Bond graph modelling of exergy in integrated energy systems

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Abstract

Integrated municipal or district energy systems are one facet of the effort to support sustainable energy systems that work towards reducing anthropogenic climate change emissions. Current energy systems — including electricity, heat, and cooling — operate mostly independently, under the control of domain-distinct industries and regulatory bodies. Operating these separate systems in a cooperative or integrated manner promises improvements in efficiency, the ability of networks to absorb renewable energy sources and storage, emissions reductions and community-based benefits.

The nature of district energy systems is that they cannot easily be modified or built upon without severe disruption to the communities they serve, so assessments of their behaviour and performance caused by potential changes must be modelled. This thesis investigates what methods can model integrated energy systems and develops a bond graph-based approach to constructing a fully-integrated system model. Although energy based methods for integrated energy system modelling exist, this thesis demonstrates that exergy can form the basis of integrated energy system models. Exergy being a measure of the usefulness of energy allows the equivalence of energy domains in a single model form, permitting development of a genuine, physically-founded integrated energy system model.

An integrated model of a residential district supplied by heat and electrical networks, based on a real UK urban area, is demonstrated in OpenModelica using the developed modelling approach. The concept of an exergy storage device is introduced to provide a mechanism for mediating energy flows between the networks. The model is used to evaluate the performance of the test network, using trial cases to investigate how transferring exergy between energy domains through the mediating storage affects the overall system energy and exergy efficiencies. Operational regimes that transfer energy from the electrical to the thermal sub-system using the mediating storage are found to improve the exergy efficiency of the system.

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Finally, to Keith and Geof — I got there in the end!

Contents

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Acronyms

AC alternating current. 103, 106

aCAES adiabatic compressed air energy storage. 20

ADE Association for Decentralised Energy. 12, 67, 68

BCT Byker Community Trust. 54, 57–59

CAES compressed air energy storage. 18–20, 24

CERT Carbon Emissions Reduction Target. 59

CESI National Centre for Energy Systems Integration. 6, 8, 63, 64

CESP Community Energy Savings Programme. 57–59

CHP Contract Heat and Power. 55

CHP combined heat and power. ix–xi, 3, 12, 13, 22, 54, 57, 59, 68, 69, 72, 88–93, 95–98, 149, 165, 179, 200–202, 204, 206, 208, 209

CIBSE Chartered Institute of Building Services Engineers. 67, 68

CPVT concentrated photo-voltaic / thermal. 22

CSB coefficient of structural bonds. 43

CTES cold thermal energy storage. 17, 18, 24

DC direct current. 99, 103, 106, 144

DECC Department of Energy and Climate Change. 69, 97

DEFRA Department for Environment, Food & Rural Affairs. 1

DH district heating. 13, 58, 64

DNO distribution network operator. 160

DOE Department of Energy. 18, 19

DPs design parameters. 45

DUoS Distribution Use of System. 62

ECO Energy Company Obligation. 59

EPRI Electric Power Research Institute. 18

EPSRC Engineering and Physical Sciences Research Council. 6

ERDF European Regional Development Fund. 59

ESL Energy Supplies Limited. 56

FMI functional mock-up interface. 40, 159

FMU functional mock-up unit. 159, 168

FRs functional requirements. 45

GPE gravitational potential energy. 18

HITL hardware-in-the-loop. 42

ICT information and communications technology. 60

IEA International Energy Agency. 18

IED Industrial Emissions Directive. 1

IMechE Institution of Mechanical Engineers. 2, 12, 14, 17, 18, 35

IPC Integrated Pollution Control. 55

KCL Kirchoff's Current Law. 99, 100, 102, 104, 110, 111

KVL Kirchoff's Voltage Law. 99, 100, 104

LCOS levelised cost of storage. 19, 81

LCPD Large Combustion Plant Directive. 1

LCTP Low Carbon Transition Plan. 1, 6

LPG low pressure gas. 64

LTES latent thermal energy storage. 17

MIT Massachusetts Institute of Technology. 50

MNA modified nodal analysis. 99–103, 106, 110, 111, 131

NA Nodal Analysis. 101

NEA National Energy Action. 68

NIFES National Industrial Fuel Efficiency Service. 55

OE Office of Electricity. 18

ORC organic Rankine cycle. 25

ORIGIN Orchestration of Renewable Integrated Generation in Neighbourhoods. 64

PCM phase change material. 24, 25

PHES pumped heat energy storage. 18, 20, 81, 84, 85

PHS pumped hydroelectric storage. 20

PI-ES Physics-Integrated Energy System. 8

PV photo-voltaic. 24, 74

PV/T photo-voltaic / thermal. 22, 74

RDF Refuse-derived Fuel. 56, 57

RHI Renewable Heat Incentive. 58, 59, 70

RMSE root mean squared error. 115

RPG resorption power generation. 83–85

RSM Response Surface Methodology. 114

SLES smart local energy system. 46, 77, 183

STES sensible thermal energy storage. 17

SysML Systems Modelling Language. 44, 53, 76, 78

TES thermal energy store. 21–23

TSB Technology Strategy Board. 5, 6

UML Unified Modelling Language. 44

UPS uninterruptible power supply. 19

VRF vanadium redox flow. 20

Chapter 1. Introduction

1.1 Context

1.1.1 Climate change and energy use

Concerns about climate change caused by carbon dioxide emissions from fossil fuels, security of fuel and energy supplies and energy cost volatility has resulted in a series of worldwide political initiatives aimed at addressing these environmental and societal problems [1,2]. The UK government's response was the development of its Low Carbon Transition Plan (LCTP), which it published in 2009 [3]. Underpinned by a series of national and European Union laws which compel the government to enact a programme of pollution reduction, the LCTP presents a new strategy for energy supply founded on a transition to a low-carbon economy. The UK Climate Change Act 2008 established a commitment to "reducing [carbon] emissions by at least 80% in 2050 from 1990 levels." [4], while the EC Renewables Directive 2009/28/EC established a mandatory target of 20% of all EC consumed energy to be produced by renewable sources by 2020 [5]. The UK's commitment under this legislation has been set at 15% of national gross final consumption, and the LCTP sets out a strategy for achieving this.

While the management of CO_2 emissions is directly addressed by these pieces of legislation, the Industrial Emissions Directive (IED) 2010/75/EU (superseding the Large Combustion Plant Directive (LCPD) 2001/80/EC on 1st January 2016) further controls atmospheric pollution by sulphur dioxide (SO_2), nitrogen oxides (NO_x) and particulates from industrial combustion processes [6]. Combustion pollutant control is creating pressure on older power stations — particularly oil and coal-fired ones — to have technology installed which limits atmospheric pollutants. Operators unwilling or unable to take the appropriate measures have the choice to opt out of the legislation under a limited life derogation which imposes a maximum number of running hours and a requirement to close non-compliant plant by 2023. A 2014 report by the Department for Environment, Food & Rural Affairs (DEFRA) [7] lists 41 plants of all types which are expected to close under the derogation. The Energy Act 2013 furthermore introduced carbon floor price support, which sets a rising price for carbon, and an Emissions Performance Standard, which sets a CO_2 production limit for new generation plant, both of which are designed and likely to accelerate the further closure of older plant [8].

1.1.2 Centralised vs decentralised energy production

It is apparent that the strict control of atmospheric pollution and carbon dioxide emission is starting to change the way in which all forms of energy are produced in the UK. At the same time that existing fossil fuel power plant stock is being depleted it is increasingly being replaced with renewable energy supplies particularly in the form of on- and off-shore wind farms, solar-produced energy at various scales, and biomass combustion. Most of these renewable energy sources are individually much smaller than traditional fossil-fuel power plants and are embedded in a distributed fashion within current energy networks. Although the majority of fossil fuel power plant is used to generate electricity, and residential and business heating is still dominated by natural gas, the redistribution of energy production from a centralised to distributed configuration creates an opportunity for a more integrated approach to energy management.

Renewable energy supply by nature is more geographically distributed than the large plant that it replaces. A 2009 report published by the Institution of Mechanical Engineers (IMechE) [9] argues that the creation of a managed distributed energy system will be a requirement for a functioning future energy network, and that a distributed energy system will necessarily be composed of a series of local energy systems. This report further defines a distributed energy system as "a collection of energy sources, energy storage and distribution networks linked to local demand" and a local energy system as an individual element of this collection. A local energy system will be "independent but would be interconnected to a distribution network to either receive energy to meet peak demand or to sell or donate energy during periods of low demand." A further IMechE report in 2015 re-iterated the need to consider heat, and not just electricity, in future energy systems, arguing that the UK government should "Tackle the provision of larger pieces of national heat infrastructure, as well as the interconnection and integration of heat systems with other energy networks." [10]. In 2014 the IMechE additionally produced a report which highlighted storage as "the missing link in the UK's energy commitments" [11]. These three works highlight the interconnected and interdependent nature of energy systems, and the need to consider joined, local solutions.

While large scale grid interconnectedness remains desirable for reasons of stability, security and economies of scale, there is a counter-argument which posits a strong incentive to produce, retain and use energy locally where possible. Close integration of local supply and demand has the potential to reduce fuel and energy transportation costs and losses, and create opportunities for economic waste energy re-use. For example low-temperature heat, which is otherwise not economically transportable over long distances, is a more viable source of energy in a local energy system.

1.2 Aim and purpose of the work

1.2.1 Motivation

Given the likelihood that future energy systems will consist of interlinked local energy networks containing mixed renewable, waste-reclaimed and fossil-fuel supplies, a range of energy demands, and some form of energy storage, some method of simulating and analysing such networks will be required. This thesis explores the underlying properties and factors that are important in modelling such mixed integrated energy networks and investigates potential methods of describing them in a unified and consistent way. Of particular importance to any such method is that the modelling strategy can routinely incorporate components from any energy domain (e.g. heat, electricity, or cold), and is able to ensure that during energy conversions between domains that the inherent quality, or potential usefulness, of the converted energy is preserved. This idea of potential usefulness of energy is important when comparing energy held in different forms. *Exergy*, commonly defined as "the useful work potential of a given amount of energy at some specified state" [12], is such a measure of the potential usefulness of energy. Exergy can be defined for any form of source energy (thermal, electrical, gravitational, kinetic, chemical, or radiative) and is a combination property of a system defined relative to a reference environment. In this thesis, exergy is regarded as a fundamental requirement for expressing the make-up of multi-domain energy systems, and the topic will be introduced and described more formally in Chapter 2.

The overall aim of a suitable multi-domain energy modelling method will be to provide a general scheme or framework for modelling and simulating any multi-vector integrated network. A suitable method would allow the incorporation of network control schemes and enable the creation of metrics on the network describing its fitness for purpose. The regulation of flow between the energy vectors is a particular source of opportunity in integrated systems; one way in which this is achievable is through multi-vector storage, which allows energy created in one domain to be stored and converted to another. How multi-vector storage should be considered and modelled as a mediating entity in integrated networks is a major motivating theme of the thesis and is explored in detail. It is important to the development of the strategy that fundamental design elements of integrated networks are examined, and that some elements of networks containing mixed thermal and electrical components are developed.

At this point an illustration of what a generic small-scale energy system might look like would be useful. Such a system has been presented by Dőry and Gróf [13], and is reproduced here as Figure 1.1. This is a representation of an integrated energy system which supplies heating and electricity to consumers at a district level; a cooling network might also additionally be added. Missing from this diagram is a connection between the electrical and thermal parts of the model, other than during energy production at the biogas combined heat and power (CHP) plant. For instance, an absorption chiller could be run from the thermal store to supply cooling and electricity, stored electrical energy could be used to drive a heat pump, or heat from the electrical energy storage inverters might be stored for later use. The creation of a scheme which permits the modelling of these kinds of physical interactions is a goal of this thesis.

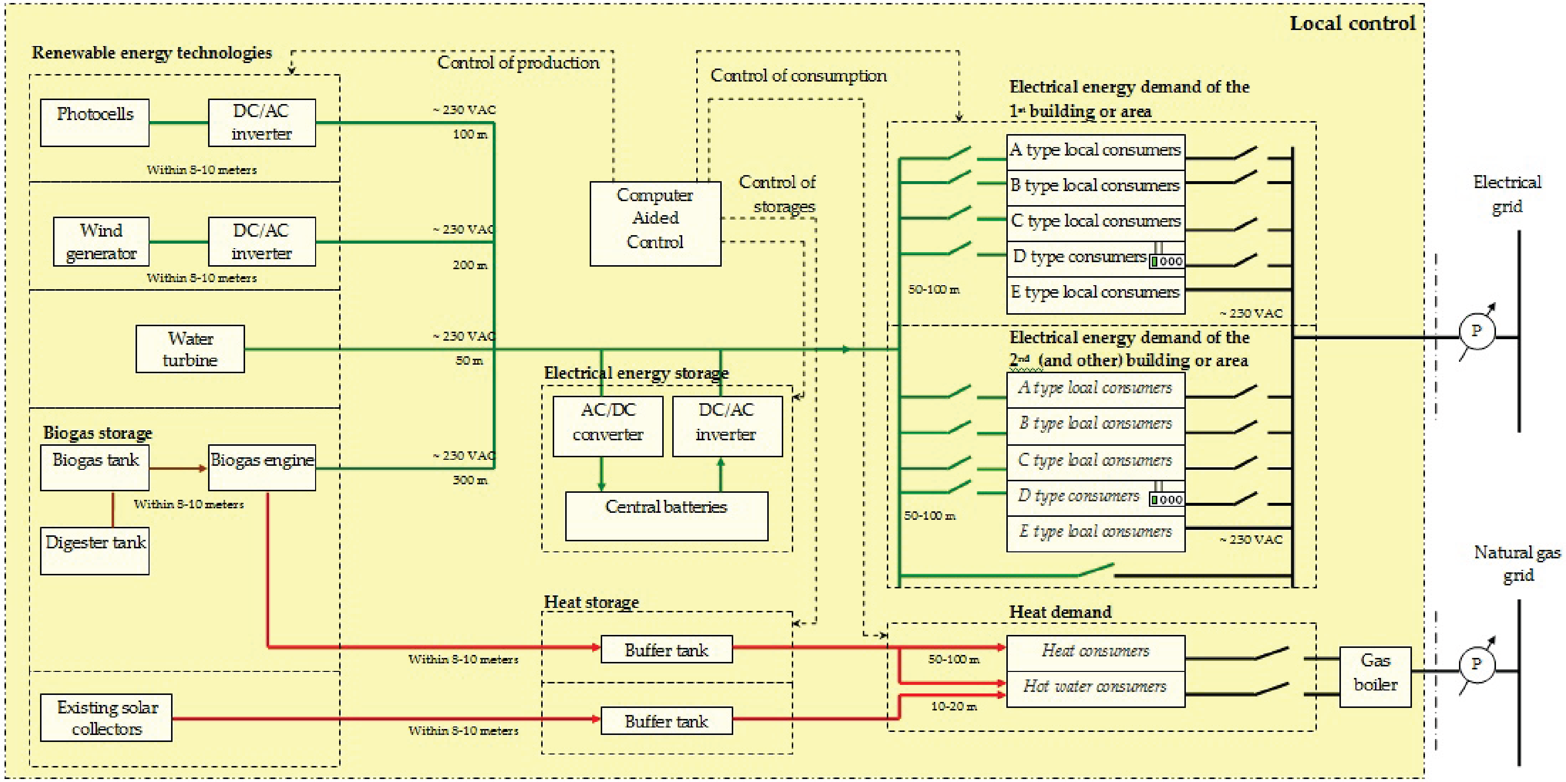


Figure 1.1: Schematic diagram of a local energy system (reproduced from [13])

1.2.2 Relevance and impact

A number of authors have approached the subject of modelling whole energy systems with the purpose of understanding operational limits and parameters.

Weitemeyer *et al.* [14] and Heide *et al.* [15] present a whole-systems energy approach to modelling the integration of grid level renewables with storage. These papers aim to estimate the degree of possible renewables integration as a function of storage, for the whole of the European electrical network. The analysis is limited to electricity production and storage (i.e. without heat or other energy domains), and, as the scope of the work is in estimating continental integration needs rather than local multi-domain networks, the authors work with idealised and simplified storage, transmission and distribution models, and normalised demand and generation. This is in contrast to the more physically-based, small-scale and multi-energy domain analysis that is pursued in this thesis.

Work on process integration methods using pinch analysis by McKenna [16] and Oh *et al.* [17] seeks to improve the efficiency of local energy systems by careful management of heat exchanger networks; these methods concentrate on heat demand and production and the use of waste heat from industrial processes. Methods using mixed integer linear programming to optimise energy networks are common, such as for example in a paper by Moreno *et al.* [18] who assess UK-wide electrical storage requirements. Local systems control methods are also addressed by some authors such as in [13] by Dőry and Gróf, who examine a fuzzy-logic technique.

The work presented in this thesis is different to these previous studies, which have not attempted to construct a unified energy domain modelling method bringing together heat, cooling and electrical demands through a mediating energy storage mechanism, and rationalising this through the use of a series of design principles. The proposed scheme allows the exploration of to what degree it is possible to treat different energy types as interchangeable with respect to storage, and how this interchangeability can be used to manage and control local energy systems. To illustrate the interchangeability of energy domains in a local energy system Figure 1.2 shows a schematic diagram of power flows through heat (red) and electrical (yellow) sub-networks. A variety of sources supply energy to the network, some of which is stored before ultimately being consumed. The dashed line highlights the area of the system where stored energy is either delivered directly to the end-user, converted directly to another form of storage, or converted during distribution.

A number of scientific initiatives in the UK are looking at integrated energy systems as a critical component of energy supply infrastructure for the future. In April 2015 the UK Government launched an Energy Systems Catapult through the UK's innovation agency Innovate UK (formerly the Technology Strategy Board (TSB)). The aim of the Catapult is to focus on "the challenges and opportunities for new technology-based products and services created by the transformation and improvement of energy networks – electricity, combustible gases and heat"; and to pursue the goal of "making the UK the leading place worldwide to develop and launch new solutions". Additionally, in June 2014 the

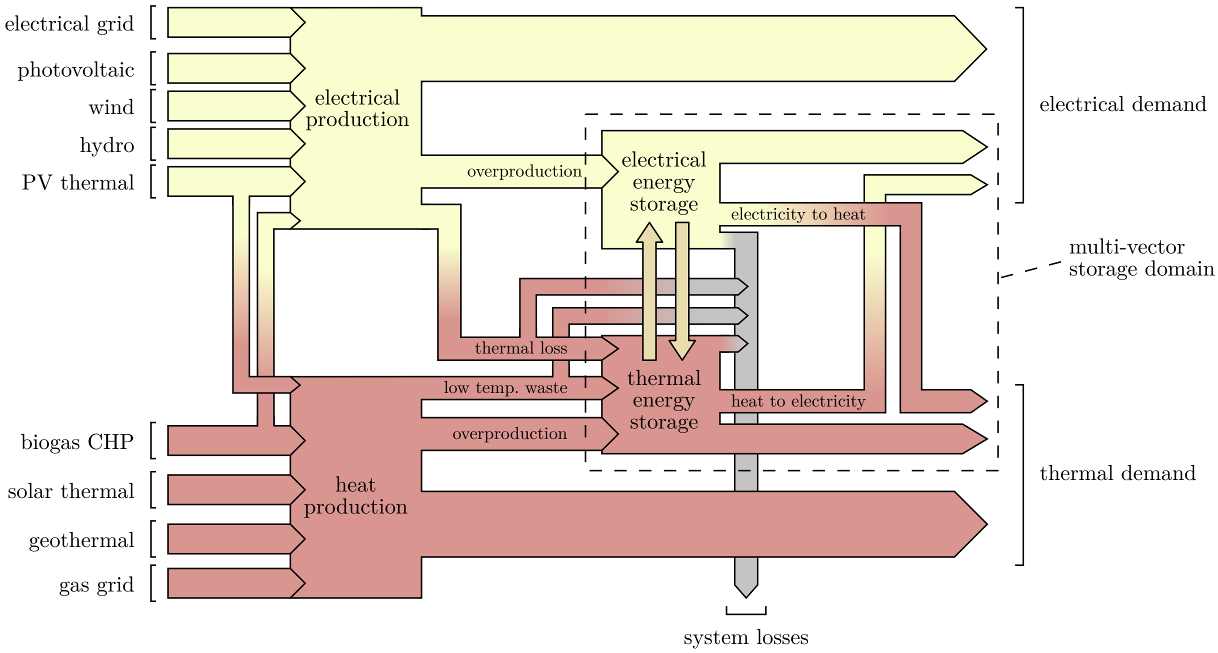


Figure 1.2: Electricity and heat energy flows for a generic local energy system

TSB announced the results of its competition "Localised energy systems - a cross-sector approach - collaborative R&D" which awarded £11.5m to projects from the EPSRC and Innovate UK. In 2016 the Engineering and Physical Sciences Research Councils (EPSRCs) National Centre for Energy Systems Integration (CESI) was launched as a £20m partnership between Newcastle, Heriot-Watt, Sussex, Edinburgh and Durham universities, with the remit of investigating flexible smart energy infrastructure, the role of consumers, and methods for meeting the UK's low-carbon targets. These schemes are aiming to improve academic understanding of integrated systems and produce commercial solutions enabling the goals of the LCTP to be met, and it is intended that the outcomes from this research will help to inform these projects.

1.3 Original contributions to knowledge

The work in this thesis describes a method for modelling and evaluating integrated energy systems in a way which has not been considered, to the best of the author's knowledge, in the existing literature. The method attempts to put the multiple energy domains - e.g. electricity, heat, cold, chemical and so on - that might be found in an integrated energy system, on an equal footing and allowing a true equivalence to be seen between the energy domains. Commonly, integrated energy systems are represented by separate domain-specific models, and the resulting disconnected nature of the overall system model can inhibit the understanding of the relative quality, or value, of the energy contained in each domain, and make it difficult to compare the quality of energy across the domains. The equivalencing of energy domains is achieved by evaluating the *exergy content* of each domain in the integrated system and to use this to compute conversions between domains. The advantage of this approach is that exergy can be used as the transactional quantity between domains, irrespective of the technology used to perform the transfer or any storage methods that might be used to temporarily hold energy that is being transferred. The use of exergy equivalencing in this way allows the idea of an abstract exergy storage device to be used to move energy around an integrated energy system, which focuses attention on how energy might be being degraded in the system during conversion processes. Often the main driver of energy conversion is financial and the use of exergy refocuses the analysis on to the underlying physical energy content and its intrinsic value as a finite resource.

In developing a method which uses exergy as the principal means of equating energy in a multi-domain integrated energy system, extensive use is made of *bond graphs* as a modelling method. Bond graphs are a generalisation of physical systems models and are able to represent all energy domains through a single unified notation. Thus, rather than using specialised schemes for electrical networks, hydraulic systems, thermal designs and so on, the integrated energy system can be represented uniformly using a single representation. This has the advantage that no single energy domain has primacy in the model, and side effects — such as thermal losses in electrical systems — are automatically included within the model, instead of being externalised. As defined in the literature, a "proper" bond graph model is thus entirely energy conserving; there is no concept of losses, as energy "lost" merely appears elsewhere in the model in the correct domain. Of course, engineering system modelling and simulation has a long and detailed history of computational techniques and bond graphs models do not necessarily improve simulation speeds or representation in individual domains. However, the bond graph method does permit a much more coherent and integrated model form to be developed for integrated energy systems, which has advantages for model consistency but particularly for the understanding of the energy flows and conversion processes in complex energy systems. The ability to maintain all energy domains within a single physically-concise model form, without resorting to analogies (such as is found in electrical circuit equivalents of heat networks) is extremely useful in communicating and understanding system energy flows and states. This method is not an approach that has, as far as the author is aware, been used before in the general energy systems modelling literature. Work by Lubega *et al.* [19] investigates the energy-water nexus using bond graphs, but this work does not attempt to use a unified bond graph-specific tool, does not consider exergy values of the different domains, and electrical network analysis is achieved using an external program.

The work in Chapter 3 on the applicability of axiomatic design foundations to energy system design has been applied to a demonstrator project. The Smarthubs Smart Local Energy System (SLES) project funded by UKRI[1] explored multi-vector approaches in the design and operation of SLESs. The axiomatic design approach investigated in this thesis was applied to the SLES project demonstrator network to develop a set of operating principles for the network as a "large flexible system". The results of this exercise were

[1] `https://gtr.ukri.org/projects?ref=104980`

published as Wardle *et al.*, “Axiomatic design of smart local energy systems”, at the 12th International Renewable Energy Conference (IREC) 2021 [20].

Work in this thesis on storage technologies and their categorisation and suitability contributed to a paper by Smallbone *et al.*, “Levelised cost of storage for pumped heat energy storage in comparison with other energy storage technologies” [21].

The conceptual development of the bond graph and network representations of integrated energy systems has been used in a modelling framework developed by the author within the CESI at Newcastle University, UK. This framework, called the Physics-Integrated Energy System (PI-ES), used a web interface to a simulator built around the principles of a unified energy domain network presented in this thesis. Sample models of the Findhorn Ecovillage (discussed in Chapter 4) and oil pipelines in Kuwait were developed to test the modelling method and developed software.

1.4 Thesis aims and objectives

This research aims to investigate to what extent energy storage can be used in an integrated energy system to mediate energy flows between the domains present in the system. To do this, answers to the following questions are pursued.

- How can integrated energy systems be studied? What kinds of experiments and models can be made in order that the effect of embedded storage systems can be investigated and evaluated?

- What are the current views from the literature, and from industry, on the potential for more localised and integrated energy systems? How do these align with decarbonisation goals?

- How can energy storage be represented? What kind of physical behaviours do storage units exhibit, and how can these be represented? What kind of storage is needed to mediate between energy flows across energy domains?

- What sorts of formal design and modelling principles can be introduced to the design of integrated energy systems? Are there any systematic ways of approaching the merging of traditionally different energy domains into a single system?

- How should the performance of integrated energy systems be measured? What kind of quantities are important?

- Can an example model of a storage-integrated energy system demonstrating the discoveries found in the previous questions be constructed? What are its properties, and what does it show?

The thesis addresses these objectives in seven major chapters. The first chapter — this one — has introduced the background and motivation to the project, and explained where its outcomes are likely to be useful. Chapter 2 presents the results of a literature review examining the way in which integrated energy systems are discussed and defined within the literature, and how energy storage is classified, what physical principles are involved, and how it is used in practice. The survey of the literature reveals how energy quality, or *exergy*, is a vital aspect of energy management in general, and so Chapter 2 continues with an exploration of the relationship between exergy, and energy storage and integrated energy systems. The fundamental principles of exergy analysis and its relationship to energy systems and storage are elaborated to highlight the factors that should be considered in the development of the schemes within the rest of the thesis. The conclusion of Chapter 2 suggests that a deeper investigative exercise with field practitioners ought to be conducted, the results of which are presented in Chapter 4.

Chapter 3 describes the overall research methodology used within the thesis. A discussion of system modelling as an activity in itself is presented, and thus how this relates to and is important for the investigation of integrated energy systems. This discussion leads into a more detailed overview of the model types that were identified in the literature and are being investigated by the thesis, along with the factors that are to be evaluated as important for integrated energy systems models.

Principles of design for integrated energy systems are the subject of Chapter 4. Three integrated energy system case studies, as well as the results of a series of interviews with active energy systems practitioners, are presented here. From these case studies and interviews the principles of Axiomatic Design are used to extract and categorise common or canonical elements of integrated energy systems. The resultant elements are combined into reference systems designs using the systems modelling language SysML. The reference elements describe the components and their interconnectivity that an eventual modelling tool should be able to represent effectively.

Chapter 5 is a detailed use and evaluation of the three major modelling approaches identified in Chapter 3. Each approach is used to model an element or elements of one of the case study systems presented in Chapter 4 to demonstrate how viable the approach is in the general case. Of particular importance is that the modelling approach is able to represent the canonical design elements from Chapter 4, and is able to incorporate energy streams of different vectors which can be inter-converted using a multi-vector storage device.

Chapter 6 describes the construction of a basic representation of a part of one of the case study networks to illustrate the preferred method from Chapter 5 of constructing integrated systems with exergy-considered multi-vector storage. The development environment is described along with how the system elements are built and how the simulation is carried out. The operation of the storage device and how this can be used to mediate between energy vectors is examined.

Chapter 7 concludes the thesis with a recap of the findings of the literature survey, the constitutive elements of multi-energy integrated networks, and how a formal design method can be used to construct archetypal components for integrated energy systems. The modelling method deemed to be the most appropriate is explored further with component examples and how these can be applied to models of the case-study networks. Finally, some further suggestions of how additional research could develop from the work within this thesis are proposed.

Chapter 2. Literature Review

2.1 Overview

Chapter 1 described the principal motivation for this thesis as one of seeking an understanding of how energy storage can be used effectively in district energy systems. The district energy systems of interest were defined to be ones in which multiple energy types, also termed energy vectors, are merged within the same system. Such integrated systems concepts are seen as being of fundamental importance to future energy system designs in order to assist in meeting climate change goals. Within this overall motivation it was clear that the work within this thesis would concentrate on frameworks that would allow such systems to be modelled and represented, and which could incorporate energy storage as a mediating device between energy vectors.

This chapter reviews and analyses energy systems and storage literature, with the above motivation in mind. The review covers three main themes.

Firstly, the nature of integrated energy networks is explored, with definitions of exactly what constitutes an energy network and what fits within its boundary (and what does not) are investigated. Exploration of the structure and use of energy networks reveals to what extent and in which situations energy storage is important. The subject of energy storage itself is the second theme, which includes what storage is, why it is important in the management of energy, the physical principles used to store energy, and the technological realisations of storage that exist today.

The subject of *exergy* then forms the final theme of the literature review. Exergy is a thermodynamic concept of the usefulness, or quality, of an energy source, irrespective of that energy source's origin as thermal, electrical, chemical, mechanical or otherwise. As will be described in Section 2.5, not all forms of apparently equal amounts of energy are capable of being put to work in equivalently-useful ways, with exergy serving as the metric of usefulness. The need to consider exergy in the management of energy in systems containing multiple energy domains becomes apparent during the review of integrated networks and energy storage literature, which is described in Section 2.4. The theme of exergy is split into two sections: first, a review of how exergy analysis is treated in the literature on energy systems and storage links the previous two sections covering networks and storage; then, a review of the thermodynamic theory of exergy explains how an exergy-centred analysis leads to approaches that place the value of energy uppermost in energy systems analysis.

2.2 Integrated energy systems

2.2.1 Definitions and context

The concepts of integrated energy systems and energy storage have been introduced previously, but further clarification and definition are needed. More detailed discussion on energy storage will take place later in the next section in this chapter. This section will deal with integrated energy systems and their definitions.

To begin with, some definitions of what a local integrated energy system is are needed. *Local*, *district*, *regional*, *urban* and *distributed* are all words found in the literature (e.g. Roskilly *et al.* [22], Magnusson and Djuric Ilic [23], Rezaie *et al.* [24], Keirstead and Shah [25], and the Institution of Mechanical Engineers (IMechE) [9]) to describe systems of energy provision (generation, supply and demand) having a limited geographical spread. This limited geographical spread is determined by defining a *system boundary*, within which lies the entirety of the system of interest. Although the concept of a boundary is a common one within engineering studies, defining the boundary of an energy system is something of a nebulous concept. The difficulty of adequately describing what a "limited geographical spread" might be for an energy system is examined by Keirstead and Shah in their exploration of thermodynamic models of urban energy system [25], in which they describe a series of geographical definitions of the boundaries of a system. All of these definitions are valid, but none are found to be definitive. Rather than being drawn into an irreconcilable definitional problem, Keirstead and Shah opt instead to bypass the geographical argument in favour of referring to energy systems in urban environments having an open thermodynamic boundary. This pragmatic and functional approach is used in this thesis. Lubega and Farid's observation [26] that sub-systems to be included within the boundary should not be subject to an external marketplace is also sensible.

In the UK, there are a number of district energy schemes (mostly combined heat and power (CHP), with some cooling) in existence or in proposal or development. The Association for Decentralised Energy (ADE) publishes a map of existing UK schemes [27], from which it can be seen that these are overwhelmingly city- or town-based, supplying large estates or isolated large settlements, universities or hospitals. Sheffield, Southampton and Nottingham all have mature (20+ years) heat networks supplying civic buildings and residential properties. Birmingham's new scheme (2007 onwards) supplies a number of city-centre buildings, and Leicester's scheme (with 14 km of pipework laid) supplies 3000 dwellings alongside more than 19 civic buildings [28]. London has published a city heat map and a "manual" [29] to support local authorities and developers in the creation of decentralised energy systems as the UK capital moves towards its goal of producing 25% of its energy from decentralised sources by 2025. In the North East of England, Gateshead began power generation from a new heat and power network in 2016, while Newcastle upon Tyne is in the planning and development phase of a system which will link existing schemes and supply key sites in the city centre [30, 31].

What is common to all of these schemes is the principle of a mixed customer base (private business, public sector, and residential) supplied by generation situated a relatively short distance from the demand. Such co-location of demand and generation coincides with what is normally a heating and cooling system design requirement, as heat is difficult to transport over significant distances. The demand is also located within what would commonly be denoted as a civic or town environment or isolated dwelling. In other words, heat, electricity and cooling are being produced at the point of demand. Some of the generation sites are quite close to or are in city centre locations, in former mill, warehouse and industrial sites. Therefore, in any analysis of appropriate storage solutions and technologies those suitable for deployment in these locations will be of most importance.

2.2.2 Thermal networks

Thermal networks are a particular type of district network as the product (heat, or cold) is difficult to transport over any distance. In the UK, heat networks have had a chequered past. In a series of papers, Russell [32], Hawkey *et al.* [33], and Hawkey and Webb [34,35] analysed the history of district heating, cooling and combined heat and power in the UK, exploring why during the 20th century district heating (DH) such systems failed to gain any real foothold in the UK. The authors suggest that resistance and apathy from the incumbent energy suppliers (gas and electricity networks) and the limited ability of regional government to implement district infrastructure schemes with wide scope and effect form the principal causes of the lack of significant investment in DH schemes in the UK. Other localised difficulties, such as a lack of trust (as embodied by the scandal involving contaminated fly ash at Newcastle upon Tyne's Byker DH site), the unreliability (perceived or real) of district schemes, and the lack of standards and price regulation, have also contributed to the perception of DH and by extension CHP as being undesirable.

In their 2014 analysis, Hawkey and Webb predict that the failures of the past are about to be repeated in the present government-backed drive for an expansion of district heat in light of climate concerns. In comparison with other countries, notably Germany and Denmark, Hawkey and Webb see local government constraints as being particularly problematic. However, it is apparent that new district schemes are nevertheless being constructed, in spite of this prediction. Two of these are in Newcastle upon Tyne and Gateshead, while a third existing scheme, also in Newcastle, is undergoing significant upgrade and renovation. Thus, a deeper investigation of the current environment surrounding district energy and co- and tri-generation schemes would be an important addition to a study of the literature. This investigation manifested as a series of informal interviews with relevant stakeholders, and is presented in Chapter 4 as part of the development of energy networks design principles alongside three detailed case study descriptions.

2.3 Energy storage

2.3.1 Overview

Energy storage is a term that covers any process in which energy is captured and held through a physical process until it is needed, when it is released for productive use. In his book *Energy Storage*, Jensen [36] provides a textbook general introduction to the subject; although dated, many of the topics, theoretical foundations and challenges described within this work are unchanged in the present day. Jensen introduces the subject of energy storage in very general terms: "Energy storage is, in one way or another, part of all the events both in nature and in man-made processes". Within the context of this thesis however the term 'energy storage' is used in a the more restricted sense of referring to storage as it relates to engineered energy systems supplying heat, electricity and cooling processes to sites of human activity or dwelling. Even within this limited scope of engineering systems, energy storage is a very broad topic indeed, and an exhaustive review of the subject is outside of the scope of this thesis. However, relatively recent comprehensive overviews of the field and the state of the art have been produced by Sabihuddin *et al.* [37], the IMechE [11], and Roskilly *et al.* [22], which explore the challenges and opportunities presented by energy storage technologies. The term "energy storage" itself in the engineering system context explicitly excludes primary fuels [36]. The energy density obtained within conventional or extractive fuels (nuclear and hydrocarbons) is created over geological time-scales, and the energy such fuels release cannot be easily re-accumulated over anthropocentric time spans. As an exception, Sabihuddin *et al.* [37]) do point out that although fuel cells consume produced storage fuels (for example, hydrogen or ammonia), the fuels used do not fit into the definition of an extractive fuel that accumulates over an extremely long time period. Primary fuels consumed by fuel cells — potentially produced locally by an electrolyser to create a storage system — are therefore correctly included within the category of engineering system energy storage.

Energy can be stored in a number of physical forms, i.e. electrochemical, chemical, electrical, mechanical (including kinetic and potential), thermal (including "hot" and "cold" forms) and magnetic, and converted to and from these forms. Real conversion processes involve a cost, the potential types and definitions of which are broad and which may include financial expenditure, energy lost during the conversion process, the production of pollutants, or the degradation of plant or storage vessels. A huge range of technologies are available with which to implement energy storage and conversion.

The management of energy systems in general is an exercise in matching supply to demand. Demand is dynamic and generally contains periodic (e.g. seasonal and diurnal) and transient components [37]. Energy supply systems must therefore normally contain a mix of supply elements that can operate at different time-scales in order to satisfy these diverse components of demand. Across the range of generation technologies, speed of response and overall power delivery capacity vary greatly, and it is not usual for a single device to be able to respond to all demands. The variable aspect of demand therefore introduces cost and complexity into an energy supply system; additional control systems, multiplicity of plant, installed overcapacity, and curtailment of generation are the result. The introduction of energy storage ("buffers") into a system between the supply and demand decouples the two somewhat and would, it is hoped, reduce the complexity of energy supply design; the storage copes with the demand fluctuations. With larger systems, aggregated demand tends to smooth somewhat and become more predictable, but in smaller or local systems the effect of individual demands is more pronounced, and it is in such systems that energy storage would be expected to have a greater effect. Indeed, the usefulness of energy storage in a local energy system in managing energy flow might be an argument in favour of storage, but an argument against local energy systems themselves. This debate will not be pursued further here and it will be assumed that there is a genuine need to develop and manage energy supply at a local level.

Notwithstanding these issues of scale and extent of an energy system, the introduction of renewable energy sources into a system brings specific challenges to the management of energy supply. It is argued by some authors [22, 36] that energy storage is an important component of systems containing renewable energy sources as it allows the incorporation of "wrong-time" energy flows [11]. Wrong-time energy flows — energy supply occurring when there is no demand, and vice versa — are not merely a system design issue; they are fundamentally characteristic of renewable energy resources. As well as wrong-time flows it is also possible to have "wrong-type" energy. This occurs in co-generation or tri-generation processes (for example, simultaneous generation of heat and electricity, or heat, cooling and electricity, respectively) where the demand energy vector mix does not often match the planned generation energy vector mix. Co- and tri-generation plant's advantage over single energy type production is that it increases the overall thermal efficiency of the plant; however, the produced energy flows must still have an end-use, yet finding such an end-use becomes more difficult at larger scales and where the (thermal) energies must be transmitted over large distances. Hence co- and tri-generation becomes more attractive at a district or local level. The management of wrong-type energy then becomes an aspect of the design space for localised systems, with energy storage featuring as a possible solution [36].

The conclusion to the above discussion is thus. Adding energy storage to local energy systems will allow the optimal operation of multi-generation plant and systems, increasing their overall thermal efficiency by ensuring that the products of generation can always be used. It will also permit the integration of more renewable energy sources at a local level by allowing such generation plant to operate when the renewable sources are available. A potential new flexible type of energy storage, termed *multi-vector storage* would provide "right-type right-time" flexibility service to the energy system. An ideal multi-vector storage system or device would be able to receive and store any form of energy, and later release that stored energy in the form required by the demand. As well as the benefits to the operation of multi-generation and conventional renewable sources, multi-vector storage also enables non-conventional sources to be included in an energy system, in particular the scavenging of other waste energy which can be stored and re-processed into other forms of energy that are more valuable. Bao *et al.* [38]) describe one such device which is able to reprocess waste heat into electricity and cooling forms.

2.3.2 Energy storage technologies

In this section, the types of energy storage technologies that are in use in engineering systems, as well as the physical principles on which these technologies are based, are examined. A comprehensive overview of the state of energy storage technologies has been produced by Sabihuddin *et al.* [37]; in particular they provide a critical evaluation of the application domains of each storage type. Sandia National Laboratories [39] examine storage technologies from the perspective of the services they can provide to electrical networks, while Roskilly *et al.* [22] broadly examine technologies from an integrated energy system viewpoint, including transport. The remainder of this section will explore which technologies the literature sees as being useful to an integrated local energy supply system.

Much like the primary generation technologies described previously, the behaviours of energy storage technologies are constrained by the physical principles used as the storage mechanism. Sabihuddin *et al.* [37], Jensen [36] and Roskilly *et al.* [22] divide storage technologies into four general areas of physical effect: Chemical; Mechanical; Thermal; and Electromagnetic. Table 2.1 shows how individual technologies are categorised in the literature according to the principal physical effect used to store energy; each of the references cited above contribute. Classification by physical effect emphasises the prediction and understanding of the general and ideal behaviours of a given storage device, irrespective of the technological implementation. Generally, technology- or physics-led approaches represent a solution-oriented approach.

Chemical Storage	Mechanical Storage
Electrochemical Cells Liquid Metal and Molten Salt Batteries Metal Air Cells Fuel Cells Flow Batteries	Flywheels (Kinetic Energy) Pumped Hydro (Gravity) Other Potential Energy Compressed Air
Thermal Storage	**Electromagnetic Storage**
Sensible Heat Latent Heat (Ice, PCM[1]) Reaction Heat	Superconductors Supercapacitors Capacitors / Inductors

Table 2.1: Landscape of energy storage solutions (from [37])

Sabihuddin *et al.* also propose a subdivision of energy storage technologies by application, parametrised by storage duration (seconds to years) and storage scale (1 W to

[1]phase change materials

1 GW). This is also similar to the approach taken in [39], which examines technologies in light of their ability to satisfy a suite of electrical networks services. This view of storage represents a problem-oriented approach.

Thus two complementary categorisation schemes are apparent in the literature: a solution-oriented perspective which emerges from the application of physical principles; and a problem-oriented one which is the result of the desire to rectify an issue within an energy system, and for which energy storage is seen as a solution. The merging of these two outlooks leads to a possible solution space. The IMechE [11] presents the result of the merging of these two categorisation methods in chart form, which is reproduced in Figure 2.1. This chart overlays the technology and application domains on axes of discharge time and energy capacity. In fact, there is a third dimension, discharge power, which is not shown here but which appears in the work in [37] instead of energy capacity. Not all possible technologies nor application domains are shown on this chart; those specific to integrated local energy systems are explored further below.

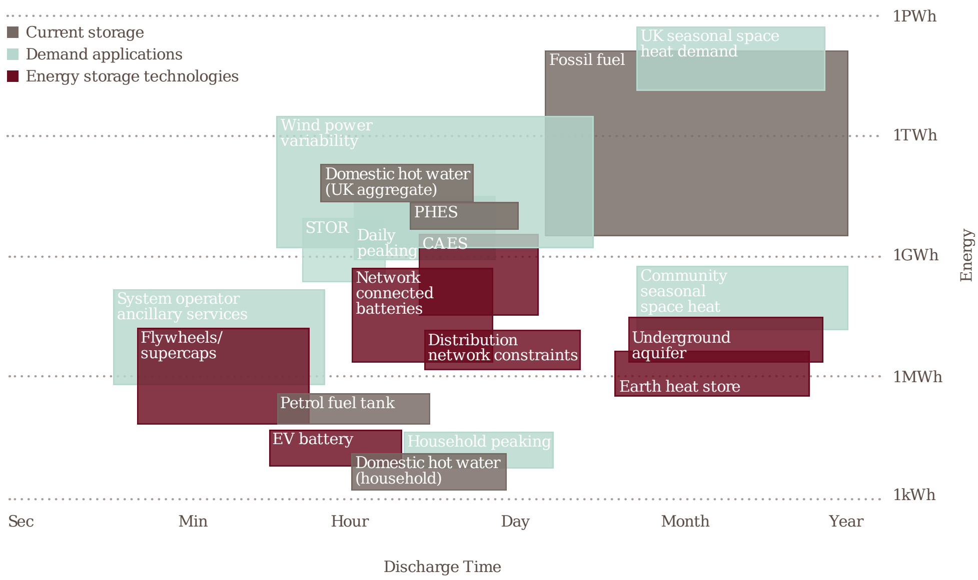


Figure 2.1: Capacities / discharge times for energy storage systems (reproduced from [11])

In [37] the authors suggest that technologies possessing storage capabilities in the mid-range time domain (minutes to hours) are suitable for what they term "bridging power" applications. Although longer-timescale storage within local integrated energy systems would be of value, the primary use of storage would be as suggested earlier the balancing of wrong-time wrong-type energy from multi-generation and renewable sources within the daily cycle. Therefore, the remainder of the review will concentrate on "bridging power" applications. Within this range Sabihuddin *et al.* place sensible thermal energy storage (STES), latent thermal energy storage (LTES), nickel-iron, nickel-zinc and nickel-metal hydride batteries, and sodium nickel chloride and sodium sulphur molten salt batteries. cold thermal energy storage (CTES) systems are positioned in the longer-term energy management and medium power class; however, given the promising nature of tri-generation systems using sorption technologies (see e.g. Best and Rivera [40], and

Cot-Gores *et al.* [41]), the "bridging power" category should be expanded to include CTES systems for local energy system applications. Referring to Figure 2.1, the IMechE [11] also places network-connected batteries, along with compressed air energy storage (CAES), pumped heat energy storage (PHES) and domestic hot water storages in the bridging-power category.

It is useful to reference the worldwide context of installed energy storage here. The U.S. Department of Energy (DOE) Office of Electricity (OE) Global Energy Storage Database [42] is a crowd-sourced online portal which provides a comprehensive record of operational storage programmes worldwide. Knowledgeable parties are able to submit information about energy storage projects to the database controllers, who verify the accuracy of the information through a third-party before adding it to the collection. The data from this source are summarised in Table 2.2 to show the global number of sites and installed power for the main storage technology classes[2]. A number of reviews of worldwide installed storage e.g. Sabihuddin *et al.* [37], Luo *et al.* [43] and the International Energy Agency (IEA) [44] reproduce data and figures provided by Rastler [45]; however the sources of the data in this report are unattributed[3]. While the data do corroborate with that published for 2009 / 2010 by the U.S. Energy Information Administration and DOE, the Energy Storage Database offers a more reliable, transparent and up-to-date source of information for research.

Table 2.2 shows that overwhelmingly the largest form of installed and operational storage worldwide is pumped-hydro storage, which at 168 GW is two orders of magnitude larger than the next biggest installed base (thermal storage) and represents 97% of all installed energy storage power. Pumped-hydro storage is not generally seen as being a suitable storage technology for local energy systems, as its low-energy, high-power characteristic is more suited to a fast-response electrical grid balancing role. Additionally, pumped-hydro is highly dependent upon geographical factors. Individual pumped-hydro schemes produce power in tens to hundreds of megawatts, with a smaller number of larger sites producing >1 GW output power. Unfortunately the low density and hence low gravitational potential energy (GPE) of water produces a relatively low energy storage density, which at a local level tends to require too much physical space for economic viability. However, using the stored GPE of a solid mass to pressurise water has been used in the past as a local energy storage device, and Sabihuddin *et al.* [37] cite a recent (at the time) GPE storage proposal. London's Tower Bridge, opened in 1894, was designed with hydraulic accumulators which used the weight of iron rams to pump water through an engine at high pressure to lift the bridge decks. Thus GPE in a more general sense should perhaps not be written-off as a possible low-duration, high power local energy storage medium.

[2]Most recent update of the database at the time of writing was 17/11/2020.

[3]Personal correspondence with Electric Power Research Institute (EPRI). It is tempting to attribute the large number of citations of Dan Rastler's figures in academic and popular science literature to the citation of his report by Wikipedia.

Storage Class	Type	Operational Sites	Installed Power
Electro-mechanical	Pumped hydro	325	167,790 MW
Thermal	ALL	206	2,444 MW
Chemical	Li-ion battery	451	1,380 MW
Electro-mechanical	Flywheel	42	931 MW
Electro-mechanical	CAES	13	724 MW
Chemical	ALL except Li-ion	403	549 MW
Chemical	Hydrogen (incl. fuel cell)	9	17 MW

Table 2.2: Worldwide installed storage base (as of 17/12/2020)

Compressed air storage is more associated with larger scale energy storage, for example to smooth fluctuations in wind farm electricity production [46], and the preferred large-scale storage location is evacuated salt caverns or similar. However, the additional heat released and absorbed during a cyclic gas compression process has synergies with heat storage in local energy systems, and CAES is flexible enough to be developed at small scale. However despite the apparent maturity of the technology however only a small number of commercially operating sites exist. Flywheel storage is a very mature technology with a high round-trip conversion efficiency [37] and is eminently usable in a local energy system. Its relatively high leakage rate may make it less attractive than other storage devices in local energy systems, however its high response rate may prove useful. Current applications tend to be short-duration high-power applications such as uninterruptible power supplys (UPSs) for data centres, voltage regulation, or pulse power provision for large research laboratories.

