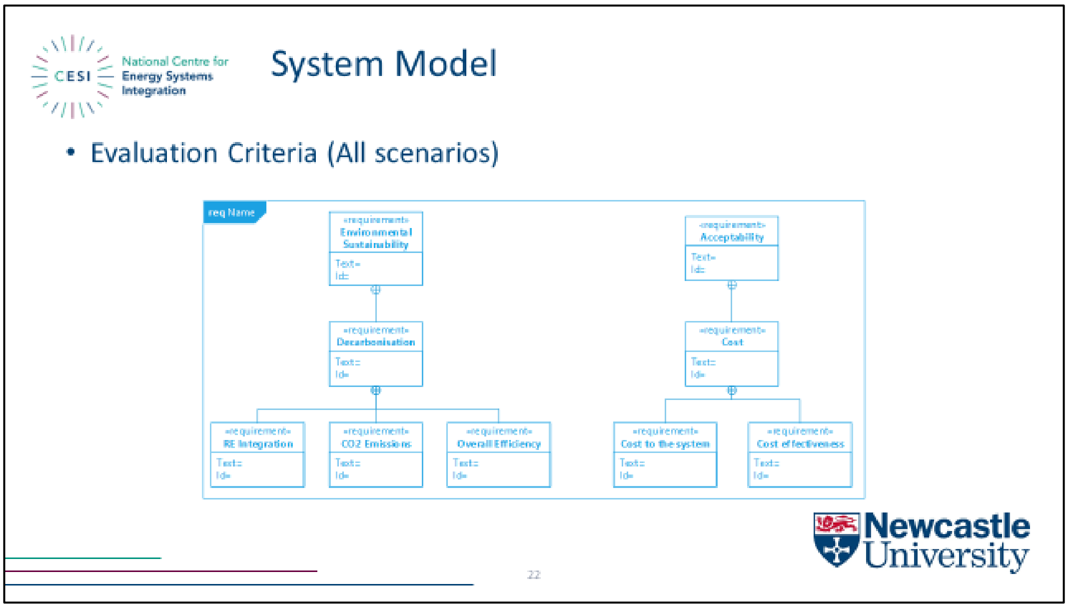
National Centre for Energy Systems Integration
CESI
System Model
• Evaluation Criteria (All scenarios)
req Name
«requirement» Environmental Sustainability
Text= Id=
«requirement» Decarbonisation
Text= Id=
«requirement» RE Integration
Text= Id=
«requirement» CO2 Emissions
Text= Id=
«requirement» Overall Efficiency
Text= Id=
«requirement» Acceptability
Text= Id=
«requirement» Cost
Text= Id=
«requirement» Cost to the system
Text= Id=
«requirement» Cost effectiveness
Text= Id=
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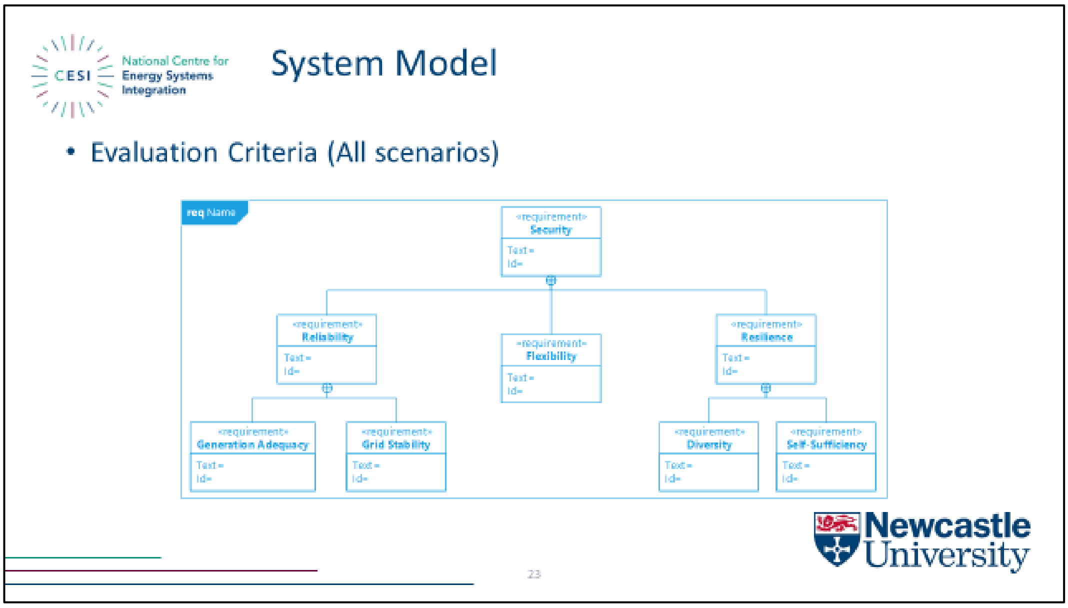
National Centre for Energy Systems Integration
CESI
System Model
• Evaluation Criteria (All scenarios)
req Name
«requirement» Security
Text = Id=
«requirement» Reliability
Text = Id=
«requirement» Flexibility
Text = Id=
«requirement» Resilience
Text = Id=
«requirement» Generation Adequacy
Text = Id=
«requirement» Grid Stability
Text = Id=
«requirement» Diversity
Text = Id=
«requirement» Self-Sufficiency
Text = Id=
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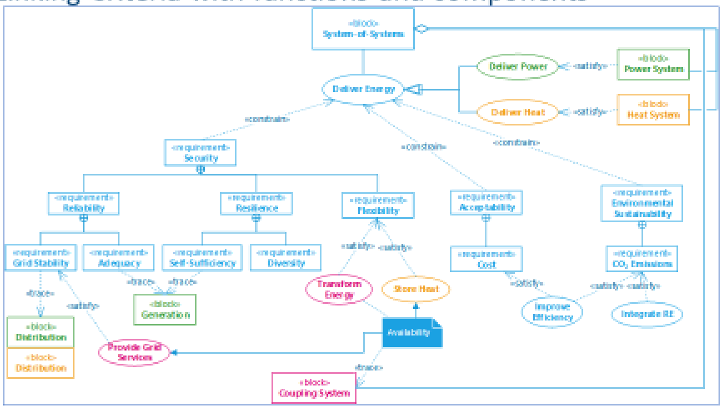
System Model