Table 2.3 shows a more detailed breakdown of the worldwide operating storage sites, excluding hydroelectric installations, as reported by the DOE. Unknown technology types are not reported in the detailed breakdown but are included in the category totals. In terms of installed power, it can be seen that lithium-ion batteries and molten salt storage storage technologies very much dominate the smaller district scale installations, with CAES and flywheels making up most of the rest of the currently-operating installations. Despite the diversity of potential technological solutions, and the range of potential applications, that a handful of technologies make up most of the worldwide storage installations suggests that factors other than engineering suitability are critical; relative cost being one, but also, speculatively, political programs, established supply chains, technological readiness, marketing, environmental issues and materials availability. This topic is not in the scope of this thesis however and will not be pursued further here.

Although storage costs will not be factored into the demonstrator system assessment in Chapter 6, it is still useful to consider the varying costs of different storage technologies in this literature review. Work by Smallbone *et al.* [21] on the levelised cost of storage (LCOS), while not covering all of the technologies shown in 2.3, provides an indicative view. The LCOS evaluation is instructive because it provides a generalised cost of storage per kWh (or per kW) which includes the capital cost of the storage equipment and the lifetime operating cost. Figure 2.2 shows the levelised cost of storage for some major tech-

Storage Type	Operational Sites	Installed Power	Percentage
Electro-chemical	768	1,786 MW	30.3%
Electro-chemical capacitor	25	31 MW	0.5%
Flow battery	69	47 MW	0.8%
Lead-acid battery	85	69 MW	1.2%
Lithium-ion battery	451	1,380 MW	23.4%
Lithium polymer battery	48	12 MW	0.2%
Nickel based battery	6	30 MW	0.5%
Sodium based battery	68	204 MW	3.5%
Electro-mechanical	55	1,656 MW	28.1%
CAES	13	724 MW	12.3%
Flywheel	42	931 MW	15.8%
Hydrogen	9	17 MW	0.3%
Thermal	206	2,444 MW	41.4%
Chilled water	25	137 MW	2.3%
Heat	19	117 MW	2.0%
Ice	124	72 MW	1.2%
Molten salt	34	2,042 MW	34.6%
Thermal storage	3	76 MW	1.3%

Table 2.3: Worldwide installed storage base - detailed (as of 17/12/2020)

nologies, including PHES, pumped hydroelectric storage (PHS), adiabatic compressed air energy storage (aCAES), glsdcaes, vanadium redox flow (VRF), lead acid (Pb), lithium-ion (li-ion), hydrogen storage (H_2) and methane storage (CH_4). In this evaluation, it can be seen, interestingly, that the mechanical storage types PHS, glsphes, CAES compare very favourably with current electrochemical battery storage (Pb, li-ion) and gas storage (H_2, CH_4)technologies, and continue to compare favourably with projected 2030 electrochemical technologies, at least in terms of storage capacity cost. The assessment illustrated is for a 100 MW/400 MW h system with 365 cycles per year, and including an assumed electricity price of 3 € ct/kWh [21].

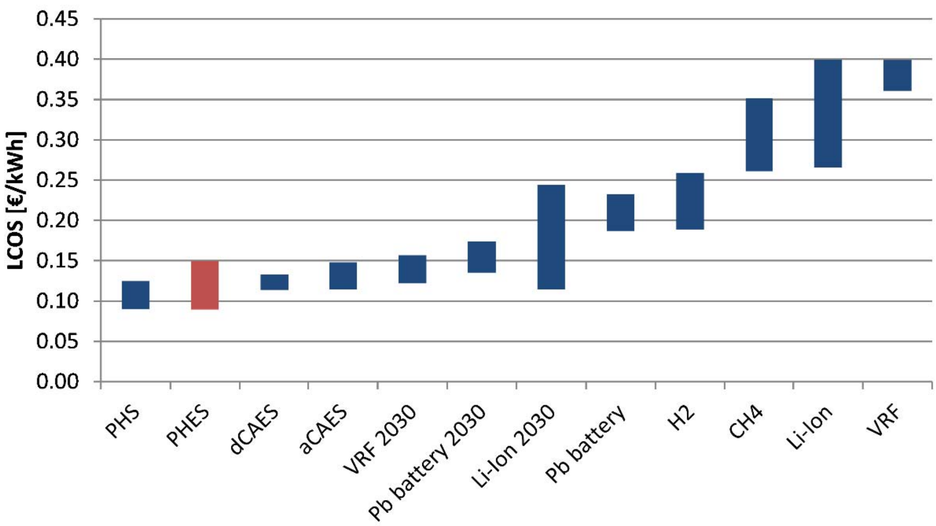


Figure 2.2: Levelised cost of storage for some major technologies (reproduced from [21])

2.4 Exergy in storage and systems

2.4.1 Exergy as a stored quantity

It has been argued by many authors (for example, Bejan and Bejan [47], Kotas [48], Sciubba [49], among others) that the processes of consuming and storing energy should be regarded instead as a process of consuming and storing exergy. Consider storing the exhaust from a 250 °C steam process which is vented to the atmosphere at 20 °C. The internal energy of the vented steam is not lost; it is transferred into the atmosphere, which has "stored" the energy contained within the steam exhaust. However, this energy is now dispersed and not available for any practical purpose.

In a proposed multi-vector storage device the exergy destruction associated with the energy storage and recovery processes, as well as the effect of the storage medium, is important. A representation of a general system ought to separate the storage medium from the energy conversion and transfer processes, so that the physical energy containment methods can be separated from the means of transferring energy to and from them. For example, a sensible heat store (e.g. a large tank of water) could be heated by either heat exchange with another hot fluid, or by electrical work in the form of a resistance heater, or mechanical work in the form of a rotating paddle. The amount of exergy stored in the water tank is dependent upon the form (vector) of the energy source and the machinery used to perform the conversion. Electrical source energy could be used to either heat the water through resistance heating, drive an electric motor attached to a stirrer, or by driving a heat pump. Each of these storage mechanisms will have different characteristics depending on the energy source and the storage medium.

A review of how the literature treats exergy in the context of storage technologies and conversion processes is presented next. Work in the literature broadly falls into four sections — integrated district energy schemes, energy storage technologies, energy conversion processes, analytical methods — and the rest of this section is divided into these topic areas. Some overlap between these subjects will be seen, particularly when considering storage and conversion, which tend to be interdependent in practice.

2.4.2 Integrated district energy systems

Interest in the exergy performance of district energy schemes involving the supply of heat and electricity from renewable or decentralised sources, or from co-, tri- or multi-generation systems, with or without storage, is evidenced by a number of publications which are examined below. The motivation for these studies is primarily to apply exergy-based analysis methods to district or local energy supply systems to create a new system design or suggest an improvement to an existing design.

In [24], Rezaie *et al.* conduct a case study of a district energy scheme supplied through gas boilers and solar collectors and using a thermal energy store (TES) to moderate supply to the system's customers, with the objective of determining the impact of adding the TES to the system. Shin *et al.* [50] analyse the design of a proposed district energy network consisting of a co-generation plant and distributed electrical generation powering heat pumps supplying a thermal energy store. The authors use exergy analysis to demonstrate that the new system will offer improved exergy performance over an older system design. In [51] Bagdanavicius *et al.* investigate four possible energy supply designs (variations on biogas-fuelled gas and steam turbine CHP) for a community energy supply system. The authors apply exergoeconomic analysis to the designs, arguing that while exergeo-economic studies are often used at large scale, they are rarely used for small or medium scale energy systems. Their analysis demonstrates that an exergo-economic study is able to identify the most exergy-efficient supply technology for supplying the community scheme. Calise *et al.* [52] examine an existing multi-generation system consisting of a photo-voltaic / thermal (PV/T) generator, a concentrated photo-voltaic / thermal (CPVT) generator, a biomass heater, a single-stage absorption chiller, and a desalination system, which covers the base load of an isolated community. The authors present a detailed exergetic, economic and environmental analysis and demonstrate an optimisation of the overall system exergy efficiency and profitability. In particular they note that the system optimum leads to non-optimum designs for one of the components (PV/T). This result demonstrates the importance of optimisation at a whole system level when considering exergy destruction as a design requirement. Coskun *et al.* [53] propose a new hybrid system design for improving the efficiency of an existing geothermal district heating system which combines a biogas-fuelled electrical generator, a water-to-water geothermal heat-pump, and biogas production from waste heat. The authors examine the system exergetically and suggest that the new system offers an energy and exergy efficiency improvement of 7.5% and 13% respectively. In particular the authors note that the low-temperature, low-exergy waste heat from the CHP process is ideally suited to biogas production rather than heating applications.

The exergy content of heat is of particular note, as exergy diminishes as temperature approaches ambient, and two papers examine heat networks specifically. In investigating possible design variants for a district heating system in Denmark, Elmegaard *et al.* [54] present a study of generic district heating networks providing domestic hot water at varying heating fluid temperatures. The authors study the conventional district heating solution (high-temperature fluid), and four different supplementary heating solutions for low-temperature supply designs: direct electric heating and three heat pump solutions. The authors are able to show through exergetic analysis that the conventional solution at the lowest possible temperature is the most efficient, and that the best low-temperature system uses a heat pump with hot water storage on the district heating side. Li and Svendsen [55] carry out an energy and exergy analysis of a low-temperature district heat network, identifying through this analysis the system components exhibiting the largest exergy destruction rates and proposing design changes which would improve the overall system exergy efficiency.

2.4.3 *Storage technologies*

In the analysis of real energy storage systems, finite-time thermodynamic analysis can be an appropriate method for obtaining process performance bounds that are closer to the behaviour of real systems than those provided by classical quasi-equilibrium methods [56]. A number of studies examine the exergy destruction performance of thermal, thermochemical, and mechanical energy storage processes.

In [57] Dinçer and Rosen provide a systematic exergy evaluation of a number of thermal systems: a Closed TES System; Aquifer TES Systems; Thermally Stratified Storage; Cold TES Systems; Optimal Discharge Periods for Closed TES Systems; and Solar Ponds. Biyikoğlu [58] analyses and optimises a sensible heat cascade thermal energy storage system using exergy as the analysis and optimisation parameter. The author specifically references the device as storing exergy rather than energy, and builds specifically on work by Krane [59] and Bejan. Caliskan *et al.* [60] analyse the exergetic performance of latent, sensible and thermochemical building storage schemes, particularly in terms of sensitivity to the definition of the thermodynamic condition called the *dead state*. The term dead state is used in thermodynamics to refer to an environmental reference state. A material in the dead state is in thermodynamic equilibrium with its surroundings. The mechanical, thermal, chemical and electrical state properties of a material at the dead state (temperature, pressure, speed, elevation, chemical potential, voltage and so on) are equal to that of those of the dead state, and the material thus has no work-producing potential. The thermal properties of the dead state are arbitrary but are usually taken to be 298.15 K (25 °C) and 1 atm [12].

The authors find that exergetic performance improves as the dead state temperature is lowered. Dinçer [61] discusses methods and applications of describing and assessing TES systems in buildings. The author presents energy and exergy analysis of thermal energy storage systems for use in system design and optimization and gives an illustrative example showing how "exergy analysis provides a more realistic and meaningful assessment than the conventional energy analysis of the efficiency and performance of a thermal energy storage system."

Shirazi *et al.* [62] develop a mathematical model of an ice thermal storage system and apply thermodynamic, economic and emissions costs to it, using a genetic algorithm[4] to obtain optimal design parameters of the plant with the exergetic efficiency of the plant as the thermodynamic objective. In another study of cold storage, Rosen *et al.* [63] assess the thermodynamic performance of cold thermal storage systems using energy and exergy analyses. The authors conclude that "exergy analysis provides more realistic and accurate assessments of the efficiency and performance of cold thermal storage systems

[4]A genetic algorithm is an iterative optimisation process inspired by natural selection. A large number of possible solutions to the problem, characterised by 'genetic parameters', are generated to form an initial solution population. These possible solutions are combined using genetic ideas of crossover and mutation. Subsequent solutions which are a better 'fit' to the problem, measured using a fitness function, are selected to iterate into successive populations. Eventually an evolutionary stopping criteria is reached and the most 'fit' solution is held to be the overall most appropriate solution to the problem.

than those given by the more conventional energy analysis. In addition, exergy analysis is conceptually more direct since it treats cold as a valuable commodity." Rismanchi *et al.* [64] review analyses of CTES systems. The authors find that energy and exergy analysis helps designers make better informed judgement due to the wide variety of parameters in such systems. The authors show also that in their opinion "exergetic efficiency analysis can show a more realistic picture than energy efficiency analysis". As a result of researchers conducting rigorous exergy-based analysis of CTES systems, the authors conclude that based on total exergy efficiency, ice-on-coil (internal melt) CTES systems is the "most desirable CTES system."

Abedin and Rosen [65] provide an analysis of a thermochemical process using energy and exergy analysis, backed up by an experimental case-study. In a related work, Abedin and Rosen [66] determine "efficiencies based on energy and exergy ... for the overall storage cycle and its charging, storing and discharging processes." for a thermochemical process. The authors suggest that "there is a significant margin for loss reduction and efficiency improvement for closed and open thermochemical storages, since the exergy efficiencies of both are significantly lower than the energy efficiencies.". Li *et al.* [67] describe an experimental investigation into the energy and exergy performance of a residential adsorption storage system.

Meunier *et al.* [68] conduct a second-law analysis of sorption heat pumps (liquid absorption, solid adsorption and chemical reaction), finding that an entropy production analysis reveals that "thermal coupling irreversibilities in solid sorption systems and other internal irreversibilities in liquid sorption systems with solution heat exchanger are dominant in the actual COP degradation with respect to the reversible Carnot COP."

Arabkoohsar *et al.* [69] provide an example of using exergy and energy analysis to examine the energy and exergy efficiency of a 100 MWp solar photo-voltaic (PV) system connected to a CAES storage system. Bagdanavicius and Jenkins [70] examine the heat generated during the compression stage of a CAES using exergy and exergoeconomic analysis. The authors claim that their study shows that "CAES-TS has the potential to be used both as energy storage and heat source and could be a useful tool for balancing overall energy demand and supply."

In [71], Caliskan *et al.* model hydrogen and electricity production and storage systems through exergy, energy and sustainability approaches.[5].

Jegadheeswaran *et al.* [74] present an exergy-based review of phase change material (PCM) latent heat storage systems. The motivation for the paper is the increase in interest in exergy-based evaluation methods in the literature (as opposed to energy-based evaluations). It examines and evaluates various exergy-based methods used to evaluate PCM storage systems. The authors conclude that: "Exergy based performance evaluation of LHTS [latent heat thermal storage] system can be stated as more perspective measure than energy based one [sic] as it reflects the true potential of the system and the economic

[5] This paper endured a spirited challenge by Calderón *et al.* [72], and the authors provided a robust rebuttal [73]

value of the storage/recovery operation.", and that "Exergy analysis of any form should consider the complete cycle operation of LHTS systems rather than considering either storage or recovery mode alone.". The authors make a strong point concerning optimisation of PCM systems using exergy analysis, in that "Optimization of any LHTS module requires rigorous exergy analysis along with energy analysis." and "Entropy generation analysis has a significant importance especially when it comes to optimization of design and operating parameters of LHTS systems." The authors conclude that "Studies still remain on large scale especially for the comparative evaluation of various performance enhancement techniques employed for LHTS systems.", and are clear about the value of exergy-based assessments: "The installation and operation of any LHTS system can be justified only if the exergetic cost of the system is minimum and exergy based thermo-economic optimization is of greater help in minimizing the exergetic cost of the system.".

2.4.4 Energy conversion processes

It is relatively difficult to disentangle energy conversion devices from their associated storage processes and physical mediums, as they tend to be closely interconnected within the design of the implementing technology. However a smaller number of papers concentrate more on an analysis of energy conversion itself rather than the energy storage system that the conversion process sits within.

Gebreslassie *et al.* [75] examine the exergy performance of water-lithium bromide absorption cycles and are able to demonstrate how exergy analysis can help improve device designs by deducing that the largest exergy destruction occurs in the absorbers and generators. Wang *et al.* [76] describe the exergy performance of an ammonia resorption cycle co-producing electricity and refrigeration, and derive an exergy efficiency for the cycle of 0.9. Al-Sulaiman *et al.* [77] model the exergetic performance of a tri-generation system using solar collectors and an organic Rankine cycle (ORC) engine. They consider four modes of operation of the device and analyse the exergetic performance of each mode. The study demonstrates the value of exergetic analysis by showing that the main sources of exergy destruction rate are the solar collectors and ORC evaporators, which would lead to possible re-design of these components.

2.4.5 Analytical methods

Later in the thesis, Sections 2.5.1 and 2.5.3 will describe the general body of literature which describes exergy analysis theory. This section will describe the ongoing work in this area that is resulting in new developments in exergetic analysis methods and their application. Although exergy analysis is a relatively established field, new developments take place when new problem areas become active and more detailed analysis tools and results are required to analyse them.

Kelly *et al.* [78] describe an approach for splitting exergy destruction into endogenous and exogenous parts and explain how the method can be used for analysing general exergy conversion systems. The endogenous part of exergy destruction comes from irreversibilities within the conversion process itself, while the exogenous part comes from the relationship between the conversion process and the rest of the system that it sits within. This decoupling of the process from its environment can, claim the authors, lead to a better understanding of interactions between energy system components and “provides very useful information for improving an exergy conversion system”. The authors investigate a number of different approaches to splitting exergy destruction and conclude they all generate “comparable and acceptable results” except for one, which they advise against using.

In [79], Silveira *et al.* propose “a thermo-economic optimization methodology for the analysis and design of energy systems.” It uses an objective function based on exergetic production costs and illustrates the method with two case studies. Further investigation would be needed to understand what distinguishes this method from other thermo-economic optimisation methods.

In examining the use of exergy for the analysis of thermodynamic systems, Jentsch takes a different approach in his 2010 PhD thesis [80]. Having examined the state of the art of exergy analysis Jentsch suggests that exergy analysis of reversible systems would be well-served by separating the quality and quantity aspects of exergy, and proposes two new properties which he terms *transformability*, a measure of energy quality, and *transformation energy*, the measure of quantity. However the resulting theory is quite complex, and it is not clear without a very detailed examination whether this splitting of exergy into two separate quantities offers significant advantages over more straightforward exergy analysis.

Kim introduces a concept called “wonergy” in [81], “wonergy” being a portmanteau of “worth” and “energy”. This is an attempt to unify cost allocation, cost optimisation and cost analysis approaches from thermo-economics and accounting into a single quantity, the wonergy, which is a quantity that can “equally evaluate the worth of each product [of the system].” In this work, the flow equations for an energy system are unified, with the “wonergy” concept becoming a generalised replacement for energy, exergy, or other assessment of value within a thermo-economic system. However, to date this concept does not seem to have become widely used, in contrast with more established methods such as presented by Lazzaretto and Tsatsaronis [82], who propose “A systematic and general methodology for defining and calculating exergetic efficiencies and exergy related costs in thermal systems”. These authors describe “how to obtain detailed definitions of exergetic efficiencies using separate forms of exergy (thermal, mechanical and chemical) and how, according to these definitions, to conduct an evaluation of costs associated with all the exergy streams entering and exiting a system component.” The resultant framework consists of a generalised matrix method implementing this generalised exergy stream cost evaluation.

Although not originating a methodological approach in itself, the 2003 paper by Sieniutycz [56] presents "a study of thermodynamic limits on production or consumption of mechanical energy in various practical and industrial systems." This comprehensive review of finite time thermodynamics (e.g. as described by Andresen [83]) and entropy generation minimisation (see e.g. Bejan [84]) examines the equivalence of these two approaches, and demonstrates results for the limits for a number of real heat and mass transfer processes that take place in finite time.

2.5 Exergy theory

2.5.1 Exergy analysis

In order to understand the application and control of storage devices and energy conversions in an energy network, some fundamental concepts from thermodynamics and the field of exergy analysis are important. In the following, as in the literature, although the the term *exergy* is preferred, the older term *availability* is sometimes used interchangeably. Other terms used for exergy in the past are; available energy, available work, potential work, useful energy, and potential entropy, among others, and these are sometimes still seen in the literature, particularly in work originating in the USA [85]. In their 2007 paper "A brief Commented History of Exergy From the Beginnings to 2004", Sciubba and Wall [85] present a comprehensive account of the history of the development of exergy analysis, and their work in this area will be summarised below.[6].

While Sciubba and Wall's study seems at first to be limited by the fact that they consider published material only up to 2004, they argue that the development of the concept of exergy began in 1824 with the publication of Sidi Carnot's work "Reflections on the Motive Power of Fire" [86], and reached a modern maturity in the early 1990s. Sciubba and Wall's paper is therefore up-to-date for any practical purposes. Figure 2.3 shows the number of exergy-related engineering research papers[7]) published by year between 1964 and 2020 inclusive. The steady increase is indicative of the continuing and growing awareness and importance of this subject to the analysis of efficient energy systems. Çengel and Boles [12] define exergy as "the useful work potential of a given amount of energy at some specified state". Exergy can be defined for any form of source energy (thermal, electrical, gravitational, kinetic, chemical, or radiative) [85] and is a combination property of a system, being defined relative to a reference environment (or "dead state"). As noted above, the foundations of the understanding of thermodynamic availability began with Carnot in 1824. Sciubba and Wall propose that following work by Clapeyron, Rankine and Thomson through the mid 19th-century, Gibbs [87] was the "first to explicitly introduce the notion of available work" in 1873 [85]. Efforts by Gouy, Stodola and Jouget in the period 1889–1909 introduced ideas of entropy generation and "dissipated work" (or exergy destruction as it is termed today) [85]. The resulting Guoy-Stodola equation,

[6]Sciubba and Wall indicate that their research covers over 2600 citations and the full list can be found online at `https://dergipark.org.tr/en/download/article-file/65699`

[7]From Scopus: `http://www.scopus.com/`

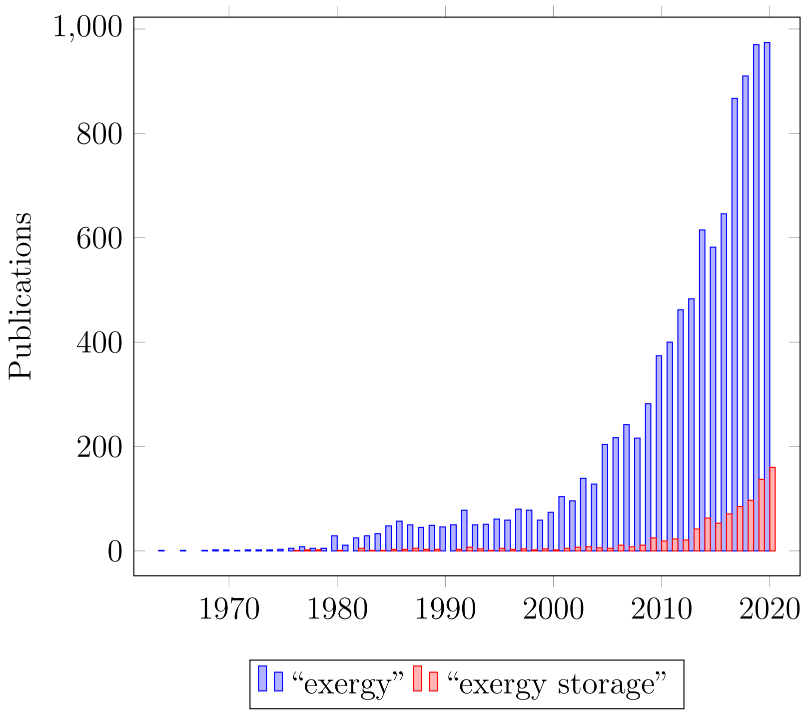


Figure 2.3: Exergy-related publications in Engineering, by year (to December 2020)

$\dot{W}_{\text{lost},0} = T_0 \dot{S}_{\text{gen}}$, is an important expression in availability analysis that states that in a given energy system, the rate of exergy loss, $\dot{W}_{\text{lost},0}$, is proportional to the rate of entropy production, $\dot{S}_{\text{gen}}$ [84]. The constant of proportionality T_0 is the "dead state" absolute temperature for the system. This expression highlights the equivalence of exergy loss and entropy production methods in energy systems analysis; either can be used to equal effect.

The foundations of what is now considered to be modern exergy analysis can be traced to Darrieus [88] and Keenan [89], whose work introduced the concept and methods of second-law analysis to a wider population of engineers and physicists. Significant work by Tribus [90], Evans [91, 92], Rant [93] and others in the 1930s through to the 1960s advanced the field and provided more detailed examples of process and systems analysis. Most particularly, the term exergy itself was proposed in 1953 by Zoran Rant in an attempt to unify the state of the art and reduce the preponderance of variant terminology.

Continuing work by Kotas, Tsatsaronis, Moran, Bejan and others [85] reformulated efficiency expressions in terms of the second law of thermodynamics, and developed applications of the theory. In his 1969 thesis Evans [92] showed that existing measures of potential work — availability, exergy (which was at that time defined in a slightly different form to the modern one), available work, Gibbs free energy, Gibbs chemical potential, Helmholz free energy, and kinetic, potential and electrical energies — are special cases of exergy (which he termed "essergy", for the "essence of energy"). This important result unified work potential measures and gave value to the exergy concept. This and other theoretical developments coincided with advancement in process analysis methods and results through the 1950s and 1960s which led to much improved understanding of engineering process irreversibilities.

By 1970, widespread application of exergy analysis was still "slight if not absent at all" [85]. In a 1973 paper in Nature, Wilkie [94] describes the development and use of the concept of exergy, indicating that at that time and despite the efforts of these researchers — and the fact that Gibbs first used its general expression in 1873 [95] — it remained still something of a little-appreciated quantity, and continued to be re-discovered by new researchers unaware of its history. Between 1970 and 2000 however application of exergy analysis to systems optimisation grew significantly. Sciubba and Wall provide an overview which lists developments in the diverse fields of: theory; theoretical applications in the field of energy conservation and efficiency improvements; theoretical progress in chemical processes; design tools; material properties and standard reference states; tutorials; and case studies in various engineering processes, engines and chemical systems.

A secondary development of exergy analysis is one linking exergy destruction (or entropy production) with the idea that irreversibility in energy conversion processes ought to be accountable in some form. This field of study is known as *thermo-economics* or *exergeo-economics* and is examined in more detail in Section 2.5.3.

In the context of this thesis, particular use is made of the work of Kotas [48], Bejan, Tsatsaronis and Moran [96], Bejan [47, 84, 97], El-Sayed [98], Boehm [99], Dincer and Rosen [100], Çengel and Boles [12], and Wall [101], which provide complete and concise orientations on theory and applications of exergy and entropy analysis.

2.5.2 Exergy fundamentals

This section recapitulates the basics of exergy theory, as this will be used in subsequent chapters and in particularly in Chapter 6. Specific reference is made here to the work of Çengel and Boles [12].

In order to understand and quantify energy quality degradation during energy flow processes, a general description of *unsteady flow processes* is needed. To begin this analysis, a control volume (cv), and a *process* on that control volume, are defined. The control volume specifies a region in space and the material which occupies that space, while the process defines how the control volume exchanges matter, heat and work with its surrounding, and the time period Δt over which this occurs. At the start of the process the control volume is in a given physical state (state 1), and at the end of the process it is in a different state (state 2). The term "unsteady" means that energy accumulates within or dissipates from the control volume during the process. A control volume state is defined by its state parameters, viz. internal energy U, velocity v, and height relative to a baseline z.

The unsteady flow process is illustrated in Figure 2.4, which shows a control volume (cv) undergoing a transition from state 1 to state 2. The upper sub-figure depicts the control volume at state 1 (at a time t), while the lower sub-figure shows the control volume at state 2 (time $t + \Delta t$). At state 1, the control volume contains a mass of material given by m_1. During the process, material flows into and out of the control volume, the control volume experiences a rate of heat transfer of $\dot{Q}_{\mathrm{cv}}$, and does an amount of work $\dot{W}_{\mathrm{cv}}$. At the conclusion of the process at state 2 the control volume contains a mass m_2.

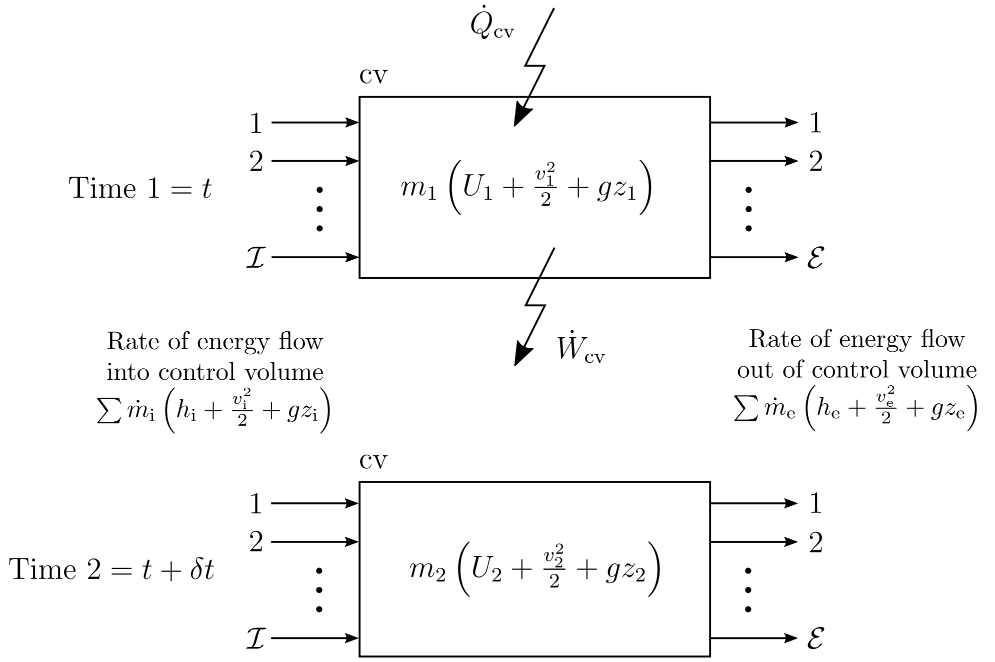


Figure 2.4: General material flow through a control volume (adapted from [12])

During the course of the process, $\mathcal{I}$ inlet material streams flow into the control volume, and $\mathcal{E}$ exit material streams flow out, with the suffixes i and e denoting the ith inlet and eth exit stream respectively. These material streams are specified by their physical properties: rate of mass flow, $\dot{m}$; enthalpy, h; mean velocity, v; and the height of the control volume inlet or exit relative to some baseline, z. Acceleration due to gravity is denoted by g and is assumed to be the same at all inlets to and exits from the control volume. An application of the conservation of mass principles to the system process gives

$$\Sigma m_i - \Sigma m_e = (m_2 - m_1)_{\mathrm{cv}}. \tag{2.1}$$

It can be seen that for a steady flow process where $m_2 = m_1$ then this expression reduces to $\Sigma m_i = \Sigma m_e$, i.e. the total exit flow mass is equal to total inlet flow mass. Applying the first law of thermodynamics to the system produces the expression

$$Q_{\mathrm{cv}} - W_{\mathrm{cv}} = \sum_{e=1}^{\mathcal{E}} E_e - \sum_{i=1}^{\mathcal{I}} E_i + \Delta E_{\mathrm{cv}}, \tag{2.2}$$

which is a statement of energy conservation between states 1 and 2, irrespective of the process that occurs between the two states. Here, the quantity ΔE_{cv} refers to the net change in energy within the control volume during time δt as the system moves from state 1 to state 2, E_i is the energy in the ith inlet stream, and E_e is the energy in the eth exit stream. The quantities E_i and E_e are the accumulated total of the energies entering and exiting the control volume during the process time Δt, where

$$E_i = \int_t^{t+\Delta t} \left(h_i + \frac{v_i^2}{2} + gz_i \right) \dot{m}_i \, dt = \int_1^2 \left(h_i + \frac{v_i^2}{2} + gz_i \right) \delta m_i \tag{2.3}$$

$$E_e = \int_t^{t+\Delta t} \left(h_e + \frac{v_e^2}{2} + gz_e \right) \dot{m}_e \, dt = \int_1^2 \left(h_e + \frac{v_e^2}{2} + gz_e \right) \delta m_e \tag{2.4}$$

The complete expression for energy conservation during the process is thus

$$Q_{\text{cv}} - W_{\text{cv}} = \sum_{e=1}^{\mathcal{E}} \int_1^2 \left(h_e + \frac{v_e^2}{2} + gz_e \right) \delta m_e - \sum_{i=1}^{\mathcal{I}} \int_1^2 \left(h_i + \frac{v_i^2}{2} + gz_i \right) \delta m_i + \Delta E_{\text{cv}} \tag{2.5}$$

Further development of this expression to account for the work lost during the process requires the second law of thermodynamics. The second law statement for flow through a control volume is given in its equality form in Equation (2.6) — proof of this can be found in [12]. Note that $\dot{Q}_{\text{surr}} = -\dot{Q}_{\text{cv}}$ (heat loss into a system is defined positively), and $\dot{S}_{\text{gen}}$ is the rate of entropy generation for the process.

$$\dot{S}_{\text{gen}} = (S_1 - S_2)_{\text{cv}} + \sum_{e=1}^{\mathcal{E}} \dot{m}_e \, s_e - \sum_{i=1}^{\mathcal{I}} \dot{m}_i \, s_i + \frac{\dot{Q}_{\text{surr}}}{T_0} \tag{2.6}$$

The first and second law statements governing the unsteady flow process (Equations (2.5) and (2.6)) can be combined by eliminating Q_{cv}. Assuming that the control volume undergoes no change of kinetic or gravitational potential energy, then $v_1 = v_2$, $z_1 = z_2$, and thus $\Delta E_{\text{cv}} = (U_2 - U_1)_{\text{cv}}$. Then,

$$\begin{aligned} W = &\sum_{i=1}^{\mathcal{I}} \int_1^2 \left(h_i + \frac{v_i^2}{2} + gz_i - T_0 s_i \right) m_i - \sum_{e=1}^{\mathcal{E}} \int_1^2 \left(h_e + \frac{v_e^2}{2} + gz_e - T_0 s_e \right) m_e \\ &+ \left[(U_1 - U_2) - T_0 (S_1 - S_2) \right]_{\text{cv}} - T_0 S_{\text{gen}} \end{aligned} \tag{2.7}$$

The actual work done by the control volume on its surroundings as a result of a volume change during the process is $W_{\text{surr}} = P_0(V_2 - V_2)$. This allows the reversible work (the maximum possible work for the process) W_{rev} to be calculated by subtracting W_{surr} from W. The condition of maximum possible work also implies that $S_{\text{gen}} = 0$ and so the above expression reduces to

$$\begin{aligned} W_{\text{rev}} = &\sum_{i=1}^{\mathcal{I}} \int_1^2 \left(h_i + \frac{v_i^2}{2} + gz_i - T_0 s_i \right) m_i - \sum_{e=1}^{\mathcal{E}} \int_1^2 \left(h_e + \frac{v_e^2}{2} + gz_e - T_0 s_e \right) m_e \\ &+ \left[(U_1 - U_2) + P_0 (P_1 - P_2) - T_0 (S_1 - S_2) \right]_{\text{cv}} \end{aligned} \tag{2.8}$$

Equation 2.8 provides a way of calculating the *maximum possible work*, or the exergy, of an unsteady flow process operating under the weak restrictions that the control volume must undergo no change in kinetic or gravitational potential energy. In order to simplify this equation, two new quantities are defined: ξ, the *stream exergy*; and Φ, the *closed-system exergy*. Both of these quantities are state functions and are measured at the inlets and exits of the control volume.

$$\xi_i = h_i + \frac{v_i^2}{2} + gz_i - T_0 s_i \tag{2.9}$$

$$\xi_e = h_e + \frac{v_e^2}{2} + gz_e - T_0 s_e \tag{2.10}$$

$$(\Phi_1 - \Phi_2)_{\text{cv}} = [(U_1 - U_2) - T_0 (S_1 - S_2) + P_0 (V_1 - V_2)]_{\text{cv}} \tag{2.11}$$

Heat exchange between the control volume and K other bodies (the sign is determined with respect to the other bodies) [12] creates an additional heat transfer work term $W_{\text{rev},Q}$, which quantifies the exergy value of these heat exchanges and is given by the Carnot cycle expression

$$W_{\text{rev},Q} = \sum_{k=1}^{K} Q_k \left(1 - \frac{T_0}{T_k}\right) \tag{2.12}$$

Finally, Equation (2.8) can be written in the general *exergetic* form:

$$W_{\text{rev}} = \sum_{i=1}^{\mathcal{I}} \int_1^2 \xi_i \, \delta m_i - \sum_{e=1}^{\mathcal{E}} \int_1^2 \xi_e \, \delta m_e + (\Phi_1 - \Phi_2)_{\text{cv}} - W_{\text{rev},Q} \tag{2.13}$$

Recall that this applies to a control volume undergoing a thermodynamic process during a time Δt, at a constant kinetic and gravitational potential energy, with $\mathcal{I}$ inlet and $\mathcal{E}$ exit material flows, and exchanging heat with K other bodies. The material flows need not be constant in rate in this general form. This general exergetic flow equation can be simplified for special cases:

$$W_{\text{rev}} = \sum m_i \, \xi_i - \sum m_e \, \xi_e + (\Phi_1 - \Phi_2)_{\text{cv}} - W_{\text{rev},Q} \qquad \textit{Uniform Flow Systems} \tag{2.14}$$

$$W_{\text{rev}} = \sum m_i \, \xi_i - \sum m_e \, \xi_e - W_{\text{rev},Q} \qquad \textit{Steady Flow Systems} \tag{2.15}$$

$$W_{\text{rev}} = (\Phi_1 - \Phi_2) - W_{\text{rev},Q} \qquad \textit{Closed Systems} \tag{2.16}$$

An analysis of the irreversibility of an energy process involves the derivation of a suitable process-specific expression for ξ or Φ for the system in question, either analytically or using numerical methods. Once found, this will give the exergy destroyed during a process (or the rate of exergy destruction, if time is introduced into the expressions through material flow rates) and hence by using the Gouy-Stodola equation, the entropy or rate of entropy production which occurs during the process. The subsequent value of the evaluated exergy destruction rate is to be found in its use in systematic methods aimed at reducing the exergy destruction (or entropy generation) within the process under analysis. This will normally involve the use of optimisation or design-related methods with the exergy destruction incorporated as a component of a system objective measurement.

Note that the above formulation neglects chemical potentials; these can be added to Equation (2.13) as $-\sum_i^N \mu_{i0} N_i$, where N_i is the mole number of substance i having potential μ_{i0} at the dead state [102].

2.5.3 Thermo-economics

Thermo-economics is an established body of knowledge that brings together thermodynamics — primarily exergy analysis — and economic principles as a means of analysing and designing energy systems. Central to the theory is the assertion that exergy is a true measure of the value of an energy source within an energy system and, as such, exergy should be used as the defining quantity when evaluating costs in thermal systems.

Sciubba and Wall describe a comprehensive history of the development of thermo-economics [85]. The first forays into the linking of thermodynamics and costs in engineering processes and systems were made in the early 20th century. Lotka [103] and Keenan [89] among others first expressed the idea that entropy should be somehow linked to process monetary economics. In the 1950s and 1960s attempts were made to correctly account for cost allocation between co-produced heat and power, and a general principle of Exergo-Economics or Thermo-Economics began to be created which allocated prices to energy streams by the specific exergy instead of the unit mass. Valero *et al* [104–106] showed how it is possible to produce a generalised plant cost function, a compact form of which is reproduced in [85] as Equation (2.17). In this expression C_0 is the evaluated cost calculated by the function Φ, which has as parameters x_j (thermodynamic parameters), π_k (material properties), d_i (hardware design parameters) and a_m (allocation criteria).

$$C_0 = \Phi\left(x_j, \pi_k, d_i, a_m\right) \tag{2.17}$$

According to Sciubba and Wall this can be used in two modes: firstly, to find the specific cost per unit of exergy of each process product, given a particular system configuration (Tribus-Evans-El Sayed formulation); secondly, to use a constrained optimisation procedure to find the optimal system design, where the design variables are features of the system under investigation, e.g. configuration parameters or process variables (Kotas-Evans-Gaggioli-Frangopoulos formulation). Sciubba and Wall declare that a more formalised and modern approach is provided by Valero, with work by Tsatsaronis, Szargut and Krane being functionally similar but "in essence their approach is embedded in Valero's formulation." [85]. This latter claim has been disputed by Tsatsaronis [107]. In any case, there exists a substantial body of work describing how thermodynamics and economics can be connected in order to correctly value the energy that is transformed and used by energy systems. This approach is not without controversy however. In [107] Sciubba and Wall refer to Szargut's 1978 paper, "Minimization of the Consumption of Natural Resource" [108], noting that Szargut prefers to conduct assessment of an energy system *purely on its primary energy consumption*, with no cost factors at all.

There are at least two viewpoints on exergetic cost revealed here: Valero's generalised plant cost function (Equation (2.17), which is itself subject to variable attribution of cost weightings in the parameters; and Szargut's "pure" exergy measures. The allocation of an exergetic "cost" for a system is not entirely objective therefore, and the motivations and biases of study authors and analysts must be taken into account when reviewing research using exergetic cost measures. In particular, lifecycle and environmental cost factors themselves have no objective definitions and the incorporation of exergetic costs into such measures must be evaluated carefully.

2.5.4 Exergy in energy systems

It will be useful to have a working definition of an *energy system*. One such definition might be that an energy system is a collection of entities which generate usable energy — generally through conversion from a fuel or from a natural system such as the wind — supply it to a point of demand, and consume it. Of course, energy is not destroyed or created, and as will be apparent from the previous sections it is in fact the exergy which is harnessed from natural sources and used up in conversion and end-use processes. While the term "energy system" remains appropriate it is important to remain aware of the fundamental difference, despite the apparently interchangeable terminology. Although energy systems encompass a very broad range of fields (e.g. food, crops, mining, transport, and so on), this thesis is limited to the study of the supply of heat, cooling and electricity to residential and commercial buildings. Furthermore, as discussed previously, a *local energy system* is limited geographically; an example would be a university campus, or a city.

The examination of thermo-economic theory in Section 2.5.3 showed that energy quality, or exergy, should be allocated a value, even if that value is the raw exergy itself; and that energy system cost accounting methods ought to be based on exergy, rather than energy. According to Rosen [109], "Cost accounting applied to energy systems normally considers unit costs based on energy.", but that "Many [authors] recommend that cost accounting and pricing are better based on exergy than energy. For instance, costs based on exergy are more rationally distributed among outputs, since exergy-based unit costs are more meaningful than energy-based ones." Thermo-economic principles thus suggest using exergy as a cost measure in examining how energy systems ought to be structured and designed in order to extract the largest amount of useful energy out of primary supplies.

Bejan and Bejan [97] discuss two contrasting strategies for managing the supply of energy within an energy supply system. They argue that a demand-led or end-use matching approach which is typical of current energy use scenarios leads to unnecessary exergy destruction, and that a supply-led approach should be pursued instead. Keenan argues a similar point in [102]; that a measure other than energy — entropy, in this case — should be used to measure the efficiency of fuel usage and system performance, and that strong attempts need to be made to organise energy demand in a way which maximises the potential of the source. Keenan illustrates this by reference to seawater distillation plants organised such that processes occur in a series, in order to permit the extraction of more useful work than is the case in a simple process (thirteen times more, in the example given). Rosen [109] argues that “Prices for a commodity based on exergy usually parallel its physical value, while prices based on energy do not. Prices of physical resources can thus be more rationally set based on exergy.”, while in [110] Wall illustrates the difference between energy and exergy losses in a series of power and heat generation processes. In 2014 report the IMechE [11] recommend that “The UK must reject its obsession with ‘cheapness’ in the energy sector.”, arguing that energy prices have been kept artificially low. Although this is a situation peculiar to the UK in comparison to other European countries, it is another indication that market prices for energy can have little to do with the real value of that energy.

The connection or lack thereof between energy supply and its true cost is again addressed by Bejan and Bejan [97], who assert that “fuel prices do not reflect fuel exergy content”. They propose that rather than approaching the subject through a market price optimisation approach, the overall policy problem should be defined as a minimisation of the exergy destroyed (or the work lost) in the system,

$$\min_i (\Xi)_{\text{lost}} = \sum_i T_0 \left(\frac{Q_i}{T_i} - \frac{Q_i}{T_{f_i}} \right) \tag{2.18}$$

where exergy destruction process i occurs between temperatures T_i and T_{f_i} with heat transfer of Q_i into the process; Ξ is the exergy. Keenan furthermore [102] presents a similar argument, that the “economic optimization usually performed by either consumer or industry is faulty”, and that it “would be valid only if the prices of capital goods and fuel reflected their total social costs.” In a Policy Briefing Note [111], Newcastle University researchers argue that in the UK at least, energy (specifically electricity) is priced too cheaply, and that “The Government needs to work with the energy industry to fundamentally change the way energy is priced”; suggesting that there is a mismatch between what the true value of the energy (or exergy) should be, and its market price. Rectification of this state of affairs again would require an optimisation of (2.18) with a correctly-priced value of entropy.

This thesis will take the view that exergy conservation (or entropy generation minimisation) is a general basic principle to be followed. If the market pricing of fuel is not indicative of the value of fuel and may change in any case, and as engineering scientists are primarily interested in seeking to improve the efficiency of systems and processes, then physical considerations should take precedence. As shown earlier, this point of view is espoused by, for example, Szargut [108]. By highlighting the fundamental performance of engineering systems, thermo-economics then makes it possible to evaluate economic structures which seek to preserve the fundamental value present in the energy sources. Under a supply-led approach, a configuration of a system which makes best use of the exergy supplied by the primary source can be sought, emphasising a managed and cooperating ensemble approach to exergy use. In the terminology of Section 2.5.3 this thesis will

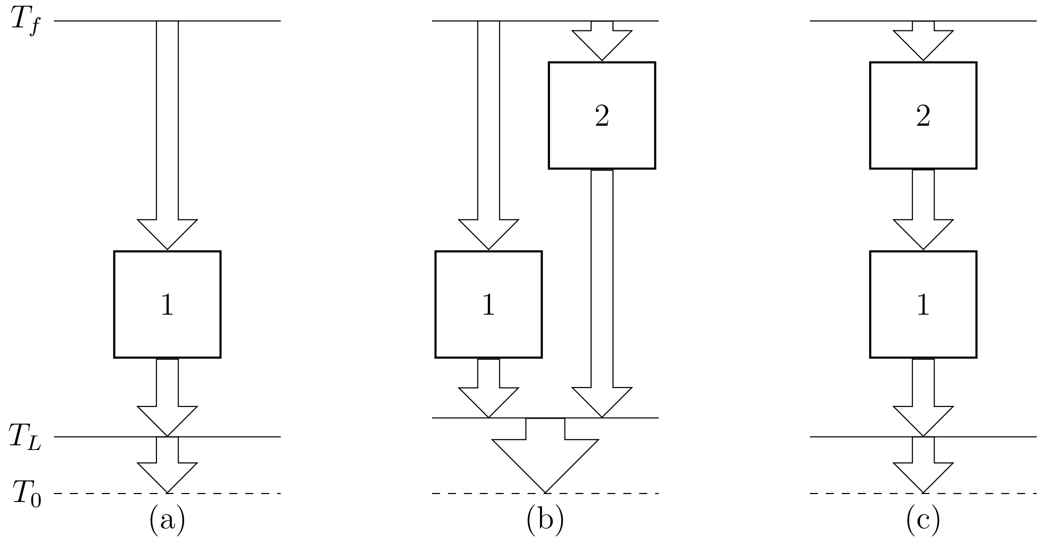


Figure 2.5: User clustering and exergy efficiency (reproduced from [97])

primarily follow the Tribus-Evans-El Sayed approach of using exergy costs as a system metric.

Note that many of these arguments are not new, but the debates surrounding the efficient use of energy do seem to be continually to be re-discovered. Keenan *et al.* in [102] state that “It is a curious fact that topping of industrial heating with power production was more common 40 years ago than it is today.”. This paper is a reprint of an article first written in 1973, i.e. during the 1970s energy crisis. Investigating to what extent this and similar statements are still true today would be a further piece of research that is outside the scope of this thesis.

In a system involving multiple energy conversions in a multi-vector energy system with storage, selecting a combination of storage mediums and conversion processes which best preserve the quality of the energy while meeting end-use demand will tend to be a common objective. The resultant *exergy loss cascade* aims to arrange end-users of the exergy in order to minimise overall exergy destruction within the system. A representation of this is shown in Figure 2.5, where processes 1 and 2 are more exergy efficient in scenario (c) than in (a) and (b) because advantage is taken of the progressive reduction in temperature of the heat from the primary fuel. Exploration of demand reconfiguration in the context of transferring energy between energy domains is explored in this thesis, as part of the demonstrator model of Chapter 6.

2.6 Literature review conclusions

The literature review presented in this chapter has covered three main themes; integrated district energy systems, energy storage, and energy quality (or *exergy*). The first two themes derive from the aims of the work presented in Chapter 1, while the idea of using energy quality as a means of equivalencing energy in different energy domains emerged while investigating the literature on the first two themes. These topics are summarised in the rest of this section.

The topic of integrated district energy systems was surveyed in an attempt to understand how such systems are defined and how they are perceived within the academic and industrial communities. The variety of terms used to describe such systems — local, district, regional, urban and distributed all being found within the literature — indicates a degree of vagueness as to what the systems under study might consist of. A pragmatic statement of our system being one consisting of a mixed energy consumer base with co-located supply and demand, and having an open thermodynamic boundary, was settled on.

The second topic in the review looked at energy storage, of interest in being able to mediate energy flows between, and decouple operations of the domains of, an integrated energy system. An overview of current storage technologies and applications, and the worldwide installed base, illustrates the landscape of district-level energy storage. During this investigation it became apparent that by mediating energy flows between energy domains, the quantity of thermodynamic exergy represented a more general means of equivalencing energy of different types, and thus the third theme of exergy studies forms the final part of the review topic.

The third theme is subdivided into two. Firstly, expanding on the ideas in the first two themes with respect to exergy, the principle of exergy storage and the exergy analysis of systems were explored. The expansive body of literature reviewed here suggests that exergy is the correct quantity for equivalencing and evaluating the behaviour and performance of systems which involve energy from multiple domains. Storage devices can be partitioned somewhat into the storage medium itself and the process by which energy is stored, which suggests a way of dealing with exergy storage devices in an integrated energy system analysis. Finally, a section on exergy itself was presented, covering the degree to which exergy is used as an analysis tool in the literature, some thermodynamic fundamentals, the thermo-economics of exergy, and the degree to which an understanding of exergy shapes the perception of the use of energy within a system. This latter section highlighted the importance of considering exergy destruction (or entropy generation) within an energy system, and demonstrated that for many authors in the field, exergy, and not energy, is the primary economic unit of an energy system.

The literature review thus informs the rest of the work in this thesis as follows. Firstly, that the investigation of the behaviour of an integrated energy system ought to at least comply with some form of definitional framework, and thus that some form of minimal framework should be developed. This idea is presented in Chapter 4 where a design-based representation of an integrated energy system is proposed. Secondly, that a model framework which uses exergy as a principal means of exchange of energy between domains and system evaluation should be explored to represent and analyse integrated energy systems. Chapter 5 describes an assessment of integrated energy systems modelling methods, with Chapter 6 showing a practical model illustrating this method. Finally, investigation of the literature revealed some gaps in current industrial thinking about integrated energy systems, in particular heat systems. To fill this gap, some case studies of working integrated energy systems were carried out, and an informal expert elicitation exercise was conducted. The results of these two pieces of research are presented in Chapter 4.

Chapter 3. Research Methodology

3.1 Introduction

Chapter 2 examined literature relevant to integrated energy systems and the movement of energy between energy domains in such systems. The important concepts of exergy and energy storage were covered, along with the general ideas contained within the subject of integrated energy systems. This chapter moves beyond the literature study and expands on the methods and techniques that will be used to examine and model integrated energy systems. Firstly, a rationalisation is provided for why modelling, rather than experimentation on real or laboratory systems, is necessary for integrated energy systems. Some system design theory based on *axiomatic design* is then presented to give a set of principles by which integrated energy systems can be reasoned about. This theory is subsequently used in Chapter 4 to expand on the system design theory presented here and apply it to some case study systems. Finally, a brief overview of model types appropriate to the modelling of integrated energy systems is given, as an introduction to the much more in depth treatment of the subject in Chapter 5.

3.2 Integrated energy system modelling

3.2.1 Overview

It was established in Section 2.3 that the management of wrong-type and wrong-time energy using energy storage as a controlling mechanism can be of great value when performed effectively in an integrated energy system at district level. In general, understanding the behaviour of energy systems producing wrong-time and wrong-type energy, and the development of strategies for the operation of appropriate control mechanisms, will require a simulation approach. The case for computer modelling and simulation as a principal approach of this thesis is investigated in the next section. A critical feature of useful simulation models will be their ability to integrate power flows from any energy domain, and so it is necessary to look for a model form that can represent any kind of power flow, represent any kind of network structure and represent storage as an abstract device with distinct storage and conversion components.

The work presented in this thesis examines *integrated* network model structures. Under these structures, the entire system is represented in a unified way using a systematic and consistent form. An alternative approach is to model systems using a modular and closed representation where different models are "soft-linked" or interfaced. Interfaced models are also often referred to as "co-simulated" models. The two approaches offer advantages and disadvantages, presented here and discussed in more detail later in this chapter.

- Interfaced models can be constructed from existing mature simulation environments.
- Interfaced models require a more refined scheme for co-simulating the models that make up the system. For example, the functional mock-up interface (FMI) specification describes a way of co-coordinating and co-simulating a series of packaged models.
- Integrated models require first principles development although this is eased by using re-usable (systems-of-systems) components.
- Integrated models allow more insight into the internal model structure, and flexibility with respect to addition and modification of components.
- Integrated models allow more built-in direct control over model components, e.g. for control systems. For a network, this may extend to e.g. topological reorganisation.

While the modular approach offers some pragmatic and computational advantages, it is proposed here that the integrated approach offers a better opportunity to appreciate and understand the basic and fundamental operation of entire integrated, mixed energy domain networks. Three types of basic methods for accomplishing this are described in Section 3.5.1.

3.2.2 Why model?

What is a model?

Models are incomplete representations of a system within the world. They are an approximation to, and can never behave exactly like, the real thing. Models of physical systems are themselves often not physical, being digital representations in a computer. A digital model has the advantages of being easy to modify, physically compact, and able to be experimented on easily. But a digital prototype of an object is still less representative of the real object than is a physical model.

Engineering is also an iterative endeavour. The construction of an actual energy network that operates successfully first time and which satisfies the various specified design aims and constraints is extremely unlikely. A good alternative is to construct a digital model of the system and to study that instead. Adjustments can be made to the model and eventually the model will behave acceptably well and if the model is a good enough representation of the real thing when it is built, then the real network will also behave acceptably. In the rest of this thesis, a “model” of an energy system means “a computer model”.

Physical prototypes and test-beds

In many cases it is essential and in fact easier to construct a prototype of the object or system of interest itself, and to experiment on that, than it is to build a computer model. This kind of approach works well for laboratory-sized projects which aim to prove operational principles. For example, a resonant pulse-jet engine design can be constructed in a lab and modified through a series of experiments until the required performance is attained. But energy networks are large, geographically spread out, require large amounts of capital investment and planning, cause upheaval and disruption to communities during their construction, and can by definition only ever exist once. It is not possible to build a full-scale prototype energy network that is identical (including in its location) to the planned one.

Living labs

As it is not possible to build and refine an actual network until it behaves acceptably, using an existing network might be considered — either in the existing location of a newly-planned design, or at a location that is similar to the proposed construction — to act a surrogate experimental test-bed. These kinds of set-ups are often termed *living labs* or *demonstrator networks*. A living lab is a real place that functions normally and within which the inhabitants go about their normal business, but which is subject to some sort of experimental intervention.

A number of recent examples illustrate the possibilities of living lab experiments in the field of energy networks. The Customer-Led Network Revolution project [112] examined a range of customer- and network-centric trials. These covered a number of user acceptance of demand response schemes and appliance management, and network control of voltage, frequency and equipment ratings. The Triangulum project [113] included a centralised controller concept which communicated with municipal building management systems to manage heating and cooling, with the objective of optimising energy consumption and reducing carbon production. The InTEGReL research facility at Newcastle University [114] consists of a synthesised demonstrator facility housing integrated energy, transport, habitation and water system that will study the benefits of the coupling of these systems. These three demonstrators, while examining different aspects of energy network function, are similar in that they all use real energy networks as their experimental environment.

By definition, living labs operate within their existing regime and construction, and in a stable state. This is helpful for studying current operational policies and for emulating a degree of out-of-the-norm operation, which can be used in developing system control strategies. For example, Yi and Lyons [115] describe triggering control actions in electrical networks without risking or inducing an actual voltage excursion, through a method of reducing the tolerances for voltage excursions to well within the statutory limits. This approach has some limitations however. Out-of-design situations cannot be adequately reproduced because of the risk of damage or loss to the system or users. Alternative scenarios for the network cannot be explored because the system exists “as-is”, complete with its current occupants and users. Likewise, design variants cannot be examined as they would require significant and potentially detrimental change to the system function.

Finally, there are ethical issues surrounding the subjection of the living lab inhabitants to speculative modes of system operation. In fact in the paper cited above, Yi and Lyons go on to supplement the living lab trials with additional computer simulation exploring these additional issues.

Limitations of laboratory simulation

Laboratory demonstrators are small-scale physical models of a real or proposed network design. They are closer to the form of the real network but they are still models. Laboratory simulation can include full replication of the actual network, including scaling effects, and may also include real-time simulators and hardware-in-the-loop (HITL) experiments, HITL being a fusion of digital and physical modelling and simulation. Laboratory simulation is particularly useful for the testing of the dynamic behaviour of discrete devices connected to a simulated environment where the behaviour of the real device and its subsequent effect on the environment is of interest. The simulation of an entire network in a laboratory is a trickier prospect, although it is achievable[1]. The main disadvantages of laboratory simulation are: the topology of the network is fixed and can be difficult if not impossible to change; space is likely to be an issue for adding new elements to the network; some network types (e.g. thermal) are difficult to construct because they have no natural energy sink, unlike the electrical grid which absorb excess electrical energy; and experiments must be conducted in real time and possibly over a long period of time. The latter can make the selected study of seasonal performance difficult without dedicated additional environmental simulation.

Reverse modelling

Engineering design models exist to assist in finding a practicable solution to a particular problem, either by creating a new design for a new problem, or by altering a known solution to meet a new need. Most integrated energy networks development will take place within existing environments, and "green-field" new design optimal approaches are likely to be limited, except to possibly explore theoretical limits. Energy networks models are likely to be used for design iteration, or for stress-test or scenario analysis; the latter involving the extrapolation of a series of changes in order to discover some fundamental system limitation — either a point is reached where no more change possible, or the system fails in some way. It would be common for stress-scenarios to be devised using methods that lie strictly outside of the engineering modelling domain as they normally involve concepts of social and technological transitions. This approach can be considered to be *reverse modelling*, in that a computer model of a known system is used to determine some limit of the system that may not have been previously understood.

An extension of reverse modelling is in using a computer model to explore extreme and optimal system configurations. The digital model allows purely speculative designs

[1]See, for example, the Smartgrid Laboratory at Newcastle University

to be created which can serve as part of design space exploration and optimisation studies. The results of these studies, while possibly not practically realisable, can provide a configuration boundary and serve to reveal fundamental truths about the system. This type of study cannot be performed at all using physical models or field trials, because they involve the creation and evaluation of many possible systems, some of which might involve parameters which cannot presently exist in reality.

3.2.3 Modelling strategies

Energy systems or networks modelling is by no means a new subject. In general however, energy systems modelling efforts tend to the domain specific, as modelling tools and solvers exploit particular aspects of physical properties and behaviour within the domain of interest. However there is a case for exploring modelling approaches that accommodate multiple energy domains within a single modelling and solution environment, and to move away from the need to integrate different tools and solvers. Why would such an approach be taken? In discussing thermo-economic system optimisation, Kotas [48] presents a mechanism called the coefficient of structural bonds (CSB) by which the effect of the optimisation of a single system component on the overall exergy performance of a system can be evaluated. The CSB provides an index value which highlights whether gains made in the optimised component produce positive or negative gains in other system components, and hence whether the overall system's exergy performance is improved as a result. It illustrates that isolated component optimisation may produce an overall worse system and thus should be avoided in favour of whole system approaches. Calise *et al.* [52] report similar findings and conclusions in their study of a poly-generation system.

It must be acknowledged that a generalised simulation environment focused on an integrated whole-system representation can produce tools which lack the focused solution strategies found in more specialised solvers. Thus there exists a trade-off between generalisability and solution efficiency. In many cases this will not be of concern — for example if the problem is small enough that computational effectiveness is irrelevant, or if a global system optimisation is more important than time of solution — but it must be borne in mind.

Therefore, it is expected that an integrated energy systems modelling environment will work best when a number of criteria are met. Firstly, that the modelling level of detail is somewhere in between highly abstract models, such as in energy hub type models, and very detailed physical models. While the essential physical behaviour of the system is to be preserved, a very detailed representation is not required. This mid-detail level representation strategy then automatically dictates that the energy systems to be modelled are relatively simple in their constituent parts, i.e. constituent models are relatively easy to compute, quick to construct, and do not require very many defining parameters, which are likely to be difficult to obtain for district-level models. Additionally the models are more likely to be scalable. Ultimately the integrated system representation will retain essential physical properties while permitting “rapid” evaluation of global performance.

3.3 System design foundations

Analysis of a complex engineering system such as an integrated energy network can only be done effectively if the system is understood in sufficient detail. In particular, the fundamental purpose of the system and the form it will take must be described accurately and in an organised way, using a formal language or framework. Such a framework provides the means of defining and codifying the structure of a system, and the methods by which its behaviour can be assessed, tested and communicated. Two such frameworks are used within this thesis.

Axiomatic Design by Nam Suh [116] is a rational method for designing engineering systems which, starting from a set of *design axioms*, leads to a methodological framework for tackling engineering design problems. Suh describes axiomatic design as “a scientific foundation for design”, intending its application to be an aid to reducing errors in the design process and to allow formal study of proposed or completed designs. This thesis uses axiomatic design principles to determine the functional requirements of integrated energy networks, and lists the physical devices that implement these functions in real systems. In this way, a comprehensive and correct description of the design of a generalise integrated energy network can be attempted, and, from this, the structure of any particular integrated energy network can be understood in the context of the general design.

The Systems Modelling Language (SysML) is a systems-oriented offshoot and generalisation of the Unified Modelling Language (UML), which is a general-purpose software modelling language. As a language, SysML is a way of encoding and communicating the details of a system design in a form which can be understood and translated by other designers, or perhaps by computational and manufacturing tools. A number of sources describe SysML in detail but Friedenthal [117] and Weilkiens [118] provide excellent and comprehensive texts. In this thesis SysML is used to create an exemplar or reference system description which embodies an ideal of an integrated energy network. This approach follows that given by Lubega and Farid [26] in which the authors develop a system reference model for what they term the “energy-water nexus”; although what the authors describe in their paper is more accurately seen as the “electricity-water” nexus. This thesis extends the concept described by Lubega and Farid to modelling the form of the integrated “electricity-heat-cooling nexus” and attempts to understand the role of exergy within such a system.

An explanation, elaboration and critique of the use of axiomatic design and SysML is given now. Lubega and Farid [26] use SysML as a primary tool for developing the functional requirements of their energy-water nexus system. However SysML itself is a representational tool to describe and to communicate a design; it is not a method or process in itself. The functional requirements and design parameters are found here using axiomatic design and then mapped into SysML constructions, which more clearly maintains the distinction between the design method and the design representation. Lubega and Farid do incorporate the principles of axiomatic design in their system analysis but not explicitly separated from the SysML representation (see below). While a number of design techniques exist (see for instance a comprehensive review of design process types by Wynn and Clarkson [119]), axiomatic design is chosen as a means of developing design principles for integrated energy networks because of its generality and strong foundational approach, which strives to anchor engineering design on a strong logical basis. Suh describes the logical framework of the method as "engineering science for synthesis", which complements the more recognisable "engineering science for analysis" responsible for the physical models used in simulation and prediction. The two types of analysis mirror each other. The purpose of SysML is then to allow the design constructed through the axiomatic design process to be instantiated and communicated.

Lubega and Farid argue that there is "a need and an opportunity to augment the study of the energy-water nexus with hybrid physics-based systems of systems models." and that physics-based models are able to provide greater insight than black-box empirical models. Previous discussion in this thesis around the usefulness of exergy as a fundamental measure of integrated energy systems, and demonstrated weaknesses of certain non-physical models, to be highlighted in Chapter 5, support this assertion. At a certain level real engineering design is inescapable and for this reason the work in this thesis positions itself within the realm of physically-based simulation.

This thesis will also take a different approach to the formulation of the system design to that pursued by Lubega and Farid. The derivation of system functional requirements (FRs) and design parameters (DPs) in [26] appears to have been carried out mostly through literature survey. Here literature is also used but the principal analysis method is one which analyses the three motivating case studies described in the Chapter 7 to provide a set of FRs and DPs for an integrated energy network. The case studies are described in some detail in the next section, followed by the design analysis.

3.4 System design theory

3.4.1 Axiomatic design process

A summary of the principles of axiomatic design is given here to provide a background to the analysis in Section 4.4; the reader is referred to [116] for further technical detail.

The fundamental basis of axiomatic design is Suh's principle that a "good" design should adhere to two design conditions, or axioms.

Axiom 1: The Independence Axiom. *Maintain the independence of the functional requirements (FRs).*

Axiom 2: The Information Axiom. *Minimize the information content of the design.*

By definition the design axioms are not provable; Suh deduces them from a set of principles and observations describing conditions required for the production of a "good" design.

A design process founded on axiomatic design requires the specification of four *design domains* that Suh identifies as the general components of designs as a whole, and the production of a set (or "vector") of requirements for each domain. Within each domain the design is captured through a vector of requirements, while the domains are related to each other by a mapping process. The domains and their relationships are illustrated in Figure 3.1 and consist of: the customer domain (produces customer attributes, {CA}); the functional domain (produces functional requirements, {FR}); the physical domain (produces design parameters, {DP}); and the process domain (produces process variables, {PV}). The customer domain contains the needs and requirements that the beneficiary or end-user of the design is looking for. The functional domain lists the functional properties that the design must have in order to satisfy the needs of the customer. The physical domain then specifies the practical design parameters that must be created (in the physical world) in order to create the functions in the functional domain. Lastly, the process domain states the process variables that are needed to produce the physical item or product specified in the physical domain. It can be seen that the specification of each domain serves to drive that of the one following, although it is important to note that the domain relationships are statements of dependency, and do not represent a process. The creation of the requirement sets tends to be a highly non-linear process in reality as information about how the design ought to be created is accumulated, and how knowledge about the relationships between the domains increases over time.

Work by Wardle *et al.* shows how the four knowledge domains can be practically constructed for a smart local energy system (SLES) [20]. The authors study a real-life integrated demonstrator system, creating taxonomies of components for each of the knowledge domains. Table 3.1 from [20] shows the breakdown of the four knowledge domains for a SLES. It can be seen that the {CA} domain captures customer-oriented requirements such as financial concerns, stakeholders, and performance-related issues, while the {PV} domain describes the bodies and tools that are needed to implement the system. The {FR} and {DP} domains contain the necessary functional aspects and design elements (primarily engineering, financial and communication) needed to realise the system functions. In the detailed analysis of systems in this thesis the {PV} vector will be ignored, as practical construction of integrated networks is not considered here. Of course, it would be vital to include the process domain when considering assembly of a real integrated energy network, as shown in the work by Wardle *et al.* [20]. The {CA} vector will similarly not be pursued further. The main application of axiomatic design to integrated energy networks in this thesis will be in the construction of the {FR} and {DP} vectors through analysis of the case study networks and literature in Chapters 4 and 2 respectively.

Customer Attributes	
System Users	heat, electricity & transport users; demand-side responders; generators; system operators; virtual power plant; aggregators; user preferences; asset owners
System By-products	carbon emissions; particulate emissions
Financial	stakeholder value; user income; contracts; DSO markets; price of energy; other markets
Flexibility	daily and seasonal flex; energy vector substitution availability
Locality	internal vs external energy consumption; % controlled by local authorities
Temporality	25-year "vision"
Functional Requirements	
Transport Energy	transport heat; transport electricity
Supply Energy	supply thermal comfort, hot water, heat, electrical power; charge electric vehicles; provide mobility
Produce Energy	accept embedded heat & electrical generation; excess electrical generation to grid
Store Energy	store heat and electrical energy; release heat and electrical energy
Receive Energy	receive grid gas; receive grid electricity
Finance	attribute cost; attribute revenue
User Services	frequency control; balancing mechanism; cater for user preferences; energy consumption time advance; energy consumption time delay
Constraints	reduce system losses, reduce user energy cost, minimise technical losses, reduce air pollution, reduce export, increase self-produced energy consumption
Design Parameters	
Control & Mediation	control in-place; local controller; cloud comms; local comms gateway; VPP
Electrical Energy	residential, front-of-meter, behind-the-meter batteries; distribution network connection; solar PV; solar canopies
Thermal Energy	[not defined]
Energy Converter	air-source & marine-source heat pump; EV chargers; electrolyser
Market & Financial	market layer; residential tariffs
Process Variables	
Asset Owners	system asset owning companies
Asset Installers	system asset installing companies
Asset Operators	system asset operating companies
Residents	councils; householders; EV drivers; businesses; landlords
System Design & Modelling	universities; consultants; system designers
Sponsors & Associates	Innovate UK; UKRI; ERIS; Energy Systems Catapult
Consultants	consulting companies
Academic	EnergyREV; CESI; Newcastle, Coventry and Cardiff Universities
Projects	PFER; SmartHubs; other

Table 3.1: Knowledge domains for a smart local energy system demonstrator (from [20])

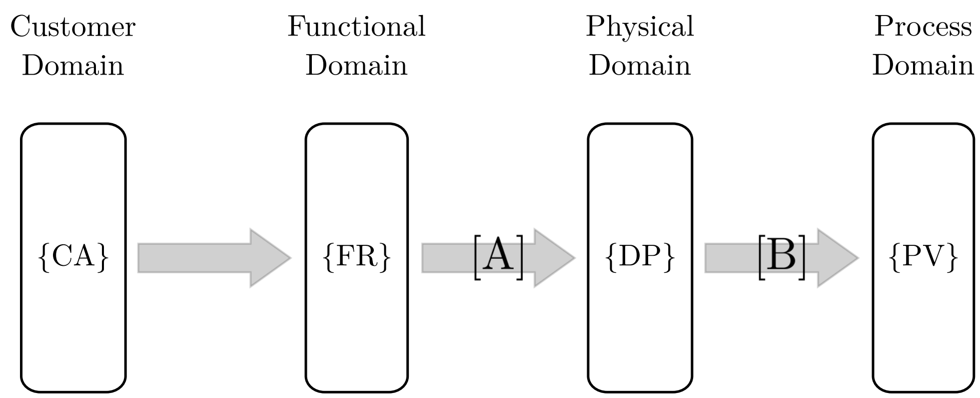


Figure 3.1: Axiomatic design domains

3.4.2 Design matrices

The previously-described design domains are related through a loose mathematical representation as a *system design matrix* and a *process design matrix*. The system design matrix is given the symbolic representation $[A]$, with the process design matrix being denoted as $[B]$. These matrices are used to create relationships between the design domains, as in Equation (3.1). In fact, this relationship might be better expressed through a dependency graph, but this concept will not be explored further in this thesis.

$$\{\text{FR}\} = [A]\{\text{DP}\} \qquad \{\text{DP}\} = [B]\{\text{PV}\} \tag{3.1}$$

The elements of $[A]$ represent the relationship between physical components of the system and the function that they provide, and the elements of $[B]$ represent the relationship between the physical components of the system and the means by which they are created. These matrices can take various forms, but careful consideration of the design axioms reveals that the matrices of a good design will be square, and either diagonal or triangular. In the case of a diagonal or triangular design matrix $[A]$ individual FRs are satisfied and controlled independently, or at least serially independently in the case of a triangular matrix, by individual DPs. The same argument holds for $[B]$ and the relationship between the DPs and PVs. An interesting corollary of this is that in a "well-designed" system, optimisation in the sense of compromise between competing FRs is not needed; neither is any rank prioritisation of the FRs. These principles can be used to examine the generic integrated energy system design matrix to see how well it matches the axiomatic design definition of a "good design", although this is not pursued in this thesis.

It is important to note that, as referred to earlier, the application of the design process is not a linear process and a degree of to-and-fro between the FRs and the DPs (what Suh calls "zigzagging") is required, along with knowledge of technologies and physical principles involved. That is, the uncovering and specification of the function and form of a system design will proceed in something of a parallel fashion.

3.5 Investigation of model types

3.5.1 Types of models

A number of possibilities exist for modelling energy networks. This section describes an overview of and rationale for three modelling strategies to be investigated in detail in Chapter 5.

As mentioned earlier in this chapter, modelling environments may be integrated, in a faithful representation of the real system, or discretised, in a form commonly referred to as co-simulated or soft-linked. In co-simulated environments each individual network is solved separately using one of the above techniques, with boundary conditions between the networks resolved through a mediating algorithm. For integrated models the entirety of the solution calculations must be carried out within a single framework. Thus for integrated models the solver must be able to represent all energy domains of interest; while for co-simulated models each solver is free to concentrate on problems specific to that domain.

3.5.2 Energy hub models

Energy hub models are a form of input-output model where the input-output relationship is described by conversion plant energy efficiency values, and the inputs and outputs are energy streams. These models are used and described by for example Chicco and Mancarella [120], Geidl and Andersson [121], Liu *et al.* [122] and Moghaddam *et al.* [123]. In these models energy streams are abstracted and can represent any physical quantity, i.e. electricity, heat, natural gas, and so on. Energy hub models are able to represent integrated energy systems at the energy stream level as matrix equations, which are subsequently most often used for dispatch optimisation studies using linear programming methods. Energy hub models are static load models, and they are commonly used to represent nodes in an electrical system [124]. In contrast to bond graph and circuit models, energy hubs measure only the quantity of energy or power transferred through the system, i.e. separate effort and flow (current and voltage in electrical systems) are not distinguished. Figure 3.2 shows an example energy hub containing a number of system components which manage a supply of gas and electricity to provide heat and electricity to a demand [124].

As noted, energy hub models are used principally for optimisation problems in steady-state networks where plant parameters are known and (in general) constant. Because the formulation considers energy only, energy hubs are not a suitable representation where the analysis of more detailed physical behaviour is required and / or where an understanding of the conjugate variable components of energy (e.g. voltage & current) is important. Nevertheless energy hubs find use in hub topology optimisation studies and particularly in generation and storage dispatch optimisation problems. An energy hub model consists of a transfer matrix made up of a component coincidence matrix and plant conversion

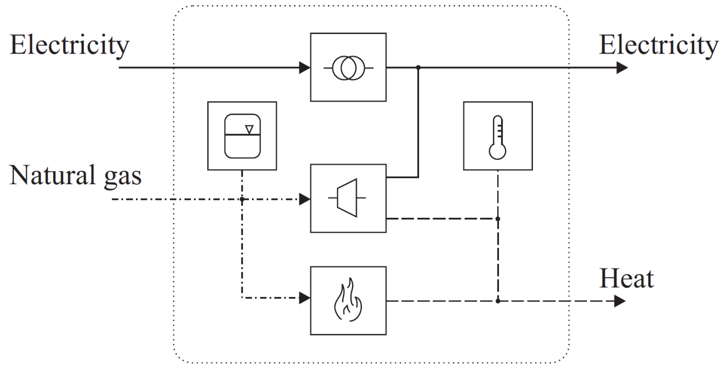


Figure 3.2: Example energy hub (from Geidl and Andersson [124])

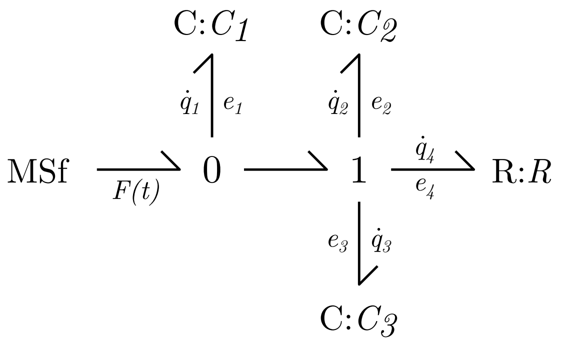
factors, and optimisation studies typically use this in a mixed-integer linear programming approach to determine optimal dispatch schedules. In such studies the selection of constraints and objective functions are crucially important.

3.5.3 Bond graph methods

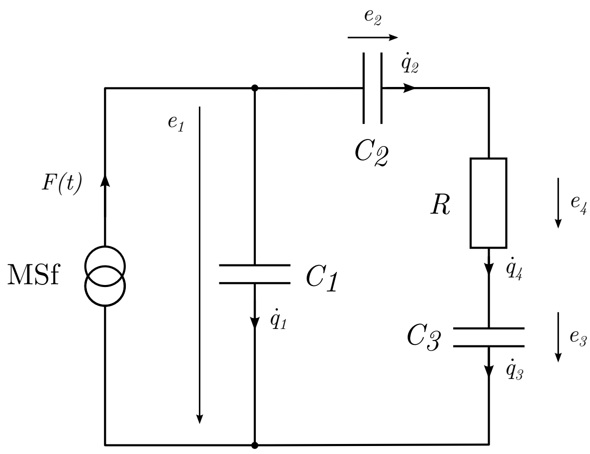
Bond graphs are a graphical technique for representing the energy flow structure of a general physical system. They present a completely generic framework and can be used to represent a (lumped) system in any domain. As described by Borutzky [125], "Bond graphs fit into the spectrum of graphical model representations as a formalism that is particularly suited for engineering systems with effects from multiple energy domains.". With this in mind, bond graphs seem especially suited to representing district energy networks and their components where incorporation of component physical behaviour is important. Bond graph models are usually implemented implicitly (i.e. non-causally), with the resultant equation sets being solved using general time-series simulation techniques.

Bond graphs were invented by Professor Henry Paynter at Massachusetts Institute of Technology (MIT) in 1959 [126] and have developed into a recognised modelling discipline with their own annual conference, the International Conference on Bond Graph Modeling and Simulation. Although they do not enjoy the recognition and support that other modelling methods possess, particularly compared to system block diagrams, they in many ways provide a more fundamental way of describing energy systems. Figure 3.3a shows the energy flows in a RC electrical circuit using bond graphs, with the equivalent electrical circuit diagram shown in Figure 3.3b [125]. In this example, it will be recognised from the circuit diagram that $\dot{q}_2 = \dot{q}_3 = \dot{q}_4$; in the bond graph, as explained later in Section 5.4, it is the '1-junction' which enforces this relationship.

A bond graph describes a dynamic system and is made up of elements that exchange energy with each other. The formalities of the graphical method proscribe the types of links that can be made between these elements, and how subsystems can be created. The resultant bond graph is a graph whose vertices describe basic elements, subsystems or components, and the edges between them describe the instantaneous power transfer between the nodes. These edges are called power bonds. The bond graph of a system



(a) Bond graph



(b) Electrical circuit diagram

Figure 3.3: Example bond graph and equivalent circuit diagram (from Borutzky [125])

reflects the actual physical structure of the real engineering system, and as such the physical topology of the system being modelled is normally a good starting point for the construction of a bond graph representing it.

Bond graphs offer a number of advantages for modelling energy systems, and some disadvantages. Energy networks can be represented by universal conjugate-valued (*effort* and *flow*) variables, irrespective of the energy domain under consideration. This meets the criteria for representing an integrated energy system in a unified way. The network elements and connections can be created from a first-principles analysis in a non-causal form at whatever degree of detail is required, and fundamental dynamic equations can be reduced in form when steady-state solutions are required. Mature languages and solvers (for example Modelica and Dymola) are available for creating and solving systems of interest. Unfortunately the bond graph method is not well-known in comparison to other system solution methods (such as block diagrams), rendering its terminology and methods unfamiliar and difficult to follow or communicate to many modellers. Some of the tools are less well-developed than more widespread ones and lack sophistication, integration add-ons, and appeal. Lastly, some of the simple bond graph methods break down when dealing with material flows and additional more complex representations must be introduced in order to adequately simulate such systems.

3.5.4 Network models

Electrical networks, both linear and non-linear, are commonly represented using Kirchoff's voltage and current laws along with constitutive equations for circuit components. Mature algorithms such as modified nodal analysis are used to construct the system equations, which are then solved either directly or iteratively. Static and dynamic solutions are both possible. Although circuit models historically emerged from efforts to predict the behaviour of direct and, more generally, alternating current electrical networks, they have also been adapted for the analysis of networks in other domains through an electrical equivalence, e.g. fluid flow, bulk heat transfer or exergy, among others (see e.g. Saloux

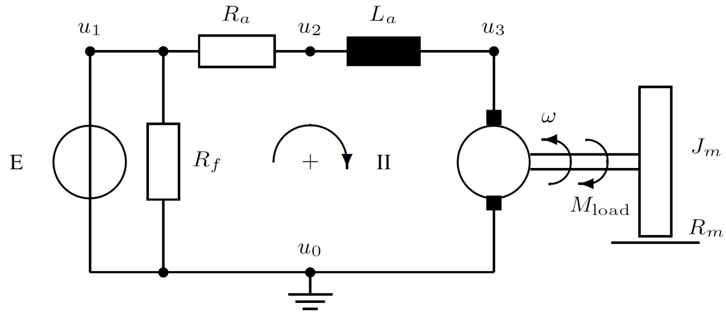


Figure 3.4: Example network model (shunt motor, from Borutzky [125])

et al. [127]). Litovski and Zwolinski [128] provide a comprehensive introduction to the subject of circuit simulation.

A network is defined as a series of branches connected at nodes; the branches represent physical connections and (lumped) devices within the network such as equipment and materials, while nodes are non-physical and represent the connection points between the lumped elements. Physical elements of the network are represented as these lumped elements. Lumped parameter circuit theory is often used to approximate continuous systems, for example transmission lines. A lumped parameter approach in energy systems modelling is appropriate because the elements of the network — generation plant, transformers, demand sites — often are genuinely discrete and distinctly geographically located. For those elements which are not discrete, for example pipes and cables, a lumped parameter approximation is suitable for steady-state or low-frequency analysis. Figure 3.4 shows an example network model, a familiar circuit diagram for a shunt-wound electric motor [125]. In this particular model the mechanical load sits outside of the electrical network representation and is not part of the circuit model.

In network models energy flow is represented as two conjugate variables and has the unit of power. This is a fundamental result in a Lagrangian analysis of energy and is also the central result of bond graph methods. These variables are in the abstract termed "effort" and "flow" and which have specific meaning depending on the domain of interest. For example in a mechanical system the effort is commonly taken to be force, and the flow to be velocity; in electrical systems the effort is usually voltage, while flow is current. Effort and flow are generally time-varying, but can also be represented as Laplace-transformed (frequency-domain) values in the steady-state. For electrical networks especially the corollary of this is that the network components are described by impedances. For much of the work in this thesis however, network flows and efforts will be real-valued and the resultant networks will be equivalent to d.c. networks. This is a reasonable approximation at for example distribution network level, but may become unsupportable in other situations.

Network models are similar to bond graphs in many ways, in that they offer a non-causal physically-based representation of an energy system. Unltimately the set of system equations to be solved are the same as that produced by bond graph analysis. Established methods (e.g. modified nodal analysis) can be used to derive the system of equations describing any non-linear or linear network. One advantage that circuit representations have is that they are familiar to most engineers, and can also be reduced to representations that are intuitive to non-engineers too.

3.6 Conclusions

Integrated energy systems are too large to build prototypes or meaningful physical scale models of, existing demonstrator labs notwithstanding. That leaves computer modelling and simulation as the means to design, analyse and predict the behaviour of integrated energy systems. The pursuit of a fully-integrated modelling environment was identified as a goal of this thesis.

From this premise that the investigation of integrated energy systems will require the analysis of computer models, and that these models should furthermore be of a "whole-system", then three principal types of models have been described; energy hubs, network models, and bond graphs. The approach taken in this thesis is to investigate the suitability of each of these approaches for physically-based integrated energy systems modelling and analysis and to use the most promising one to demonstrate an application to a sample network. The criteria for assessing the methods and the assessment process itself is described in Chapters 5 and 6. It is recognised that co-simulation approaches have particular strengths, but a comparison between co-simulation and integrated approaches as described in Chapter 2 will not be pursued within the scope of this thesis.

The engineering design theory of axiomatic design is proposed here as a method which can underpin the rational design of an integrated energy system. Rather than arbitrarily select components to make up a system, axiomatic design provides a framework for identifying functional requirements and design parameters that can be used to form a palette of functions and solutions out of which the integrated energy system model can be built. In Chapter 4 these principles will be used in an analysis of three case study integrated energy systems to reveal these functional requirements and the design parameters which fulfil them. SysML is subsequently used as a descriptive language for tying these elements together into reference systems.

The next chapter will describe some of the principles of energy networks design. The work in this chapter uses the methodological tools outlined in this chapter to explore the designs of integrated energy networks and to develop a set of reference model components. The findings of interviews with industry practitioners are presented to fill gaps in the literature search and to suggest some avenues of development of an integrated energy system model.

Chapter 4. Integrated Energy Networks Design Principles

4.1 Introduction

This chapter describes a set of case studies which expand on the themes developed in Chapters 2 and 3. Following on from the design theory presented in Section 3.4, the case studies are used to extract design elements integral to integrated energy systems design frameworks. A series of interviews with industry practitioners are presented in Section 4.3 to enhance the findings from literature, which revealed that heat networks are perhaps being overlooked in favour of attention on electrically-based solutions. Finally, these elements are brought together to construct elements of an integrated energy system reference model that can be used to inform modelling choices, which is a topic pursued in Chapter 5.

4.2 Motivating case studies

4.2.1 Byker district heating network

Overview The Byker District Heating System is a district heating system serving Byker, an eastern suburb of Newcastle upon Tyne, UK. The heat generation system is a mixed-equipment plant and includes a combined heat and power (CHP) system, gas boilers and a biomass burner. Operations and project management officials from the Byker Community Trust (BCT), who own and manage the heat network, have informed this thesis with planning, technical and operational detail alongside information about the plant itself, illuminating the past, present and future of the site.

In researching the heating network at Byker, particular credit must be given to the work by Paul Mobbs entitled "The Byker RDF Plant and the Contamination of Land in Newcastle upon Tyne with Incinerator Ash" [129]. This document was commissioned by the Byker residents to provide some independent insight into the events surrounding the contamination of surrounding land with incinerator ash during the 1990s. Mr Mobbs has collected a very detailed record of official documentation and plant history, which is a valuable aid to understanding the present-day design of the system. While recognising the grey literature status of this report, the current section draws on its contents extensively.

The district heating system at Byker in its current form is a consequence of legacy and pragmatism. The design by Ralph Erskine of the Byker estate (the construction of which started in 1968 and was completed in 1982) featured a district heating system intended to operate by incinerating municipal waste, which was at the time considered to be a virtually cost-free fuel. A similar system can be seen in the city of Sheffield, UK [130]. With the benefit of hindsight however, two flaws can be observed in this assumption. Firstly, the design was deemed to be "good enough" for the time, in that it provided a cheap heating solution for social housing which would be replaced by something more technologically advanced [129]. Inevitably, the fundamental system has never been replaced; it has functioned "well enough" and thus the desire to embark on a disruptive and expensive whole-system replacement programme has never been very compelling. Only relatively recently has a programme of system upgrades been undertaken. Secondly, because heat for the network was to be generated from waste, an expectation or promise of free residential heating was created by the original system constructors. If this was ever true, given that municipal waste still needs to be collected, transported, stored, and processed, which is not without cost, it is not true now. The heat for the network is presently created by the burning of natural gas and biomass at a non-negligible cost to the network's users.

The early incentives for developing a district heating system emerged from the North East Regional Planning Committee's efforts in the late 1960s to reduce the cost of landfill waste disposal by incinerating the waste instead, a method which had been popular in Victorian times but which had fallen out of favour. Subsequent to a decision to construct an incinerator at Byker, Newcastle Council insisted on pollution abatement methods and a district heating system to be added to the design. In 1968 the National Industrial Fuel Efficiency Service (NIFES) and Newcastle's City Engineer's department jointly authored a report entitled *Refuse Incineration at Newcastle upon Tyne — Project Appraisal Study*, the outline objectives of which were given as:

> "To carry out a detailed appraisal of the incineration problems of Newcastle upon Tyne and to prepare a joint report covering:
>
> "a). the advantages and disadvantages of one incineration depot as opposed to two, and the selection of site or sites;
>
> "b). the feasibility and economics of utilising the heat produced by the burning of refuse."

Mobbs notes that "In November 1976 the City Council's Housing Committee agreed to go ahead with the development of a pilot heat station, to be developed as part of the Byker Wall development. During the early stages of the Byker development, hot water was raised with a gas/oil-fired plant to the north of the Byker development. As the Byker plant was developed the heat load was gradually switched over to the current 'heating plant'." Thus the twin requirements of Erskine's social housing development at Byker, and the city council's desire to reduce landfill waste costs, came together to produce the Byker Heat Network development. By June 1992 the then owners Contract Heat and Power (CHP), which is a moderately confusing name in the context, stated in their Integrated Pollution Control (IPC) application that the aims of the heat plant were to "a). Provide heat for the residents of the Byker District Heating Scheme at costs which are lower than those arising from the use of fossil fuels.

"b). Dispose of 33% of the City of Newcastle Municipal Waste by using the extracted light fraction, wood, cardboard, paper and light plastics, as fuel.

"c). Generate electricity for sale to the Non-Fossil Fuel Purchasing Agency under the Government's initiative to produce electricity from Non-fossil and Renewable alternatives."

and also that

> "It is fundamental to the success of this project that the environmental aspects at all times show an improvement by comparison to the existing methods of waste disposal and power generation."

It is clear from this that by 1992 the original aims of the plant — to provide cheap heating for Byker estate residents and to provide cheap waste disposal for the council — were still being maintained in principle at least, along with an additional electricity-generating component. Mobbs questions whether these objectives, taken as a whole, were practical. The at-that-time lack of metering and control rendered it difficult for the residents to maintain stable temperatures, and the heating costs were regarded as high and with a regressive unit costing (the more heat used, the cheaper it is per unit). The combination of the uncorrelated objectives of domestic waste incineration and domestic heat demand creates too much heat when there is no demand, with the residents experiencing an over-hot supply and an inability to regulate or turn it off in summer. The use of light domestic waste as fuel has also been calculated to be uneconomic in comparison to fossil fuels[1]. The viability of the co-generation proposal is a topic that Mobbs doesn't tackle directly, only noting that "In June 1994, ESL applied for planning permission for the '*erection of an electricity generation plant*', but this application was subsequently withdrawn. The position with regard to the planning permission for electricity generation is itself unclear. The company records for ESL, as part of the mortgage agreement on the plant, list a letter from the '*Newcastle upon Tyne Development Corporation*', dated the 19th July 1991, stating that changes to the plant to facilitate electricity generation would not be require [sic] planning permission."[2](original author italics). It is not clear whether such a proposal would have been worthwhile.

It is apparent then that originally the plant was designed to burn municipal waste (Refuse-derived Fuel (RDF)) with residential heat provided as a side-effect. As recorded by Mobbs [129], the Byker Heat Station opened on 21st April 1980 with one boiler. Two more boilers were added in June 1982, and 24-hour operation started in 1983. Apparently,

[1]Mobbs's assessment of heating costs doesn't take into account maintenance costs. It also doesn't price carbon.

[2]Energy Supplies Limited (ESL)

the original boilers were coal-fired designs and had difficulties burning the RDF, and were replaced later. Coal was sometimes used during the 1990s.

A scandal involving refuse-derived ash being used on allotments and for construction in the Newcastle area is well documented by Mobbs [129], and Pless-Mulloli *et al.* [131,132]. Mobbs quotes a Newcastle City Council press release from 7th April 2000:

> "Ash from the Byker Heat Station has been used for the construction of surface footpaths, bridleways and hardstandings at various locations in the city though mainly for paths in allotments since 1994."
>
> "This process was ceased in mid-1999 after fears were raised about the chemical composition of the ash and Newcastle University was commissioned by the City Council, with advice from the health authority, to sample and analyse the ash at a number of allotments. Initial results have now been received from this analysis which show, in some cases, raised levels of some metals and dioxins."

As a result of the ash scandal, the details of which are not reiterated here, the burning of RDF ended in 1998 [133]. The plant then burned coal until conversion of the boilers to natural gas began around 2003, this work being completed by 2005. The three gas boilers are still present and used within the facility today, but their operation is now supplemented by a biomass boiler and a CHP unit both of which were installed in 2012.

2012–2013: Biomass and CHP upgrade As alluded to earlier, one of the main historical criticisms of the heat plant at Byker has been that the heat supplied to the residents of the Byker estate has always been more expensive than heat provided by domestic gas boilers. Figures provided by Mobbs [129] show that, on average, heat network customers were in 2000 paying $1/3$ to $2/3$ more per kWh of heat than domestic gas boiler owners, although this figure does not include maintenance and replacement costs. The original ethos behind the installation of a RDF-burning district heat network was that heating would be "essentially free", which made the subsequent relatively high cost of the produced heat somewhat unpalatable. The volatility of wholesale gas prices also left the residents vulnerable to external fuel market forces, providing an incentive to develop a secondary source of fuel and heat production.

In order to renovate the plant and to reduce these costs for the residents, the BCT embarked on a renovation programme in 2011 and 2012 which would see a 1 MW biomass boiler and 1 MW gas-fired combined heat and power plant installed on the site. Minutes from the Byker Community Trust board meeting in 2012 [134] state that "The first phase [of renovation] — renewal of the main boiler plant and changing the fuel source — could attract substantial funding via the Community Energy Savings Programme (CESP) and secure a grant of approximately £2 million to cover the costs of the proposed works." This would mean that the entirety of the works could be subsidised by Community Energy Savings Programme (CESP) funding. The second phase was to be covered by the Community Trust investment programme. The time-line for the system upgrade was thus primarily driven by the 31st Dec 2012 deadline for CESP funding submissions. It is interesting to note that in the BCT minutes it is stressed that the biomass boiler is not a heat-from-waste option, illustrating the depth of sensitivity still surrounding the ash contamination episode.

The biomass-plus-CHP option was evaluated by the contractor to provide the largest annual heat savings (£236,170) over the current gas boiler configuration. Part of these savings would come from income derived from Renewable Heat Incentive (RHI) payments, and electrical export sales from the CHP unit. The biomass boiler output is capped at 1 MW because of an unusual break-point in the RHI funding; above 1 MW the per-MWh subsidy rate falls from ~2.6p/MWh to ~0.8p/MWh, on the entire energy generated, which would paradoxically make a larger generator less economic. This would seem to be a flaw in the RHI subsidy scheme although no further investigation into this has been undertaken here.

The plant currently operates in a break-even fashion, i.e. the estate residents cover the cost of fuel and operations through bill payments to the BCT. As of late 2015, there had been a 4-year freeze in fuel bills for the residents coinciding with an increase in gas prices, which was regarded as a success for the new plant[3]. Bills are still apparently "slightly higher" than they would be for a household with natural gas heating. Second-stage renewals works in 2016 (described below) were aimed at reducing this discrepancy.

It is of note that the Byker Estate itself acquired Grade II* Listed status in 2006/2007. Listed building status often serves to constrain somewhat the work that can be carried out on that building, although in this case it has not prevented proposed refurbishment, as evidenced by the BCT schedule of maintenance and upgrading.

2016–present: Controls, infrastructure and capacity upgrade A recurring problem with the Byker DH system has been the lack of controls present in the heat network. This has led to over-heated houses, and, as a result of a fixed residential heating charge, over-use of fuel; the residents have been unable to control their heating even if they wanted to, and in any case the flat rate for heating has provided no incentive to be frugal with heating energy. This lack of metering or plant heat controls thus drives up fuel costs and wastes primary energy. There are further complicating factors to the straightforward introduction of metering however. Communications with an officer from the BCT indicate that there is evidence from other UK DH plants having introduced metering and thus decoupled its heating charges from its standing charges and rent, that this can result in increasing non-payment of fuel bills, and a dramatic drop in DH plant revenue. Non-payment of fuel bills is not grounds for eviction in the way that non-payment of rent can be. Community or district heating networks tend to be ideally suited to social housing installations, and so this complication could be a consideration at a national level when planning heat network costing.

[3]Personal communications with the BCT district heating (DH) programme manager

The issues of controls is more straightforward. From 2016 to 2018 the BCT has been upgrading storage tanks, heat substations, house heat controls and plant controls in order to permit a more refined use of the system and bring operational costs down further while improving the residents' comfort. In particular the pipework in general is too small for high demand, and the new controls will help to reduce the cost of generation of the heat (fuel costs) and reduce demand overall. Despite the lack of cost incentive without metering there is nevertheless a comfort incentive to residents, and the new controls will reduce the wastage of heat caused by production when there is very little to no demand, particularly in the summer months.

As well as the controls and infrastructure upgrade the construction of a new 4 MW biomass boiler is planned to deliver another £250k annual saving to the Trust and residents. The new plant will cost £4.5m and would have been subsidised by the Energy Company Obligation (ECO) scheme, which replaced Carbon Emissions Reduction Target (CERT) and CESP in January 2013; however with the removal of the low-carbon incentive from the most recent ECO funding scheme, the BCT is currently seeking other forms of funding including matched European Regional Development Fund (ERDF) funding. A number of risks are still inherent in the construction (including further vulnerability to funding schemes, and site clearance and civil works costs in particular) but the project is in the planning stage. Part of the construction will see some thermal storage attached to the new plant, and private electricity sales to local businesses and potential long-term heat network expansion are also under investigation.

Plant layout and operation The plant consists of three natural gas boilers (3 x 6 MW heat), a biomass boiler (1 MW heat), and a CHP unit (1 MW heat, 1 MW electricity). Figure 4.1 shows a general view of the configuration of the plant. This is also approximately how the plant is laid out physically within its enclosing building.

The biomass boiler and the CHP plant supply the heating system base-load, with the biomass boiler operating continuously and the CHP plant operating from 7am-7pm daily in order to maximise feed-in-tariff revenue and minimise operating and maintenance costs. Per kWh produced these generation units are more expensive to operate than the gas boilers, but the RHI back-tariff and electricity sales to the grid renders them cheaper overall. In 2014 for example, biomass fuel costs were £190k with a RHI back tariff providing £160k to the BCT in subsidy. The three gas boilers now operate only when necessary to provide top-up heat load or to provide heat during maintenance of the biomass boiler or CHP unit; no more than two, and typically only one, will be operating at once, and during summer the single operating boiler will be on an idling schedule.