- Linking Criteria with functions and components



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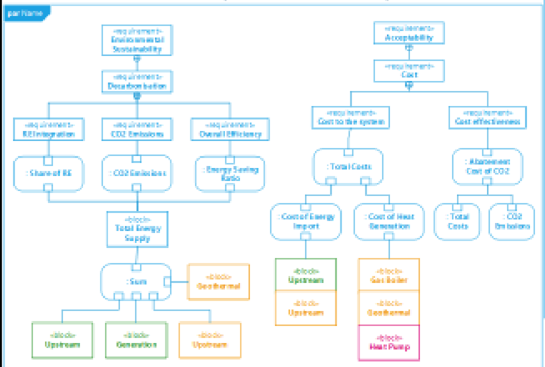
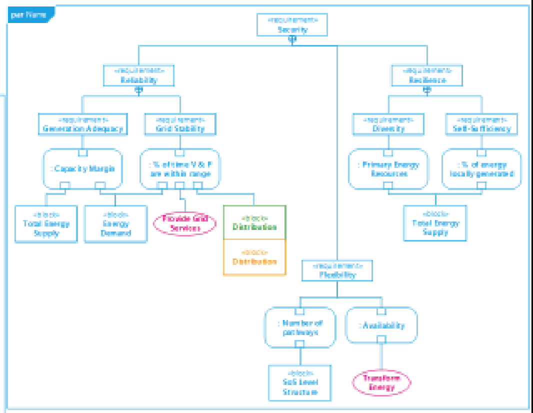
System Model

- Indicators (All scenarios)





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Framework Application

- Results for all scenarios

Scenario	Environmental Sustainability		
	Decarbonisation		Efficiency
	CO2 Emissions (tCO_2 eq)	RE Integration (% of RE from total gen)	Energy Saving Ratio
1	30.59	21.66	10.29
2	41.63	11.25	
3a	33.9	16.62	-12.83
3b	11.97	42.61	-51.13
4a	1.63	95.21	-4.05
4b	15.06	64.27	19.04
5	30.15	6.63	69.72
6	15.86	63.07	21.31
7	19.92	62.01	19.35

Scenario	Acceptability		
	Cost		Land
	Cost to the System (£)	Cost Effectiveness (£/tCO2 reduced)	Land use (m^2)
1	9,400.73	124.26	133.17
2	8,028.51		133.17
3a	7,453.66	-74.37	133.17
3b	6,864.04	-39.26	133.17
4a	14,563.99	163.36	294.37
4b	12,895.57	183.14	175.66
5	21,595.25	1,181.27	165.29
6	14,681.44	258.13	175.66
7	14,017.91	275.86	175.66

Scenario	Security					
	Reliability		Resilience		Flexibility	
	Generation Adequacy	Grid Stability	Diversity	Self-Sufficiency	Pathways	Availability

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Session 2: Discussion

- Why do you think the framework procedure is, or is not, robust and consistent?
- How much does the framework output (the system model) achieve the intended purpose of addressing the evaluation principles?
- What could be the most useful way to visualise and interpret the results for informing decision making?

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Part 3: Reference System Architecture

- High-level architecture; Usefulness
  - rather than going through the process again and again
  - readily available to use as a reference for evaluation
  - generic to include all possible stakeholders and components to pick from
- Other potential uses, basis for:
  - design and validation of future integrated energy systems
  - define and enhance the roles of different actors involved
  - examine cyber-physical interfaces of the whole system, and issues related to interoperability, cyber-security and data sharing

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Session 3: Discussion

- What do you think of using the reference system architecture concept for evaluation?
  - Would it be more useful to have a readily available system architecture model than to go through the framework process to develop one?
- Can you think of other applications that a reference system architecture would be useful for?
- Closing Question: Overall, what do you think are the strengths and weaknesses of the proposed framework?

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Appendix E: North of Tyne Integrated Networks Model

This appendix presents the mathematical formulation and algorithms included in the integrated networks simulation model used for the North of Tyne case study in addition to the network map in the region.

E.1. Model Algorithms

Figure E.1 shows the model inputs, outputs and underlying equations used for the optimal gas and power flow analysis in MATLAB.

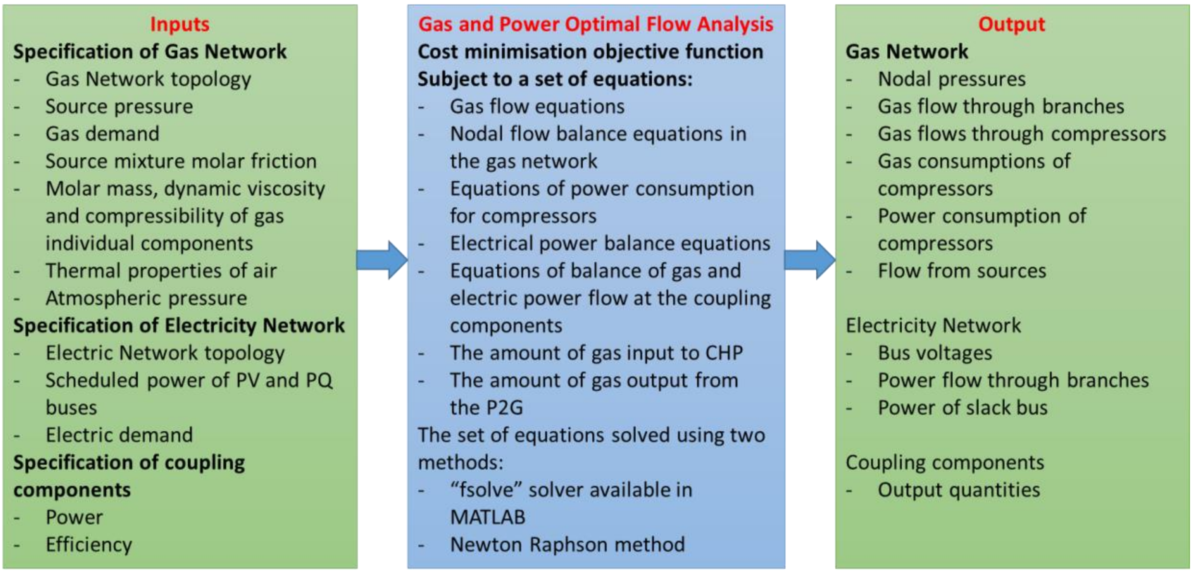

Figure E.1 Overall schematic of the North of Tyne model implementation algorithm

Two methods are used to solve the gas and power flow in these integrated networks. The first one is to use the "fsolve" solver of MATLAB to solve the set of nonlinear equations and find the values of the unknown variables. Once the values of nodal pressures and the values of bus voltages are obtained the values of the flows of the gas pipelines and the power flow through electricity branches are calculated using the gas and power flow equations. The second method of calculation is a general approach executing a single gas and power flow analysis in a unified framework based on the Newton–Raphson formulation. The set of equations are solved by forming a Jacobian matrix in the iterations.