The plant serves 2000 households on the Byker estate, one primary school, one church, some community buildings and a social services home. Only around ten private households have their own gas heating installed. The extent of the primary heat network is shown in Figure 4.2 which shows the plant (circled number '01'), the piping as a black line, and the heat substations as circled numbers '02' to '14'. The pipe network from the substations

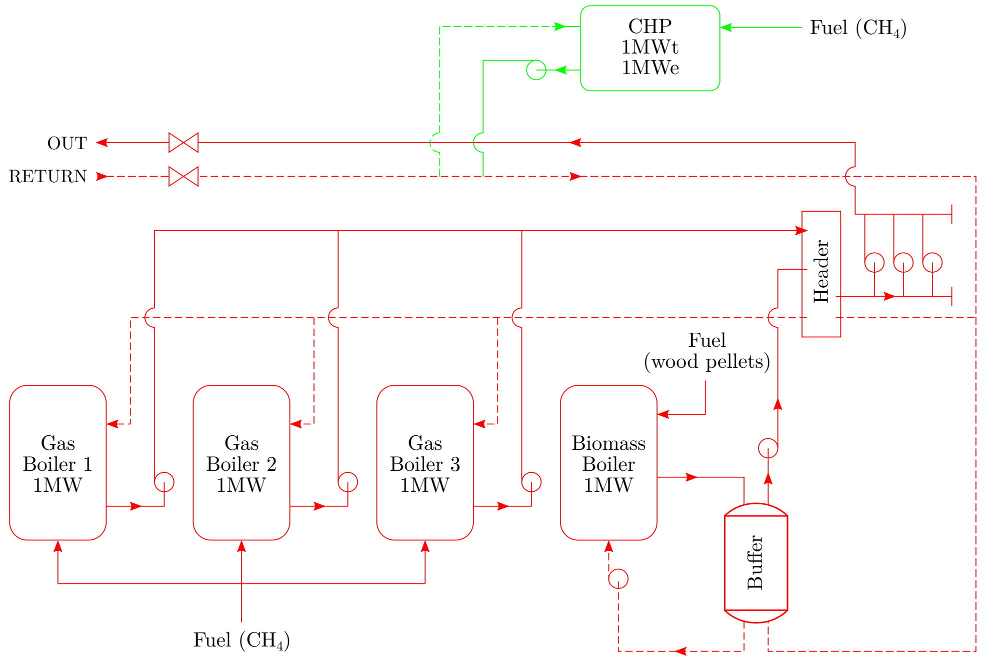


Figure 4.1: Byker heat plant schematic diagram

to the end-users is extensive and not shown. This illustration is used in Section 4.4 as part of the functional and design element extraction exercise, and in Chapter 6where the thermal demand data from each substation collected by the network monitoring system is used to synthesise an overall system demand.

4.2.2 Manchester town hall extension and library

The Manchester (UK) Central Reference Library and attached Town Hall Extension are of interest as a motivating case study as they form part of Manchester's demonstration or living lab contribution to the Triangulum Project, which is a European Smart Cities and Communities Lighthouse Project [135]. The Triangulum project sites are intended to test ideas of how smart cities might operate and what kind of components they might need to function. The results of the Triangulum project include possible models for transport, energy, information and communications technology (ICT) and business systems, as well as how these should be integrated. Only the energy system and its operation within an extended system-of-energy-systems is of interest to this thesis and connections to the other systems are not investigated. The construction and operation of the energy system, and the project trials, were investigated through a series of interviews with staff working for the trials operators Siemens.

The library and town hall extension house a sophisticated multi-energy vector energy system that supplies electricity, heat and cooling to the staff and customers of the buildings. The overall heating and cooling architecture is shown in Figure 4.3; the electrical network is not shown explicitly but it is connected to the various devices and pumps shown. A series of trials being conducted under the Triangulum project examine possible *modes of operation* of the energy system. These modes of operation essentially dictate

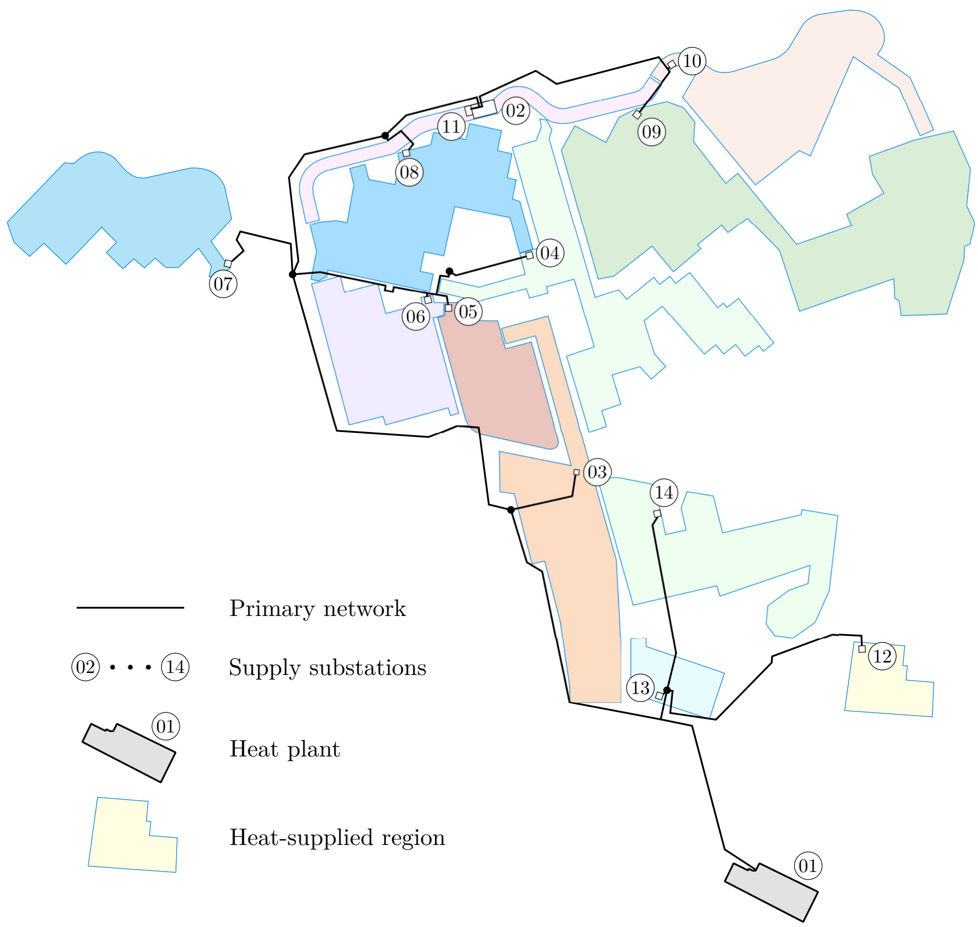


Figure 4.2: Byker heat network — primary system, substations and supply regions

a control policy for the energy system and correspond to a constrained optimisation or control problem. A mode determines an objective function with a set of associated constraints, while additional constraints exist within the system itself. Often constrained optimisation problems are constructed with fairly arbitrary objective functions, but a set of well-defined operational modes would be a useful way of comparing different control or topological schemes in a systematic way. The modes of operation defined within the project are:

- Energy cost reduction by Distribution Use of System (DUoS) charge reduction
- Peak demand flattening
- Renewable energy usage increase
- Carbon emission reduction

The heat produced on-site is managed by a series of control policies. The system is designed to operate in one of three modes[4].

- Absorption cooling mode, which is the system's normal operational mode. Here, heat produced by the CHP engine is used by the absorption chiller to produce chilled water.
- Electric cooling mode, used during chiller maintenance or during a mismatch between cooling demand and supply.
- Business continuity mode, used during a mains supply failure where the system effectively becomes islanded. The CHP unit operates at a practical maximum capacity and supplies electricity to essential services, with all un-needed heat produced being rejected to atmosphere.

The library and town hall extension is an interesting illustration of the difficulty of conducting living lab experiments, which was discussed earlier in this thesis. Because the buildings are in constant active use it is difficult for the trials operators to perform radical experiments with the energy system. Additionally, at the time of the trials the main town hall was undergoing refurbishment and staff were being relocated to the extension, which caused the occupancy pattern within the town hall extension to be in flux. Uncontrollable system parameters such as the occupancy pattern are another difficulty of living lab experiments as they can render a generalisation of trials findings very difficult.

4.2.3 Findhorn Ecovillage

Findhorn Ecovillage is a settlement in Moray, Scotland, near the village of Findhorn and on the River Findhorn that empties into the North Sea between Inverness and

[4]Reference drawing no 1200-NGB-SM-56-ALL01 10/12/2013 NG Bailey

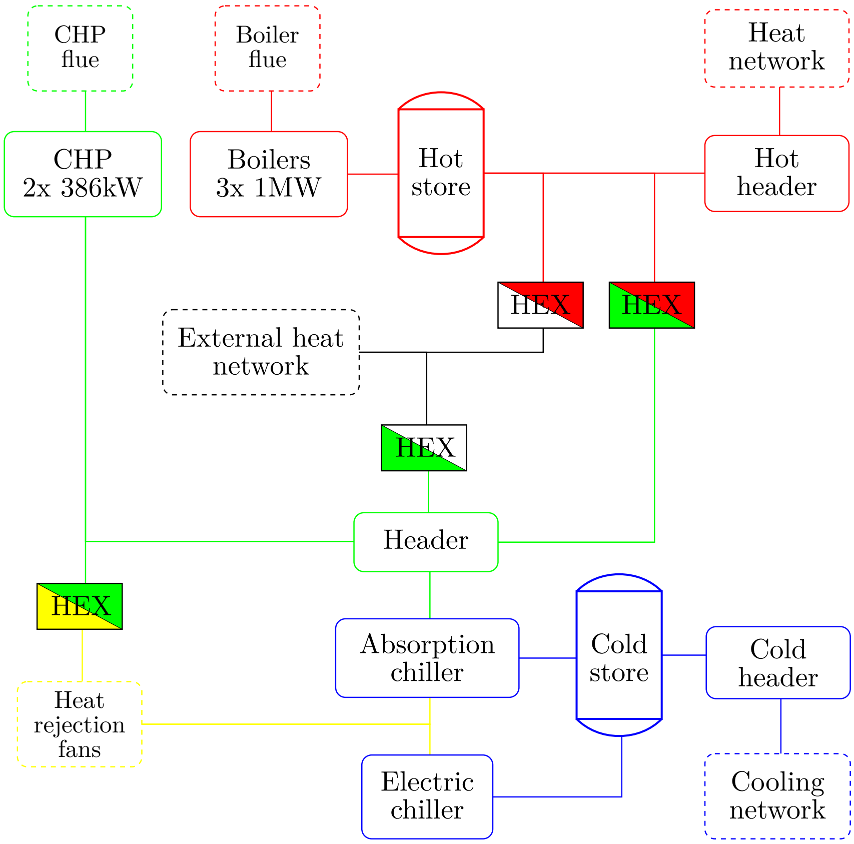


Figure 4.3: Manchester tri-vector supply system schematic diagram

Lossiemouth. The settlement was founded initially in 1962 as an experiment in sustainable habitation and low-environmental-impact existence although, at least to begin with, it was not envisioned as an "intentional community" [136]. As of 2018 the Ecovilalge consisted of 102 domestic dwellings and 20 commercial buildings, and with 20 new houses being built. It combines low-carbon and environmentally-conscious enterprises in building codes, food provision, renewable energy and water systems as well as in social practices and values, in order to demonstrate a sustainable way of organising human living. Findhorn Ecovillage forms a case study within the scope of National Centre for Energy Systems Integration (CESI), an academic and industrial partnership head-quartered at Newcastle University. Details about the village including systems diagrams, housing stock, monitoring data and information about the energy supplies were available through an extended working partnership with the project undertaken during the course of the research described in this thesis. The Ecovillage participates heavily in energy monitoring, renewable energy trials and educational programmes and can be regarded as an example of a closed living laboratory.

As an experiment in sustainable existence, Findhorn Ecovillage's development is predicated on finding low-impact solutions to energy and material supply while maintaining a regular quality of life for the inhabitants. To achieve this the village's energy supplies are designed as a mixture of external energy connections and embedded energy generation. Electricity for lighting, consumer goods, commercial processes and heating by direct electric element and heat pumps is supplied from an 11kV/400V grid connection through two secondary substations, and augmented by two renewable energy sources: an on-site wind array comprised of three 225 kW turbines; and 30 domestic PV installations supplying a total of 70 kW generation capacity. Primary heating for most residents is supplied by combustion of fuels, with imported oil and low pressure gas (LPG) forming the bulk of the supply. Domestic wood burners, three district heating networks, and solar domestic hot water (installed at 60 houses) make up the remainder. There is no gas grid connection; heating oil and gas is supplied by tank and bottle. Other than heating fuel containment and hot water buffering within individual dwellings, commercial buildings and DH plant, no other primary energy storage was present on the site during the period of study (2018)[5]. A map of the Ecovillage with the constitutive components of its energy system by region is shown in Figure 4.4 (based on data courtesy of the Findhorn Foundation and the Centre for Energy Systems Integration).

Findhorn Ecovillage's residents are reported to have an ecological footprint that is half of the UK average and, out of those communities which have been measured, the lowest in the industrialised world [137]. The Ecovillage is therefore often presented a worthy exemplar for the construction and operation of a sustainable settlement, both as it stands in the present day and under certain imagined futures [138]. Under the assumption then that Findhorn Ecovillage can be used as a potential model community for future energy systems within the UK, this thesis leans on the Ecovillage as a motivating case study for the exploration of multi-vector energy systems. Note that it is not clear whether the spiritual and other alternative community aspects of Findhorn Ecovillage are a pre-requisite to the development of such a community, nor to what degree the Ecovillage's hinterland and external connections for trade and development are sustainable in themselves, but these topics are not explored further within this thesis. Work by Forster [139] suggests that the ecological and spiritual aspects of the village are not necessarily interdependent.

Findhorn Ecovillage has also formed part of a study into demand response through novel energy control architecture. The Orchestration of Renewable Integrated Generation in Neighbourhoods (ORIGIN) project [140] investigated the use of financial incentives and automated control to encourage an increase in community electricity consumption when export of the on-site wind generation to the national grid would otherwise have been curtailed by external grid constraints[6]. The project final report concludes that "ORIGIN highlighted that, even with the encouragement of financial incentives, there is a need for repeated engagement with the end users to relate the ongoing impact of consumers' their participation in the demand response management of their energy lifestyles", and that "The project results suggest that a viable business case can be made for a forecast informed actuated community scale demand response initiative if the community can trade

[5]Refer to `http://www.ecovillagefindhorn.com/` and the CESI document *CESI Findhorn Ecovillage Study 2017-06-19 Findhorn Ecovillage Study: System Description*

[6]See https://cordis.europa.eu/project/id/314742 and also http://www.ectp.org/project-database-list/project-details/orchestration-of-renewable-integrated-generation-in-neighbourhoods/ for official details.

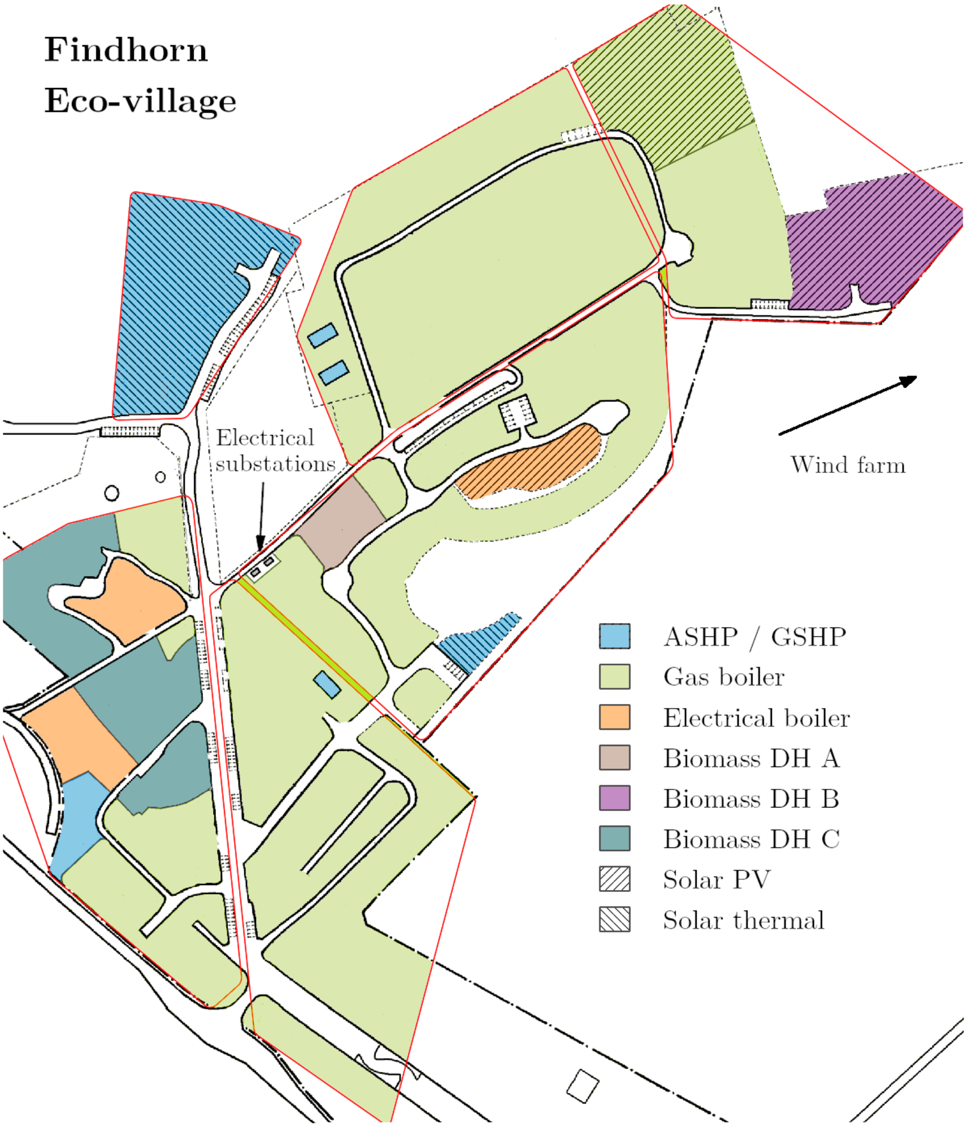


Figure 4.4: Findhorn system component map

with the local DNO.". Some of the automated demand response mechanisms were to use the generated electricity to provide space and water heating, which can be categorised as a wrong-time, wrong-type energy issue (as described in Chapter 2) within the Ecovillage. While the financial and control mechanisms are not explored further in this thesis, the project's conclusions reinforce the idea that a form of cross-vector conversion and potentially storage is important for semi-islanded or semi-autonomous energy networks. The specific energy flows, equipment and demands within the Findhorn Ecovillage are investigated in more detail in Section 4.4.

4.3 Expert perspectives on thermal networks

As mentioned in Chapter 2, the literature surrounding district heat networks in the UK suggests a troubled past. Further evidence from the case study presented in Section 4.2.1 shows the progress that is being made but also provides some deeper reasons behind the relative difficulties that district thermal networks have been faced with. While the main issues in the past have been with thermal networks the barriers and opportunities extend to all forms of district energy.

Thus in order to obtain a flavour of the mood surrounding district energy in the UK, six informal interviews with industry and local government stakeholders were conducted. These stakeholders were: a district energy programme manager; a director of a large-scale commercial heat pumps manufacturer; a city council energy planning manager; two district energy operations and project managers; and an innovation manager from an international engineering company.

The interview process was informal, with a small number of participants, and so no formal coding, analysis or evidential system has been used. Taking the interviews as a whole however, it was nevertheless possible to identify six general themes, these being: a comparison between the UK and international approaches; incentives and drivers; government policy and organisation; challenges for future development; the role of storage in district energy schemes; and the nature and importance of operational objectives. Contributions from the interviewees as well as relevant contributions from literature have been gathered under each theme, the presentation of which forms the rest of this section. A possible avenue of further work beyond the scope of this thesis to investigate each of these themes more comprehensively is discussed in Secion 7.4.

4.3.1 International comparison

Scandinavian countries such as Sweden and Denmark are regularly held to be exemplar developers of district energy schemes, and are regarded as representing a model that the UK should be following. One interviewee suggested that the experience of these countries has been different to that of the UK, in that they did not have the same reserves of North Sea gas as the UK has had. Also, local pollution caused by the burning of oil for heat in Scandinavian countries resulted in their governments investing in heat networks as an alternative to individual residential heating devices.

Hawkey [34] shows that district heating has also been more successful in the Netherlands and Germany because of their more autonomous local government arrangements. While recent changes (see next section) appear to be increasing the flexibility of UK local government in this regard, the permissible schemes are still subject to restrictions which the more autonomous northern European local governments are not subject to. The net effect is that control of development in the UK is still mainly centralised — with national government deciding where flexibility is permitted — creating a subsequent potential lack of ability to tailor investment at a regional level, precisely where the ability to take advantage of the local environment and opportunities (physical, societal, economic) is necessary.

4.3.2 Past and current incentives and drivers for constructing district energy schemes

With reference to the Byker District Heating scheme as a case study, two interviewees indicated that government incentives are the prime driver of investment. Reducing energy bills for social housing residents by reducing dependency on a volatile and increasing gas price, as well as receiving generation feed-in-tariff revenue from renewable energy sources, are the main areas of concern for the operators of this scheme, and it is reasonable to expect that such concerns are to be a common feature of such schemes in the UK at present. Side effects of such a strategic approach is that plant procurement is opportunistic and short-term (particularly within the span of a particular government incentive scheme), and that renewable incentive scheme technical limitations (for example, on minimum or maximum installed capacity, or on tariff structures) are not necessarily aligned with the technical and engineering requirements of the particular generation site and its attached distribution network.

A focus on "getting pipes and wires in the ground" was reported by one interviewee as being of crucial importance, moreso than the design of primary energy conversion plant, because this aspect of infrastructure development is the most disruptive to the community and the most difficult to gain governmental planning approval for. The planning of the energy production plant itself tends to be a secondary consideration because in general the plant is situated within an industrial location and can be changed "relatively" easily; but the installation of infrastructure is difficult to do and is very disruptive to the local population.

Climate change concerns are naturally the main overall driver of change, creating the resultant commitment to district energy as a means to achieve system energy efficiency improvements. In the UK currently about 2% of district energy consumption is satisfied by district heating. The government has committed to a strategy of ensuring that district heating supplies 20% of the UK's heat demand by 2030 (which would fall within the 5th carbon budget) [141]. In order to stimulate development, £300m funding for district energy was provided in 2015-2016, this amount being aimed at funding local authority pilot schemes and development projects.

One interviewee stated that a notable difference from past efforts to expand district heating was that Chartered Institute of Building Services Engineers (CIBSE) and the Association for Decentralised Energy (ADE) (formerly the Heat Trust) has produced a code of practice and standardisation for new district energy networks [142]. The interviewee described past district heating developments as having had a tendency to have been bespoke or one-off designs, implemented with unregulated construction and operation. This lack of standardisation or compliance with industry best practices in design and development has, according to the interviewee, seen volatile prices and poor performance occurring regularly across the heat networks estate, further leading in some cases to district energy systems gaining a level of notoriety and mistrust among their customer base.

The CIBSE / ADE Code of Practice is intended to propagate a level of professionalism and standards in order to prevent such low-quality development eroding trust in district energy systems.

It is anticipated that the diminished supply of North Sea gas by 2030 will result in few or no new gas boilers (in their current form at least) being installed in the UK. One possible consequence of this is that domestic heat production will take the form of a small combi-boiler for instantaneous demand, and a heat pump for the heat baseload[7]. This does rely on heat pumps becoming acceptable to UK domestic users, because their physical size and method of operation compared to the domestic gas boiler present a behavioural and cultural barrier. An alternative possibility is that instead of heat pump installation being within individual households, large-scale heat pumps are adopted to supply district heat networks. One interviewee noted that the driver behind the take-up of large-scale heat pumps (many over 2 MW and up to $\sim$ 10 MW) is a straightforward financial assessment. Heat pumps can be operated by the half-hour within the electricity industry's settlement framework, making it possible for the owners to take advantage of market price shifts. Within this environment heat storage also then becomes an important consideration.

Local drivers for the construction of district energy schemes can emerge from a diverse range of sources. Government schemes which result in cost-effective energy production for fuel-poor residents from renewable heat and power sources are attractive. For such locations, as noted by one of the interviewees managing a district heating scheme, generation revenue and feed-in-tariffs enable the lowering of bills for residents while benefiting from large capital investment subsidies. For these operators and managers, the available incentives, the limitations that the incentive schemes place on system design (such as power or energy limits to subsidised generation), and the lifetime of the incentive schemes, both in terms of the initial application deadline as well as the revenue period, will form critical elements of the system objective and cost evaluation.

4.3.3 Government policy and organisation

One interviewee noted that UK local government has indeed become more commercially-focused and that energy has become "municipalised". Local government is now able to break into the energy market, and it is assisted in doing so by its responsibilities to its residents and tenants, as well as by a broader-scale distrust of the main UK energy suppliers. In 2010 the then Energy Minister Chris Hune was responsible for changing local government regulations to allow, for the first time, local government to receive revenue from local generation sources, CHP among them. The main restriction on this revenue is that the generation must be heat-led, but nevertheless this represented a significant break from past policies and restrictions on local authorities' independence with respect to the profitability and cost of district energy schemes.

[7] Such a possibility has been the subject of a study by National Energy Action (NEA)

In 2013 the City Deals scheme (following the demise of the Regional Development Agencies (RDAs)) was instituted to provide money to municipalities for appropriate investment in low-carbon projects piloting the feasibility of district energy [143]. Also in 2013 the UK government through the Department of Energy and Climate Change (DECC) published its future of heating strategy [141]. As part of this the DECC heat network delivery unit was charged with investing £9m into feasibility studies. As a result local governments are now able to raise revenue out of district energy. For example, Nottingham and Bristol councils have been able to offer "white label" energy supplies to other cities and towns, in competition with existing energy suppliers.

One interviewee noted that local governments have now learned to construct more robust arrangements for their district schemes. By operating a joint venture (stand-alone business) with a long term (e.g. 40 years) partner, local government is able to share the risk of the enterprise. This is in contrast to arrangements in the past where facilities have been operated wholesale by third parties and have often ended unsatisfactorily with the removal of profits and a lack of investment.

4.3.4 Challenges for future development

District heat schemes in particular tend to be used to supply densely-populated social housing areas, municipal and community properties, and light industrial and office spaces. Some facilities, such as hospitals, often maintain their own CHP plant and can add to the local supply of heat and power. Heat lost during distribution is an important aspect of the cost of a district heat and cooling system, and densely-populated locations offer excellent opportunities to reduce such losses. Privately-owned suburban properties, currently heated with individual gas boilers that are occupier-owned, are likely to prove more resistant to a shift to communal end-use heating supply. Moving heat production to a more centralised location, and changing the energy supply vector from gas to heating and cooling, will be a difficult obstacle in the UK, culturally and psychologically. Some lessons can be learned from Scandinavian countries which have not had the benefit of a historically-reliable gas supply.

4.3.5 The role of storage in district energy schemes

It is apparent that there is no "one size fits all" approach to storage in district energy schemes. The application of a particular storage technology can be an opportunistic one, and dependent on local factors such as geography, geology, and the existence of other industries and facilities (either in use or abandoned). Some examples provided by the interviewed experts are:

a) In Vojens, Denmark, an old salt mine with a 203,000 m^3 capacity has been converted to a seasonal thermal store, capturing summer solar energy and releasing it in winter. This type of storage is naturally site-specific, but where available is extremely valuable for seasonal supply-side storage.

b) Rivers are often used as a low-temperature source for heat pumps. The temperature of a river is generally perhaps slightly lower than ideally desirable, but rivers (in cities especially) have an enormous heat capacity and can be regarded as a constant temperature cold-side reservoir. This makes the efficiency of river-supplied heat pumps more predictable, leading to simpler designs and more reliable cost and revenue estimations. A potential ecological effect of river-sourced heat pumps however is that the downstream water is cooled as a result of the transfer of heat through the heat pump. For example, Metcalfe *et al.* suggest that a 0.51 °C reduction in downstream water temperature for a 4.61 MW heat pump output from the river Wensum through Norwich, a moderately-sized city in the UK. 4.61 MW is a small contributor to the heat requirements for such a city, and thus it seems unlikely that a significant amount of overall heating demand can be provided by river-sourced heat pumps without creating a severe ecological disturbance.

c) Sewers and mines are able to provide a constant temperature heat source for heat pumps; their concentrated nature makes them suitable for district schemes only.

d) In Cranbrook, Exeter, UK, a demonstration project using a 2000 sq. m solar array which supplements an existing gas-powered district heating scheme and combines with heat pumps is under evaluation. A 55 °C store is supplied from the solar thermal array, cooling from 55 °C to 30 °C to heat the network overnight. Its drawback is that it is expensive, and it attracts no RHI. Additionally the large ground area needed for the solar panels restricts the possible deployment opportunities.

e) In Heerlen in the Netherlands a mine water storage scheme uses the mine water as a thermal store for heat produced during the cooling of a data centre, among other sources; the scheme does not use a conventional centralised plant, instead receiving heat from a variety of sources attached to the network.

Heat pumps in particular almost certainly require thermal storage facilities to operate to the satisfaction of heat consumers. Heat pumps operating in a district energy system that take advantage of half-hourly electrical price fluctuations will absolutely require some form of storage, either at the supply or the production side of the plant. Network thermal stores (e.g. as exhibited in Scandinavian systems) permit heat pumps to be worked harder in their optimal operating region, with the heat pump being controlled through a simple on-off cycle. Storage acts as an inertial element in the system which serves to smooth the fluctuations caused by this on-off cycle. One of the interviewees expressed an interest in the possibility of using the building fabric itself as a storage option for heat-pump supplied facilities. This is an open research question.

Whether or not storage is useful within a district energy system depends very much on what question is being asked and the perspective of the system operator. A large number of measures of efficiency, optimality or cost effectiveness can be defined and which are each important to different observers of the system. An examination of the usefulness of a multi-vector storage that is used to transfer energy between energy domains will be explored in Chapter 6. The main evaluation criteria considered in this model will be system efficiencies and possible side effects created by using the storage device.

Local conditions also absolutely affect the range of storage solutions available to a district energy scheme. Some technologies might generally always be available, such as off-the-shelf latent or sensible heat storage or chemical batteries; while others, for example geologically-based storage, will depend upon the site. The performance of the building stock itself also factors into the storage design, helping or hindering the solution depending on installed levels of insulation and the types of materials used in construction.

4.3.6 Operational objectives

Intriguingly, the purported goals of an energy system were found to be as diverse as the selection of interviewees. Financial concerns tend to be most important to city management and governance, especially with reference to tackling issues of fuel poverty, customer billing, and public sector expenditure. In general stakeholders were interested in seeking some form of "optimal" performance for a district energy system, with the meaning of "optimal" varying depending on the respondent. One particularly interesting line of thought that emerged from one interviewee was that of optimising for "modes of operation". A town- or city-wide energy system, or a large industrial location constituting its own energy system, may not require only a single optimisation objective, nor even a static multi-target objective function, but could require "modes" of operation which are used in particular circumstances. For instance, operation under an islanded situation may be a mode; or a high-resilience mode might be required for a particular operation-critical purpose. Other modes might emphasise financial considerations, or environmental commitments. This concept was illustrated in the case study in Section 4.2.2 and will inform some of the operational conditions used by the demonstrator model in Chapter 6.

4.4 Identification of FRs from the Motivating Case Studies

An integrated energy system probably qualifies as a *large flexible system* by Suh's definition [116]. A large flexible system is one which has a large number of FRs at the highest level, but which must only satisfy a subset of the FRs at any given time. Different FR subsets are required to be satisfied at different points in time, and Suh states that such systems must be able to reconfigure themselves in order to be able to satisfy the different FR sets during the lifetime of the system. Lubega and Farid [26] concur with this description, although they do not attempt to provide a fully-complete knowledge database of solutions. Large flexible systems may have multiple DPs which are able to satisfy each FR. For example, in an integrated energy network a "provide electricity" FR can potentially be supplied by a grid connection or by a solar panel, or a number of other technologies. The definition of what qualifies as a "good design" is modified for large flexible systems.

Ordinarily in an axiomatic design process the generation of the design will proceed roughly linearly from the specification of the customer attributes, to the subsequent identification of functional requirements, through the determination of design principles to meet these functional requirements, and finally to the devising of process variables in order to physically realise the design. However this thesis proposes that by examining the motivating case studies as exemplar energy systems, a typical set of design principles can be composed, and from this a set of functional requirements can be deduced. Essentially this is a reverse engineering process using existing real system examples to produce a set of functional requirements for a general integrated energy network.

The following sections describe the decomposition of the three case study systems to create a set of possible energy network components and functions. This is done by examining the system descriptions presented earlier, particularly with reference to the system schematic diagrams (Figures 4.1, 4.2, 4.3 and 4.4) to establish the physical devices present in each system, which represent the system DPs. This decomposition is then "reverse mapped" to discover the FRs that these devices provide. The final decomposition is given in Table 4.1. No *a priori* set of functional requirements was contrived or assumed before starting the decomposition; instead, this set was built up through discovery while examining each system component in turn.

In the following sections, *italics* are used to highlight a design parameter (DP), while text in **bold** identifies a functional requirement (FR). Note that minor energy supply connections such as for services, instrumentation, monitoring and so on are not included in this analysis.

4.4.1 Byker Heat Network FRs

The larger components of the heat network plant are the *gas boilers* and *natural gas CHP engine*. Both of these types of devices **produce heat**, and the CHP engine also is used to **produce electricity**. The gas boilers and CHP engine are both supplied from an *external gas grid connection* which is used to **distribute fuel (natural gas)**, while the CHP engine is additionally connected to an *internal electrical network*, in turn connected to an *external electrical grid connection*, both of which are used to **distribute electricity**. The gas boilers have a *natural gas boiler flue* and the CHP engine has a *natural gas engine flue*, both of which are used to **remove waste heat**. Additional cooling of the CHP engine is achieved by an array of *cooling fans* which also **remove waste heat**.

The bulk of the base heat demand for the heating circuit is supplied by the *biomass boiler* which is again used to **produce heat**. The fuel for the biomass boiler comes from a *biomass hopper*, the function of which is to **distribute biomass**. The supply chain for biomass beyond the boundary of the hopper is not considered further, other than to regard it as part of the biomass distribution system. Lastly within the plant there is a *hot thermal buffer water store* which serves to **store heat (short-term)**. A series of *electrical pumps*, again connected to the *internal electrical network*, serve to **distribute heat** along with the *primary heat loop*, which consists of the piping and valves of the water circuit.

Outside of the plant, on the heating network loop, the primary heating loop is connected to a series of *secondary heat stations*, which **transform heat** to a state suitable for distribution on the *secondary heat loop*, the function again of which is to **distribute heat**. The secondary heat loop is finally connected to individual buildings through *dwelling heat exchangers* which also **transform heat**, at which point a **consume heat** function can be assumed to occur in the *dwelling*. The dwelling heat exchangers can be considered to lie on the system boundary and thus how consumption happens beyond this point is not part of this decomposition. Dwellings are connected to the external electrical grid and **consume electricity**.

4.4.2 Manchester town hall extension and library FRs

The Manchester system is more complex than the Byker one; it contains more energy vectors and more conversion processes. Three *natural gas boilers* **produce heat** and their *natural gas boiler flues* **remove waste heat**. Two *natural gas CHP engine* units also **produce heat**, and additionally **produce electricity** while their *natural gas CHP engine flues remove waste heat.* A *hot thermal buffer water store* is used to **store heat (short-term)** but there is an additional *hot water store* which provides a **store heat (longer term)** function. The CHP engine requires cooling and is connected to a *heat exchanger* (for **transforming heat** and subsequently to an array of *heat rejection fans* which allow the CHP engine to **remove waste heat**.

The natural gas boilers and the CHP engine are both connected to a *natural gas grid connection* which **distributes natural gas**; the CHP engine is additionally connected to an *internal electrical network* and subsequently to an *external electrical grid connection*, both of which **distribute electricity**. The internal and external electrical networks are joined through an *electrical transformer* which **transforms electricity**.

The heat produced by the boilers and CHP engine enters a *primary heat loop* which **distributes heat**, with the assistance of *electrical pumps* connected to the *internal electrical network*. The primary heat loop is also connected to a *heat exchanger* which **transforms heat** into an *external heat network*, which also has the purpose of **distributing heat** to locations outside of the boundary of the network. The external heat network is connected through a *valve* which can be used to **isolate external heat distribution**.

The main feature that is different to the Byker system is the addition of a cooling system. An *absorption chiller* and an *electric chiller*, both powered from the internal electrical network, are used to **produce cold**. A *cold water store* allows the system to **store cold (longer term)**. These devices are connected to an *internal cooling network* which **distributes cold** to the building complex. Excess heat from the *chiller exhaust* is connected to the heat rejection fans which again **remove waste heat** from the system.

4.4.3 Findhorn Ecovillage FRs

The Findhorn network is of a larger scale than the Manchester one and includes more variety of technologies. The system serves to **produce heat** primarily through three *biomass boilers* which use *stored wood* as fuel (**distribute biomass** function). Heat is supplied to residents through *heating loops* which **distribute heat**; the residents then **consume heat** within their dwellings. A *biomass boiler flue* is used to **remove waste heat** in the produce heat process. A small natural gas CHP engine **produces heat** and **produces electricity**, the heat being supplied to a small group of residents through a *heat loop* (**distribute heat**).

The Ecovillage is connected to an *external electrical grid connection* which **distributes electricity** through an *electrical transformer* **transforming electricity** to be used in the village's *internal electrical network* (**distribute electricity**). A number of devices are connected to the internal electrical network. Solar photo-voltaic (PV) installations on residents' dwellings are used to **produce electricity** for the internal electrical network, as are solar photo-voltaic / thermal (PV/T) installations which also **produce heat**. Heat from the PV/T installations is consumed within the dwelling (**consume heat**). An on-site *wind park* consisting of a number of wind turbines **produces electricity** for the internal network. All dwellings on the site **consume electricity** from the internal electrical network.

In addition to the biomass boilers a number of other heat sources exist. *Heat pumps* are powered from the internal electrical network and **produce heat** for consumption at a dwelling level. Some dwellings use *propane burners* to **produce heat** for single dwellings; the supply of *propane fuel* is from bottles and can be regarded as part of an external **distribute fuel (propane)** function.

4.4.4 Summary of FR identification process

The FR decomposition exercise above has generated a set of functional requirements for an integrated energy system. These are

- produce heat
- produce electricity
- distribute fuel (natural gas)
- distribute electricity
- remove waste heat
- distribute biomass
- store heat (short term)
- distribute heat
- transform heat
- consume heat
- consume electricity
- store heat (longer term)
- transform electricity
- isolate external heat distribution
- produce cold
- store cold (longer term)
- distribute cold
- distribute fuel (propane)

These FRs re-occur with different DPs and in various ways in the different systems; a variety of devices are commonly available to meet each FR and the specific one used depends on other design and customer parameters (e.g. cost, operating region, performance etc.) which are not covered in more detail in this thesis. The useful outcome of the FR decomposition exercise is that it isolates the FRs from any actual technology and can focus the purpose of an integrated energy network on what functions it needs to provide to the users of the system, independent of any particular solution. By concentrating on function the fundamental operation of the system can be understood without bias, and appropriate technologies can be procured or researched as needed to fit the performance requirements.

Study	Technology (DP)	Function (FR)
Byker / Manchester / Findhorn	Ext. electrical grid connection	distribute electricity
Byker / Manchester	Ext. nat. gas grid connection	distribute natural gas
Byker / Manchester / Findhorn	Natural gas boiler flue	remove waste heat
Byker / Manchester / Findhorn	Natural gas engine flue	remove waste heat
Byker	Secondary heat station	transform heat
Byker	Dwelling heat exchanger	transform heat
Byker / Manchester / Findhorn	Electrical transformer	transform electricity
Byker / Findhorn	Biomass boiler	produce heat
Byker / Manchester	Natural gas boiler	produce heat
Byker / Manchester	Natural gas engine	produce heat / electricity
Byker / Manchester / Findhorn	Heat loop	distribute heat
Byker	Secondary heat loop	distribute heat
Manchester	Cooling loop	distribute cold
Byker / Manchester	Hot thermal buffer water store	store heat (short-term)
Manchester	Hot water store	store heat (longer-term)
Manchester	Cold water store	store heat (longer-term)
Manchester	Absorption chiller	produce cold
Manchester	Electric chiller	produce cold
Findhorn	Solar PV	produce electricity
Findhorn	Solar PV-T	produce electricity / heat
Findhorn	Heat pump	produce heat
Findhorn	Propane burner	produce heat
Findhorn	Wind park	produce electricity
Byker / Manchester	Cooling fans	remove waste heat

Table 4.1: DP to FR mapping for the three case studies

4.5 A system reference model

4.5.1 Representation

The commonality set of functional requirements extracted from the case studies presented suggests a systematic approach to defining integrated energy systems. An appropriate representation would capture the general nature of the primary energy systems and their interconnectedness, and allow a detailed physically-based analysis. It would also contain the essential elements of the system such that general behaviour can be deduced and the effect of loads, perturbing effects, and structural changes can be calculated. Such a representation is commonly referred to as a *reference model*. Such models exist in for example computer networking (OSI network model [144]) and electrical distribution networks (IEEE reference network models [145]), however no such reference model exists for an integrated heating, cooling and electrical network, particularly with the inclusion of multi-vector storage at the junction of the three domains.

Work by Saloux *et al.* [127] and Frank *et al.* [146] in classifying electric heaters, heat pumps and thermal collection systems in integrated energy systems demonstrates a systematic approach to a configurable system architecture. The methods described in these papers are limited by the range of applications presented, and a more generally applicable approach is required to describe a broader integrated energy system. Lubega and Farid's 2014 and 2016 papers [19, 26] explore the intersection of two energy systems to form a larger and comprehensive integrated "energy-water nexus". In their work they suggest using a system-of-systems approach to define a reference model for such systems, in order to capture the complex interactions between the two sub-domains and to explore the wider behaviour that results and that is not visible when studying either system in isolation. SysML is used as the language to define their system reference model. The central foundation of Systems Modelling Language (SysML) lies in three main parts, which are familiar from systematic design principles [116, 147] that is: specification; form; and function. In SysML these are termed *requirements*, *structure* and *behaviour*. Although any representational form can be used in a realisation of the systematic design principles, SysML has the advantage of being a mature and well-recognised language for describing model-based systems engineering problems. Using the formal language of SysML enables the development of a generalised form for the individual and combined district electricity, heating and cooling networks found in integrated energy networks, providing a consistent framework for the development and connection of physical component models and the exploration of variant designs and system parametrisations.

The difficulty in attempting to capture the essential form and function of a system without using a formal language is addressed by Friedenthal *et al.* [117]. The main traditional alternative to the use of a formal language is to adopt a document-based approach, which has a number of limitations. Requirements, analysis and design elements are distributed across multiple physical documents, making it difficult to maintain the consistency, completeness and accurate relationships between them. The degree to which elements are included or excluded from the system definition depends upon the bias, knowledge and interest of the individuals compiling the system definition, making the document body as a whole vulnerable to an *ad hoc* approach. Even given a rigorous documentation management scheme, synchronisation of document elements and maintaining the relationship between requirements and design at different levels of the document hierarchy is difficult.

Without a model-based approach that formalises the fundamental purpose of the system and how this purpose is to be met, details of implementation (the DP set) can unwittingly become the driver of the design rather than the solution. In studies of existing systems, the current designs and technologies involved can present tempting "obvious" solutions, preventing the discovery and understanding of alternative and innovative concepts. With reference to the systems considered in this thesis, the author has found that integrated energy systems debates often revolve around the electrical network and its technologies, despite the provision of heat representing a much larger challenge to the system. The electrification of heat is then often taken as a natural and obvious approach when in fact the link between the function of the system — to provide energy in multiple vectors — and the realisation of that function through particular types of devices is not actually well-established.

4.5.2 System boundary

A system to be modelled and studied cannot be infinitely large. A *system boundary* must be defined that specifies what is inside and what is outside of the system of interest. The flow of information, material and energy across the boundary is also an important consideration and must be determined in as much detail as is necessary. In energy system studies, the modelled system will rarely be isolated and will be connected to a larger network of energy supply and demand. The externally-connected systems operate as a load-balancing mechanism for the modelled system — supplying or absorbing energy according to the shortfall or abundance of energy supplied within the system — but other forms of energy and information exchange can take place at the boundary. For instance, the modelled network may be able to act as a buffer energy store providing services to the wider networks. Such services include the absorption and supply of energy in itself as demand-side response service, frequency-response services for electrical networks, and carbon-reduction strategies (where the flow across the boundary is financial), among others. A taxonomy of some of the sorts of flexibility services that can be offered by a type of energy system termed a smart local energy system (SLES) are explored by Wardle *et al.* [20] and Mullen *et al.* [148]. In these works the authors consider the services that the system may offer or receive both internally and externally, with the externally-connected services requiring a definition as part of the system boundary. Naturally, the expected cost or revenue of a system-supplied service across its boundary is a very important factor in establishing the financial viability of the system flexibility services.

The system boundary must be large enough to capture the essential behaviour and interactions within the system, but it must also be small enough to allow meaningful conclusions about the behaviour to be drawn. Boundaries may be geographical, conceptual, political, or based on some other important feature of the system. This thesis is mainly concerned with boundaries based on energy vector and geography.

Section 2.2 examined how urban or local energy systems can be identified and defined in the literature. A pragmatic and functional solution to the definition of such a system proposed by Keirstead and Shah [25] is adopted in this thesis; that is, an integrated energy system in an urban environment is one with an open thermodynamic boundary.

This solution also contains an understanding that the term "urban" or "local" retains its common-sense meaning of a settlement of somewhat finite size and connectivity, even if the exact geographic boundary is something which cannot be precisely determined. It was also noted in Section 2.2 that Lubega and Farid also proposed a sensible definition that the sub-systems to be included within the system boundary should not be subject to an external marketplace [26].

The three case studies presented in this thesis also provide guidance as to what should be considered a boundary for integrated energy systems. In examining the case studies it may be useful to borrow a term from computing science. "Duck typing" refers to a method of type classification that defines the features of a group of objects from the properties of those objects, so that if a new object exhibits those properties then it can be considered to be of that class[8]. Similarly, under the assumption that the case studies are recognisable as integrated energy systems, then their boundaries can be assumed to define a generic system boundary, and other systems which look like the case study reference systems can be considered to be classified by the same type of system boundary. This approach avoids the need for a pedantic and unworkable classification scheme. Therefore, using an approach similar to that presented by Lubega and Farid, the system boundary for a district-scale integrated energy system which contains the three case study networks is given in Figure 4.5.

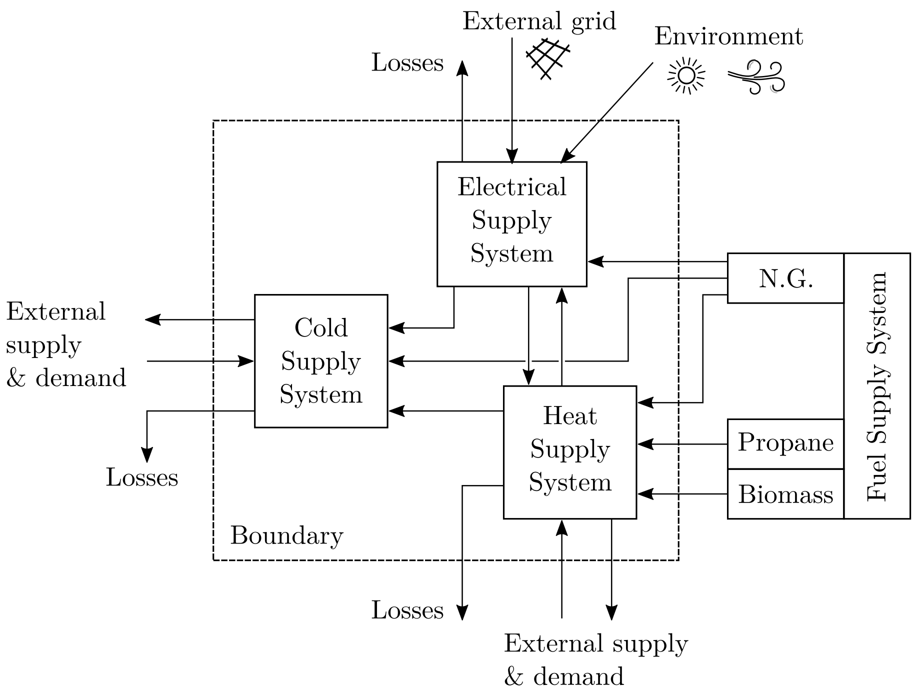


Figure 4.5: Integrated energy system boundary

Using the principles of axiomatic design and the representational techniques of SysML, a systematic decomposition of the tri-vector (heating, cooling and electricity) energy system can then be undertaken using the case study components as a reference point. Figures 4.6, 4.7 and 4.8 show the resultant SysML activity diagrams.