E.2. Mathematical Formulation

The mathematical formulation of the gas and electricity optimal power flow analysis can be expressed as

$$Min\ (Cost\ of\ non\ gas\ electric\ genertation$$
$$+ Cost\ of\ gas\ electric\ generators\ supplied\ from\ another\ gas\ network \quad (1)$$
$$+ Cost\ of\ gas\ supply\ )$$

Subject to:

$$h(x) = 0 \quad (2)$$

$$g(x) \leq 0 \quad (3)$$

where x is the state vector which includes the angle and amplitude of the voltage of all the electrical network buses, the active and reactive power of the all the generators including the renewable resources and CHP, the power set-points of the considered P2G assets, the pressure of the different nodes in the gas networks, and the amount of the gas imported from upstream networks, $h(x)$ and $g(x)$ are the equality and inequality constraints, respectively.

The equality constraints are given by the following equations.

The gas flow equation:

$$q = S_{ij} M_k \sqrt{S_{ij}\left(p_i^2 - p_j^2\right)} \quad (4)$$

$$M_k = \eta_{pk} \frac{18.062\ T_n D^{8/3}}{P_n \sqrt{S_g L T Z_g}} \quad (5)$$

where:

S_{ij} Flow direction, where $S_{ij} = 1$ if $P_i > P_j$, and $S_{ij} = -1$ if $P_i < P_j$,

q Gas flow in Standard Temperature and Pressure (STP) conditions,

M_i Molar mass of the component i in the gas mixture

T_n Standard temperature

P_n Standard pressure

D Pipe diameter

S_g Gas gravity

T Average gas temperature

z_g Average gas compressibility factor

η_{pk} Pipeline efficiency

p_i Absolute gas pressure at the sending end of the pipe

p_j Absolute gas pressure at the receiving end of the pipe

L Pipeline length

The mass flow balance equation at each node can be written in matrix form as

$$Aq_p + Uq_C + W - T\tau = 0 \quad (6)$$

where:

q_p Vector of flow rate through pipelines,

q_c Vector of flow rate through compressor,

A Branch-nodal incidence matrix,

W vector of gas supply and demand at each node,

T Matrix represents where gas is withdrawn to power the gas turbine of the compressor,

τ Gas supplied to the gas turbine of the compressor,

U Matrix describes the connection of compressors and nodes.

In addition to the matrix A, which represents the interconnection of pipelines and nodes, we define the matrix U, which describes the connection of compressors and nodes. In this matrix, the item U_{ik} is +1, if the *k*th compressor has its outlet at node i, and -1*;* if the *k*th compressor has its inlet at node i, 0 otherwise. The vector of gas injections W is obtained by

$$W = W_S - W_L \quad (7)$$

where:

W_S A vector of gas supplies at each node;

W_L A vector of gas demands at each node.

The matrix T and the vector τ represent where gas is withdrawn to power a gas turbine to operate the compressor. In the matrix T, the item T_{ik} is +1; if the kth compressor's turbine gets gas from node i, and 0 otherwise. Analytically, the gas supplied to the gas turbine of the compressor k can be approximated as

$$\tau = \alpha_k + \beta_k BHP_k + \gamma_k^2 BHP_k^2 \tag{8}$$

where $\alpha_k, \beta_k, \gamma_k$ are compressors gas consumption coefficients.

An AC power flow model is used to represent the electricity network. The steady state operation of a power system is formulated by stipulating that, at each system's bus, the power injected by generators, the power demanded by loads, and powers exchanged through the transmission elements connected to the bus must add up to zero. This applies to both active and reactive powers. Consequently, the real and reactive power injections at bus i need to satisfy the following equations:

$$P_{G_i} - P_{L_i} - P_i(V, \theta) = 0 \tag{9}$$

$$Q_{G_i} - Q_{L_i} - Q_i(V, \theta) = 0 \tag{10}$$

where:

P_{G_i}	real power generation at bus i,
P_{L_i}	real power load at bus i,
Q_{G_i}	reactive power generation at bus i
Q_{L_i}	reactive power load at bus i,
P_i	real power injection at bus i,
Q_i	reactive power injection at bus i,
V	Bus voltage magnitude vector,
θ	Bus voltage angle vector.

The relationship between the natural gas and electricity networks is provided by Power-to-Gas and the gas-fired turbines' generators i.e. gas turbines or the CHP, which act as energy converters. This coupling is mathematically formulated by Equations (11) and (12).

$$q_{generator} = \frac{3600\ P_{generator}}{\eta_{generator} * 37.26} \tag{11}$$

$$q_{P2G} = \frac{P_{P2G} \times \eta_{P2G}}{11.57} \tag{12}$$

where:

$q_{generator}$ gas flow supplied to the gas-fired turbines' generator,

$P_{generator}$ generated real power,

$\eta_{generator}$ Generator efficiency,

q_{P2G} Gas flow produced by the P2G unit,

P_{P2G} Real power supplied to the P2G unit,

η_{P2G} efficiency of P2G unit,

The impact of the coupling components will be considered into Equation (6), (7) and (9), where these components affect the items (W_s), (W_L), (P_L) and (P_G).

The integrated gas and power flow formulation of the natural gas and electricity infrastructures is obtained by combining the stated flow models considering the link between both infrastructures through gas-fired power plants connected to gas pipelines and power-to-gas units using electrical energy. Hence, the set of nonlinear equations that must be solved for the state variables of both infrastructures. The proposed solution approach consists of applying Newton-Raphson's method (or using the" fsolve" function in MATLAB) to provide an approximate solution to the total set of equality constraints. The Jacobian matrix used in Newton's solver is given by Equation (13):

$$J = \begin{bmatrix} \frac{\partial \Delta q}{\partial p} & \frac{\partial \Delta q}{\partial BHP} & \frac{\partial \Delta q}{\partial P_G} & 0 & 0 \\ \frac{\partial \Delta BHP}{\partial p} & \frac{\partial \Delta BHP}{\partial BHP} & 0 & 0 & 0 \\ 0 & 0 & \partial \Delta P_G / \partial P_G & 0 & 0 \\ 0 & \partial \Delta P / \partial BHP & \partial \Delta P / \partial P_G & \frac{\partial \Delta P}{\partial \theta} & \frac{\partial \Delta P}{\partial V} \\ 0 & 0 & 0 & \frac{\partial \Delta Q}{\partial \theta} & \frac{\partial \Delta Q}{\partial V} \end{bmatrix} \quad (13)$$

Note that the number of equation which is $NN - NS + NC + N_{coupling} + 2 * nbb$ equations, must equal to the number of unknown decision variables ($NN - NS + NC + N_{coupling} + 2 * nbb$), where:

NN : The number of the nodes of the gas networks,

NS: The number of gas sources,

NC: The number of compressors,

$N_{coupling}$: The number of coupling components, and

nbb : The number of buses in the electrical network.

This is a necessary condition to solve the integrated gas and power flow by using Newton-Raphson or other iterative methods.

In addition to these equations, the following equality equations are used to calculate the amount of gas input to CHP estimated in m^3, and the amount of gas output from the P2G also estimated in m^3.

- Amount of gas input to CHP coupling the gas node *k* and the electric bus *i*:

$$W_L(k) = \frac{P(i)*3600}{\zeta_{CHP}*GCV} \tag{14}$$

where:

$W_L(k)$	Amount of the gas input to the CHP connected to the gas node k
$P(i)$	Amount of the output power from the CHP connected to the bus i,
ζ_{CHP}	Efficiency of the CHP
GCV	Gas caloric value

- Amount of gas out from the P2G coupling the gas node *k* and the electric bus *i*:

$$W_S(k) = \frac{P(i)*3600}{GCV} \tag{15}$$

where:

$W_S(k)$	Amount of the gas output from the P2G connected to the gas node k
$P(i)$	Amount of the input power to the P2G connected to the bus i,
GCV	Gas caloric value