[8]If it walks like a duck, swims like a duck, and quacks like a duck, then it probably is a duck

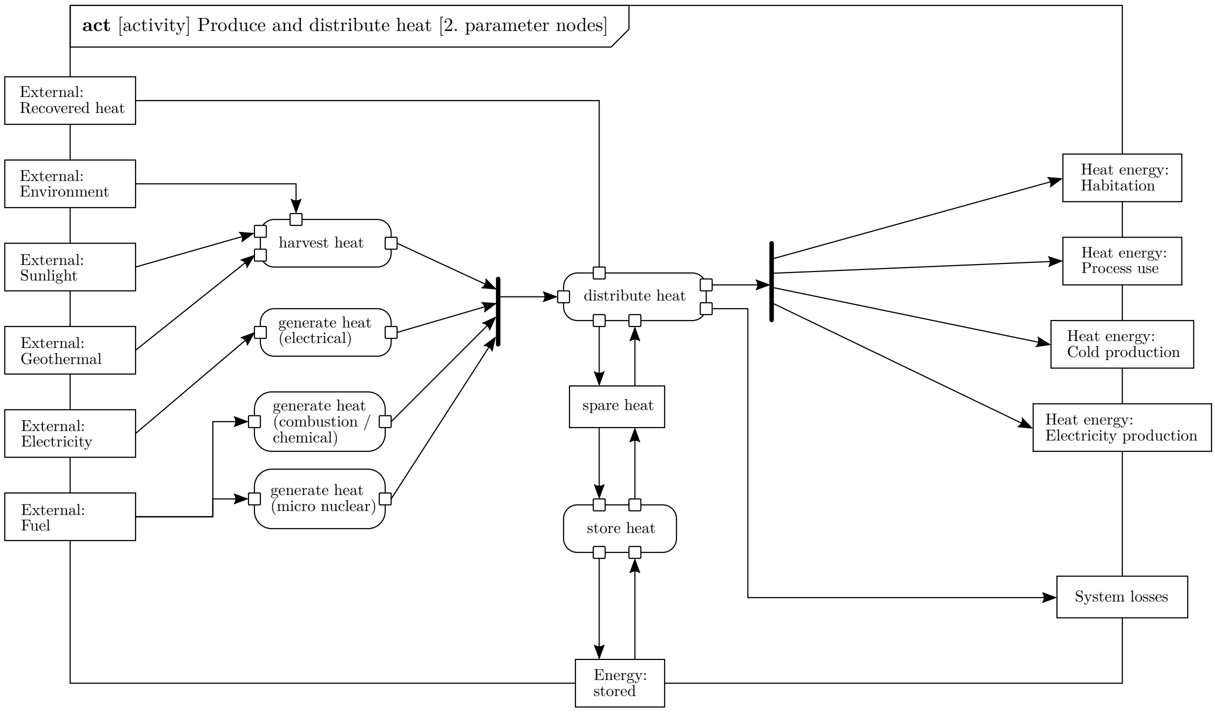


Figure 4.6: SysML produce and distribute heat

4.6 Conclusions

This chapter has presented a case for using systematic design methods for the construction of components used in integrated energy systems modelling. Three case studies of integrated energy systems were used to identify a set of standard components that can be used in integrated energy systems studies. These standard components were re-cast in terms of the functional requirements that they meet, using principles of axiomatic design. These standard components were compiled into reference systems using SysML as a systems communication and design language. These standard components are to be used in the modelling exercises presented in Chapters 5 and 6.

To augment the case studies and fill in some gaps in the literature review presented in Chapter 2, a short series of interviews with industry practitioners was conducted. These interviews revealed that, in the UK at least, government policies, historical fuel reserves and societal views on community energy supplies are colouring the perspectives on future integrated energy systems involving district heating and large scale deployment of storage and currently-uncommon devices such as heat pumps. It is apparent that there is no “one size fits all” approach to storage in particular.

With the interview perspectives in mind, the integrated system reference model does not represent an ideal system or a complete system design for all integrated energy systems. Rather, it provides a reference point for the analysis of existing systems or the development of new ones, from which possible solutions and domain combinations can be proposed.

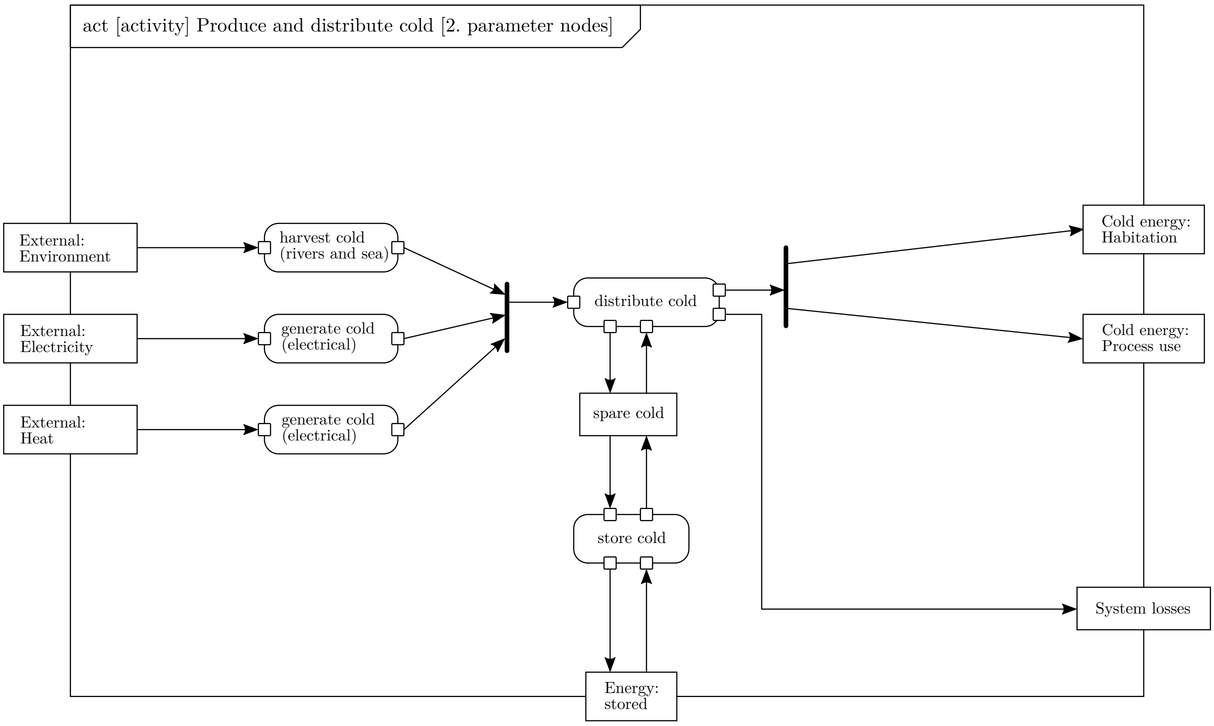


Figure 4.7: SysML produce and distribute cold

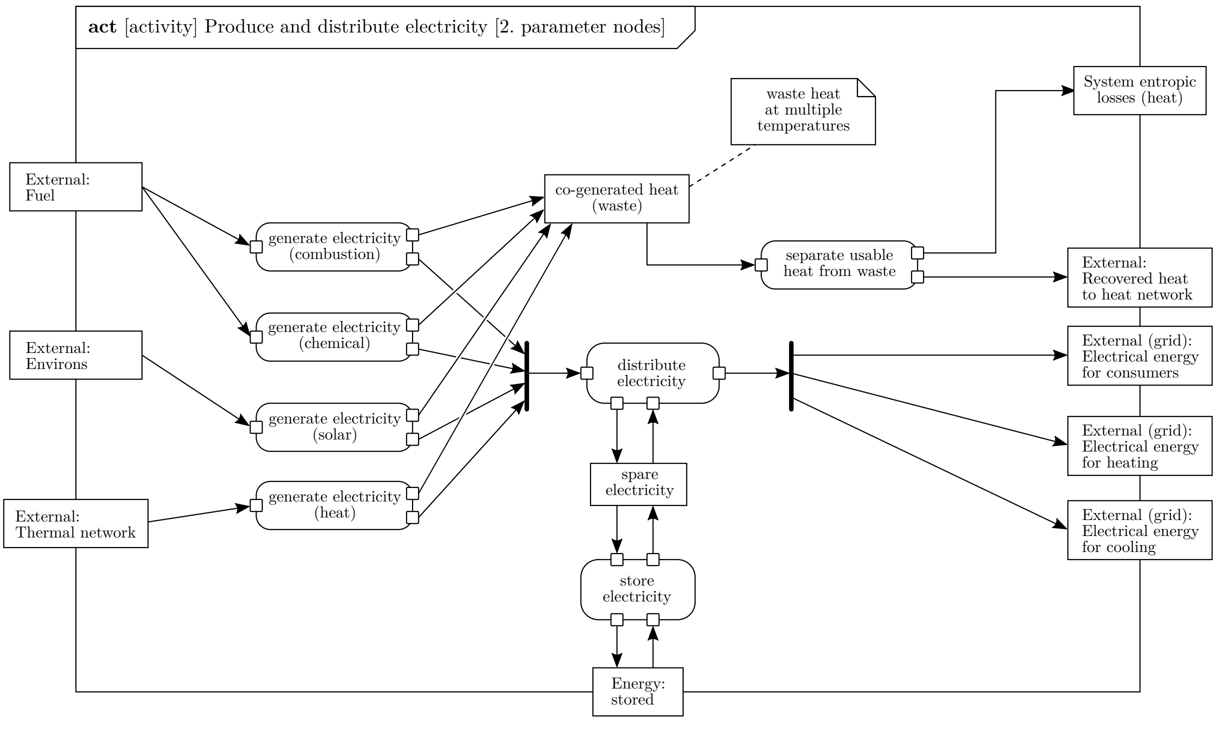


Figure 4.8: SysML produce and distribute electricity

Chapter 5. Integrated Energy Networks Modelling

5.1 Overview

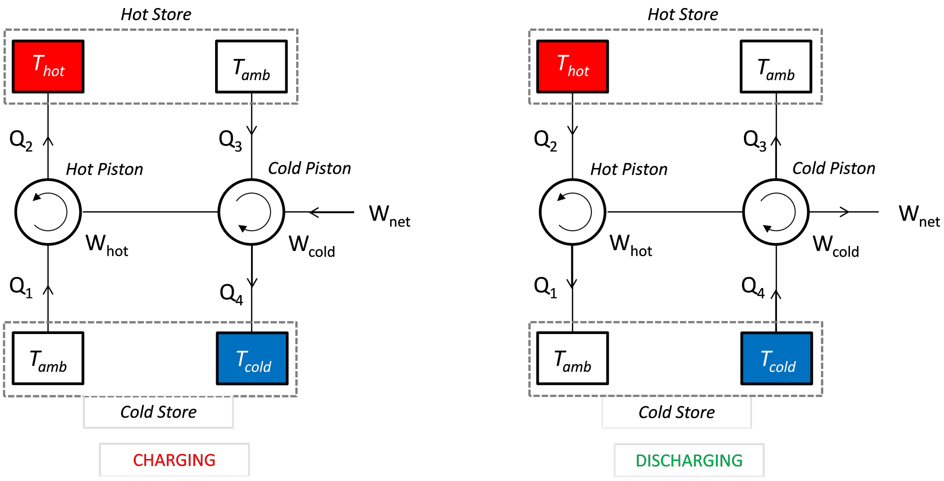
The previous chapters examined integrated energy systems as described by the literature, and explored the structure of three integrated mixed-vector case-study energy networks and the recurring elements that were found in these networks. These elements were explained from an engineering design point of view and it was shown how the recurring elements can be used as primary design elements for reference and case-study integrated multi-vector systems. The importance of exergy as a meaningful quantity in multi-vector systems, particularly with respect to the interchange of energy between vectors using storage as a mediating device, was explained.

This chapter will explore three methods of implementing models for simulating integrated energy systems. The degree to which each model class can adequately represent integrated systems is judged on the properties explored in the previous chapters; that is, their ability to represent standard design elements in a systems approach; their ability to adequately represent physical behaviour required to incorporate exergy measurements on the system; their ability to represent multiple domains of energy flow; and to what extent they can incorporate storage models that accurately consider cross-domain exergy exchanges.

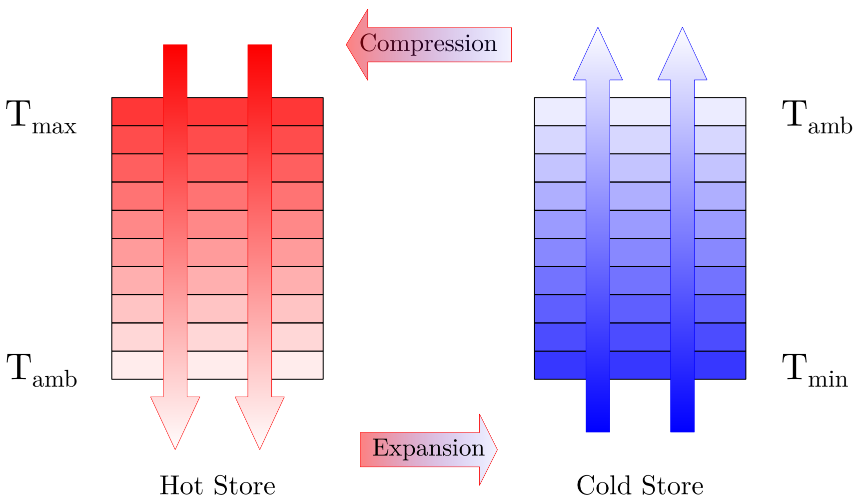
5.1.1 Multi-vector generation and storage devices

This chapter will begin with a study of two real multi-generation and storage devices: a pumped-heat energy storage device; and an adsorption tri-generation unit. Understanding the behaviour of these devices will reveal the design features a system-level model should have if it is to be incorporated into an integrated energy system model.

Pumped-heat energy storage Smallbone *et al.* [21] describe the operation and economics of a pumped heat energy storage (PHES) system, with the principal aim of examining the levelised cost of storage (LCOS) value of the system. Only the mechanical details of the machine described in this paper are of interest here. The PHES system is used to store electricity as sensible heat in two storage vessels, using a reciprocating machine which can operate as a heat pump converting electrical energy to heat, or as a heat engine converting heat energy to electrical. The machine operates on a working fluid (argon in this particular case) in a closed compression-expansion cycle. Figures 5.1a (taken from [21]) and 5.1b show the general operating principle of the storage system, which is used in the following modes.



(a) System operating principle (reproduced from [21])



(b) Stratified store

Figure 5.1: Pumped heat energy storage system

- **Charging:** Operating as a dual heat pump, the reciprocating engine alternately compresses and expands the working fluid to move heat from the environment to a stratified hot store, and from a stratified cold store to the environment. The stratified stores consist of a stack of independent sensible heat units as shown in Figure 5.1b, through which the heated / cooled working fluid passes.

- **Discharging (electrical out):** In this mode the operation of the reciprocating engine is reversed and it functions as a heat engine. The piston arrangement turns an electrical generator to produce an electrical output.

- **Discharging (heat out):** Here the stored exergy in the hot store can be released at the stratification temperatures, which range between the atmospheric temperature and the maximum temperature of the store. Note that the output stream temperature will drop as energy is extracted from the store.

- **Discharging (cold out):** Similarly, exergy stored in the cold store can be released at temperatures between ambient and the store minimum. The output stream temperature will rise as energy is added to the store.

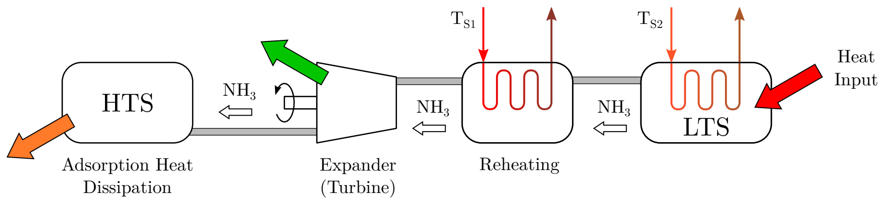
When empty, the storage units are at ambient temperature; and when full, the temperature of the two stores is uniform throughout and at a maximum / minimum dependent upon the working fluid material properties and the expander and compressor design.

It would also be possible for the system to support incoming heating and cooling streams at temperatures corresponding to the stratification layers, but the particular device in this instance does not support this mode of operation.

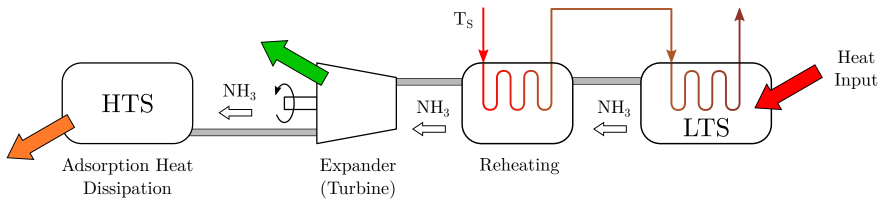
Resorption tri-generation Bao, Ma and Roskilly present a thermochemical process which enables the possibility of a device which can store and convert electricity and heat energy to and from stored chemical energy, often simultaneously [149]. The device uses what the authors call an “advanced resorption power generation (RPG) cycle”, which is an ammonia-based chemical absorption cycle that can be used in either a refrigeration or a heat pump capacity. The system presented here also uses an intermediate heating process to dry out the ammonia and improve the power of the cycle.

The authors present three potential operating cases for the device, which are shown diagrammatically in Figure 5.2. “LTS” refers to the low-temperature sorbent, and “HTS” to the high-temperature material. The working fluid in this device is shown as ammonia (NH_3).

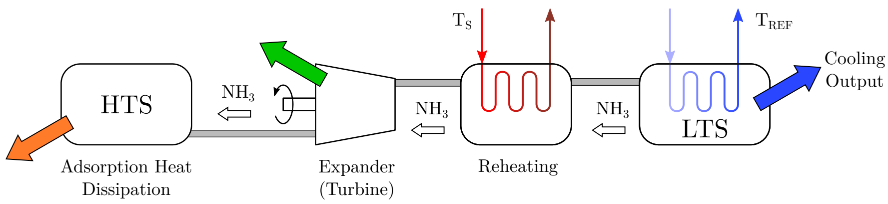
Figure 5.2a shows a process which uses two heat streams at different temperatures which perform the desorption process (T_{S2}) and the reheating process (T_{S1}) — such a case might be found in an industrial site having multiple process waste heat streams at different temperatures. The process in Figure 5.2b uses only a single stream, assumed to be at a much higher temperature than the desorption temperature, which is used to first



(a) Two heat sources at different temperatures



(b) A single heat source



(c) Single heat source with cooling output

Figure 5.2: Resorption power generation device operational modes

perform reheating (T_{S2}) and then to drive the desorption process. Finally, Figure 5.2c shows a situation where the device's desorption temperature is lower than the ambient temperature: the desorption process cools the incoming stream to provide a cooling effect, while a separate hot stream is also used to perform the re-heating stage. In all cases, power is produced through a turbine attached to an electrical generator as the desorbed ammonia undergoes expansion.

Systems representation Both the PHES and RPG devices can, from a systems standpoint, be considered to be black boxes able to receive and deliver electricity and heating or cooling. The PHES device is able to receive electrical energy and release electrical, heat and cold energy. The RPG device is able to accept one or more incoming thermal streams (it would possible to include multiple re-heating stages) and produce electrical power, possibly a cooling effect, and some residual low-temperature waste at the adsorption side.

5.1.2 Connecting energy domains with multi-vector storage

As explored in earlier chapters, one of the principal supposed benefits to integrating energy systems vectors, particularly through storage devices, is that the resultant integrated system should be able to respond better to wrong-time and wrong-type energy provision. An "ideal storage device" in such a system would sit at the nexus of the vectors and be able to convert energy freely from one domain to another, and store and release energy as required. Although such a device does not exist in reality, the study of an ideal model provides an important starting point for understanding what essential features such a device might possess without these being obscured by detail. From this starting point, it is then possible to go on to consider the additional constraints and limitations of real devices, such as the PHES and RPG devices examined above, and under what circumstances these might need to be accounted for in a model. *Multi-vector storage* is therefore defined to be an energy storage principle that allows conversion of energy from one form to another, mediated by a storage medium. In reality, energy must be stored in some physical form, but in the conceptual model it is convenient to regard multi-vector storage as a store of pure exergy. This is justified as follows.

As stated in Chapter 2, this thesis is concerned with integrated energy systems involving cooling, heating and electrical energy only, and so the the multi-vector storage device is required to sink and source energy in only these forms. In a real device, energy would be stored as latent heat, sensible heat, kinetic energy, chemical bonds, or in some other physical form, but the approach taken here will be to select a universal quantity which is equivalent irrespective of the energy domain. Following the discussion in Chapter 2 it is argued here that the most appropriate quantity is the exergy value of the stored energy. Exergy (or reversible work) is a state property common to each of the different physical forms that might be used to store energy, therefore providing a common measure between energy domains. Exergy streams from different vectors will add linearly to an exergy store, thus providing a consistent and easily-quantifiable method of connecting distinct energy systems.

Definitions An *ideal multi-vector storage device* is a device which is able to reversibly convert any energy stream to and from its pure exergy content for subsequent storage or release. An ideal multi-vector storage device is free to absorb and release an infinite amount of energy at an infinite rate. Real devices will have restrictions on their storage capacity and their rates of energy storage and release, and will cause some energy to be lost during their conversion processes. They are also likely to exhibit some time-dependent energy loss characteristics. In order to account for these restrictions, this thesis proposes a gradation of exergy storage models into four tiers according to the degree of realism they exhibit.

- Type 1: Reversible and infinite. The storage device can absorb and produce an infinite amount of energy at an infinite rate, with no loss.
- Type 2: Reversible, but with limits on storage capacity and power (energy rate) delivery.
- Type 3: Irreversible, i.e. the process of energy storage and recovery results in some exergy destruction. The device also has the capacity and power delivery limits of a type 2 model.

- Type 4: As Type 3 but with additional constraints on the relationship between the in- and out-flows relating to the technology being modelled.

This thesis only considers multi-vector storage devices connected to thermal and electrical flows, but the principle is applicable to any type of connected energy domain. Derivations will be presented here for these two cases.

Referring back to the exergy fundamentals in Section 2.5, it can be seen that if in a differential time dt a specific quantity of energy δq enters the storage device via a heat stream (denoted by the suffix h), and the storage device already contains a quantity of exergy, Ξ_h, then the differential specific exergy, ξ_h of the heat stream entering the storage is defined as

$$d\xi_\mathrm{h} = \left(1 - \frac{T_0}{T}\right)\delta q \tag{5.1}$$

$$= \left[(h - h_0) - T_0(s - s_0)\right] \tag{5.2}$$

Then in the limit,

$$\frac{d\Xi_\mathrm{h}}{dt} = \dot{m}\left[(h - h_0) - T_0(s - s_0)\right] \tag{5.3}$$

where Ξ_h is the exergy content of the store contributed to by thermal energy, $\dot{m}$ is the instantaneous stream mass flow rate into the store, h, s and T are the specific enthalpy, entropy and temperature of the stream respectively, and the subscript 0 refers to the dead state. For heat streams flowing out of the store, it is necessary to select a flow rate and the temperature and pressure of the stream, from which the specific enthalpy and entropy may be determined. This selection of the flow rate and temperature is an operational choice and will either be calculated from another state of the system, or set as control parameters.

Conceptually, the thermal streams entering the store can be considered to be feeding a reversible heat engine converting the thermal energy to work, which is then stored. On recovery, a reversible heat pump is used to recover the work energy to a thermal stream at whatever temperature and flow rate is selected to be the output of the store. Note that the energy is always conserved, and the exergy is converted appropriately according to the temperatures of the in-flowing and out-flowing streams. An in-flowing stream at a temperature T_L will store a particular amount of exergy, which can be later recovered at a different temperature with a different out-flow rate. A higher out-flow temperature of T_H would be compensated by a lower out-flow rate than the in-flow rate at the lower temperature; and vice versa.

Electrical streams by definition are already in the form of work and therefore transfer energy into the store (per phase) as

$$\frac{d\Xi_\mathrm{e}}{dt} = VI\cos\phi = \Re(P * Q^*) \tag{5.4}$$

where V and I are the (line-to-neutral) voltage and current phasor magnitudes at the store and $\cos\phi$ is the phase angle, or alternatively, P and Q are the complex power flowing into the store with * indicating the complex conjugate. Again, in order to extract exergy from the store three of the quantities in the above expression need to be provided by the model or control system, commonly through the system demand and constitutive equations of the connected network.

The total rate of change in the exergy contained within a store connecting n heat and m electrical streams is then given by

$$\frac{d\Xi}{dt} = \sum_n \frac{d\Xi_{\mathrm{h}}^n}{dt} + \sum_m \frac{d\Xi_{\mathrm{e}}^m}{dt}, \tag{5.5}$$

which can be implemented as a difference equation within a simulation model to obtain the change in exergy stored per unit time.

As incoming energy is converted to an equivalent stored exergy value, the device will be able to receive and deliver energy from and to any other domain, possibly simultaneously. Referring back to the list of storage types above, it is apparent that Type 1 devices are purely theoretical, as they represent an instantaneous and infinite conversion from one domain to another. These would be useful in, for example, baseline energy hub models. Type 2 devices could be used to represent realistic theoretical limits of a real device. Type 3 devices are useful as the first practical multi-vector storage representation where losses are represented in some form. Type 4 devices would be a suitable representation for example a co- or tri-generation device which is able to co-produce heat and electrical power from a high-temperature input, and which has a strict relationship between the produced heat and power output. The selection of the model type representing the store will depend on the application and degree of complexity required in the model.

5.1.3 Chapter objectives

This chapter will present three studies of model frameworks potentially useful for integrated energy systems representation: energy hubs; nodal analysis methods; and bond graphs. The modelling of integrated energy systems within this thesis is predicated on the following criteria:

- The model should be able to incorporate all energy domains using a single unified component representation.
- All components identified in the design abstraction exercise in Chapter 4 must be representable.
- Physically meaningful properties of the networks and components should be accessible. This is in order to be able to evaluate and control the exergy content of energy streams.
- The model should be amenable to a system-of-systems approach so that multi-level

architectures can be created. This will promote computational re-use of components and the construction of larger-sized systems based on small components.

- Components and links in the network will model large-scale devices and a bulk, lumped-parameter uniform treatment of system properties will be acceptable and appropriate.
- A piecewise steady-state time solution is adequate. Any system dynamics are of a shorter timescale than the steady-state solution period.
- The boundary of the system is definable and energy entering or leaving the system within the boundary can be represented in an appropriate fashion. Cellier [150] describes energy sources within the context of an electrical circuit as "... actually a non-physical element. Power cannot be generated, only transported and converted. However, a *system* never denotes the whole of the universe. It denotes a piece of the universe. Sources are interfaces between the system and the universe around it." Such sources for other energy domains should be definable and represented at the system boundary.

In the rest of this chapter, each of the three modelling frameworks are used to construct illustrative components an integrated energy system, drawing on the reference systems described in Chapter 4. Chapter 6, in presenting the development of an integrated energy network model which incorporates a multi-vector exergy storage model that can be used to connect the different domains of the integrated network, will examine the applicability of each of these modelling approaches. The most suitable approach is used to develop the integrated energy network model.

5.2 Energy hub models

5.2.1 Overview

A number of authors (e.g. Chicco and Mancarella [120, 151], Geidl and Andersson [121, 124, 152, 153], Liu *et al.* [122], and Moghaddam *et al.* [123], among others) describe a class of model used in representing integrated energy systems called an *energy hub* model. An energy hub is a spatial location where energy conversion takes place, and typically the overall energy system is constructed from interconnected energy hubs. The energy hub is a type of input-output model where the input-output relationship is described by conversion plant energy efficiency values, with the inputs and outputs being energy streams. The energy streams are able to take any physical form, i.e. electricity, heat, natural gas, and so on. Figure 5.3 shows an example of an energy hub, studied by Geidl and Anderssen in [124], which contains an electrical transformer (T), a combined heat and power (CHP) unit (CHP) and a natural gas boiler (B), along with some thermal (e_h) and electrical (e_e) storage. The energy hub receives electrical and gas energy input, and supplies heat and electrical power.

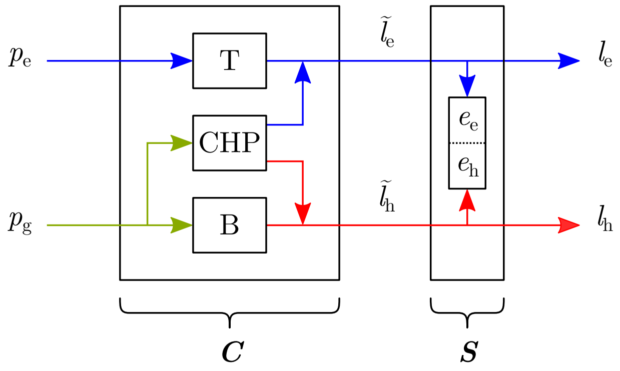


Figure 5.3: General representation of a CHP plant

Energy hubs form a class of model of the form shown in Equation 5.6, which expresses the time-dependent energy conservation for the system using the notation of Geidl and Andersson from [124].

$$\boldsymbol{l}^t = \boldsymbol{C}^t \boldsymbol{p}^t - \boldsymbol{S}^t \dot{\boldsymbol{e}}^t \tag{5.6}$$

During time interval t, $\boldsymbol{l} = (l_1, l_2, ..., l_n)$ is the system load vector (power), $\boldsymbol{C}$ is the system conversion matrix, $\boldsymbol{p} = (p_1, p_2, ..., p_m)$ is the power input (supply), $\boldsymbol{S}$ is the system storage matrix (referred to the output), and $\dot{\boldsymbol{e}} = (e_1, e_2, ..., e_n)$ is the storage energy flow vector. Using this notation, the configuration shown in Figure 5.3 has the definition

$$\begin{bmatrix} l_{\mathrm{e}}^t \\ l_{\mathrm{h}}^t \end{bmatrix} = \begin{bmatrix} \eta_{\mathrm{ee}}^t & \eta_{\mathrm{ge}}^{\mathrm{CHP}} \nu^t \\ 0 & \eta_{\mathrm{gh}}^{\mathrm{CHP}} \nu^t + (1-\nu^t)\eta_{\mathrm{gh}}^{\mathrm{B}} \end{bmatrix} \begin{bmatrix} p_{\mathrm{e}}^t \\ p_{\mathrm{g}}^t \end{bmatrix} - \begin{bmatrix} \eta_{\mathrm{e}}^{-1} & 0 \\ 0 & \eta_{\mathrm{h}}^{-1} \end{bmatrix} \begin{bmatrix} e_{\mathrm{e}}^t - e_{\mathrm{e}}^{t-1} \\ e_{\mathrm{h}}^t - e_{\mathrm{h}}^{t-1} \end{bmatrix} \tag{5.7}$$

where the subscripts e, g and h refer to electrical, gas and heat energy respectively, with double subscripts referring to conversion processes between the first and second subscript, and

η_{ee}^t is the energy efficiency of the transformer

$\eta_{\mathrm{ge}}^{\mathrm{CHP}}$ is the energy efficiency of the CHP gas-to-electrical conversion

$\eta_{\mathrm{gh}}^{\mathrm{CHP}}$ is the energy efficiency of the CHP gas-to-heat conversion

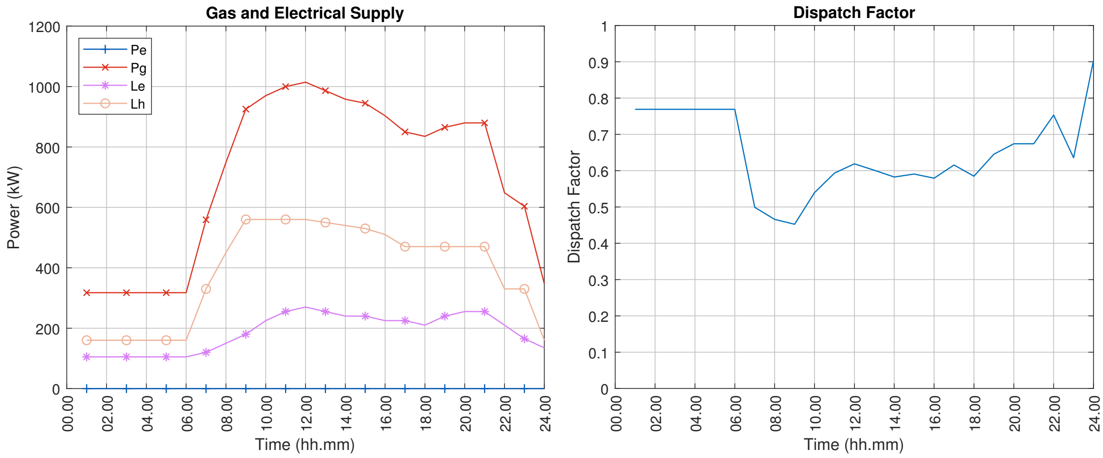
$\eta_{\mathrm{gh}}^{\mathrm{B}}$ is the energy efficiency of the boiler gas-to-heat conversion

η_{e} is the electrical energy storage charging efficiency (inverted when discharging)

η_{h} is the heat energy storage charging efficiency (inverted when discharging)

ν^t is the ratio of gas diverted to the CHP plant instead of the boiler (dispatch factor)

Energy hub models are commonly applied to *dispatch problems*, in which the values of the input power and dispatch factors ν^t that should be chosen to satisfy the load vector $\boldsymbol{l}^t$ are determined. Because the energy hub system of equations (Equation 5.6) is non-linear and under-determined, an optimisation approach is appropriate. For the problem



(a) System energy flows

(b) CHP dispatch factor

Figure 5.4: Single-day energy hub optimisation

represented by Figure 5.3 the objective function

$$\min_{\forall t} \mathcal{F} = p_{\mathrm{e}}^t + p_{\mathrm{h}}^t \tag{5.8}$$

would suffice. This objective function measures the total primary energy demand of the hub, with $0 <= \nu <= 1$ and $p_{\mathrm{e}}^t, p_{\mathrm{h}}^t >= 0$, but with no other constraints. The determination of dispatch factors is quite a common exercise in the optimisation of energy networks operations. As an example, the DEMS energy management system developed by Siemens has a dispatch forecasting facility which attempts to produce a half-hourly dispatch schedule given expected system loading and plant availability. Through an understanding of the optimisation space and the system constraints, the energy hub model can be used to show, for a fixed CHP heat-to-power ratio, how the system storage should be operated.

An example dispatch study of the system shown in Figure 5.3 was conducted using a mixed-integer linear programming algorithm driven by the objective function in Equation 5.8. The results are shown in Figure 5.4. Graph (a) shows the system load and supply powers in kW, and graph (b) illustrates the corresponding dispatch factors required to minimise Equation 5.8 over a single day (24 hours on the x-axis). The load data (l_{e} and l_{h}) is taken from [120]. It can be seen that for such a system, use of the CHP is preferred (high ν^t) but, being primarily driven by the electrical demand, operation of the gas boiler is still required to meet the heat demand. Also the storage unit is not prioritised at all — as primary energy consumption is the only objective requirement, the inefficiencies of energy conversion incurred during the storage process will merely increase losses. In general, one of p_{e}^t, p_{h}^t or ν^t will be at a limit for all t, depending on the load mix; in this specific case $p_{\mathrm{e}}^t = 0$ which indicates that the electrical demand is fully satisfied by the CHP device.

This example optimisation shows that hub models are a useful approach to dispatch optimisation but only when the system constraints and objective functions are well-understood. Otherwise, the dispatch schedules found by the optimisation algorithm can be misleading or otherwise unusable. In the example, the storage unit remained unscheduled because the objective function contained no information that would enable it; the addition of a time-dependent price term would be one way of accomplishing this. Also, the dispatch schedule for the CHP unit is not one which any real CHP plant would operate under. Here, some constraints on its operation are needed. A further example of this can be seen in the paper by Moghaddam *et al.* [123], which show a series of operating points for a CHP device which are unlikely to be achievable in practice.

Because energy hub models are based solely on energy flows, they may not be a suitable representation when knowledge of the physical behaviour of the network and network components is needed, either for control reasons or if the physical properties are part of the design parameters. There is additionally a fundamental difficulty with the application of energy hubs in certain circumstances. This is the "CHP plant problem" and is described below.

5.2.2 Energy hub CHP plant analysis

A CHP plant is a common component found in energy hub models. In some circumstances however the energy hub representation does not correctly capture the physical behaviour of the plant. To illustrate this "CHP plant problem", the Byker District Heating system (described in detail in Chapter 4) is represented and analysed as an energy hub. To recap: the heating system supplies approximately 2000 residential properties (mostly social housing) alongside a small number of municipal buildings and some commercial properties. Heat is supplied to the district network by three 6 MW natural gas boilers, a 1 MW biomass boiler and a 1 MW(e) / 1 MW(h) CHP unit.

As a first approximation the plant can be modelled in the same form as the energy hub described earlier in this chapter and shown in Figure 5.3. In this basic configuration the biomass boiler is ignored and only one of the gas boilers is considered to be operational; this situation often arises in practice when the biomass boiler is undergoing maintenance in summer months and there is only a small heating load on the system. In the actual plant the electricity produced is exported directly to the distribution network but it is possible to imagine the plant electricity production directly supplying the estate, with any shortfall being made up from the grid connection. In fact, inspection of primary substation records show that the plant is more than adequate in size for the estate and can supply surrounding residential areas too. This does not alter the basic analysis. The plant component energy and exergy efficiencies, denoted by η and ψ respectively, are derived in Appendix A and are summarised in Table 5.1. The suffix labels comb, e and h refer to combustion, electrical and heat production efficiencies respectively. It is noticeable that while a change in loading has a significant effect on the system energy efficiencies, it creates much less variation in the exergy efficiencies.

The simplified plant layout is shown in shown in the Appendix, Figure A.2. In this system the CHP unit heats the loop return water in series with the boiler using jacket

Boiler	Feed @ 80 °C Feed @ 100 °C	$\eta_{\text{comb}} = 0.926$ $\eta_{\text{comb}} = 0.926$	$\psi_{\text{comb}} = 0.187$ $\psi_{\text{comb}} = 0.206$
Engine	Load 100%	$\eta_{\text{e}} = 0.327$	$\psi_{\text{e}} = 0.314$
		$\eta_{\text{h}} = 0.487$	$\psi_{\text{h}} = 0.083$
	Load 75%	$\eta_{\text{e}} = 0.318$	$\psi_{\text{e}} = 0.306$
		$\eta_{\text{h}} = 0.508$	$\psi_{\text{h}} = 0.087$
	Load 50%	$\eta_{\text{e}} = 0.300$	$\psi_{\text{e}} = 0.288$
		$\eta_{\text{h}} = 0.551$	$\psi_{\text{h}} = 0.094$

Table 5.1: Overall efficiencies for Byker heating plant CHP and gas boiler

cooling, and is incapable by itself of heating the loop supply water to its design temperature of 130 °C. Although the CHP jacket coolant is a principal component of the heat recovery system, the primary purpose of this circuit is nevertheless to cool the CHP engine block. The heating loop return temperature of 80 °C, coupled with the limiting design temperature of the CHP engine jacket of 100 °C and with the need to maintain a heat transfer temperature gap in the heat exchanger, limits the temperature gain in the CHP cooling circuit. As a result, the temperature gain in the main heating loop from the CHP sub-system is also limited.

Therefore, the energy hub system illustrated in Figure 5.3 is not an accurate representation of the real system. Heat energy is portrayed as being supplied in an additive fashion, but in the actual plant the loop water after the CHP unit heating section is at approximately 100 °C. The boiler is then needed to raise the temperature of the water further so that it reaches the outgoing loop design temperature. To correctly represent this, the energy hub model would need to be modified as shown in Figure 5.5 by the addition of an extra *fictitious* heating device, B'. This fictitious device is a convenient modelling mechanism that is not present in the real system, added to allow the energy hub problem to be solved properly because the energy hub model does not include temperature states into account, only energy flows. The (fictitious) physical system that would correspond to this energy hub model is shown in Figure 5.6. There is a discrepancy between the real system and the energy hub representation caused by the way in which the energy hub input-output elements function. The addition of the fictitious heating device is to demonstrate how the energy hub problem can still be solved, but at the expense of the model no longer matching the real system physically. The fictitious device needs to be capable of heating the loop water from 100 °C to 130 °C (under pressure at 10.35 barg). "barg" is a common abbreviation for "bar (gauge)", i.e. a gauge reading of pressure which neglects atmospheric pressure. The absolute pressure in bar is the barg value plus the atmospheric pressure. The real boiler B still heats the loop water from 80 °C to 130 °C. In reality even this is not a correct representation because in the real plant a mixing process occurs at the exit from the CHP heat exchanger, but it is a reasonable first approximation.

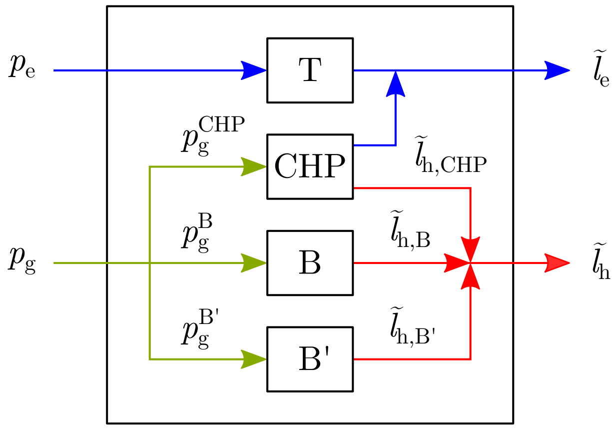


Figure 5.5: Modified system energy hub representing the Byker CHP plant

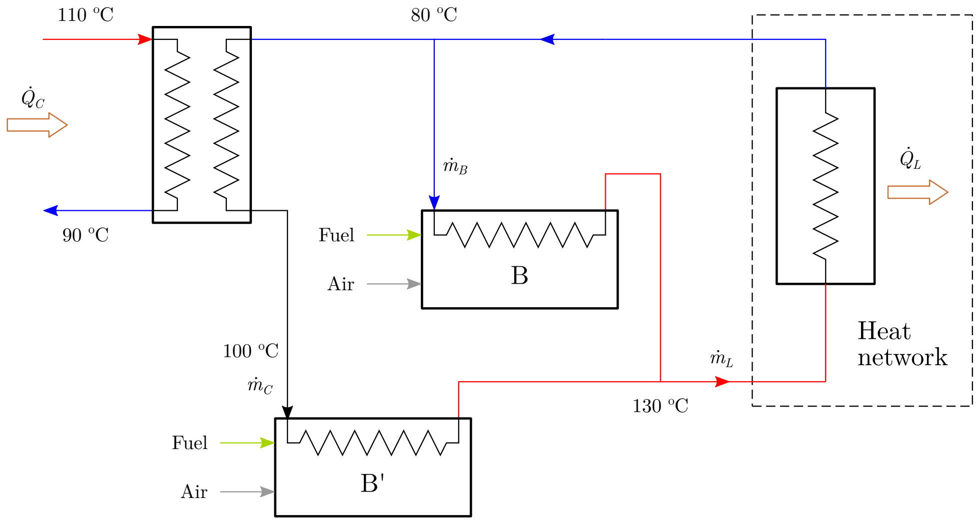


Figure 5.6: Modified energy hub model — equivalent physical system

The energy balance for the modified system is

$$\tilde{l}_{\mathrm{h}} = \tilde{l}_{\mathrm{h,C}} + \tilde{l}_{\mathrm{h,B}} + \tilde{l}_{\mathrm{h,B'}} \tag{5.9}$$

$$\tilde{l}_{\mathrm{h}} = \eta_{\mathrm{gh}}^{\mathrm{CHP}} p_{\mathrm{g}}^{\mathrm{CHP}} + \eta_{\mathrm{gh}}^{\mathrm{B}} p_{\mathrm{g}}^{\mathrm{B}} + \eta_{\mathrm{gh}}^{\mathrm{B'}} p_{\mathrm{g}}^{\mathrm{B'}} \tag{5.10}$$

An additional constraint is required because the mass flow rate of the fluid is common to both the pseudo-boiler B' and the CHP unit C by definition (they are in series). This continuity constraint is given by

$$\frac{\eta_{\mathrm{gh}}^{\mathrm{CHP}} p_{\mathrm{g}}^{\mathrm{CHP}}}{\eta_{\mathrm{gh}}^{\mathrm{B'}} p_{\mathrm{g}}^{\mathrm{B'}}} = \frac{\Delta h(\mathrm{CHP})}{\Delta h(\mathrm{B'})} \tag{5.11}$$

where Δh is the fluid specific enthalpy increase provided by the pseudo-boiler B' and the CHP unit, respectively. These specific enthalpy changes can be calculated from the system temperatures on exit and entry to these heat exchange elements, as already presented. An example case is now examined to illustrate how this fictitious device works.

In order to demonstrate the method, suppose the system operates with the CHP unit at 75% load, and all of the demand is to be supplied by the CHP plant. Therefore there is no external electrical connection, the gas boiler B is inactive, and the gas supply to the CHP unit and the boiler B' is to be calculated. It is supposed that the energy efficiency of the pseudo-boiler B' is equal to that of the boiler B. The electrical load is given as 817.3 kW (75% of the rated maximum) and the heat demand will follow the resulting heat supply. Using the numerical values presented in Figure 5.5 and Table 5.1 for this case, it can be seen that:

Given: $p_{\mathrm{e}} = 0$ kW, $p_{\mathrm{g}}^{\mathrm{B}} = 0$ kW, $\tilde{l}_{\mathrm{e}} = 817.3$ kW, $\eta_{\mathrm{ge}}^{\mathrm{CHP}} = 0.318$, $\eta_{\mathrm{gh}}^{\mathrm{CHP}} = 0.508$, $\eta_{\mathrm{gh}}^{\mathrm{B'}} = 0.926$

Temperatures: $T_1 = 80\,°\mathrm{C}$, $T_2 = 100\,°\mathrm{C}$, $T_3 = 130\,°\mathrm{C}$

Thus

$$\frac{\Delta h(\mathrm{CHP})}{\Delta h(\mathrm{B'})} = \frac{h_{@100\,°\mathrm{C}} - h_{@80\,°\mathrm{C}}}{h_{@130\,°\mathrm{C}} - h_{@100\,°\mathrm{C}}} = 0.633$$

Then:

i) $p_{\mathrm{g}}^{\mathrm{C}} = \frac{\tilde{l}_{\mathrm{e}}}{\eta_{\mathrm{ge}}^{\mathrm{CHP}}} = \frac{817.3}{0.318} = 2570.1\,\mathrm{kW}$

ii) $\eta_{\mathrm{gh}}^{\mathrm{CHP}} p_{\mathrm{g}}^{\mathrm{CHP}} = 0.508 \times 2570.1 = 1305.6\,\mathrm{kW} = \tilde{l}_{\mathrm{h,C}}$

iii) $\frac{\eta_{\mathrm{gh}}^{\mathrm{CHP}} p_{\mathrm{g}}^{\mathrm{CHP}}}{\eta_{\mathrm{gh}}^{\mathrm{B'}} p_{\mathrm{g}}^{\mathrm{B'}}} = 0.633 = \frac{\Delta h(\mathrm{CHP})}{\Delta h(\mathrm{B'})} \implies \tilde{l}_{\mathrm{h,B'}} = 1968.68\,\mathrm{kW}$

iv) $p_{\mathrm{g}}^{\mathrm{B'}} = \frac{\tilde{l}_{\mathrm{h,B'}}}{\eta_{\mathrm{gh}}^{\mathrm{B'}}} = \frac{1968.68}{0.926} = 2126.0\,\mathrm{kW}$

The total heat power supplied in the form of gas is thus $2570.1\,\mathrm{kW} + 2126.0\,\mathrm{kW} = 4696.1\,\mathrm{kW}$. Assuming no heat is lost during distribution to the load, this means that the mass flow rate to the load is

$$\dot{m} = \frac{\tilde{l}_h}{h_{@130\,°\mathrm{C}} - h_{@80\,°\mathrm{C}}} = 15.47\,\mathrm{kg/s}.$$

The overall energy efficiency is

$$\eta = \frac{817.3 + 1305.6 + 1968.68}{4696.1} = 0.871.$$

Thus, the fictitious boiler device can be used successfully to calculate an overall efficiency for the CHP unit that can be used within an energy hub model.

5.2.3 Extension to an exergy hub

One of the purposes of this thesis is to examine the potential for using exergy analysis more extensively when analysing mixed-vector integrated energy systems. It is then natural to examine whether the energy hub model can be transformed into an exergy hub model with the energy flows converted to exergy flows. An examination of the system leads to the conclusion that the resulting *exergy hubs* for the systems shown in Figures 5.3 and 5.5

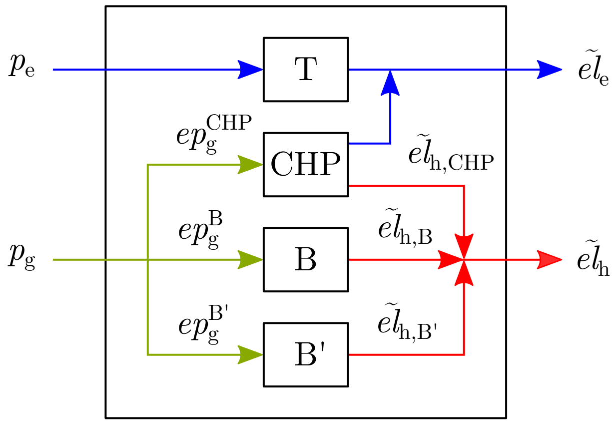


Figure 5.7: Modified system exergy hub representing the Byker CHP plant

have the same system topologies, but with the device energy efficiencies being replaced with exergy efficiencies. This is especially noticeable in that the boilers B and B' have a different exergy efficiency, while maintaining the same energy efficiency. The resulting exergy hub is shown in Figure 5.7. In the exergy hub system, the supply and load powers $\boldsymbol{p}$ and $\boldsymbol{l}$ are replaced with exergetic supply and load powers, $\boldsymbol{ep}$ and $\boldsymbol{el}$ respectively.