The inequality constraints $g(x)$ are:

$$V_{i\,min} \le V_i \le V_{i\,max}$$

$$I_{kmax}^2 \ge I_k * I_k^* \tag{16}$$

$$P_{Gi\,min} \le P_{Gi} \le P_{Gi\,max}$$

$$Q_{Gi\,min} \leq Q_{Gi} \leq Q_{Gi\,max}$$

$$1 \leq P_{p2g,k} \leq P_{\text{p2g,max},k}$$

$$p_{i\,min} \leq p_i \leq p_{i\,max}$$

$$Ws_{i\,min} \leq Ws_i \leq Ws_{i\,max}$$

where:

V_i	Voltage magnitude at bus i,
$V_{i\,min}, V_{i\,max}$	minimum and maximum voltage magnitude at bus i respectively,
I_k, I_{kmax}	current through branch k, and the maximum value of this current,
P_{Gi}, Q_{Gi}	Active and reactive power of the generator G_i,
$P_{Gi\,min}, P_{Gi\,max}$	Minimum and maximum active power generated by the generator G_i,
$Q_{Gi\,min}, Q_{Gi\,max}$	Minimum and maximum reactive power generated by the generator G_i,
$P_{p2g,k}, P_{\text{p2g,max},k}$	Power set-point of P2G k and the maximum value of this set-point respectively,
p_i	Pressure at node i,
$p_{i\,min}, p_{i\,max}$	Minimum and maximum pressure at node i,
Ws_i	Supplied flow from gas source i,
$Ws_{i\,min}, Ws_{i\,max}$	Minimum and maximum flow supplied from the source i, respectively.

The method used to solve the optimal power problem is based on the interior point algorithm.

E.3. Network Map

Figure E.2 shows the map of the electricity and gas networks nodes where the topology data is currently available. The colour code used in Figure E.2 is given as follows.

For the electricity network:

- Crimson indicates grid supply points
- Turquoise indicates bulk supply points
- Navy indicates primary substations

For the gas network:

- Grey indicates nodes and governors
- Yellow indicates the InTEGReL site

Note that the gas network extends beyond the map in Figure E.2, North to Saltwick in Northumberland and South to Bishop Auckland in County Durham. This area contains the site for the Integrated Transport Gas Electric Research Laboratory (InTEGReL) in Low Thornley, Gateshead. InTEGReL is planned to be the UK's first multi-vector integrated energy systems research and demonstration facility investigating utility scale infrastructure, with a joint operation between Northern Powergrid and Northern Gas Networks, the electricity and gas distribution componies, respectively. Figures E.3 depicts the integrated gas and electrical networks in the NoT CA area.