The exergy amounts supplied by each plant element add, either through enthalpy increase through sequential heating, or through a bulk increase caused by the addition of mass, and thus

$$\tilde{el}_{\mathrm{h}} = \psi_{\mathrm{gh}}^{\mathrm{CHP}} ep_{\mathrm{g}}^{\mathrm{CHP}} + \psi_{\mathrm{gh}}^{\mathrm{B}} ep_{\mathrm{g}}^{\mathrm{B}} + \psi_{\mathrm{gh}}^{\mathrm{B'}} ep_{\mathrm{g}}^{\mathrm{B'}} \tag{5.12}$$

The relative enthalpy constraint applies as before, but now there exists a relative exergy gain constraint. Again because the CHP and pseudo-boiler heat the water in series the mass flow is common, and

$$\frac{\psi_{\mathrm{gh}}^{\mathrm{CHP}} ep_{\mathrm{g}}^{\mathrm{CHP}}}{\psi_{\mathrm{gh}}^{\mathrm{B'}} ep_{\mathrm{g}}^{\mathrm{B'}}} = \frac{\Delta e(\mathrm{CHP})}{\Delta e(\mathrm{B'})} \tag{5.13}$$

Using the same example as before, then

Given: $ep_{\mathrm{e}} = 0$ kW, $ep_{\mathrm{g}}^{\mathrm{B}} = 0$ kW, $\tilde{el}_{\mathrm{e}} = 817.3$ kW, $\psi_{\mathrm{ge}}^{\mathrm{CHP}} = 0.306$, $\psi_{\mathrm{gh}}^{\mathrm{CHP}} = 0.087$, $\psi_{\mathrm{gh}}^{\mathrm{B'}} = 0.206$

$$\begin{aligned}\frac{\Delta e(\mathrm{CHP})}{\Delta e(\mathrm{B'})} &= \frac{e_{@100\,^\circ\mathrm{C}} - e_{@80\,^\circ\mathrm{C}}}{e_{@130\,^\circ\mathrm{C}} - e_{@100\,^\circ\mathrm{C}}} \\ &= \frac{(h_{@100\,^\circ\mathrm{C}} - h_{@80\,^\circ\mathrm{C}}) - T^0\,(s_{@100\,^\circ\mathrm{C}} - s_{@80\,^\circ\mathrm{C}})}{(h_{@130\,^\circ\mathrm{C}} - h_{@100\,^\circ\mathrm{C}}) - T^0\,(s_{@130\,^\circ\mathrm{C}} - s_{@100\,^\circ\mathrm{C}})} \\ &= 0.509\end{aligned}$$

Then:

i) $ep_{\mathrm{g}}^{\mathrm{CHP}} = \frac{\tilde{el}_{\mathrm{e}}}{\psi_{\mathrm{ge}}^{\mathrm{CHP}}} = \frac{817.3}{0.306} = 2670.9\,\mathrm{kW}$

ii) $\psi_{\text{gh}}^{\text{CHP}} ep_{\text{g}}^{\text{CHP}} = 0.087 \times 2670.9 = 232.4\ kW = \tilde{el}_{\text{h,C}}$

iii) $\frac{\psi_{\text{gh}}^{\text{CHP}} ep_{\text{g}}^{\text{CHP}}}{\psi_{\text{gh}}^{\text{B'}} ep_{\text{g}}^{\text{B'}}} = 0.509 = \frac{el_{\text{h,C}}}{el_{\text{h,B'}}} \implies \tilde{el}_{\text{h,B'}} = 456.6\,\text{kW}$

iv) $ep_{\text{g}}^{\text{B'}} = \frac{\tilde{el}_{\text{h,B'}}}{\psi_{\text{gh}}^{\text{B'}}} = \frac{456.6}{0.206} = 2226.4\,\text{kW}$

The total exergy rate supplied in the form of gas is thus 2670.9 kW + 2226.4 kW = 4897.3 kW, and the total heat exergy rate supplied to the load is 232.4 kW + 456.6 kW = 689.0 kW. Assuming no heat is lost during heat distribution, this means that the mass flow rate to the load is

$$\dot{m} = \frac{el_{\text{h}}}{e_{@130\,°\text{C}} - e_{@80\,°\text{C}}} = 15.48\,\text{kg/s}$$

which is the same as that calculated through energy considerations in the previous section. The overall exergy efficiency is

$$\psi = \frac{817.3 + 232.4 + 456.6}{4897.3} = 0.308$$

The combined exergy efficiency is lower than the overall exergy efficiency of the CHP unit, but remember that the CHP is unable to produce the absolute exergy demand on its own. The fictitious boiler is able to, but has a lower exergy efficiency at 0.206. Thus it can be concluded that the combined CHP-boiler plant is the more efficient configuration. However, it must be remembered that the boiler used to enhance the CHP's heat production does not actually exist, it is a computational device required to elevate the temperature of the stream leaving the CHP system so that it matches the temperature of the stream leaving the real boiler, so that stream mixing can occur properly. Despite then being able to solve an exergy dispatch problem for the modified energy hub using this device, it is not clear how this should translate into a real operating plan for the plant.

5.2.4 Observations

What has been demonstrated in the previous section for the energy hub representation of a real CHP-boiler plant feeding a heat network and electrical grid, is that a naïve application of the energy hub concept fails to capture the real behaviour of the plant. The basic energy hub model does not capture energy quality and in particular temperature, and it also ignores heat energy transfer via mass transport. Geidl and Andersson recognise this point, stating that "The simplified model, which corresponds to a network flow or transportation model ..., is believed to provide sufficient accuracy for overall system design studies. However, for other purposes detailed power flow models may be required to obtain meaningful results" [121]. Nevertheless, even in acknowledging the limitations of the energy hub model, the specific weaknesses are unclear.

In the real plant under study, the CHP unit by itself is not capable of producing heat at the required temperature, even though its raw heat energy power output may be enough

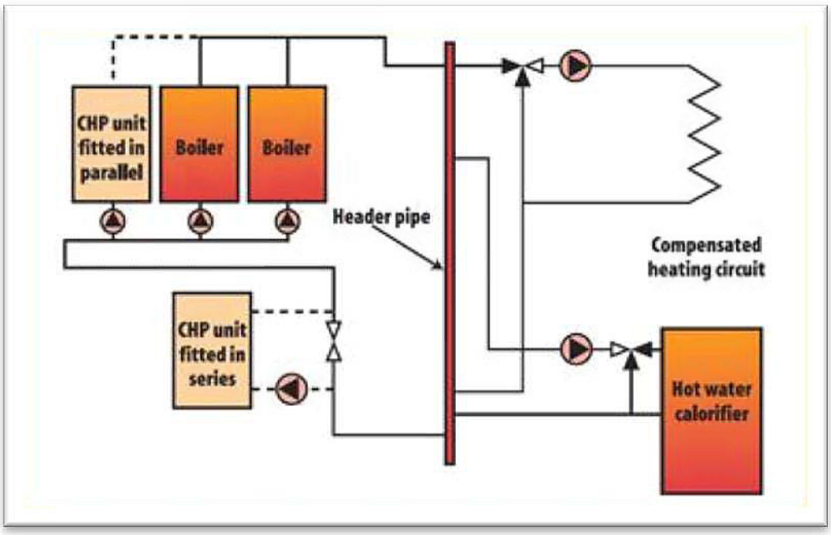


Figure 5.8: CHP system standard installation locations (reproduced from [154])

to satisfy the demand. This is because the CHP unit operates as a low-temperature pre-heating / waste heat reclamation unit rather than a primary heat-and-power device. Figure 5.8 shows two standard methods for CHP plant installation from Department of Energy and Climate Change (DECC)'s guidance document for CHP developers [154], the case under study here being of the series retro-fitted type. Heat is transferred from the engine via the cooling jacket and exhaust heat exchange in series; however, the maximum operating temperature of the engine jacket limits the amount of heat that can be added to the coolant, which in the case study unit is given by the manufacturer as 99 °C. Although indications from the plant are that in practice it does run slightly hotter than this, insufficient data were available to accurately determine the temperature. In any event, the precise temperature is not important to this analysis. At this temperature, coupled with the high return temperature of the water from the district heating loop of 80 °C, there is little heat transfer flexibility and thus a high mass flow rate of coolant is needed through the engine to limit the temperature gain. This in turn limits the temperature gain from the exhaust heat exchanger and thus the temperature gain that can be supplied to the heating loop, despite the apparent transfer of all (assuming ideal heat transfer) heat energy from the engine to the heating loop. A straightforward rule however can be deduced from the study. Heat production plant operating in parallel and producing equivalent-quality heating can be added at the output within the energy hub model. Heat production plant operating in series must be supplemented by an auxiliary, fictitious, unit which makes up the heat quality shortfall and may (especially in the exergy hub case) operate at a different efficiency. Assuming that power output can be modulated through mass flow control and that system temperatures are fixed, the energy and exergy hub model can therefore still be used; but it is unclear how the fictitious heating device should translate to control of the real plant. A specific exergy model might also perhaps make the best representational form, rather than the energy representation.

The systems described by some authors in the literature are however unrealistic in other respects. While the presentation of a general theoretical and optimisation framework in e.g. [124] is a sound method for high-level anstract system studies, individual applications often do not take into account some critical aspects of real engineering systems.

- Prime movers tend to operate at reduced efficiency at part-load (or potentially increased efficiency for heat), and thus the constant-efficiency assumption of the energy hub model is inaccurate. The generation efficiencies do not necessarily change proportionally as a function of load either, as can be seen by the studied CHP engine. This applies equally to non-heat engine prime movers. Exergy efficiencies reduce less under load.

- A realistic operational schedule must be accounted for within the system constraints. This would normally be implemented as a system constraint. For example, the CHP engine in the case study only operates on weekdays between 7am and 7pm, in order to maximise revenue from generation feed-in tariffs while reducing fuel and plant maintenance costs. Some studies (e.g. [123]) produce optimised CHP operational schedules that are highly variable and thus unrealistic in real-plant operation.

- Some form of buffering storage tends to be a firm requirement for practical hot water loops. The buffer decouples production from demand and enables demand fluctuation to be managed. However, this buffering store is not featured in many of the case examples presented in the literature.

Thus although it is possible to implement a general energy and exergy hub with series and parallel heating, the simplified approach does not adequately capture the real system and potentially produces results that do not translate back into an operational strategy for the real system. As well as requiring a load-efficiency curve for each plant component, system temperature and pressure fluctuations in series circuits are not captured by this model without an additional set of pre-calculated enthalpy or exergy ratios, and for more complicated hub topologies this begins to erode the benefits of the energy hub approach as a simplified non-physical flow model. Ultimately the overall heat delivery from energy hub units depends on the contributory temperatures and mass flows. Other more physically-based approaches are examined in the rest of this chapter.

Finally, it is worth considering briefly the types of objective functions used in energy hub studies. Different authors studying energy hub optimisation strategies use different objective function formulations, which limits the comparisons that can be drawn between different energy hub studies. One possible solution to this would be to construct a set of standard "operational modes" for energy hubs which have a clearly-defined objective function and set of constraints. The idea of an "energy trilemma" also forms a more consistent way of evaluating energy systems. An energy trilemma is a general statement of intent for the management of energy systems which makes explicit the trade-offs that exist due to the competing priorities of the energy system. The World Energy Council defines a Trilemma Index which is "an annual measurement of national energy system performances across each of the three trilemma dimensions: Energy Security ... Energy Equity ... [and] Environmental Sustainability" [155]. Papers by Singh *et al.* [156] and Heffron *et al.* [157] describe the trilemma in more detail and some means by which it can be addressed. The general topic of the energy trilemma is beyond the scope of this thesis; however it does contribute to the subject by providing a means of measuring and modelling the environmental sustainability part of the trilemma through a better understanding of exergy in energy networks.

5.3 Nodal analysis methods

5.3.1 Overview

Electrical direct current (DC) circuit theory combines the interconnection expressions known as Kirchoff's Current Law (KCL) and Kirchoff's Voltage Law (KVL) with circuit component constitutive equations, and a number of solution methods are known for solving the resulting equation sets (e.g. see [128, 158, 159]). The idea of using a DC circuit model approach is explored as a method for approximating general integrated energy networks which consist of other domains of energy in addition to the electrical domain. Modelling techniques that are used for electrical components are extended to non-electrical domains, and component models which transform energy between domains are developed.

Although a number of approaches to analysing electrical circuits are available, the technique used in this work to construct models of general energy systems that can be described as a graph or network is known as modified nodal analysis (MNA). The method is described in the following sections, with e.g. [128] providing a more comprehensive description. The general MNA method is explained along with the concept of an *element stamp*, and how a system matrix can be built up from the stamps of the branch elements in the system. A (non-exhaustive) set of individual stamps that can be used in a general mixed domain energy system are then presented.

In applying electrical circuit theory to general energy networks, a few assumptions have been made which constrain the types of networks that can be represented. The behaviour of system elements is assumed to be static, i.e. element constitutive equations do not change with time. Transitions in fluid phase and flow regime are assumed not to take place and the constitutive equations of elements representing fluids are also constant. This is generally an acceptable assumption for large-scale engineering networks where the state of the system is designed and known and where distinct phases can be separated in a lumped fashion. For studies in which phase transitions occur depending on operational conditions this assumption no longer applies, and a further iterative step is needed to evaluate the correct state. This is not pursued in this thesis.

5.3.2 Modified Nodal Analysis

Modified nodal analysis is a technique for the creation of a representation of a network or circuit in matrix form. In circuit theory and in the more general sense in the generalised representation of power networks described by bond graphs, three types of equations are needed to be able to describe an energy network:

- equations describing equality of flows, using KVL
- equations describing equality of efforts, using KCL
- the constitutive equations of network branches

Section 5.4 covering bond graph models will show that these are equivalent to the bond graph 1-junction, 0-junction and 1-port elements respectively.

Additional more complex expressions which relate branches to each other, e.g. bond graph n-port elements such as transformers and gyrators, extend the fundamental graph scheme. MNA was introduced by Ho *et al.* [160] and is described in detail by Litovski and Zwolinski [128], with the terminology introduced by Litovski and Zwolinski being adopted for this thesis. This terminology is specifically related to electrical networks problems and thus the effort values are labelled voltage, while the flow values are labelled current. However the voltage and current symbols can be assumed to refer respectively to any relevant effort or flow in a power network.

A network is defined as a set of branches that connect to each other at nodes. The branches represent the main physical content of the network, while nodes are the points at which branches interact. It is evident that a network is a lumped-parameter approximation of a system. For a static problem or at a given discrete time in the solution of a dynamic system the nodes of a network have an effort value relative to some reference point, while the flow through a branch is fixed. One of the nodes in the network is chosen as the reference or ground node; the total number of nodes in the network is given as $n + 1$, with n non-reference nodes, and the ground node customarily being labelled as node zero. There are evidently then n independent 0-junction or KCL equations which describe the behaviour of the flows at the nodes. In addition, each branch requires a constitutive equation which relates the nodal efforts at either end of the branch to the flow through the branch.

Figure 5.9 shows the kth node of a general network [128]. The network is described by a set of equations which describe the topology (KCL equations) and the constitutive relations of the branch, that is

$$f_k\left(\mathbf{i}_k\right) = \sum_{l=1}^{L_k} i_{kl} = 0 \text{ for } k = 1, 2, ..., n \tag{5.14}$$

$$g_{kj} \cdot (v_k - v_j) = i_{kj} \tag{5.15}$$

i_{kl} is the lth current leaving the kth node, there are L_k branches connected to node k, and $\boldsymbol{i}_k$ is the vector of currents leaving the kth node. g_{kj} is a general relationship between the effort difference across the branch and the flow through it. For a conductive branch for example, $g_{kj} = G_{kj}$ where G_{kj} is the branch conductance.

By combining the node and branch constitutive equations, the branch flows can be eliminated and the set of equations solved for the node efforts. Evidently as a set of n equations in n unknowns the these can be written in matrix form,

$$\boldsymbol{G} \cdot \boldsymbol{v} = \boldsymbol{i} \tag{5.16}$$

where $\boldsymbol{G}$ is commonly referred to as the nodal admittance matrix. The $\boldsymbol{i}$ vector provides the system excitation while $\boldsymbol{v}$ are the nodal efforts which are to be found.

This method of network solution is known as Nodal Analysis (NA). NA however breaks down when effort sources or excitations are present in the system. In such a case, for an ideal effort source between two nodes,

$$v_k - v_j = E_{kj} \ , \tag{5.17}$$

and because there is no flow variable in this equation the nodal KCL equations for the nodes at either end of this branch cannot be formulated. The solution is to introduce a new variable, the effort source flow. Intuitively as well as mathematically this makes sense, because the ideal effort source must also provide a flow in order for there to be a supply of power to or from the source. The introduction of an additional variable creates a solvable set of equations; in addition to the nodal efforts, the effort source flows are also now unknowns to be found. This method is called MNA.

It might be noticed that in the original problem formulation above, the flows through the branches are not provided as a result of solving the nodal admittance matrix equation. These can however be solved when the vector $\boldsymbol{v}$ has been found, by substitution into the branch constitutive equations. Alternatively, the flow through any branch can also be found directly in the same way in which the effort source flow is found; by its addition as a new variable into the $\boldsymbol{v}$ vector, along with the appropriate constitutive equation in the admittance matrix. In any case, the outcome is the same, but it may be more expedient or convenient to include unknown flows of particular interest into the $\boldsymbol{v}$ vector directly. This

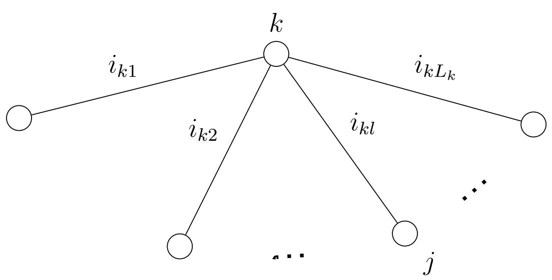


Figure 5.9: kth node and attached branches

topic shall be returned to when the topic of non-linear branch elements is investigated.

With the addition of effort source flows the generalised MNA system is given a particular standard form, as presented in [128]:

$$\boldsymbol{A} \cdot \boldsymbol{x} = \boldsymbol{z} \tag{5.18}$$

where

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{G}_r & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{bmatrix} , \ \boldsymbol{x} = \begin{bmatrix} \boldsymbol{v} \\ \boldsymbol{j} \end{bmatrix} , \ \boldsymbol{z} = \begin{bmatrix} \boldsymbol{i} \\ \boldsymbol{e} \end{bmatrix} \tag{5.19}$$

$\boldsymbol{G}_r$ is the $n \times n$ nodal conductance matrix; $\boldsymbol{B}$ is the $n \times m$ matrix of derivatives of the nodal equations with respect to the new (flow) variables; $\boldsymbol{C}$ is the $m \times n$ matrix of derivatives of new flow equations with respect to the node efforts; $\boldsymbol{D}$ is the $m \times m$ matrix of derivatives of new flow equations with respect to the new (flow) variables; $\boldsymbol{v}$ is the vector of n node efforts; $\boldsymbol{j}$ is the vector of m new branch flows; $\boldsymbol{i}$ is the vector of ideal current sources; $\boldsymbol{e}$ is the vector of ideal voltage sources. The "new" flows are those introduced as additional variables whenever an ideal voltage source is added to the network.

5.3.3 Algorithm for matrix creation

The regularity of the matrices described in the previous section suggests an automated method for their creation, and such a method does indeed exist. The technique uses a way of representing the network branches referred to as "stamps". The stamp method is an additive method for populating the system matrix [128] and is presented briefly here.

It might be recognised that the matrix $\boldsymbol{G}_r$ represents a nodal connectivity matrix, whereby an entry in the (k, j)th row and column indicates a branch connection between nodes k and j. In some network analysis methods this nodal connectivity matrix is defined explicitly in an initial step but this is not necessary with MNA. Because KCL applies, the entire network can be constructed by superposition and thus each branch can be added one at a time into the global connectivity matrix. Thus the stamp for a branch element is independent of all other branch elements and can be determined by considering the branch contribution in isolation. The process is illustrated by an examination of a conductance branch [128]. The implementation of stamps for use in general energy systems modelling will be given later in this chapter.

A general conductive branch is shown in Figure 5.10. It can be seen that irrespective of the form of the rest of the network, the contribution of this branch is purely additive and is given by Equations 5.20.

$$\begin{aligned} k &: G_{kj}v_k - G_{kj}v_j + \Sigma_k = 0 \\ j &: \ - G_{kj}v_k + G_{kj}v_j + \Sigma_j = 0 \end{aligned} \tag{5.20}$$

These equations can be succinctly described in a tabular form known as the element's stamp, shown in Table 5.2. The stamp shows that the conductance value G_{kj} is added to

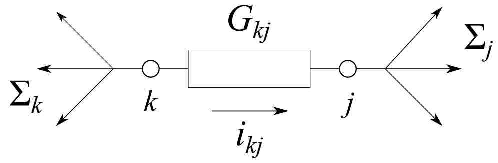


Figure 5.10: A general conductive branch

	v_k	v_j	RHS
k	G_{kj}	$-G_{kj}$	
j	$-G_{kj}$	G_{kj}	

Table 5.2: A conductance stamp

the kth column of the kth equation, and to the jth column of the jth equation; and that the same value is subtracted from the jth column of the kth equation, and from the kth column of the jth equation.

The construction of the system matrix then follows in a straightforward way. A matrix of size $(n+m, n+m)$ is created. Then, each branch in turn is added to the matrix in the appropriate place following the element's stamp definition, which includes any additional flow variables and excitation to be added directly into the relevant matrix or vector. Note that branches can be added which do not form part of a circuit; these are still valid and the flow in these branches will be equal to zero.

5.3.4 Linear and non-linear elements

DC electrical circuit analysis concerns itself with linear resistances and conductances. Alternating current (AC) analysis is possible if the branch constitutive equations are expressed as complex impedances in the s-domain through application of the Laplace transform, creating impedance stamps, although such elements are not considered in this thesis. However, many electrical and non-electrical branch components do not follow a linear constitutive relationship. Sometimes a circuit may perform over a limited range of operation such that a linear response approximation can be considered, but for many electrical devices and mechanical systems this is not possible and a non-linear version of the MNA method and solution strategy must be considered. In this work a non-linear MNA solver was constructed from first principles following [128] to tackle some of the mixed energy system designs of interest, and the design and operation of this algorithm is described here. While the fundamental method is described in detail by Litovski and Zwolinski, the focus of that work is on VLSI electronic systems using devices such as diodes and transistors. The components explored within this work share a common foundation but are different in their form, and some unique aspects of solving networks containing these components have been discovered.

Non-linear elements The concept of *companion models* as described in [128] is used as a method for adding non-linear branch elements into a network. A companion model for a

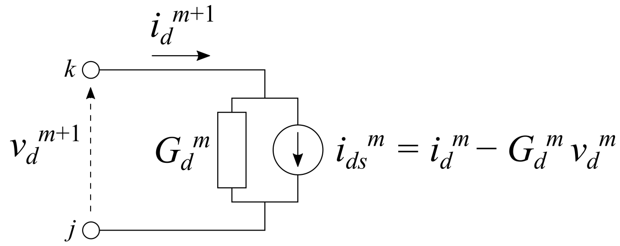


Figure 5.11: Non-linear conductance branch companion model

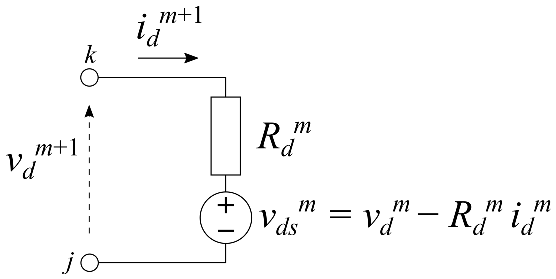


Figure 5.12: Non-linear resistance branch companion model

non-linear branch component de-constructs the model equation into a parallel conductance and current source for conductance-type branches, or a series resistance and voltage source for resistance branches. The values of the companion model components are linearised at the point of solution and are computed iteratively, with the $(m+1)$th iteration effort and flow values given as an expression in the mth iteration values. In this work a Newton-Raphson iterative approach is used to find solutions to the non-linear equations. Although other methods are available, N-R is used due to its "simplicity, easy implementation and quadratic convergence" [128]. The following sections describe the general form of companion models and how they are used to form integrated energy systems components.

It can be shown [128] that for a general conductive companion model, the relationship between the branch current for the $(m+1)$th iteration and that for the mth iteration is (with the m superscript indicating iteration number)

$$i_d^{m+1} = i_d^m + G_d^m \left(v_d^{m+1} - v_d^m\right) = G_d^m v_d^{m+1} + \left(i_d^m - G_d^m v_d^m\right) \tag{5.21}$$

and for a resistive companion model,

$$v_d^{m+1} = v_d^m + R_d^m \left(i_d^{m+1} - i_d^m\right) = R_d^m i_d^{m+1} + \left(v_d^m - R_d^m i_d^m\right) \tag{5.22}$$

with the subscript d indicating that these quantities are taken at the boundaries of the device. These expressions can be seen to be applications of KCL and KVL to the companion model branch. Schematics of the two types of companion model are given in Figures 5.11 and 5.12 (see [128]). A further substitution of

$$i_d^m - G_d^m v_d^m = i_{ds}^m \tag{5.23}$$

$$v_d^m - R_d^m i_d^m = v_{ds}^m \tag{5.24}$$

	v_k^{m+1}	v_j^{m+1}	RHS
k	G_{kj}^m	$-G_{kj}^m$	$-i_{ds}^m$
j	$-G_{kj}^m$	G_{kj}^m	i_{ds}^m

Table 5.3: A non-linear conductance stamp

	v_k^{m+1}	v_j^{m+1}	i_d^{m+1}	RHS
k			1	
j			-1	
br	G_d^m	$-G_d^m$	-1	$-i_{ds}^m$

Table 5.4: A non-linear conductance with current stamp

where the subscript ds stands for "device source" and references the device current or voltage source as appropriate, simplifies the above to

$$i_d^{m+1} = G_d^m v_d^{m+1} + i_{ds}^m \tag{5.25}$$

$$v_d^{m+1} = R_d^m i_d^{m+1} + v_{ds}^m \tag{5.26}$$

This makes clear that the companion model current or voltage is the sum of a linearised resistance or conductance and an internal current or voltage generator. The quantities G_d^m and R_d^m are the linearised conductances and resistances respectively at iteration m and derive directly from the first term in the Taylor expansion of the device equations. They are given by

$$G_d^m = \left.\frac{\partial i_d}{\partial v_d}\right|_{v_d=v_d^m} \tag{5.27}$$

$$R_d^m = \left.\frac{\partial v_d}{\partial i_d}\right|_{i_d=i_d^m} \tag{5.28}$$

The set of all branch non-linear equations that are defined in terms of the present and next iterative step form a Newton-Raphson system of the form

$$\boldsymbol{G}^m \boldsymbol{x}^{m+1} = \boldsymbol{I}^m \tag{5.29}$$

$$\boldsymbol{I}^m = \boldsymbol{G}^m \boldsymbol{x}^m - \boldsymbol{f}\left(\boldsymbol{x}^m\right) \tag{5.30}$$

The stamps for a non-linear element are the same irrespective of the actual element constitutive equation. The value of the element conductance or resistance at iteration m is given by the derivative of the constitutive equation at that iteration. The general stamp for a non-linear conductance, non-linear conductance with additional branch current, and non-linear resistance are given in Tables 5.3, 5.4 and 5.5, reproduced from [128].[1].

[1]There is an error in Table 3.1c in [128], with the br-RHS value given incorrectly as $-v_{ds}^m$

	v_k^{m+1}	v_j^{m+1}	i_d^{m+1}	RHS
k			1	
j			-1	
br	1	-1	$-R_d^m$	v_{ds}^m

Table 5.5: A non-linear resistance stamp

5.3.5 Solution methods

Linear algebraic equations

The application of the MNA method to a static DC or frequency-domain AC circuit results in a set of linear algebraic equations. Methods for solving sets of linear algebraic equations are well-documented in the literature (e.g. in [161]) and will not be explored here.

An interesting possibility for solving such equations is to perform the calculation symbolically. The matrices for anything other than a trivial computation are too complex to manipulate by hand, but computer software such as Matlab or Maple can perform symbolic manipulation of matrices. This approach was taken initially for solving the network matrices of an example energy system. However, very quickly the symbolic expressions become very large and unmanageable, and the computation very slow, despite the sparseness of the matrices. This is particularly evident in non-linear problems. While it is possible therefore to construct the initial matrices in symbolic form while performing the MNA analysis step, in order to conduct any serious computation substitution of numerical values is necessary before any solution steps are taken.

This is also a problem when evaluating the variance properties of the system of equations, which involves a calculations of the inverse of the Hadamard product of a matrix with itself; the Hadamard product in this case being a new matrix of the same size as the original matrix, with each element being the square of the original element. This is a very slow calculation to perform numerically as it stands, and impossibly slow symbolically.

Newton-Raphson iteration

In the previous sections it was explained that systems containing non-linear companion models form a set of non-linear algebraic equations and these can be solved iteratively using a Newton-Raphson algorithm. In addition to the basic algorithm some of the techniques such as iteration damping and variable tolerance evaluation in [128] were implemented. The basic algorithm is the familiar Newton-Raphson loop:

1. Initialise the $\boldsymbol{x^m}$ vector with initial estimates of the solution for $m = 0$
2. Calculate G_d^m and R_d^m values
3. Calculate values for the $\boldsymbol{x}^{m+1}$ vector

	v_k	v_j	RHS
k	$1/R_{kj}$	$-1/R_{kj}$	
j	$-1/R_{kj}$	$1/R_{kj}$	

Table 5.6: A resistance stamp

4. Repeat the above steps from 2. until the $\boldsymbol{x}^m$ and $\boldsymbol{x}^{m+1}$ are equal to within some defined tolerance ϵ.

A stopping tolerance similar to that given in Equation (3.29) in [128] was used, with a correction. The logic of the development of this value is correct but the expression as given is in error, as it gives a value of $\epsilon \approx 5 \times 10^{-4}$ irrespective of the values of n and k. A correct expression for the convergence threshold value is

$$\epsilon = 10^{-\left(\frac{3+k-log(n)}{2}\right)} \tag{5.31}$$

Here, ϵ is the desired maximum difference (error) between subsequent iterations of the Newton-Raphson algorithm, k is the number of significant figures used to represent numbers used in the calculations, and n is the number of variables in the network model.

The role of the slack connection

In energy networks, there is never an exact balance between supply and demand and this difference is accounted for in a "slack" branch. This is implemented here as a perfect constant voltage source at an appropriate part of the network, and represents say an external grid connection. For islanded systems where the over- or under-supply cannot be absorbed or sourced from the slack branch, the power into and out of the network would need to balanced through an iterative process. This would require an algorithm to realistically and intelligently adjust demands and possibly supplies to balance the power in the network. Such an approach is not pursued here and a slack branch is retained to balance the power in the system.

5.3.6 Components

Electrical

Four types of electrical branch are used in the development of the integrated energy system model; conductance and resistance branches, an ideal current source branch, and an ideal voltage source branch. The conductance stamp was given earlier in Table 5.2, while the remaining three are given in Tables 5.6, 5.7 and 5.8. These stamps can also be used in other domains for branches having similar relationships between the effort and flow in the branch.

	v_k	v_j	RHS
k			$-I_{kj}$
j			I_{kj}

Table 5.7: A current source stamp

	v_k	v_j	i_e	RHS
k			1	
j			-1	
br	1	-1		E_{kj}

Table 5.8: An ideal voltage source stamp

Power

A difficult problem arises when trying to represent components which are only defined by a power injection in to or removal out of the system. It is common in energy networks modelling to have a mixture of effort and flow sources but it is also very common that only the power of a source or sink is wanted or specified. This leads to a problem that is akin to that addressed by load flow analysis methods in electrical engineering.

A power branch can be defined simply enough using the companion model method. The constitutive relationship is

$$i_d = \frac{P}{v_d} \tag{5.32}$$

and then

$$G_d = \left.\frac{\partial i_d}{\partial v_d}\right|_{v_d = v_d^m} = -\frac{P}{v_d^2} \tag{5.33}$$

The companion current generator value is given by

$$\begin{aligned} i_{ds}^m &= i_d^m - G_d^m v_d^m \\ &= \frac{P}{v_d^m} - \left(-\frac{P}{v_d^{m2}}\right) v_d^m \\ &= \frac{2P}{v_d^m} \end{aligned} \tag{5.34}$$

When solving a system with power branches, the hyperbolic nature of the power branch constitutive equation causes some difficulties. In well-behaved constitutive equations, i.e. ones that are continuous and single-valued, the Newton-Raphson algorithm will tend to converge to a solution even with poor initial conditions. For power branches however it is necessary to initialise the problem more carefully by setting sensible values for v_d^0 and i_d^0, preferably near to the expected solution and ensuring that all of the values are different (possibly by the introduction of some randomness). This requires a degree of physical insight to do successfully. In a pseudo-static system where the efforts and flows change in time but are regarded as constant over a given time interval, even though there is no differential relationship between time periods, the solution for the previous time interval can be sensibly used as the initial values for the next.

Thermal

A district thermal network which uses piped fluids to transport heat can be represented in a much simplified form within the network framework if certain assumptions are made. Using the circuit model the return temperature from each load is assumed to be at around the same temperature, and thus the return pipe network is considered to be a "ground state". Therefore outgoing and return losses are lumped into one pipe loss factor in the outgoing pipe. Mixing on the return network is thus ignored. Pipe power losses are assumed to be proportional to the length of pipe, with a pre-determined constant of proportionality. These are quite restrictive assumptions but they are assumed to be appropriate for a first approximation of the behaviour of a heat network operating under normal conditions.

In the simplified circuit-based scheme, power elements are used to represent thermal elements in the circuit. The external temperature does not factor explicitly in the network formulation, and is instead implicit in the thermal load. Often the thermal demand is provided by separate thermal modelling studies and / or by data, which includes the temperature implicitly.

For traditional liquid heat networks where energy loss through heat transfer is much higher than that lost through pressure losses, the pressure component can be disregarded and the network elements represented by temperature and mass flow quantities alone. In reality the heat losses should be a function of the temperature; but this is not easy to fit into the branch model system. In practice, it is the thermal demand power that is known and the network will be operating at a known operational point. In this situation thermal demand end-points can be modelled using power elements. Pipe branches can also use a power branch model with the power loss being specified per-unit length.

Fluid In order to fit lumped fluid components into the circuit model, it is assumed that the type of flow is known by design, and flow is either laminar or turbulent (i.e. not transitional). Fluid networks in large-scale energy systems normally exhibit turbulent flow, for which the relationship is a sign-preserving quadratic resistive relationship, i.e.

$$p_d = R\, q_d\, |q_d| \tag{5.35}$$

$$R_d = \left.\frac{\partial p_d}{\partial q_d}\right|_{q_d = q_d^m} = R\ |q_d| + R\, q_d\, \mathrm{sgn}(q_d) \tag{5.36}$$

Note that R is assumed constant, which is not normally the case (it will be subject to an empirical relationship such as the Darcy-Weisbach relation), but if the range of operation is narrow then this will be a reasonable assumption. If this is not the case then R must also become a variable in the Newton-Raphson iteration.

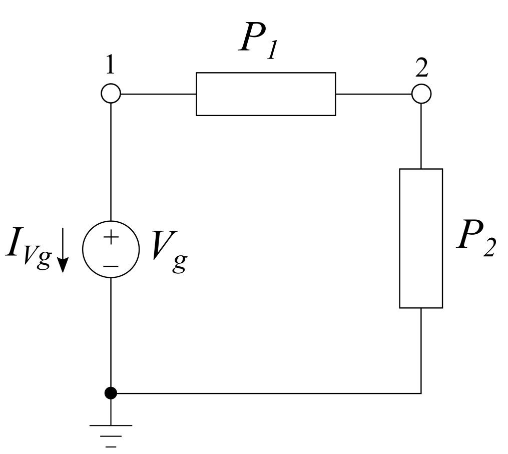


Figure 5.13: Power network system diagram

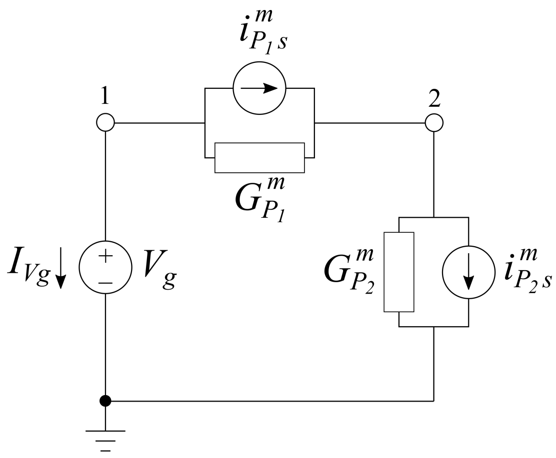


Figure 5.14: Power network companion model diagram

	v_k	v_j	i_e	RHS
k			1	
j			-1	
br	1	-1		E_{kj}

Table 5.9: Voltage source stamp

	v_k^{m+1}	v_j^{m+1}	RHS
k	G_d^m	$-G_d^m$	$-i_{ds}^m$
j	$-G_d^m$	G_d^m	i_{ds}^m

Table 5.10: Non-linear conductance stamp

For laminar flow the relationship between pressure and flow rate is linear and an ordinary resistive relationship can be used. Again this assumes that the friction factor R is constant, which will often be approximately true.

5.3.7 Example network

To illustrate the method, consider a system with two power branches as shown in Figures 5.13 and 5.14. The following sections demonstrate the assembly of the system equations using KCL as the circuit nodes, and using MNA.

(A) MNA method

i) Stamps. The stamps used in this network are the conductive branch stamp and the voltage source branch stamp, shown in Tables 5.9 and 5.10.

ii) Matrix construction
There are $n = 2$ nodes, and $m = 1$ additional branch equations. Therefore $\boldsymbol{A}$ is a 3×3 matrix and $\boldsymbol{x}$ & $\boldsymbol{z}$ are both of size 3×1.

a) Add voltage source V_g

$$\boldsymbol{A} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} V_1 \\ 0 \\ I_{V_g} \end{bmatrix}, \quad \boldsymbol{z} = \begin{bmatrix} 0 \\ 0 \\ V_g \end{bmatrix} \tag{5.37}$$

Remember that V_j for the voltage source is $0V$ and the earth node is excluded from the circuit equations.

b) Add power element P_1

$$\boldsymbol{A} = \begin{bmatrix} G^m_{P_1} & -G^m_{P_1} & 1 \\ -G^m_{P_1} & G^m_{P_1} & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} V_1 \\ V_2 \\ I_{V_g} \end{bmatrix}, \quad \boldsymbol{z} = \begin{bmatrix} -i^m_{P_1 s} \\ i^m_{P_1 s} \\ V_g \end{bmatrix} \tag{5.38}$$

c) Add power element P_2

$$\boldsymbol{A} = \begin{bmatrix} G^m_{P_1} & -G^m_{P_1} & 1 \\ -G^m_{P_1} & G^m_{P_1} + G^m_{P_2} & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} V_1 \\ V_2 \\ I_{V_g} \end{bmatrix}, \quad \boldsymbol{z} = \begin{bmatrix} -i^m_{P_1 s} \\ i^m_{P_1 s} - i^m_{P_2 s} \\ V_g \end{bmatrix} \tag{5.39}$$

Remember here that V_j for the element P_2 is zero (earth) and therefore this node does not feature in the system equations.

(B) Nodal equations with KCL. Conventional currents out of junctions are taken to be positive.

i) Node 1

$$I_{V_g} + i^m_{P_1 s} + G^m_{P_1}(V_1 - V_2) = 0 \tag{5.40}$$

ii) Node 2

$$G^m_{P_1}(V_2 - V_1) + G^m_{P_2}(V_2 - V_0) + i^m_{P_2 s} - i^m_{P_1 s} = 0 \tag{5.41}$$

iii) Voltage source

$$V_1 - V_g = 0 \tag{5.42}$$

Rearranging gives

$$G^m_{P_1} V_1 - G^m_{P_1} V_2 + I_{V_g} = -i^m_{P_1 s} \tag{5.43}$$

$$-G^m_{P_1} V_1 + (G^m_{P_1} + G^m_{P_2}) V_2 = -i^m_{P_2 s} + i^m_{P_1 s} \tag{5.44}$$

$$V_1 = V_g \tag{5.45}$$

which can be arranged into a matrix expression which is same as that derived using the MNA method.

Having derived the general matrix for this system the specific constitutive equations for the power branches can be added. The general constitutive equation for a power branch is given by $i_d = {}^{P}\!/_{v_d}$. By definition,

$$G^m_d = \left.\frac{\partial i_d}{\partial v_d}\right|_{v_d = v^m_d} \tag{5.46}$$

$$\text{so if } i_d = \frac{P}{v_d},\ G_d^m = -\frac{P}{(V_d^m)^2} \tag{5.47}$$

$$\text{Thus } G_{P_1}^m = \frac{-P_1}{(V_{P_1}^m)^2} \quad \text{and} \quad G_{P_2}^m = \frac{-P_2}{(V_{P_2}^m)^2} \tag{5.48}$$

Additionally, an expression for i_{ds}^m is needed. Again by definition,

$$i_{ds}^m = i_d^m - G_d^m v_d \tag{5.49}$$

$$\text{so} \quad i_{P_1 s}^m = i_{P_1}^m - \left(\frac{-P_1}{(V_{P_1}^m)^2}\right) V_{P_1}^m = i_{P_1}^m + \frac{P_1}{V_{P_1}^m} \tag{5.50}$$

$$\text{Also} \quad i_{P_1}^m = \frac{P_1}{V_{P_1}^m} \tag{5.51}$$

$$\text{so} \quad i_{P_1 s}^m = \frac{2P_1}{V_{P_1}^m} \quad \text{and also } i_{P_2 s}^m = \frac{2P_2}{V_{P_2}^m} \tag{5.52}$$

Finally, substituting these quantities into the system description (matrices), gives something that can be solved in terms of the vector $\boldsymbol{x}$.

$$\boldsymbol{A} = \begin{bmatrix} -\frac{P_1}{(V_{P_1}^m)^2} & \frac{P_1}{(V_{P_1}^m)^2} & 1 \\ \frac{P_1}{(V_{P_1}^m)^2} & -\frac{P_1}{(V_{P_1}^m)^2} - \frac{P_2}{(V_{P_2}^m)^2} & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{z} = \begin{bmatrix} -\frac{2P_1}{V_{P_1}^m} \\ \frac{2P_1}{V_{P_1}^m} - \frac{2P_2}{V_{P_2}^m} \\ V_g \end{bmatrix} \tag{5.53}$$

Application to a heat network The power element can be used to model heat demand, if certain assumptions are made.

i) The heat transport fluid does not change state and has a constant specific heat capacity C_p

ii) Pressure and head losses are ignored as small relative to the heat transported

iii) Losses and demand can always be expressed as a power

iv) Mixing of fluids at different temperatures on the fluid return is ignored

v) In a simplified network the power losses on the outgoing and return pipes can be approximated on the outgoing only. Alternatively the full network can be constructed but this adds to the solution complexity.

In a thermal network with these assumptions, the power through an element / section of line is given as (with the fluid mass flow rate $\dot{m}$ constant and the specific heat capacity of the fluid given by C_p)

$$\begin{aligned} P &= (h_k - h_j)\dot{m} \\ &= C_p\, \dot{m}\, (T_k - T_j) \text{ for constant } C_p \end{aligned} \tag{5.54}$$

$$\text{so } \bar{P} = \dot{m}\,(T_k - T_j) \quad \text{where } \bar{P} = \frac{P}{C_p} \tag{5.55}$$

where h is the fluid enthalpy and T its temperature, and the subscripts k and j represent the state at the kth and jth nodes to which the branch is attached. Thermal elements are thus approximated as non-linear power branches with flow $\dot{m}$ and effort T and with the power scaled by the specific heat capacity of the fluid.

5.3.8 Multi-port branches

In order to connect different domains together, multi-port elements are required. In conventional circuits these are the VCVS, CCVS, VCCS and CCCS elements, along with transformers, gyrators and similar elements. However at a high-level, e.g. the heat pump in the following section, many network devices have no real constitutive relationship between effort and flow and the relationship is purely power-based. Additional elements need to be developed to be able to add these to the system. In particular, where a power transformation exists, one of the efforts or flows at one of the ports must be specified for a solution to be possible.

A type of general power-to-power element that can incorporate a constant modulus as well as a response surface is required, which incorporates a simple (i.e. quadratic) surface directly into the system Jacobian. The material on other multi-port non-linear elements in [128] would form a the basis for this. This describes general one- and multi-port elements represented by ideal sources controlled by multiple variables, such that

$$y = f(\boldsymbol{x})$$

describes a controlled variable y defined by a non-linear function in a vector of controlling variables $\boldsymbol{x}$, which may not be circuit variables. This function can be a response surface in a series of variables outside of the circuit and will achieve the goal of representing any complex device as a quadratic response surface with error.

5.3.9 Response surfaces

When developing integrated energy systems models, it is sometimes the case that a branch constitutive relationship cannot be created directly. The underlying behaviour of the device may not be fully understood or it may be in the form of an implicit relationship. It may also be the case that the exact model is very complex and difficult to compute, and only the first-order behaviour is needed. In other cases the behaviour of the component might exist in the form of experimental data. The idea of using an approximation of a model that can be quantified by its behaviour and model uncertainty is also appealing for computational purposes. A particular part of an energy system might be adequately described by a coarse approximation that is fast to compute but which adds only a minor degree of uncertainty. In this work such models are termed response surfaces. Other terms for similar concepts include emulators, surrogates or black-box models [128]. Included in this definition are interpolated look-up table models.

The Response Surface Methodology (RSM) is a systematic data-driven way of creating an approximate model of a system, process or device. The method incorporates a means of designing experiments on the system to create a set of data that can be used to create the model, methods for designing and creating the models itself, and algorithms and methods for examining the model, for example to find optimal conditions or control points. A full exploration of RSMs is outside the scope of this thesis but Myers *et al.* [162] describe the methodology in great depth. Here, only the model creation step and the integration of response surface models into energy systems networks is pursued. By including such models it is possible to reduce the overall complexity and hence solution time of an energy system model.

A response surface is defined as an approximating relationship between a number of independent variables and one or more dependent variables, called the response. The approximating relationship does not have to bear any relationship to the actual underlying function, and in fact low-order polynomial approximations over a defined region of the system response are generally appropriate. An advantage of using a fixed-degree polynomial to approximate complicated parts of an energy system is that they are then amenable to differentiation, and thus their stamp can be directly determined and used within the system Jacobian matrix. This will be returned to later in this section.

Using the terminology in [162], the general form of a response surface is given by

$$y = f(\xi_1, \xi_2, ..., \xi_k) + \epsilon \tag{5.56}$$

where y is the response, $\xi_1, \xi_2, ..., \xi_k$ are the natural independent variables which produce the response, f is the underlying function producing y, and ϵ is variability not included in f. f is not known and is the function that is to be approximated using a response surface. As noted above, a low-order general linear model is generally sufficient; usually this is at most a second-order model.

Heat pump response surface model In order to illustrate the method, a response surface model for a heat pump is developed. A heat pump is a power-to-power type of device which is characterised by its coefficient of performance, K, which in turn is a function of two temperatures, an ambient temperature T_{amb} and a design temperature T_c. A more sophisticated model would also include the capacity and power output as factors, but this is not explored further here.

The Heliotherm HP20L-M-WEB is a split design modulating vapour-compression air-source heat pump that is capable of 27kW of heat output. The actual heat output is a function of the temperature lift $T_c - T_{amb}$, the evaporator and condenser heat exchanger temperature differential, and the compressor speed. Only the effect of the temperature lift is modelled here, with the relationship between K, T_{amb} and T_c shown in Figure 5.15 [163].

A direct general linear model using the natural variables of the relationship of the form

$$K = \beta_0 + \beta_1 T_c + \beta_2 T_{amb} + \beta_3 T_{amb}^2 \tag{5.57}$$

was created in Matlab. The independent variables were not coded in this instance. The model coefficients are $\beta_0 = 8.3763$, $\beta_1 = -0.1017$, $\beta_2 = 0.1225$ and $\beta_3 = 0.0015$, with a root mean squared error (RMSE) for the model of 0.2988. The model equation 5.57 can be used to predict a new value of K given T_c and T_{amb}, the variance associated with this being given as [162]

$$\sigma_{K_{new}} = \text{MSE} \times \left(1 + \boldsymbol{x}'_m \left[\boldsymbol{X}'\boldsymbol{X}\right]^{-1} \boldsymbol{x}_m\right) \tag{5.58}$$

where $\boldsymbol{x}_m$ is the model space prediction point $[1, T_c, T_{amb}, T_{amb}^2]$ and $\boldsymbol{X}$ is the model matrix. MSE is the mean square error, i.e. RMSE^2. A more realistic model would also incorporate the heating capacity of the heat pump as an upper limit to the heat demand.