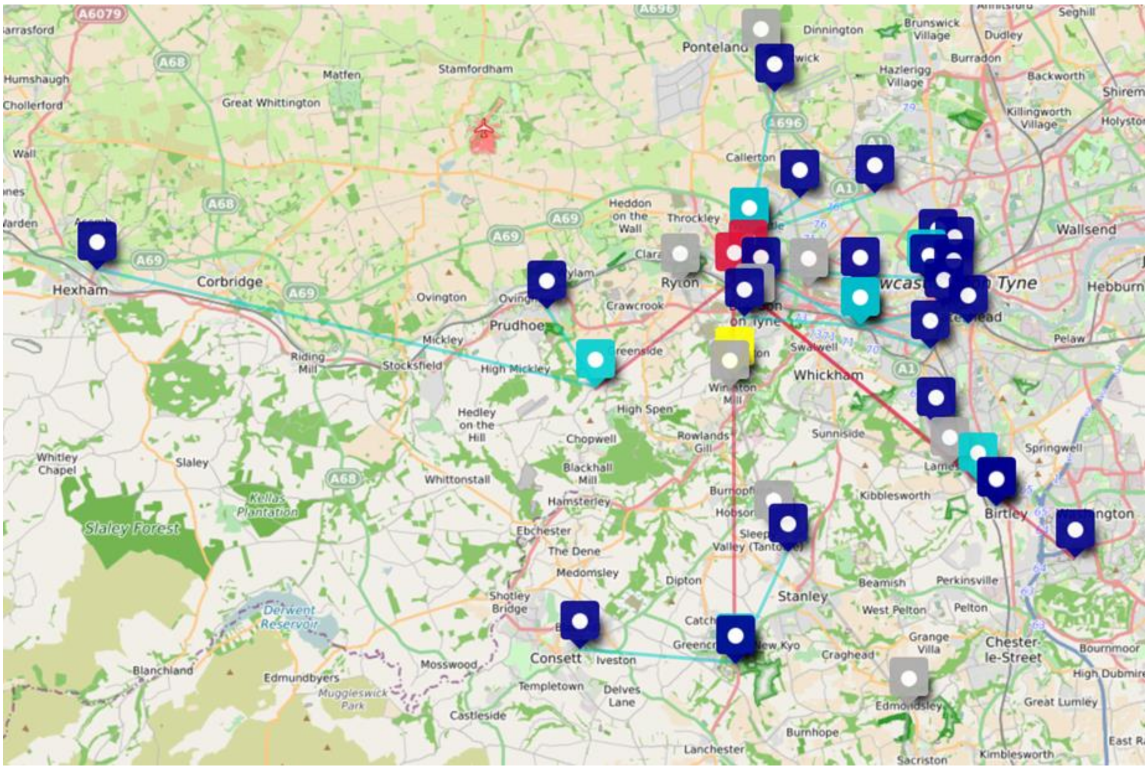

Figure E.2 Map of the electricity and gas network nodes

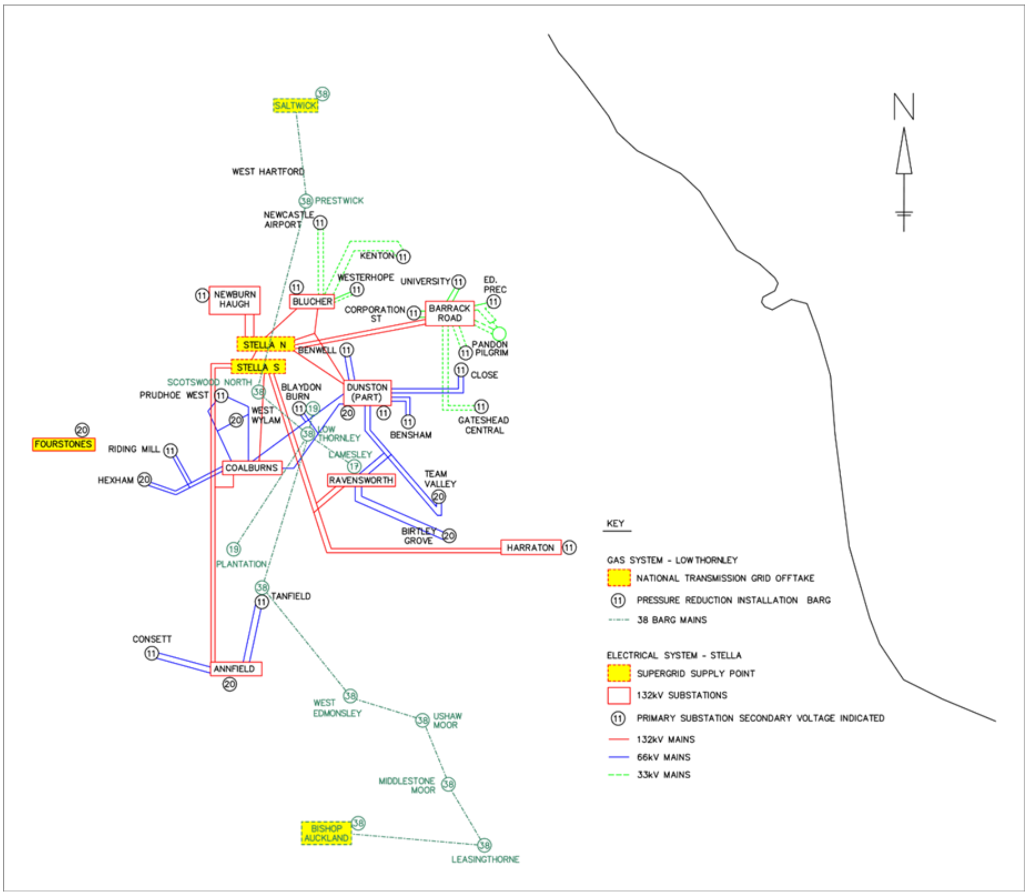

Figure E.3 Schematic of the Integrated electricity and gas network

Appendix F: North of Tyne Case Study Parameters

Table F.1 Energy load paramters

Scenario	**Final Energy Load (MWh)**			**Peak Energy Load (MW)**		
	Electric Load	Heat Load	Total Load	Electric Load	Heat Load	Total Load
1	7,039.81	26,284.82	33,324.63	358.43	1,305.01	1,622.94
2	8,156.79	23,130.64	31,287.43	431.44	1,148.41	1,547.42
3	7,039.81	26,284.82	33,324.63	358.43	1,305.01	1,622.94
4	8,156.79	23,130.64	31,287.43	431.44	1,148.41	1,547.42
5	7,039.81	26,284.82	33,324.63	358.43	1,305.01	1,622.94
6	8,156.79	23,130.64	31,287.43	431.44	1,148.41	1,547.42

Table F.2 Renewable energy generation parameters

Scenario	Wind Energy (MWh)			Solar Energy (MWh)		
	Energy used	Energy wasted	Total available energy	Energy used	Energy wasted	Total available energy
1	864.98	52.42	917.40	40.98	1.70	42.68
2	860.29	57.11	917.40	41.58	1.09	42.68
3	864.87	52.53	917.40	40.95	1.73	42.68
4	861.38	56.02	917.40	41.60	1.08	42.68
5	6,153.60	524.09	6,677.69	40.01	2.66	42.68
6	6,324.27	353.42	6,677.69	41.16	1.51	42.68

Table F.3 Coupling components parameters

Scenario	CHP				P2G				
	Electricity production (MWh)	Heat production (MWh)	Maximum capacity (MW)	Cost (£)	Input (MWh)	Output (MWh)	Losses (MWh)	Maximum capacity (MW)	Cost (£)
1	2,437.78	2,133.06	120	114,271	0	0	0	0	0
2	2,497.63	2,185.43	120	117,076	0	0	0	0	0