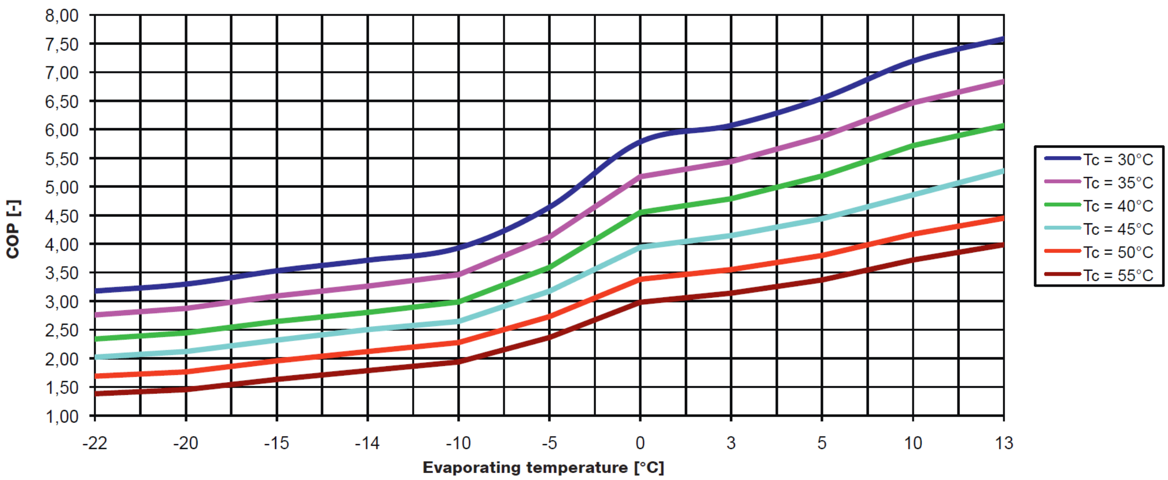


Figure 5.15: Heliotherm model HP20L-M-WEB-COP performance characteristic

5.4 Bond graphs

5.4.1 Introduction to bond graphs

Bond graphs are a graphical method for describing power systems in their very broadest sense. Originally devised in 1959 by Professor Henry Paynter, bond graphs provide a formal structure for representing physical processes and systems in any physical energy domain, and with any types of connection between the domains [126]. Bond graphs are a form of lumped-parameter model representation and consist of elements that represent the dynamic processes and power transfers that occur in the modelled system. Proper bond graphs are completely energy preserving which can be very useful as a self-validation mechanism for integrated energy systems design.

Bond graphs differ from the circuit representations in the previous section in that while circuit networks are terminal-oriented, bond graphs are power-port oriented and for some physical domains are a more accurate model representation of physical reality, while retaining a graphical structure that illuminates the flow of power through a system. The networks formed through circuit theory have by definition an inherent closed nature and obey additive laws at nodal points. Sometimes these circuit-equivalent forms can be used effectively in non-electrical domains, such as in first-order heat transfer models, but they are not always appropriate. Bond graphs use an additional node to allow for a series connection of elements in non-mechanical systems, since in bond graphs power ports are connected, while in networks terminals are connected; it is always possible to construct a bond graph from a circuit graph, but the reverse is not true.

The fundamentals of bond graphs and their relevance to integrated district energy systems modelling are explained in the following sections. Bond graphs are described by a number of authors, for example Thoma [164], Breedveld [165], Borutzki [125] and Brown [166], and the reader is referred to these more comprehensive texts for a fuller description of bond graph theory than is presented here.

5.4.2 Bond graphs for describing engineering systems

A *graph* G is a set of objects V termed vertices or nodes, and a further set E of pairs of nodes called edges; $G = (V, E)$. A graph may be undirected, where the edges have no inherent direction; or directed, where they do. Graphs can be used to describe integrated engineering systems, with the nodes of the graph denoting some kind of interesting structure or process, and the edges indicating how these structures and processes connect to each other.

Graphs form a naturally lumped-parameter approach to modelling an integrated engineering system. A lumped parameter approach is a common and suitable technique for many modelling tasks and is particularly suitable for modelling integrated energy systems. *Bond graphs* are a particular type of graph where the nodes represent large, discrete, spatially concentrated engineering devices, and the edges describe the power transmitted between them. Being graphical and hierarchical, bond graphs are also suited to component-based modelling strategies that are important in engineering systems design. These topics will be explored in this section.

Bond graphs are then a way of encoding physical engineering systems as a set of components that exchange energy. A more precise definition of bond graphs is provided by Borutzki [125]. Firstly, an *undirected bond graph* is an "undirected graph whose vertices denote subsystems, components, or basic elements, while the edges called (power) bonds represent the instantaneous energy transfer between nodes." An undirected bond graph can be used in an initial modelling stage where the relationship between the system elements are being mapped. However, for analysing the power flow through a graph a conventional direction of power flow through each bond must be defined. Borutzki's definition of a *directed bond graph* is that: "A bond graph is called a directed bond graph if a half arrow has been added to each bond indicating the positive reference direction of the energy flow across the bond." These definitions are very general and do not require the particulars of the physical energy domain to be specified. A system from any physical energy domain can be represented by a bond graph. A corollary to this is that multiple domains of physical behaviour can be represented within the same overall graph with the correct node types. These themes will be returned to later.

Bond graphs are a power port-based approach to systems modelling. Port-based approaches originated in electrical circuit analysis and were extended to other domains by Paynter [165] in the formation of the bond-graph notation. In contrast to signal-based approaches — for example, control system block diagrams — port-based approaches preserve fundamental bilateral or acausal physical relationships.

Bond graphs also lend themselves well to submodelling. A single node in a bond graph can be another entire bond graph. Borutzki notes that "If several effects are involved in a physical process, different elements will have to be composed in a bond graph submodel representing the process." [125]

5.4.3 Bonds and elements

A general graph node may have any number of edges connected to it. Edge connections to the nodes of a bond graph are more restricted than in the case of a general graph, to ensure that bond graph nodes describe meaningful physical behaviour. Bond graph nodes — generally called elements or components — are only permitted to have bonds connected to them at defined *power ports*. The number of power ports can be any number greater than zero, depending on the physical component being modelled. Zero-port components would exchange no energy with any other components and thus would be quite uninteresting. Bonds (graph edges) are connected to element power ports and are the means by which power is transmitted between the graph elements. All element power ports must be connected to another element through a bond; unconnected ports are not permitted. Bonds must also always be connected to a power port at both ends of the bond. Because power bonds transmit power instantaneously between elements, no energy is stored, produced, transformed or dissipated within a bond itself. These physical functions are the purpose of the graph elements.

In the dynamics of any physical system in any energy domain, any work (and hence power) transferred is minimally determined by pairs of conjugate variables. In bond graphs these are called *effort* and *flow*. Ordinarily the effort and flow quantities for an energy domain are assigned in a directly analogous way; for example in mechanics, force is normally denoted the effort variable and velocity the flow variable, although there can be reasons for considering alternative assignments, with Borutzki presenting a discussion of the assignment of effort and flow variables in [125], pages 23–28. Table 5.11 lists common effort and flow variables by energy domain (see e.g. [125] or [164]).

Energy domain	Effort e	Flow f
Translational mechanics	Force F (N)	Velocity v (m/s)
Rotational mechanics	Torque M (Nm)	Angular velocity ω (rad/s)
Heat transfer	Temperature T (K)	Entropy flow rate $\dot{\mathrm{S}}$ (W/K)
Electrical	Voltage v (V)	Current i (A)
Magnetic	Magneto-motive Force V (A)	Magnetic flux rate $\dot{\Psi}$ (Wb/s)
Chemical	Chemical potential μ (J/mol)	Molar flow rate $\dot{\mathrm{N}}$ (mol/s)
Hydraulic	Pressure p (N/m^2)	Volumetric flow rate Q (m^3/s)

Table 5.11: Effort and flow variables by energy domain

It was previously stated that an undirected bond graph is rendered into a directed bond graph through the addition of a *half-arrow* on each bond in the graph. The half-arrow indicates the direction of conventional positive power flow. The actual instantaneous power in a bond may be flowing in either direction along the bond, and the half-arrow denotes only the sign convention. The half-arrow convention distinguishes power bonds from *signal bonds*, which are represented by a full, filled arrow and which do not transmit any power. Conventionally the half-arrow is placed on the side of the bond line where the flow variable is notated. These diagrammatic conventions are illustrated in Figure 5.16.

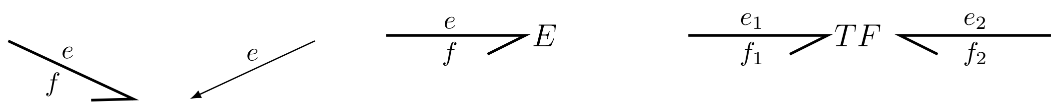


Figure 5.16: A power bond, a signal bond, and one- and two-port elements

5.4.4 Basic bond graph element types

Breedveld [165] identifies nine basic bond graph node types, which represent five groups of basic physical behaviour. These basic node types are described in this section.

Junctions A junction is an n-port topological constraint element which instantaneously transmits power to the bonds connected to each of its ports, and without storing any energy, converting energy to another form, or dissipating it. Junctions are energy conserving and obey the general principle

$$P_{in} - P_{out} = 0 \tag{5.59}$$

$$\text{or } \sum_n e_n f_n = 0 \tag{5.60}$$

where P_{in} and P_{out} is the power entering and leaving the junction respectively, and n is the number of connections. A junction can always have any number of power ports, and hence bonds, connected to it. The simplest possibilities which permit the solution of this general expression of the power balance are ones which assume either all flows are equal, or ones which assume all efforts to be equal [158]. Junctions in which all flows are equal are called *1-junctions*, and those in which all efforts are equal are called *0-junctions*. In earlier bond graph literature these are denoted s-junctions and p-junctions respectively. The graphical convention for 0- and 1-junctions is shown in Figure 5.17.

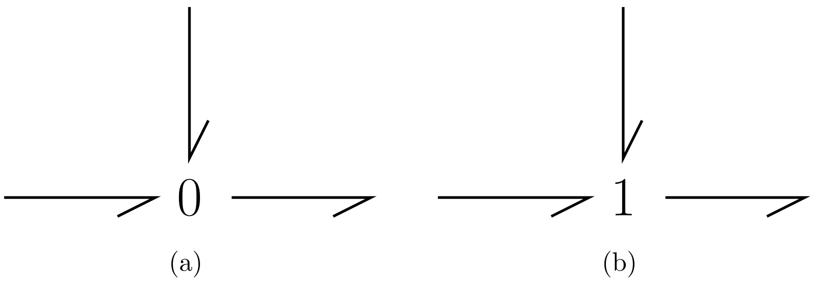


Figure 5.17: Bond graph junctions (a) 0-junction (b) 1-junction

The constitutive equations of a 0-junction are

$$e_1 = e_2 = ... = e_n \tag{5.61}$$

$$f_1 + f_2 + ... + f_n = 0 \tag{5.62}$$

and those of a 1-junction,

$$f_1 = f_2 = ... = f_n \tag{5.63}$$

$$e_1 + e_2 + ... + e_n = 0. \tag{5.64}$$

for n attached bonds and with all attached power bond flows having the same positive direction relative to the junction. It can be seen that these rules are equivalent to Kirchoff's Current and Voltage Laws respectively. Bond graph junctions serve to distribute power between elements; all such power distribution within a bond graph network can be accomplished by a correctly-connected set of junctions forming a *junction-structure*.

Sources and Sinks Bond graph source and sink elements are idealised one-port active elements which are able to supply or remove an infinite amount of energy at an infinite rate to or from the bond graph representing the system. Two types are used; an *effort source (or sink)* and a *flow source (or sink)*. Sources are further characterised by whether they supply a constant effort or flow. Technically only one element type exists — the source — with a sink being a negative source, but in practice it is useful to distinguish between the two as a statement of intent. These elements are essentially unrealistic and as such are regarded as boundary conditions to the model rather than as part of the model itself, although they remain a part of the graph. Figure 5.18 shows the graph conventions.

Figure 5.18: Bond graph sources (a) effort source (b) flow source (c) effort sink (d) flow sink

Dissipators Dissipators or resistances are passive elements which remove energy from the bond graph; they represent entropy-producing processes. The well-known linear electrical resistor is an example of such an element. Formally the dissipator is a 2-port element with the second port being connected to the thermal domain, but given certain assumptions it can be simplified to a 1-port element (this is justified in [165]). The one-port resistive element is shown in Figure 5.19 and defined [125] as

$$e(t) = \Phi_R(f(t)) \tag{5.65}$$

The familiar linear electrical resistor is defined as $\Phi_R = R \times f$ and so the constitutive relationship is the well-known $e = Rf$.

In many situations the heat that is dissipated in the resistance is of no interest, and the simple dissipator model is sufficient. However, the lost heat can be accounted for in a bond graph by extension of the dissipative element to an entropy-producing two-port RS-element. One port of the element can be in any domain, but the second port must be in the heat domain. The RS-element has the definition

$$e_1(t) = \Phi_R(f_1(t))e_1(t)f_1(t) = e_2(t)f_2(t) \tag{5.66}$$

Commonly $\Phi_R(f_1(t))$ is constant and is represented as a resistance R or a conductance $G = {}^1/_R$. The RS-element allows the heat generated from the dissipator to be correctly accounted for within the bond graph.

Energy stores Energy stores are passive bond graph elements which are able to instantaneously store and release energy and which exhibit some sort of restoring force which resists the storing effort and hence limits the amount of energy which can be stored. Two standard linear bond graph storage elements are possible with their representations shown in Figure 5.19. The one-port capacitive (C) energy store is defined [125] as

$$\int f(t) = \Phi_C(e(t)) \tag{5.67}$$

The one-port inductive (I) store is defined as

$$\int e(t) = \Phi_I(f(t)) \tag{5.68}$$

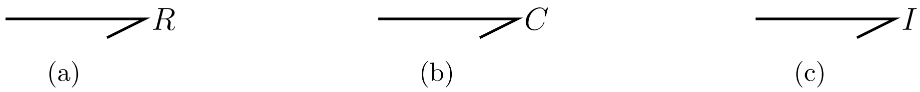


Figure 5.19: Bond graph elements (a) dissipator (b) C-store (c) I-store

Transformers and gyrators Transformers and gyrators are connective two-port elements which transfer energy between distinct sections of the energy system. The bond graph representations are shown in Figure 5.20. Generally transformers represent devices which convert energy within the same energy domain, while gyrators convert energy between different energy domains, although this is not a firm rule. A two-port transformer with effort and flow pairs (e_1, f_1) and (e_2, f_2) at its two ports follows the constraint

$$e_1(t) = T\, e_2(t) \tag{5.69}$$

$$f_2(t) = T\, f_1(t) \tag{5.70}$$

and hence

$$e_1(t)f_1(t) = e_2(t)f_2(t) \tag{5.71}$$

demonstrating that power is conserved in the device. The parameter T is called the transformer modulus and may be a constant, or it may be controllable given an external signal. Such a controllable device is called a modulated transformer.

A two-port gyrator with effort and flow pairs (e_1, f_1) and (e_2, f_2) at its two ports follows the constraint

$$e_1(t) = G\, f_2(t) \tag{5.72}$$

$$e_2(t) = G\, f_1(t) \tag{5.73}$$

and hence

$$e_1(t)f_1(t) = e_2(t)f_2(t) \tag{5.74}$$

demonstrating that power is conserved in the device as it is in a transformer. The parameter G is called the gyrator modulus and may be a constant, or it may be controlled by an external signal, producing a modulated gyrator.

Accumulators Accumulators are one-port storage elements that are not one of the basic bond graph elements. In contrast to a store, an accumulator may exhibit no restoring effort or flow inhibiting the accumulation of energy. A reservoir filled by a fluid from

(a) (b)

Figure 5.20: Bond graph elements (a) transformer (b) gyrator

above would be an example of an accumulator — the reservoir will continue to fill until it overflows, without ever impeding the flow of fluid that is filling it. An accumulator is more like a sink or source element than a store, although it may have the behaviour of both. Importantly the accumulator differs from a sink or source element in that it has a maximum and minimum capacity, and has a maximum and minimum (often zero) fill and release rate. It may also be subject to a time-dependent loss or gain of the stored quantity that can be approximated as an element parameter but which would also be more correctly modelled as a part of the bond graph.

5.4.5 Thermodynamic bond graphs

The bond graph elements presented so far are quite straightforward in that they represent real physical connections through which energy is transferred and conserved. In integrated energy systems however fluids are commonly used to transport energy, either as sensible heat or possibly in the form of a chemical solution. Energy is transferred in these systems as a mass flow. Open thermodynamic systems representing these mass flows require additional state information and the energy bonds can no longer be simply represented by two variables, which complicates the creation of appropriate bond graphs. Borutzky [125] notes that a number of potential methods for incorporating thermodynamic systems into bond graphs have been proposed in the literature, and reduces the field of possibilities to two main approaches. These are examined here.

Pseudo bond graphs separate the mass and energy parts of the physical process and thus relax the fundamental requirement for bonds to represent power flows, while retaining the other structural elements such as the basic elements and graph construction rules. Pseudo bond graphs are reported by Borutzky and other sources in the literature to have been used successfully to model a variety of systems. The pseudo-bond graph methods tend to use more recognisable engineering terms (such as heat flow $\dot{Q}$ rather than entropy flow $\dot{S}$), but as well as the non-energy-conserving bond the C-storage elements are not conservative, and the separation of mass and energy flows leads to more difficulty in connecting these models to non-thermodynamic parts of the bond graph.

True bond graphs maintain pure power bonds within the graph and require more structural development, and some new types of graph elements which extend the basic node types. However the power bonds in true bond graphs remain energy-conserving and thus offer a more general and correct approach to bond graph modelling. In particular, cross-domain transformers and gyrators can be guaranteed to be energy conserving. As integrated energy systems involve interacting energy flows from multiple domains where the conversion of power is important, it is considered that a true bond graph approach is the more suitable approach. In Chapter 10 of [125] Borutzky lists three main approaches to true bond graph construction. These will be summarised briefly here.

3-port C-field and multibonds Neglecting kinetic energy, it follows from the two-property postulate of thermodynamics that an open thermodynamic system has an extensive internal energy which is a function of the entropy S, volume V and number of moles N of the substance occupying the system.

$$U = f(S, V, N) \tag{5.75}$$

The total differential of this function is

$$dU = \frac{\partial U}{\partial S} dS + \frac{\partial U}{\partial V} dV + \frac{\partial U}{\partial N} dN \tag{5.76}$$

which results in the Gibbs' fundamental equation for the open system control volume:

$$\frac{dU}{dt} = T\dot{S} - p\dot{V} + \mu\dot{N} \tag{5.77}$$

where T, p and μ have the following definitions

$$T \equiv \frac{\partial U}{\partial S},\ -p \equiv \frac{\partial U}{\partial V},\ \mu \equiv \frac{\partial U}{\partial N} \tag{5.78}$$

The open system described by Equation 5.77 is represented in bond graphs as a 3-port capacitive element or field (introduced by Breedveld [167]) that is energy conservative, and the three terms of the equation are respectively the heat, work and mass flow into the element. Note that pressure is defined negative for positive flow into the element. The three power bonds can be treated individually and in some applications one or more of the bonds can be omitted. For example, a closed system which by definition has a constant mass may neglect to include the mass flow bond, and an adiabatic system could omit the heat flow term. In a general modelling system however the three bonds can be combined into a multi-bond [125] or thermo-bond [168], also called a bus-bond in some applications.

In regular bond graphs the capacitive field contains a single parameter, the bond-graphic capacitance, which permits the implementation of a generalised capacitive element. A generalised thermodynamic capacitive field is not possible however as the constitutive equation of the three-port capacitive field is defined according to the material that is contained within it. Borutzky provides a derivation of a constitutive equation for an ideal gas, but other materials, most notably water, steam near the saturation line, and mixed-phase materials, require individual treatment.

3-dimensional multibonds (convection bonds) Thoma describes a representation that is similar to the 3-port C-element described above [169]. In this scheme, also called convection bonds by Thoma, transported kinetic energy and phase transitions are ignored, and molar flow rate is instead written as a mass flow, which reduces the three bonds to a $(p, \dot{v})$ pair, a $(T, \dot{S})$ pair, and a signal bond characterised by the fluid mass flow $\dot{m}$.

Convection bonds Brown also considers the generalised thermodynamic capacitive field, reproducing the derivation of Equation 5.77 [166] . However Brown suggests a different approach based on the derivation of stagnation enthalpy in a fluid line and introduces a hybrid-type power bond to represent mass flow called a *convection bond* [166]. From the analysis of a fluid line through a fixed cross-sectional area, Brown shows that the product of the stagnation enthalpy h_0 and mass flow $\dot{m}$ is the total power through the cross-sectional area. However, the two-state postulate must still be met to fully-define the state of the fluid and so Brown proposes adding the pressure p_0 to the bond as an additional effort variable. The enthalpy is what Brown terms the "proper effort" while the pressure effort serves to define the computational causality of the bond. Convection bonds as defined by Brown are used by for example Lubega and Farid in their modelling of the water-electricity nexus [19]. The convection bond is not a multi-bond, rather it is a hybrid single bond which has two effort quantities which determine different aspects of the flow. Brown defines a new notation which uses an additional dashed line on the effort side to indicate a convection bond (Figure 5.21). For the types of integrated energy

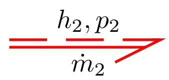


Figure 5.21: Convection bond

networks that are found in integrated energy networks, energy transport tends to occur using incompressible fluids (i.e. water) and the capacitive terms are un-needed. For such systems the convection bond approach is convenient and straightforward and it is this scheme which is used in this thesis.

State Calculation Greifeneder and Cellier in their work on bond graph convective flow modelling [170] describe a true bond graph scheme which uses Gibbs fundamental equation directly to compute the power flows and internal energy changes within a substance-specific C-field. Brown points out in [166] that such a direct scheme requires an iterative or lookup process to determine material state and offers an alternative non-iterative method; however, no attempt has been made to integrate Brown's method. Cellier and Greifeneder provide methods for calculating material state for water (liquid and vapour) and air (ideal gases), and have created a bond-graph modelling library for the Modelica language that implements the basic components; C-fields, conductive heat flow, resistive pipe flow and volume work. Some of the implementation is used directly and some is used as learning material.

An aspect that must be considered is the incorporation of equations of state into the model. In a pure bond graph approach using a triple thermodynamic bond, such as in that proposed by Greifeneder and Cellier [170], it is possible to calculate state in generalised capacitive elements. In a Brown formulation network however state and derived state quantities must be calculated locally where necessary. A common example is the need to calculate temperature in heat transfer elements. It is necessary therefore to attach an additional identifier to a convective thermodynamic bond denoting the chemical species involved in the power transfer, and to provide a programmatic means of calculating state for each species. In this work only single species power bonds are considered, and only relatively simple state calculations are applied, and the attachment of state information to bonds is not attempted. The materials considered are incompressible water; and ideal gas formulations for air and common atmospheric compounds involved in combustion, i.e. CO_2, CH_4, H_2O and N_2. However, the method is extensible to mixed species bonds and more sophisticated state calculation methods.

5.4.6 Modelling principles

It was noted earlier that a fundamental feature of bond graphs is their lumped parameter nature. The result of this is an important principle of modelling integrated energy systems using bond graphs, particularly thermal systems. The lumped nature of bond graphs indicates that the individual physical behaviours making up the system are to be modelled discretely. This can be seen clearly in elementary systems such as mass-spring-damper systems, which may be in reality a single component but which can be modelled discretely and for which approximations to the parameter of individual components can be made.

For thermal convection systems it is desirable and necessary to divide the system to be modelled into reversible and irreversible processes which can be modelled using distinct bond graph components. A convection bond represents a state of the convected fluid and state changes can only take place between bonds, i.e. within convective elements such as RS or HS element types. A general state transition can then be represented as a group of bond graph elements each of which represents a reversible process. Process losses are accounted for using irreversible components, which serve to modify the underlying reversible processes. Furthermore for a ducted fluid, say, if processes on the fluid can be separated into constant enthalpy and constant pressure processes then the resulting bond graph will feature straightforward discrete elements with clearly-defined behaviour that can be re-used from a library of such components. If this is not possible then often a new process-specific bond graph element will need to be created.

In the electrical and mechanical domains irreversible behaviour is mostly modelled by the familiar linear resistances and frictional forces respectively. In fluids (in the context of integrated energy systems), the friction of fluids in ducts will be the most commonly encountered irreversible process. These are easily handled using the RS element (which may be linear or non-linear) which has a non-thermal primary port. In the thermal domain, a special RS element with a thermal-domain primary port is required and this is described below.

The separation of processes into reversible and irreversible behaviours and into constant state processes where possible simplifies bond graph creation but also allows the resultant bond graphs to illuminate important aspects of a system's behaviour and make-up. The explicit representation of the individual process components within the graphical description lend the bond graph an important communicative strength as well as a computational one.

In the following sections, the modelling tool Dymola is used to develop and explore the component models [171].

5.4.7 Processes

Heat conduction Thoma [164] describes a bond graph model for linear heat conduction based around the RS-element, shown in Figure 5.22. This model is also reproduced by Borutzski [125], Cellier [158] and used by Cellier and Greifeneder [168, 170]. The model takes the form of a 2-port thermal resistance with both ports in the thermal domain. The constitutive equations for the RS-element used in this model are as described previously, with R as the RS-element bondgraphic thermal resistance. For the overall model, both power conservation and a way of modelling of the heat conduction process must be considered. The latter is provided by Fourier's conduction law $\theta = \frac{\Delta T}{\delta Q}$, where Q is the thermal power and θ the thermal resistivity. Then the overall graph must satisfy (ignoring the junction equations)

$$T_1\,\dot{S}_1 = T_2\,\dot{S}_2 \tag{5.79}$$

$$\frac{\Delta T}{\delta Q} = \frac{T_1 - T_2}{T_1\,\dot{S}_1} = \frac{T_1 - T_2}{T_2\,\dot{S}_2}, \quad \text{with } T_1 > T_2,\ \theta > 0,\ \delta Q > 0 \tag{5.80}$$

The RS-element itself is characterised by the expressions

$$\dot{S}_1\,(T_1 - T_2) = (\dot{S}_2 - \dot{S}_1)\,T_2 \tag{5.81}$$

$$T_1 - T_2 = R\,\dot{S}_1 \tag{5.82}$$

Comparing these, the relationship between the resistivity, efforts and flows can be seen to be

$$T_1 - T_2 = \theta\,T_1\,\dot{S}_1 \tag{5.83}$$

Comparing this with the constitutive equation of the RS-element shows that the bondgraphic resistance of the RS-element is $R \equiv \theta\,T_1$. For computational purposes it is necessary that the calculation of R is self-contained within the RS-element, for which the value of T_1 is unknown. However, because for the RS-element the value of the input effort $e_1 = T_1 - T_2$ and the output effort $e_2 = T_2$, then $T_1 = e_1 + e_2$, and the bondgraphic thermal resistance is given by

$$R = \theta(e_1 + e_2) \tag{5.84}$$

For the entire element, putting $G = 1/R$ as the thermal conductivity in J/kg K s, the entropy flows into and out of the element are

$$\dot{S}_1 = \frac{G\,(T_1 - T_2)}{T_1} \tag{5.85}$$

$$\dot{S}_2 = \frac{G\,(T_1 - T_2)}{T_2} \tag{5.86}$$

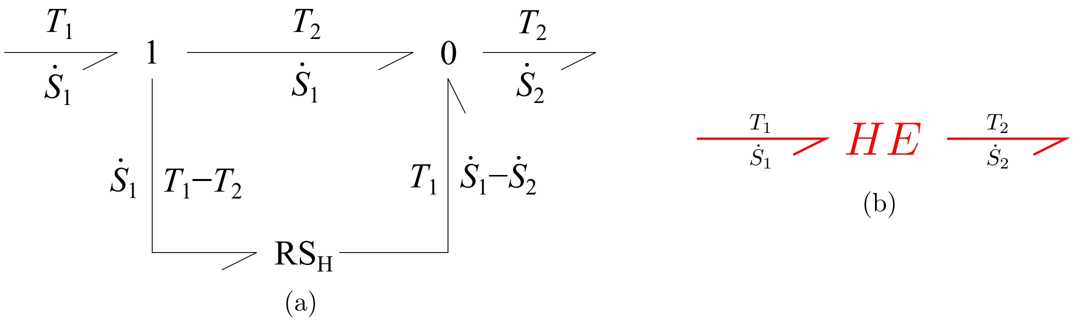


Figure 5.22: Heat conduction bond graph (a) Thoma (b) Macro-model

It is also possible to construct the model directly by using the linear conduction law (Fourier's Law), leading to a single 2-port RS conduction model with the following constitutive equations that are identical to the above. As there are two equations and four unknowns for the element, two of the quantities must be specified as boundary conditions.

$$T_1\dot{S}_1 = T_2\dot{S}_2 \tag{5.87}$$

$$T_2\dot{S}_2 R = T_1\dot{S}_1 R = T_1 - T_2 \tag{5.88}$$

This variant is given by Brown [166]. The main advantage of this direct approach over the Thoma formulation is that reverse heat flow is calculated naturally; the Thoma graph formulation requires a mirror image model for reverse power flow, with the addition of a switch to ensure that the correct model is used. The direct formulation also involves fewer equations and bond graph parts. However the Thoma formulation illustrates how a conduction model proceeds from the fundamental RS element type, and how the generated entropy is re-introduced into the heat domain part of the bond graph.

Although the heat transfer RS coupler is often shown with the same symbol as the ordinary RS element, a "H" suffix will be used here to distinguish the two as they have different constitutive equations. The macro model is given the symbol HE for heat exchange.

In [168] and [170] a bi-directional conduction model using this construction is presented which splits the incoming thermal stream through two RS-junctions to re-enter the graph at both the incoming and outgoing streams; rather than the structure presented above, where entropy produced by the RS-junction re-enters the graph downstream at the 0-junction. Unfortunately this construction is incorrect; the model assumes without justification that the two RS-elements have a bondgraphic conductivity of $G/2$ and the incoming entropy flow is split equally between them. A proof of why this is incorrect is not attempted here, but a cursory simulation reveals that the entropy generated by this model does not equal that calculated from Equation 5.80.

Heat exchange A bond graph representation of device which exchanges heat between an entropy flow and a convective fluid flow is given by Brown [166] and is shown in Figure 5.23. The system is described by six equations, ten unknowns and three parameters, and therefore four unknowns must be given as boundary conditions. An equation of state must also be provided so that the stream temperature can be calculated.

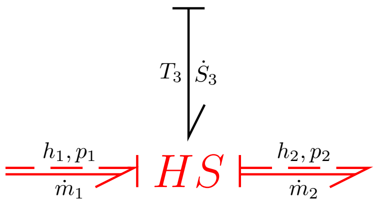


Figure 5.23: Convective heat exchanger bond graph

$\dot{m}_1 + \dot{m}_2 = 0$	mass continuity
$\dot{m}_1 h_1 + \dot{m}_2 h_2 + \dot{s}_3 T_3 = 0$	energy conservation
$p_1 = p_2$	pressure equality
$T_3 = T_2$	outlet temperature
$h_2 - h_1 = c_p(T_2 - T_1)$	equation of state

A number of combinations of unknowns are possible, including (p_1, h_1, h_2, $\dot{m}_1$), (p_1, T_1, T_2, $\dot{m}_1$), and (p_1, h_1, h_2, $\dot{m}_1$). However, p_1 and p_2 are not independent and cannot both be used as independent variables at the same time.

Combustion A gas combustion processes has been modelled using bond graphs in order to calculate the temperature of combustion products used as a heat source for boilers and heat engines. The combustion process used here is a straightforward stoichiometric-with-excess-air calculation that uses an iterative approach to find the temperature of the combustion products, as described by Kotas [48] and Çengel and Boles [12]. Only natural gas combustion is modelled, and the assumption is made that natural gas can be treated as pure methane (CH_4). The intention of the stoichiometric-with-excess-air model is to account for energy transfer and exergy destruction within a combustion process and does not account for the formation of “problem” combustion products such as NOx and SO_2 and thus cannot be used to study the atmospheric pollution caused by combustion. While these noxious products may very well be a legitimate target of heat plant analysis this is outside of the scope of this investigation. Fuel (methane gas) is supplied from the gas supply network, which is regarded to be an infinite and constant reservoir and thus is represented as a bond graph source element. A custom bond graph element describing the stoichiometric reaction is central to the combustion calculation. This is a multi-port component which performs the reactants-products energy balance calculation. Using the terminology in [48], the temperature of the combustion products is found from the energy balance

$$m_f(\mathrm{NCV})^0 = (\theta_2 - \theta^0)\sum_k n_k \tilde{c}^h_{p,k}$$

where m_f is the mass of fuel, $(\mathrm{NCV})^0$ is the per kg lower heating value of fuel, θ_2 is the temperature of the combustion products, θ^0 is the initial temperature of the fuel and air, n_k is the number of moles of product k, and $\tilde{c}^h_{p,k}$ is the mean specific heat for enthalpy of product k. The stoichiometric combustion equation for methane in excess air of ratio x is

$$\mathrm{CH_4} + 2(1+x)(\mathrm{O_2} + 3.76\mathrm{N_2}) \longrightarrow \mathrm{CO_2} + 2\mathrm{H_2O} + 2x\mathrm{O_2} + 9.776\mathrm{N_2}$$

or

$$\mathrm{CH_4} + 2\mathrm{O_2} + 2x\mathrm{O_2} + 9.776\mathrm{N_2} \longrightarrow \mathrm{CO_2} + 2\mathrm{H_2O} + 2x\mathrm{O_2} + 9.776\mathrm{N_2}$$

which results in a molar and mass breakdown of the reaction as shown in Table 5.12. Because, as mentioned above, the mean specific heat and the final temperature of the

Substance	CH_4	O_2	N_2	$\longrightarrow$	CO_2	H_2O	O_2	N_2
Moles in reaction	1	$2(1+x)$	9.776		1	2	$2x$	9.776
Molar mass	16	32	28		44	18	32	28
kmol / 100kg fuel	6.25	$12.5(1+x)$	61.1		6.25	12.5	$12.5x$	61.1
Mass (kg) in reaction	100	$400(1+x)$	1710.8		275	225	$400x$	1710.8

Table 5.12: General gas boiler combustion reaction

combustion products are both unknown and depend on each other, they are found from the energy balance equation using an iterative method. Within the Dymola environment this iterative step is performed implicitly for each time step using Newton's method. The combustion bond graph is shown in Figure 5.24, with the combustion energy balance model presented in Figure 5.25. The model contains a series of tables of values for $\tilde{c}^h_{p,k}$ for the reactants and products, which are taken from Table D.1 in [48]. Only the specific combustion reaction used in this study has been developed. The equations governing the solution of the reaction are as follows.

$$H_{\text{in}} = \dot{m}_{\text{in}} h_{\text{in}} \tag{5.89}$$

$$\dot{m}_{\text{in}} = M_1 r \tag{5.90}$$

$$r\nu_k = n_k \tag{5.91}$$

$$m_k = M_k n_k \tag{5.92}$$

$$\tilde{c}^h_{p,k} = f(T) \tag{5.93}$$

$$(T - T_{\text{ref}})\tilde{c}^h_{p,k} = M_k h_k \tag{5.94}$$

$$H_{\text{out}} = \sum_k M_k \tilde{c}^h_{p,k} \tag{5.95}$$

$$(T - T_{\text{ref}})H_{\text{out}} = H_{\text{in}} \tag{5.96}$$

In the above, reacting air (oxygen and nitrogen) has an enthalpy value of zero. Subscript k refers to species k, M is the molar mass of the species, and m is the mass in kg. H refers to enthalpy and h to specific enthalpy; $\dot{m}$ is mass flow rate. ν_k is the stoichiometric mole number for species k, n_k is the actual number of moles of the species k in the calculation, and r is the molar ratio for that species. As noted above, $\tilde{c}^h_{p,k} = f(T)$ and is the average specific heat capacity for species k between a reference state (subscript ref) and temperature T with the function $f(T)$ being computed from tabular interpolation. T is the temperature of the reaction. Suffixes 'in' and 'out' refer to the streams entering and leaving the reaction respectively.

Chemical kinetics Chemical kinetic bond graph elements are not included in the demonstrator model in Chapter 6, but a short description is included here for completeness and to indicate how they could be used in an integrated enrgy system model. A number of authors have addressed the problem of representing a chemical reaction using bond graphs. Roman *et al.* present two papers [172,173] implementing a reaction network for two combustion reactions,

$$C + O_2 \longrightarrow CO_2$$

$$CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O$$

These reaction networks are in fact a special case of a generalised reaction scheme as described by Thoma, Greifeneder [174], Brown [166], and also by Couenne [175]. The networks described by Roman *et al.*, while accurate, have disjoint thermal and input mass flow sections and require additional bonds which feed the energy increase seen at the output back into the input compliances; or separate energy accounting for the reactants, which breaks the integrity of the bond graph by introducing external computation. The

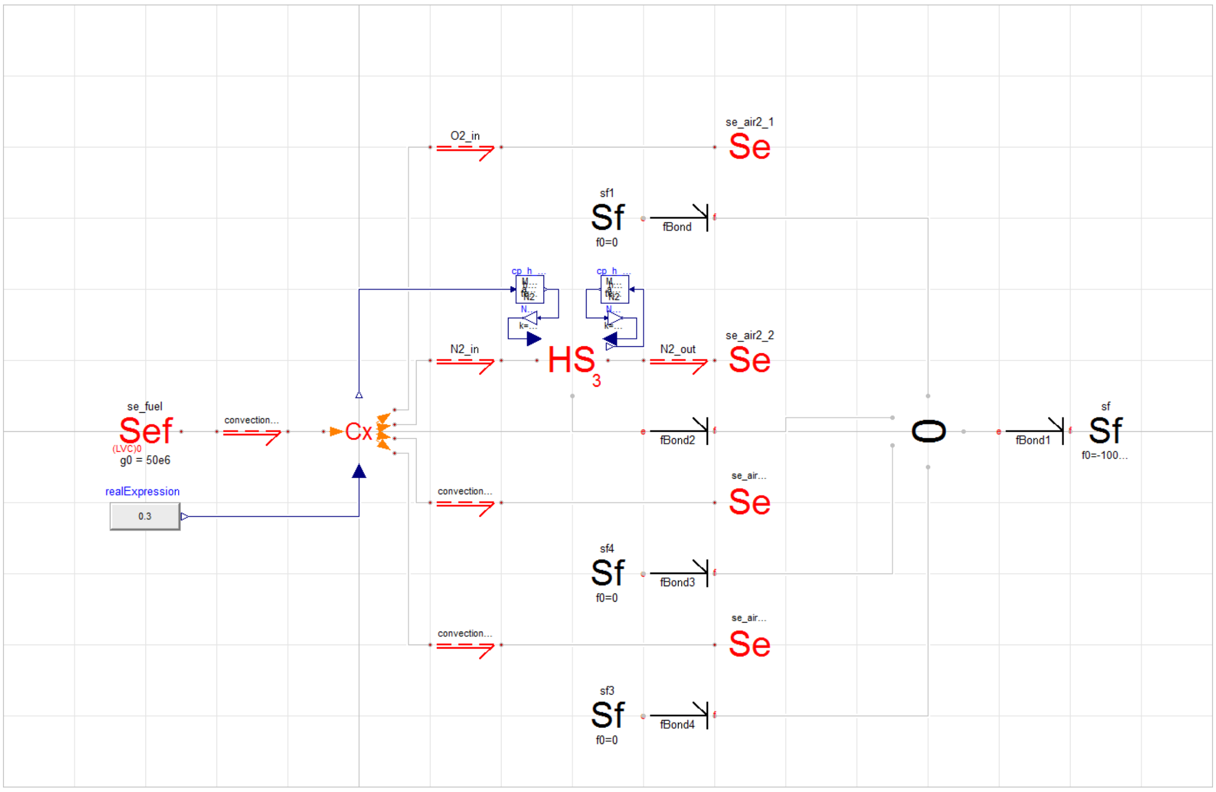


Figure 5.24: Combustion bond graph

networks also only really work for a closed system, and for fixed volume containers. The general models allow for correct accounting of energy in heating the reactants, and for open system mass flows.

The generalised reaction networks noted above all describe fundamentally the same architecture. The reaction takes place within an open system represented by a thermodynamic compliance (one-port C-element) containing the reactants and products, which are allowed to flow into and out of the system. The reaction itself is described by a network consisting of a 1-junction joined to a set of stoichiometric transformers which transform molar flows into the correct amounts for the reaction, and to a reaction rate element which controls the overall reaction rate and provides a transformer component which converts the reaction rate into an enthalpy value. The reaction rate element implements Arrhenius' equation. Finally, conservation of energy is provided by a 0-junction connected to the system compliance and the heat side of the reaction rate network. To make the chemical reaction aspect of the network distinct from the physical, Greifeneder suggests the addition of mass-to-molar flow transformers.

Stream mixing and splitting When fluids at different temperatures enter a volume and mix, the resultant fluid leaving the volume is at an intermediate temperature and has lost entropy as a result of the irreversible mixing process. This commonly occurs in heat networks where fluids mix on the return network, and which is poorly represented within a MNA method. Brown [166] provides a stream merging model that is valid for all flow directions of the three streams involved (two inlet and two outlet). This element model is

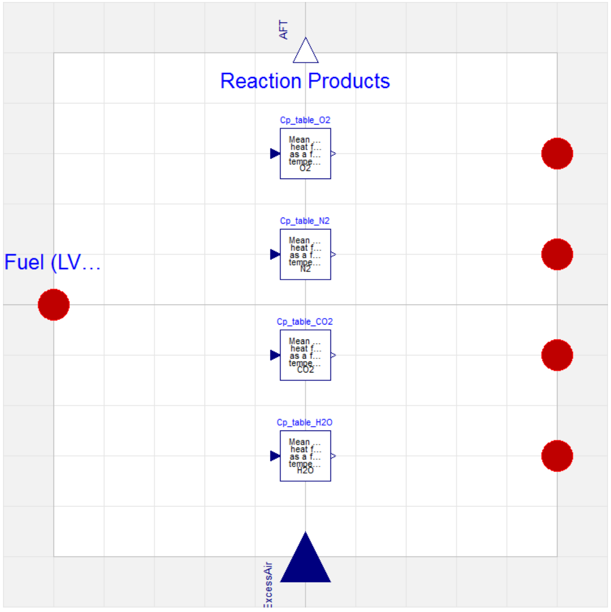


Figure 5.25: Combustion energy balance bond graph component

termed an 0S-junction as it functions like a 0-junction for convection bonds only with the addition of an entropy loss. The junction is shown in detail and as a macro-component in Figure 5.26. The lines joining the HS elements are ordinary thermodynamic $(T, \dot{S})$ bonds which serve to equalise the temperatures across the streams (a bond arrow direction can be specified if necessary); then flow continuity happens at the regular 0-junction. The presence of the heat transferring thermodynamic bonds represents the entropy loss in the process. A more general n-stream model is not addressed in this thesis.

It is possible to create a simpler model for stream splitting which requires no heat transfer elements and thus merely divides the flow at a 1-junction. This is also shown in Figure 5.26. Either one can be used, depending on the application, although care must be taken when using the splitter model as this is not valid for reverse flows unless the temperatures of all of the incoming streams are equal.

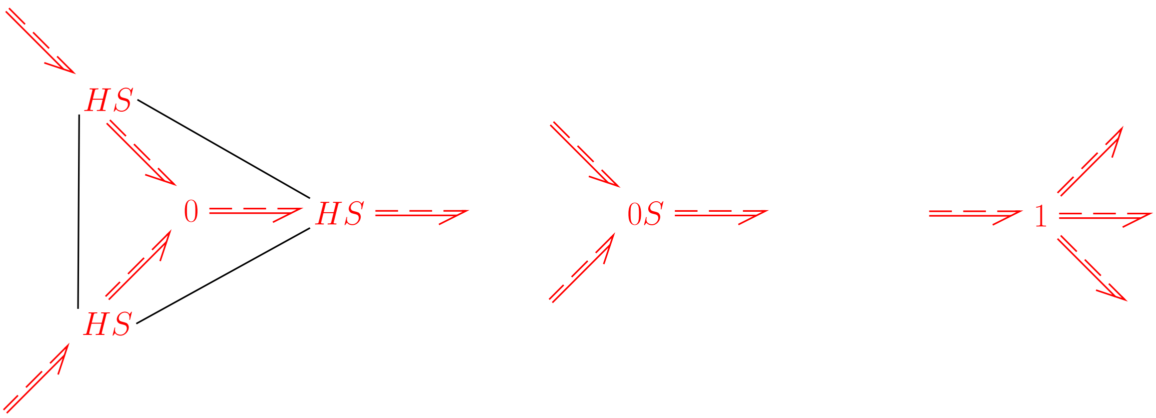


Figure 5.26: 0S junction for mixing and splitting processes

The 0S junction can be built within a modelling environment by connecting HS and thermodynamic 0-junction sub-models together into a meta-model. Alternatively, the equations can be derived for the sub bond graph model and the element implemented directly. The former approach is taken here.

5.4.8 Systems

The previous section described fundamental bond graph elements that describe physical processes and behaviours. In this section, use will be made of these fundamental elements to build up sub-systems that describe the larger components of integrated energy networks. These sub-systems model the main building-blocks — engineering structures and devices — that can be found within an integrated energy system. Given the large and diverse nature of such systems it is not possible to present an exhaustive collection, and instead the set of modelled sub-systems has been chosen to include only the systems used in the representative case studies presented in Chapter 6.

Boiler A model for a boiler is shown in Figure 5.27 and is similar to that given by Lubega and Farid [26] and uses concepts from the counterflow heat exchanger described by Brown [166]. The boiler transfers heat between two streams of fluid; the hot gases from the combustion process pass over a stream of fluid, cooling the combustion exhaust gases and heating the water. Some heat is lost to the environment through the boiler wall. Brown condenses the thermal RS and HS elements into a composite HRS element, but as this boiler model is a sub-system in its own right there is little advantage to be gained by doing this and the individual elements are retained.

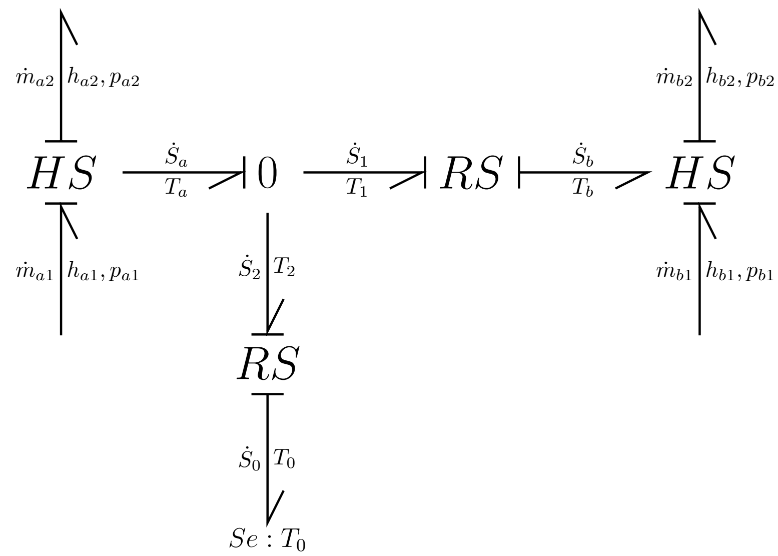


Figure 5.27: Bond graph for a boiler

Heat engine bond graphs In incorporating co- or tri-generation as bond graph models where only the output is required and not the dynamic behaviour of the engine cycle, it is useful to consider models derived from first principles using air-standard cycles and endo-reversibility assumptions. Although these models will not capture the fine detail of more complex dynamic models, they illustrate the dependence of engine efficiency on cycle type and sources of irreversibility. Such models permit the main features and the effect of controllable or design parameters of co- and tri-generation plant in a broader systems design to be included without cluttering the analysis with detail, especially where the precise plant detail is not known but where a model based on a realistically-likely engine cycle is known. These models are still much more fine-grained than the energy-based models found in for example energy hub models, permitting a study of temperature and exergy and integration into a bond graph model.

Endo-reversible studies of heat engines aim at separating the reversible and irreversible processes involved in the cycle. This approach justifies the bond graph lumped parameter methods which naturally divides energy flow into reversible and irreversible components. Gonzalez-Ayala *et al.* describe a form of endo-reversible analysis of heat engines [176] which lends itself well to adaptation into a bond graph formulation. Following the work by Gonzalez-Ayala *et al.* who analyse a Brayton engine cycle, this section will analyse Otto and Lenoir cycles as being particularly suitable for thermal engines used in energy systems and thus appearing in bond graph system models.

Gonzalez-Ayala *et al.* describe two loss factors that can be used to explain the reduction in work seen in non-Carnot heat engine cycles, one caused by the deviation of the geometry of the ideal cycle itself from the Carnot cycle, and the other caused by internally irreversible processes. The loss factors are an alternative expression for the second-law efficiency of the cycle and isentropic efficiency values in expansion and compression processes, but they offer a convenient way of separating and exploring the different losses and importantly in encapsulating these in a steady-state bond graph formulation.