3	2,449.98	2,143.74	120	114,843	18.73	14.98	3.75	8	1,030
4	2,530.48	2,214.17	120	118,616	32.05	25.64	6.41	8	1,763
5	1,778.99	1,556.61	120	83,390	573.87	459.09	114.77	160	31,563
6	2,193.94	1,919.69	120	102,841	624.21	499.37	124.84	160	34,331

Scenario	HPs		
	Energy Consumption (MWh)	Capacity (MW)	Cost (£)
1	0	0	0
2	1,116.98	73.00	40,211
3	0	0	0
4	1,116.98	73.00	40,211
5	0	0	0
6	1,116.98	73.00	40,211

Table F.4 Upstream energy parameters

Scenario	Energy imported (MWh)			CO_2 Emissions ($kgCO_2eq$)		
	Electricity Network	Gas Network	Total	Electricity Network	Gas Network	Total
1	3,879.92	30,240.58	34,120.50	986,521	7,068,280	8,054,801
2	4,937.58	27,182.79	32,120.37	1,263,848	6,365,953	7,629,801
3	3,886.22	30,244.31	34,130.53	987,741	7,069,558	8,057,299
4	4,931.52	27,210.69	32,142.21	1,265,713	6,369,416	7,635,129
5	335.04	28,748.74	29,083.77	68,968	6,688,174	6,757,142
6	910.86	26,143.53	27,054.39	198,650	6,105,927	6,304,577

Scenario	Cost (£)		
	Electricity Network	Gas Network	Total
1	107,858	284,866	392,724
2	137,666	256,062	393,728
3	108,032	284,901	392,933
4	137,376	256,325	393,701
5	8,958	270,813	279,771
6	24,836	246,272	271,108

Table F.5 Normalised indicator values

Scenario	CO_2 Emissions	RES Integration	Efficiency	Total Cost	Self-Sufficiency	Flexible Capacity
1	0.30	–0.32	0.37	0.08	−0.32	–0.39
2	0.33	–0.31	0.19	0.36	–0.23	–0.06
3	0.30	–0.32	0.36	0.09	–0.31	–0.36
4	0.33	–0.31	0.16	0.38	–0.22	–0.03
5	–0.59	0.58	–0.45	–0.62	0.38	0.25
6	–0.67	0.68	–0.63	–0.29	0.68	0.61