A general heat engine, i.e. one with an arbitrary engine cycle, has a reversible efficiency η_{rev} and actual efficiency η. The efficiency of a Carnot engine operating between the extremes of temperature of the general heat engine has an efficiency of η_C. The loss factors or 'd'-factors are given for any heat engine cycle as

$$d = d_e + d_i - d_e d_i \tag{5.97}$$

with

$$d_e = 1 - \frac{\eta_{\text{rev}}}{\eta_C} <= 1 \tag{5.98}$$

and

$$d_i = 1 - \frac{\eta}{\eta_{\text{rev}}} <= 1 \tag{5.99}$$

d_e gives the geometric closeness of the engine cycle to a Carnot cycle. The work lost in non-Carnot cycles relative to a Carnot cycle operating between the extremes of temperature of the non-Carnot cycle is as a result of an effective (irreversible) heat transfer between the Carnot reservoir temperature and the reversible heat transfer temperature of the non-Carnot engine cycle. d_i on other hand accounts for the internally irreversible processes of the cycle itself, particularly compression and expansion processes which have isentropic

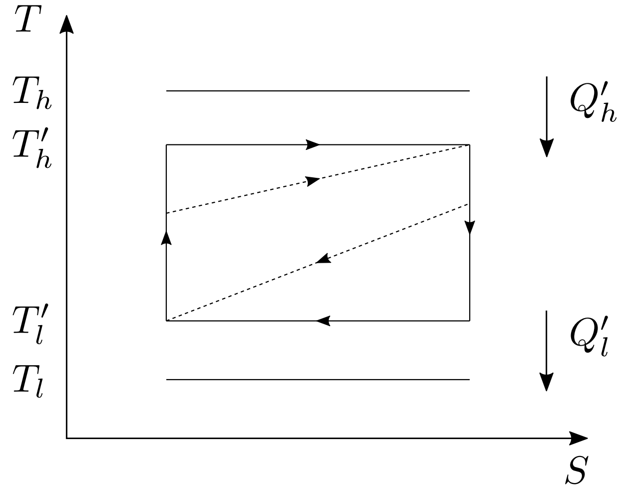


Figure 5.28: An endoreversible temperature-entropy diagram of Carnot and Diesel cycles

efficiencies of less than unity.

Figure 5.28, which shows a T-S diagram of a Carnot cycle and a Diesel cycle (dashed line), illustrates these irreversibilities. T_h and T_l represent the actual high- and low-temperature sources respectively, with T_h' and T_l' being the high- and low-temperature limits of the engine cycle. Heat transfer Q' takes place at the boundaries of the cycle; where the external temperature is different to the Carnot cycle temperature this must necessarily involve irreversible heat transfer, the theory of which is covered by endoreversibility studies pioneered by Curzon and Ahlborn [177]. The parameter d_e represents irreversibilities caused by the endoreversible behaviour of the cycle as a result of heat transfer from and to temperatures T_h and T_l rather than the Carnot temperatures T_h' and T_l', including the because of the geometry of the cycle. The parameter d_i represents irreversibilities caused by the curvatures of irreversible engine cycle processes, i.e. a non-isentropic expansion process. In the illustrated Diesel process, this would occur for deviations of the constant-S processes from the vertical. Further analysis of endoreversible engine cycles begins with Curzon and Ahlborn's 1975 paper but this is not taken further in this thesis. The coupling term $d_e d_i$ is noted in [176] but not elaborated further. This term is merely a consequence of the overlap between the externally irreversible (geometric) losses and the internally irreversible ones.

Gonzalez-Ayala *et al.* derive an expression for a Brayton cycle which gives

$$d_e(a,\tau) = 1 - \frac{1 - a\tau}{a(1-\tau)} \tag{5.100}$$

$$d_e(a,\tau,\eta_c,\eta_t) = 1 - \frac{\eta_c(1-\tau) + \tau - \eta_c\eta_t}{\eta_c(a-\tau) + \tau - a\tau} \tag{5.101}$$

The derivation of the Otto cycle loss factors follows a very similar approach to that of the

Brayton cycle. Set

$$r_v = \frac{v_1}{v_{2S}} = \frac{v_{4S}}{v_3} \tag{5.102}$$

$$a = r_v^{\gamma-1} \tag{5.103}$$

$$\tau = T_1/T_3 \tag{5.104}$$

$$\gamma = c_p/c_v \tag{5.105}$$

a)

$$|\dot{q}_{in}| = c_v(T_3 - T_2) = c_v T_3 \left[1 - \frac{T_{2S} - T_1}{T_3 \eta_c} - \frac{T_1}{T_3}\right] \tag{5.106}$$

Process 1 → 2S is isentropic, so

$$\frac{T_1}{T_{2S}} = \left(\frac{v_{2S}}{v_1}\right)^{\gamma-1} = \frac{1}{a} \tag{5.107}$$

and so

$$\begin{aligned} |\dot{q}_{in}| &= c_v T_3 \left[1 - \frac{T_1 a - T_1}{T_3 \eta_c} - \frac{T_1}{T_3}\right] \\ &= c_v T_3 \left[1 - \frac{\tau}{\eta_c}(a-1) - \tau\right] \end{aligned} \tag{5.108}$$

b)

$$|\dot{q}_{out}| = c_v(T_4 - T_1) = c_v T_3 \left[1 - \frac{\eta_e(T_3 - T_{4S})}{T_3} - \frac{T_1}{T_3}\right] \tag{5.109}$$

Process 3 → 4S is isentropic, so

$$\frac{T_{4S}}{T_3} = \left(\frac{v_3}{v_{4S}}\right)^{\gamma-1} = \frac{1}{a} \tag{5.110}$$

and so

$$|\dot{q}_{out}| = c_v T_3 \left[1 - \eta_e\left(1 - \frac{1}{a}\right) - \tau\right] \tag{5.111}$$

c) Total work output is then

$$|\dot{w}| = |\dot{q}_{in}| - |\dot{q}_{out}| \tag{5.112}$$

$$\begin{aligned} &= c_v T_3 \left[1 - \frac{\tau}{\eta_c}(a-1) - \tau - \big(1 - \eta_e(1 - {}^1\!/\!a) - \tau\big)\right] \\ &= c_v T_3 \left[\eta_e(1 - {}^1\!/\!a - \frac{\tau}{\eta_c}(1-a)\right] \\ &= c_v T_3 \left[\eta_e - \frac{\tau a}{\eta_c}\right]\left[1 - \frac{1}{a}\right] \end{aligned} \tag{5.113}$$

d) The efficiency of the process is given by

$$\eta = \frac{|\dot{w}|}{|\dot{q}_{in}|} = \frac{\left[\eta_e - \frac{\tau a}{\eta_c}\right][1-a]}{1 - \frac{\tau}{\eta_c}(a-1) - \tau} \tag{5.114}$$

For an isentropic cycle $\eta_c = \eta_e = 1$ and so the efficiency reduces to the textbook result of

$$\eta_{\text{rev}} = \frac{[1-\tau a]\left[1 - {}^1\!/_a\right]}{1 - \tau a + \tau - \tau} = 1 - \frac{1}{a} \tag{5.115}$$

$$\eta_{\text{rev}} = 1 - \frac{1}{r_v^{\gamma-1}} \tag{5.116}$$

The loss factors are given by

i)

$$d_e = 1 - \frac{\eta_{\text{rev}}}{\eta_c} = 1 - \frac{1 - {}^1\!/_a}{1-\tau} = \frac{1 - \tau - 1 + {}^1\!/_a}{1-\tau} \tag{5.117}$$

$$i.e. \quad d_e = \frac{1 - a\tau}{a(1-\tau)} \tag{5.118}$$

ii)

$$d_i = 1 - \frac{\eta}{\eta_{\text{rev}}} = 1 - \frac{\left[\eta_e - \frac{\tau a}{\eta_c}\right]\left[1 - {}^1\!/_a\right]}{1 - \tau - \frac{\tau}{\eta_c}(a-1)} \frac{1}{(1 - {}^1\!/_a)}$$

$$= 1 - \frac{(\eta_e - \frac{\tau a}{\eta_c})}{1 - \tau - \frac{\tau}{\eta_e}(a-1)}$$

$$= \frac{1 - \tau - \frac{\tau a}{\eta_c} + \frac{\tau}{\eta_c} - \eta_e + \frac{\tau a}{\eta_c}}{1 - \tau - \frac{\tau a}{\eta_c} + \frac{\tau}{\eta_c}}$$

$$= \frac{\eta_c - \tau\eta_c + \tau - \eta_e\eta_c}{\eta_c - \tau\eta_c - \tau a + \tau}$$

$$\text{so} \quad d_i = \frac{\eta_c(1-\tau) + \tau - \eta_e\eta_c}{\eta_c(1-\tau) + \tau - \tau a} \tag{5.119}$$

These loss factor expressions are identical to those determined for the Brayton cycle as presented by Gonzalez-Ayala in [176]. The factor a is equal to $r_v^{\gamma-1}$ for an Otto Cycle, while a is equal to $r_p^{\frac{\gamma-1}{\gamma}}$ for a Brayton Cycle.

The Lenoir Cycle is often used as a model for an ideal pulse-jet engine cycle, and loss factors are calculated here for this cycle also.

i)

$$|\dot{q}_{in}| = c_v(T_2 - T_1) = c_v(r_p T_1 - T_1) = c_v T_1(r_p - 1)$$

$$= c_v T_2(1 - {}^1\!/_{r_p}) \tag{5.120}$$

ii)

$$
\begin{aligned}
|\dot{q}_{out}| &= c_p(T_3 - T_1) \\
&= c_p \left(T_2 - \eta_e(T_2 - T_{3S}) - T_1\right) \\
&= c_p \left(T_2 - \eta_e(T_2 - T_2\, r_p^{\frac{1}{\gamma}-1}) - \frac{T_2}{r_p}\right) \\
&= c_p T_2 \left(1 - \eta_e(1 - r_p^{\frac{1}{\gamma}-1}) - \frac{1}{r_p}\right)
\end{aligned} \tag{5.121}
$$

Remembering that $c_p = \gamma\, c_v$, the efficiency of the cycle is given by

$$
\begin{aligned}
\eta &= \frac{|\dot{q}_{in}| - |\dot{q}_{out}|}{|\dot{q}_{in}|} \\
&= \frac{c_v T_2 \left(1 - \frac{1}{r_p}\right) - c_v \gamma T_2 \left(1 - \eta_e \left(1 - r_p^{\frac{1}{\gamma}-1}\right) - \frac{1}{r_p}\right)}{c_v T_2 \left(1 - \frac{1}{r_p}\right)} \\
&= \frac{r_p - 1 - r_p \gamma \left(1 - \eta_e \left(1 - r_p^{\frac{1}{\gamma}-1}\right) - \frac{1}{r_p}\right)}{r_p - 1} \\
&= 1 - \frac{r_p - r_p\gamma\eta_e + r_p\gamma\eta_e r_p^{\frac{1}{\gamma}-1} - \gamma}{r_p - 1} \\
&= 1 - \frac{\gamma \left(r_p\,(1 - \eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1\right)}{r_p - 1}
\end{aligned} \tag{5.122}
$$

In the isentropic case $\eta_e = 1$ and thus

$$
\eta_{\text{rev}} = 1 - \frac{\gamma(r_p^{\frac{1}{\gamma}} - 1)}{r_p - 1} \tag{5.123}
$$

The loss factors are computed similarly. Taking into account that the efficiency of the comparative Carnot cycle is

$$
\eta_c = 1 - \frac{T_1}{T_2} = 1 - \frac{1}{r_p} = \frac{r_p - 1}{r_p} \tag{5.124}
$$

then

$$
\begin{aligned}
d_e &= 1 - \frac{\eta_{\text{rev}}}{\eta_c} \\
&= 1 - \frac{r_p - 1 - \gamma(r_p(1-\eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1)}{r_p - 1} \times \frac{r_p}{r_p - 1} \\
&= \frac{(r_p - 1)^2 - r_p(r_p - 1 - \gamma(r_p(1-\eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1)}{(r_p - 1)^2} \\
&= \frac{r_p^2 - 2r_p + 1 - r_p^2 + r_p + r_p\gamma(r_p(1-\eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1)}{(r_p - 1)^2} \\
d_e &= \frac{1 - r_p + r_p\gamma(r_p(1-\eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1)}{(r_p - 1)^2} \qquad (5.125)
\end{aligned}
$$

In the isentropic case $\eta_e = 1$ and thus

$$
d_e = \frac{1 - r_p + r_p\gamma(r_p^{\frac{1}{\gamma}})}{(r_p - 1)^2} \qquad (5.126)
$$

$$
d_i = 1 - \frac{\eta}{\eta_{\text{rev}}} \qquad (5.127)
$$

$$
\begin{aligned}
d_i &= 1 - \frac{r_p - 1 - \gamma(r_p(1-\eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1)}{r_p - 1} \times \frac{r_p - 1}{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1)} \\
&= 1 - \frac{r_p - 1 - \gamma(r_p(1-\eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1)}{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1)} \\
&= \frac{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1) - r_p + 1 + \gamma(r_p(1-\eta_e) + \eta_e r_p^{\frac{1}{\gamma}} - 1)}{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1)} \\
&= \frac{-\gamma r_p^{\frac{1}{\gamma}} + \gamma + \gamma r_p - \gamma r_p \eta_e + \gamma \eta_e r_p^{\frac{1}{\gamma}} - \gamma}{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1)} \\
&= \frac{\gamma(r_p - r_p^{\frac{1}{\gamma}} - r_p\eta_e + \eta_e r_p^{\frac{1}{\gamma}}}{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1)} \\
&= \frac{\gamma(r_p(1-\eta_e) - r_p^{\frac{1}{\gamma}}(1-\eta_e)}{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1)} \\
d_i &= \frac{\gamma\left[r_p - r_p^{\frac{1}{\gamma}}\right][1-\eta_e]}{r_p - 1 - \gamma(r_p^{\frac{1}{\gamma}} - 1)} \qquad (5.128)
\end{aligned}
$$

The loss factors derived here can be used in bond graph power models which have known temperatures for the engine heat and sink. For situations where the heat or power generator uses an engine cycle and compression ratio which are known or can be inferred, the loss factors can be derived and a reasonable approximation to the engine used in a bond graph system model.

This section has presented general expression for loss factors in a steady-state heat engine, and some specific loss factors for particular heat engines were derived. The usefulness of this approach in terms of a bond graph formulation is that it permits the heat engine to be represented as a Carnot cycle element along with separate loss sections, heat transfer and storage elements. The heat engine bond graph model described in this way is a semi-ideal steady-state model that retains temperature information in the power flow sections and explicitly accounts for second-law losses. The applicability to any cycle allows a basic representation of different kinds of CHP prime movers, e.g. gas turbines, piston engines or other cycles for which an analytical solution can be derived. Such models are sufficient approximations for systems analysis in which the precise details of the prime mover are not available or necessary. The starting point for a heat engine bond graph is the Carnot cycle, which is described by Brown [166] and introduced in Chapter 6 during the development of a demonstrator system model. The further detailed development of such a model element is not pursued further in this thesis as it does not feature in the demonstrator model.

Electrical power systems In their 2015 paper [178], Núñez-Hernández *et al.* apply the bond graph formulation to steady-state electrical network power flow analysis. The authors propose a multi-bond representation of the circuit power bonds, which recasts the standard electrical power bond characterised by a single voltage and current as a two-part bond, one part each representing the real and imaginary parts of current and voltage. Núñez-Hernández *et al.* term these *phasor bonds*, resulting in a phasor bond graph or PhBG. In fact, this is the result of applying the Laplace transform to the regular time-domain bond graph model [125], resulting in an s-operator form for bonds and graph element constitutive equations. By making the regular substitution $s = j\omega$ the system is described in the frequency domain and the system passive elements become frequency-dependent impedances instead.

Umesh Rai and Umanand also describe a complex-variable bond graph approach, their method differing from Núñez-Hernández *et al.*'s in that they take a more practical implementation-oriented approach with application to power electronic control of an induction motor, rather than network power flow analysis [179]. As part of their scheme for categorising and modelling the energy-water nexus, Lubega and Farid also describe a frequency-domain electrical power transmission network integrated into their model [19]. Lubega and Farid do not however model the network explicitly using bond graphs, instead opting to describe the network (an IEE14 test network) directly in incidence matrix form with explicit coupling connections to the system bond graph. It is not mentioned explicitly but it is assumed that the power flow is solved for externally to the bond graph.

A set of electrical bond system models were implemented and tested using the Modelica environment Dymola [171]. In modelling phasors in Modelica, rather than implement multibonds specifically, a new bond type, the complex bond, has been created, which generalises the regular bond type into the complex plane. The result is the same as using a multibond, although the derivation of system state space matrices outlined in [178] requires the bond quantities and impedances to be expressed in matrix form. When using a computer solver such as Dymola however it is not necessary to derive the system state matrices directly, as the equation sorting algorithm carries out this step implicitly.

The resulting bond graph of an electrical power flow network closely resembles the regular one-line diagram of power flow analysis. Impedances are calculated using well-known formulae. Loads and generators are categorised as standard system bus types, as described by for example [180]: generator bus (GB), defined by voltage and real power; load bus (LB), defined by real and reactive power; and the slack bus (SB), defined by voltage magnitude and phase angle. Other forms are possible (e.g. [178] defines the load bus by magnitude and phase angle) but for the purposes presented here the power consumed at the demand side is of most interest for an electrical network component in a mixed energy distribution system. Figure 5.29 shows the symbol for a generation bus as a source element connected to a 0-junction, the 0-junction forming a generic equal-effort connector, hence acting as an electrical bus. The other bus elements are defined similarly.

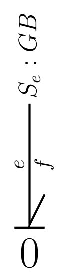


Figure 5.29: Symbol for a generation bus, with a connection via a 0-junction

In the bond graph formulation of the power flow problem, standard network components map to the bond graph form as in Table 5.13.

Components The various components of an electrical bond graph network are shown in Table 5.13. Component values are given in terms of their reactances, which must be calculated from component properties such as resistance, capacitance and so on. Note that in an electrical circuit the efforts are voltages and flows are currents, and the definitions and constitutive equations of the bond graph elements are given in terms of their bondgraphic quantities. Phase angles are denoted ϕ, and element parameters from which the bondgraphic properies are derived have the index 0.

A transmission or distribution cable is represented by the bond graph shown in Figure 5.30. The impedance is commonly resistive and inductive, however a capacitive element could be added, and the line impedance being represented by a separate sub-bond graph

Component	Symbol	Definition (Parameters)	Constitutive Equations
Resistive Impedance	RC	$Z_{R,0} = R + 0j$	$e = Z_R f$
Capacitive Reactance	CC	$Z_{C,0} = 0 - X_C j$	$e = Z_{C,0} f$
Inductive Reactance	LC	$Z_{L,0} = 0 + X_L j$	$e = Z_{L,0} f$
Bus	0	0-junction	$e_1 = e_2 = \ldots = e_n$ $\Re(f_1) + \Re(f_2) + \ldots + \Re(f_n) = 0$ $\Im(f_1) + \Im(f_2) + \ldots + \Im(f_n) = 0$
Line	see Figure 5.30	1-junction	$f_1 = f_2 = \ldots = f_n$ $\Re(e_1) + \Re(e_2) + \ldots + \Re(e_n) = 0$ $\Im(e_1) + \Im(e_2) + \ldots + \Im(e_n) = 0$
Generator Bus	$S_e : GB$	$e_0, \Re(S_0)$	$e_0^2 = \Re(e)^2 + \Im(e)^2$ $\Re(S_0) = \Re(e)\Re(f) + \Im(e)\Im(f)$
Slack Bus	$S_e : SB$	e_0, ϕ_0	$\Re(e) = e_0 \cos\phi_0$ $\Re(f) = e_0 \sin\phi_0$
Load Bus	$S_e : LB$	$S_0 = P_0 + jQ_0$	$P_0 = \Re(S_0) = \Re(e)\Re(f) + \Im(e)\Im(f)$ $Q_0 = \Im(S_0) = \Im(e)\Re(f) - \Re(e)\Im(f)$

Table 5.13: Electrical bond graph components

instead of the single impedance element Z.

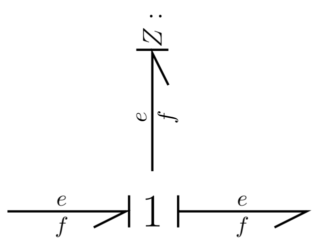


Figure 5.30: Transmission / distribution cable bond graph model

Test network The power flow problem is non-linear and solutions are routinely found by iteration, e.g. by Gauss-Seidel or Newton-Raphson (including variants such as fast-decoupled load flow). Within Dymola, at each time step a solution to non-linear expressions within the model is found using the Newton-Raphson method. Thus while the behaviour of real networks cannot be exploited for a faster-acting solution, the general solution method still holds and for the relatively small networks under study here this is not an issue.

To test the complex bond, impedance and bus component implementations in Dymola, the example network given as an exercise by Kirtley [180] is used. The one-line diagram of the network is shown in Figure 5.31. The equivalent bond graph for this network is shown in 5.32. The parameters for the test network are (all quantities per-unit):

$\boldsymbol{Z}_1 = 0.05 + j0.10$
$\boldsymbol{Z}_2 = 0.05 + j0.05$
$\boldsymbol{Z}_3 = 0.15 + j0.20$
$\boldsymbol{Z}_4 = 0.04 + j0.12$

Bus 1: $P_0 = 1$, $V_0 = 1.05$

Bus 2: $P_0 = 1$, $V_0 = 1.00$
Bus 3: $P_0 = -0.90$, $Q_0 = 0.00$
Bus 4: $P_0 = -1.00$, $Q_0 = -0.20$

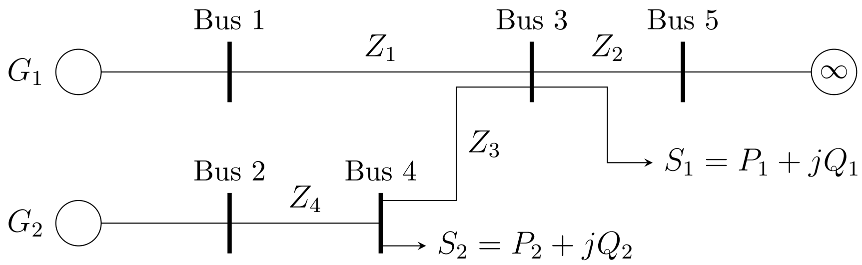


Figure 5.31: One-line diagram of example electrical network

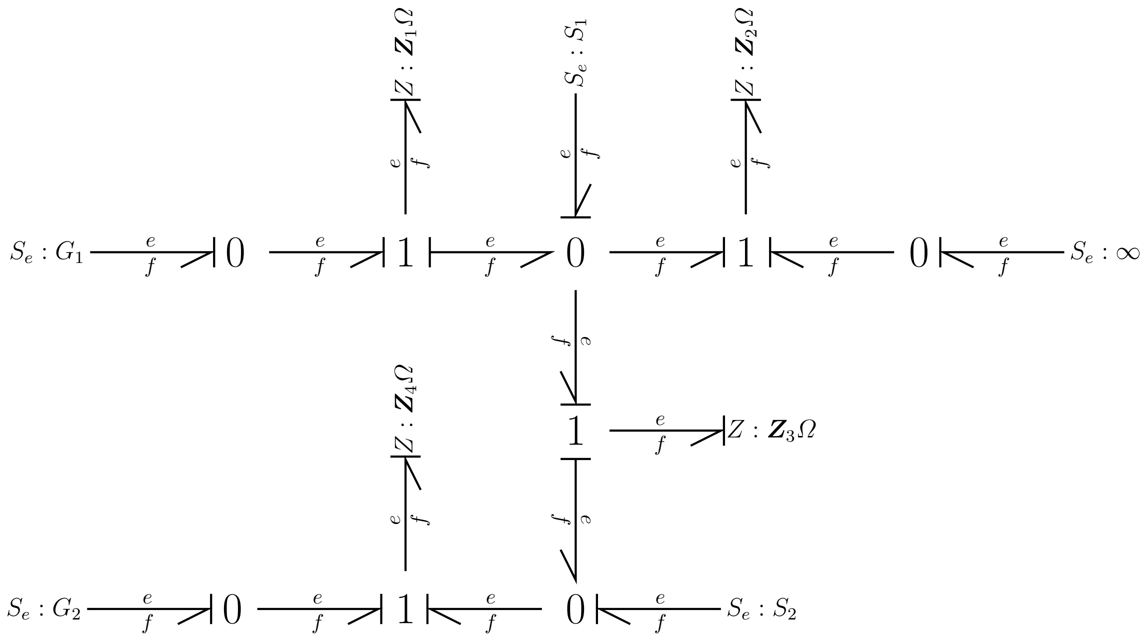


Figure 5.32: Bond graph version of Figure 5.31

The Gauss-Seidel Matlab algorithm presented by Kirtley [180] was used to solve the power flow problem in matrix form. The bond graph representation was constructed in Dymola using the developed complex-valued bond graph components, and Dymola was used to solve the system of equations. The same results were obtained using both approaches, as shown in Table 5.14. An image of the network representation as modelled in Dymola is shown in Figure 5.33.

5.5 Conclusions

This chapter has presented three major methods of developing models suitable for representing integrated energy systems. Energy hub models use an energy flow representation that links centres of production, conversion and consumption, resulting in a matrix expression for the system that is particularly well-suited to optimisation studies. Network

	Matlab		Dymola	
Bus	Voltage (V p.u.)	Power (W p.u.)	Voltage (V p.u.)	Power (W p.u.)
1	$1.0451 + j0.1015$	$1.0000 + j0.1369$	$1.0451 + j0.1015$	$1.0000 + j0.1369$
2	$0.9892 + j0.1469$	$1.0000 + j0.1457$	$0.9892 + j0.1469$	$1.0001 + j0.1457$
3	$0.9933 + j0.0074$	$-0.9000 + j0.0000$	$0.9933 + j0.0074$	$-0.9000 + j0.0000$
4	$0.9491 + j0.0255$	$-1.0000 - j0.2000$	$0.9491 + j0.0255$	$-1.0001 - j0.2000$
5	$1.0000 + j0.0000$	$-0.0065 + j0.1407$	$1.0000 + j0.0000$	$-0.0065 + j0.1407$

Table 5.14: Test network computational results

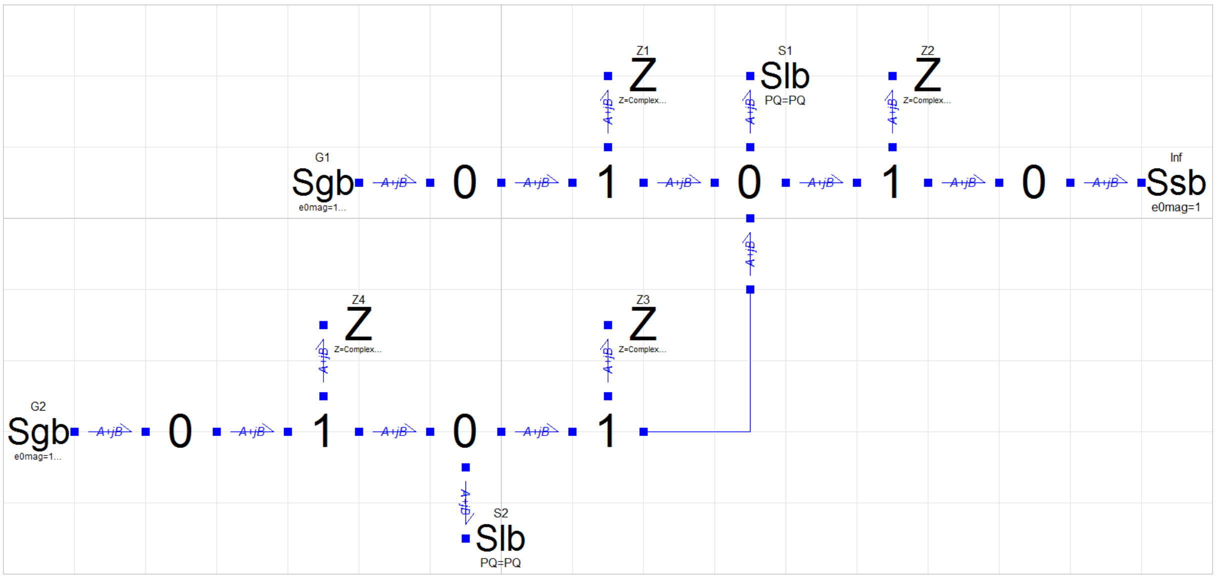


Figure 5.33: The test network in Dymola

models, developed from DC circuit theory, are a convenient analogous form for electrical and non-electrical systems that can represent a wide range of linear and non-linear system elements. However, the representation of heat flow is somewhat difficult to incorporate. Bond graphs are a general representation for energy systems in general, and can be used effectively to create system models in any energy domain. One of their main limitations is their relative obscurity compared to block-diagram and circuit forms.

A number of element models were explored for each of the three modelling forms. These element models were taken from the system reference models developed in Chapter 4, which themselves were evolved from energy network case studies and expert elicitation. The process of developing these elemental models allows the modelling criteria outlined at the start of this chapter to be assessed. The next chapter, Chapter 6, will examine the three model forms in light of the development of a demonstrator integrated energy network, and one will be selected to realise this demonstrator model. It will be seen that not all of the model elements developed during this chapter are used in the demonstrator model itself, but their development permitted the exploration of the three model types and their strengths and weaknesses. The details and theory presented in this chapter has shown how a more expansive systems model than presented in Chapter 6 would be able to incorporate more fully-developed versions of these elements.

The evaluation in this thesis of the three methods of representing integrated energy systems resulted in findings that fill some gaps in knowledge in the literature.

Investigation of energy hub models showed that they are primarily involved in input-output modelling of single-valued networks (energy transfer), and are not used to represent networks where energy needs to be represented by an effort-flow pair. As a result, the work in this chapter showed that energy hub networks struggle to accurately represent networks where the effort or flow is important for operational or design reasons, for example temperature in a heat network. Furthermore, it was shown that it is possible to naively create energy hub networks that look like they are providing a meaningful solution to an energy system dispatch problem, but on closer inspection can be seen to be physically incorrect or even impossible. Attempts to resolve this issue create a more complicated energy hub model type, losing the inherent advantages of the energy hub formulation for no particular advantage.

Additional evaluation of energy hub models in this chapter showed that *exergy hub* models are possible. The exergy hub retained the topology of the energy hub, but with the energy flows replaced by exergy. Analysis of a demonstration network in this chapter showed the equivalence of the energy and exergy hubs. Use of the demonstrated exergy hubs rather than energy hubs would open the door to a rich exergeo-economic dispatch optimisation method using that could help to place exergy as the principal-costed quantity in an integrated energy system, as proposed by some of the literature described in Chapter 2.

Development of network models for integrated energy system representation revealed that they have difficulty representing thermal networks. The network models studied were primarily intended for analysing electrical systems, but heat networks have frequently been represented by electrical analogies and this approach was taken here. However, electrical analogies of heat only really work for heat conduction, and the network models have difficulty in representing convective flow. As such, stream mixing and splitting and return flow pipework cannot be easily or accurately represented and the network model of heat results in the need for a number of approximations and non-physical compromises.

Network models as presented in the literature are effort-flow based (i.e. voltage-current, for electrical networks), but integrated energy network analysis is often power-based. The work in this thesis extends the effort-flow based foundation to include power-based representations of system elements. This required the derivation of new network element types for representing power-based elements in the network models, as well as an alteration to the Newton-Raphson solution algorithm and a development of the understanding of the physical constraints needed to correctly solve power-based formulations. Additionally, a new iteration convergence stopping condition was presented, corrected from that presented in the literature.

The work in this thesis explored some additional bond graph components that add to the types of systems that can be represented by bond graphs. While normally used to represent dynamic systems, this chapter explored pseudo-steady state bond graphs, i.e. systems that are piecewise steady-state and which have instantaneous transitions between states. Such representations are generally used to study integrated energy networks at a large scale as the dynamic transitions between states happen on a very short timescale compared to the operating schedule of the systems. As in the network models approach, the work in this thesis has developed power-based bond graph elements, as opposed to the effort-flow elements that are usually found in bond graph models. Such elements are useful for representing commonly-described energy systems which deal in power transferred rather than effort-and flow specifically. Nevertheless, the requirement to still be able to derive effort and flow values in the network, as opposed to in the energy hub case, which deals only in power and offers no effort-flow quantities, means that the bond graphs developed here are of a mixed type which offers great flexibility to systems modellers. A derivation of a modified Carnot engine bond element for more realistic prime-mover efficiencies, for use in Carnot bond elements, is also presented.

A full bond graph equivalent of a frequency-domain electrical network, equivalent to a one-line alternating current representation of an electrical system, was developed. This representation includes power-based elements — slack buses, load buses, generator buses, and lines — and principally operates in the PQ domain, with complex-valued bonds. While similar derivations by two other authors were found in the literature, it is believed that this thesis adds to the literature by demonstrating how to construct a native power-based electrical bond graph that can be naturally connected to other energy domains. Other integrated energy systems analysis using bond graphs did not take this step, instead opting to conduct the electrical systems analysis using an external electrical network solver.

Chapter 6. Demonstrator System Model

6.1 Model principles

The broader context of energy system modelling examines the purpose of modelling in general and the results which can be produced by modelling. Researchers in this field often explore the role of *scenario generation* in modelling, and the degree to which resultant scenarios affect the validity of the outputs of modelling. Scenarios in the context of energy systems analysis are defined as imagined alternative views of the future, or internally-consistent stories of how the future might look [138]. Lacking detailed scenario generation, analyses of energy systems often miss the real future which happens to that system. The production of scenarios which are likely to realistically represent the possible futures of the system being analysed is therefore an important and involved technical exercise. Such a complex undertaking is however outside of the scope of this thesis. The goal here will instead be to allow an evaluation of the state of a demonstrator energy network, for which some "typical" or illustrative operational schedules have been devised, and these illustrative schedules are not presented as being a comprehensive representation of the possible futures of the demonstrator network.

The purpose of this demonstrator case study therefore is: to examine how to construct a local energy system model in a unified fashion where all domains are present in the (unified) model; to examine how cross-linkage between energy networks could improve the overall performance of the network; and to understand how elements of the network can be controlled or specified, to permit proposed technologies or devices to exist within the network. This chapter presents a demonstrator model designed to meet these purposes.

The other purpose of the demonstrator model is to illustrate the modelling principles developed in the previous chapters of this thesis, which are used here to suggest a modelling approach for integrated energy systems. These principles are as follows.

1. The model structure should support multiple energy domains in a unified representation. This is inherent in the overall purpose of the thesis in investigating multi-vector energy systems, the value of which was discussed in Chapter 1.

2. All energy domains should be able to be represented equally well, i.e. without using analogies or compromises. It was shown in Chapter 5 that some modelling representations make it difficult to adequately represent certain energy domains. In particular, heat, and heat transport in fluids, are especially difficult to model correctly when temperature and entropy cannot be accounted for.

3. Multi-vector storage should be representable. This is inherent in the premiss of the thesis.

4. The system can be represented as a lumped-parameter form suitable for representing district energy systems. Distributed parameter representations can be more accurate, but these capture behaviours (primarily waves and transients) that are of no significant operational interest in local energy systems studies. Lumped parameter modelling reduces the complexity of the system model and enables the development of system-of-system representations (see next principle).

5. A systems-of-systems approach is preferred. Assuming as above that a lumped-parameter model is used, a system-of-systems approach permits ready scaling of a system model. Sub-models can be developed and verified and then incorporated as "black boxes" in larger systems.

6. The boundary of the system should be clearly representable. A discussion of the representation of system boundaries was presented in Chapter 2 where it was seen that an "open thermodynamic boundary" is a suitable form of system boundary for local energy systems. To adequately represent such a boundary it is important that the model contain components that satisfy boundary conditions by representing flows to and from the system.

7. The exergy, or, equivalently, entropy properties of the system components should be available to permit thermo-economic evaluation. This topic was discussed at length in Section 2.5 where it was argued that thermo-economic approaches that consider exergy as a fundamental economic unit of energy systems are important for local energy system evaluation.

8. A pseudo-steady state formulation is acceptable; that is, system change takes place at discrete time intervals on the scale of minutes, and between these times the system is in a steady-state. As pointed out above when considering lumped- vs distributed-systems modelling, transients are of no real interest in operational studies of energy systems and thus dynamic behaviour can be ignored. Then only a suitable steady-state time interval needs to be considered; long intervals reduce simulation costs, but the time interval needs to be short enough to incorporate control actions.

9. The main form of energy storage in a local energy system is accumulative storage. When considering "energy storage" in local energy systems this is normally considered to be energy accumulation rather than capacitive storage, as noted in Section 5.4. Certain types of capacitive storage such as building fabric thermal inertia may be of interest but these may be of secondary importance. Nevertheless the ability of the modelling environment to incorporate this secondary storage type should be noted.

A comparison of the model types discussed in Chapter 5 with the principles set out above are shown in Table 6.1. It can be seen that bond graphs provide the only modelling

	Energy hubs	Networks	Bond graphs
1. Unified domain representation	Y	Y	Y
2. Equality of domain representation	Y	N	Y
3. Multi-vector storage	Y	N	Y
4. Lumped parameter	Y	Y	Y
5. System-of-systems support	Y	Y	Y
6. Clear boundary representation	Y	Y	Y
7. Exergetic state properties	N	Y	Y
8. Pseudo-steady-state	Y	Y	Y
9. Accumulative storage representation	Y	?	Y

Table 6.1: Comparison of model types to the local energy system modelling principles

framework that can meet all of the principles. Energy hubs are a versatile modelling representation but the reduction of physical (effort, flow) pairs to a single quantity (i.e. energy) eliminates their ability to compute exergy values from the system's physical state, unless the entire system is redefined in exergy terms. This would require these quantities to be defined and maintained during simulation however, at which point the system is no longer an energy hub. Network model forms cannot adequately represent non-network energy domains (e.g. heat) without a reduction to an analogous form. Because of this, an investigation into the representation of accumulative storage in network models was not pursued, and remains an unanswered question.

A demonstrator model of a multi-domain energy system with accumulative multi-vector storage which meets the above principles is described in the rest of this chapter. The demonstrator model scope is given, along with the ways in which it meets the modelling principles. The mathematical description and software implementation of the model are then described in detail; here, the model element definitions found in Chapter 5 are used, along with reference system elements described in Chapter 4 to define system components from the model elements. Finally, six simulation test cases of the model are described which illustrate its use in practice. The meaning of the model outputs resulting from these simulations are discussed along with the shortcomings of the model.

6.2 Demonstrator model structure

The demonstrator model is similar in structure to the Byker heat network model described in Chapter 4 and examined as an energy hub model in Section 5.2. The scope of this model is broadened by adding the regional electrical distribution network supplying the same district as the heat network. The energy supply system consists of a combined heat and power (CHP) unit (for example a natural gas engine generator set with exhaust heat reclamation), a connection to the larger electrical grid, and a boiler supplied by gas or biomass fuel. This system generates heat and electricity which is supplied to a local district consisting mainly of off-gas residential properties along with some municipal and commercial buildings. The demand side is considered to be a single lumped load, and

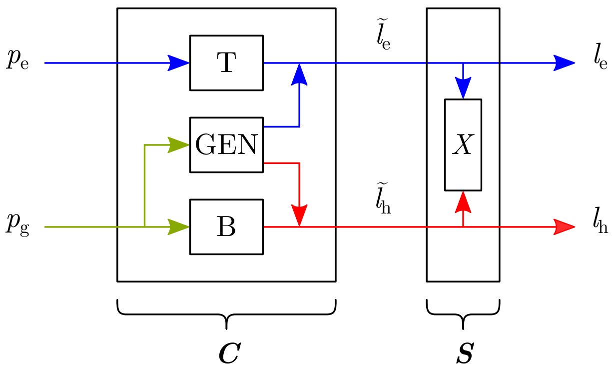


Figure 6.1: General demonstrator model

the heat transmission system (consisting of a pipe network) is ignored for the sake of simplicity.

An energy-flow schematic model of the demonstrator system which illustrates the principles described above is shown in Figure 6.1. Here, T is the electrical transformer supplying the region, GEN is a fixed-schedule CHP unit, B is a boiler, and X represents an exergy store. p_e is electrical power supplied by the electrical grid, p_g is gas supplied from the gas network, $\tilde{l}_e$ is the total electrical power produced, $\tilde{l}_h$ is the total heat power produced, and l_e and l_h are electricity and heat powers supplied to a load respectively. The collections C and S respectively refer to the plant ("energy centre") and storage components of the system. A more detailed SysML system activity diagram using the methods developed in Chapter 4 is shown in Figure 6.2. The unit components of this system within each of the subsystem boundaries are as above (CHP, electrical transformer, boiler, pipework, cabling) and come from the list of reference system components listed in Table 4.1. This demonstrates how a well-ordered system-of-systems design using SysML can be used to construct and manage integrated systems designs.

As explained in Chapter 4, distributed generation, even non-renewable, is often operated on a fixed cycle for contractual or financial reasons, and the electrical generator can therefore be considered to be an inflexible source that is to be managed by the exergetic storage. The main differences between the demonstrator model and the previously-described energy hub model of the Byker heat station plant are that the storage element is multi-vector, i.e. it can store and release energy from and to both the thermal and electrical domains, and that no stratified thermal buffer store is present. Additionally, only the boiler combustion products are included in the model; the combustion process itself is not included, the results of the analysis in Appendix A being used instead.

The demonstrator model is constructed as a bond graph using the components and methods outlined in Chapter 5. By using bond graphs to build the system model, the entropy flows that occur during energy transport and conversion processes are explicitly shown in the model structure, particularly in the parts of the system that include heat, either through heat transfer processes or through mass transport. The direct quantification of entropy production, or equivalently exergy destruction, in the model allows for an evaluation based on principles that elevate entropy production as an important economic

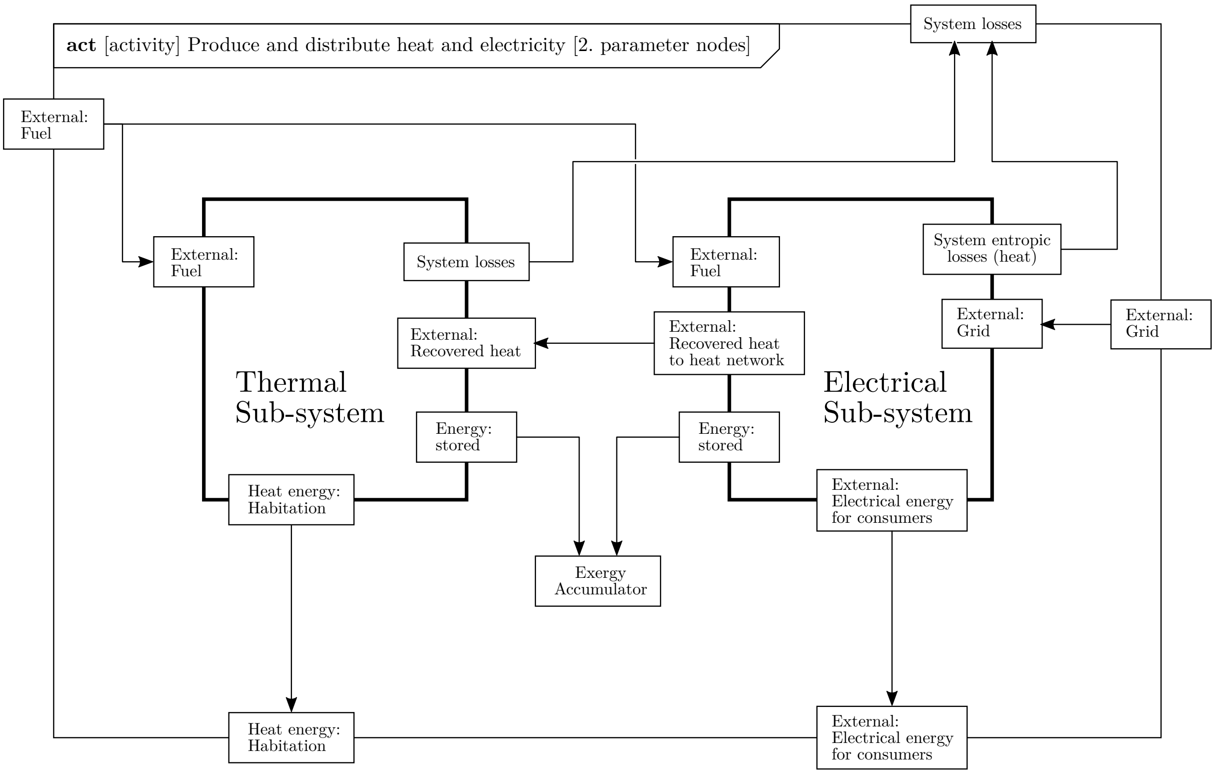


Figure 6.2: Demonstrator system SysML diagram, showing boundary connections

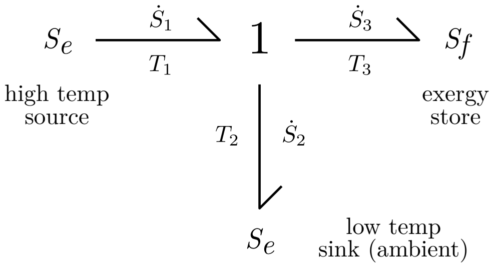
quantity. The argument for using exergy destruction measures in systems modelling and evaluation was discussed in Chapter 2 under the banner of thermo-economics.

6.3 Mathematical description

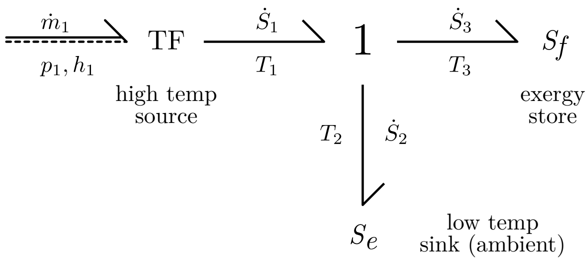
6.3.1 Exergy accumulator

It was argued in Chapter 5 that a multi-vector storage device which can convert between energy domains is an important component in the management of integrated energy systems. Section 5.1.2 discussed the merits of representing such a store (more correctly, an accumulator) as an exergy store, and presented a hierarchy of types of exergy storage models. This section will elaborate on the concepts explored there, to develop a suitable representation of exergy flow for inclusion in bond graph models of integrated energy systems. The exergy accumulator model used in the demonstrator system is a "Type 1" device, i.e. one that is reversible and infinite, and which can no limit on its energy conversion power. As discussed in Section 5.1.2. such a device is purely theoretical, but it is useful as a starting point for the type of system study illustrated by the demonstrator network. A "perfect" device allows general behaviours of the system to be observed without distraction by the technical details of real systems. For realistic analyses aimed at economic evaluations and specific technical designs, a different type of storage model should be selected from the storage classification typology in Section 5.1.2.

For exergy to be used as an equivalence measure in multi-domain energy systems, the method of conversion of energy to exergy for each domain must be established. Recall



(a) Thermal input



(b) Convective input

Figure 6.3: Bond graph Carnot cycle model

that exergy is a measure of the maximum possible work that can be obtained from an energy source. Electricity is already a form of work, and does not need to be converted further. For fuels such as natural gas, Kotas demonstrates that the lower or net calorific value can be used as an acceptable approximation (within a few percent) of its exergy value [48]. Tabulated values of the ratio of exergy to lower calorific value can be used if greater precision is required, but as natural fuels vary in their composition such precision is likely to be illusory.

Heat energy however is not in a work form, and so the exergy equivalent of heat is required. For heat conduction, i.e. energy that is present in an entirely thermal form, the exergy of the thermal supply can be evaluated using a bond graph equivalent of a Carnot cycle, shown in Figure 6.3a. This representation of an ideal thermal machine is due to Brown [166]. The 1-junction representing the Carnot engine is described by the constitutive equations, with $\dot{S}$ being entropy rate (flow) and T being the absolute temperature (effort),

$$\dot{S}_1 = \dot{S}_2 = \dot{S}_3 \tag{6.1}$$

$$T_1 - T_2 - T_3 = 0. \tag{6.2}$$

T_1 is the temperature of the engine's high-temperature source, and T_2 the temperature of the low-temperature sink, and so the usable power output on bond 3 is $T_3\dot{S}_3$, where $T_3 = T_1 - T_2$. The efficiency of the engine is calculated as $\eta = T_3\dot{S}_3/T_1\dot{S}_1 = (T_1 - T_2)/T_1 = 1 - T_2/T_1$, which is the Carnot cycle efficiency.

For convective flows, a first approximation to such a model is an extension of the Carnot cycle converter (Figure 6.3b), wherein a steady flow of material is changed to its exergy value. Here, the transformer converts from a convective to conventional bond, while the 1-junction represents an ideal Carnot engine which computes the exergy value of the flow. The Carnot cycle is as above and the transformer equations are

$$h_1 - h_{ref} = c_{\text{av}}\,(T_1 - T_{ref}) \tag{6.3}$$

$$T_1\dot{S}_1 + \dot{m}_1 c_{\text{av}}\,(T_1 - T_{ref}) = 0, \tag{6.4}$$

where h is the fluid specific enthalpy, T is the fluid absolute temperature, $\dot{m}$ is the mass flow rate of the fluid, c_{av} is the mean specific heat capacity between the fluid temperature and the dead state, and the suffix ref refers to the dead or reference state (corresponding to state 2 in the Carnot graph).

Unfortunately this appealing and straightforward device is incorrect. Each differential element of mass, dm, that enters the exergy converter does not stay at the temperature it enters with during its conversion to work; instead, assuming that the maximum amount of exergy is to be extracted from the stream, the differential mass element drives the Carnot engine as it cools, with a lower and lower efficiency, releasing less and less exergy until it reaches the dead state. Limiting the discussion to the exergy carried by an incompressible fluid as a storage mechanism, e.g. liquid water, then recall from Section 5.1.2 that the expression for the exergy flow rate, $\dot{\Xi}$, of an incompressible stream flow is given by

$$\dot{\Xi}_2 - \dot{\Xi}_0 = \dot{m}\left\{(h_2 - h_0) - T_0\,(s_2 - s_0)\right\}\,, \tag{6.5}$$

where state 2 and state 0 are the operating and dead states respectively. The kinetic and gravitational potential energies are neglected in this expression — in general these will be a lot lower than the exergy resulting from the heat content of the stream, and in this model cannot be calculated without additional information (pipe diameters, elevations) which is unknown. For an incompressible stream entering the converter and driving the Carnot engine, the volume does not change as the fluid cools, hence $dv = 0$. The entropy change in the above expression is determined from the definition for entropy in differential form,

$$ds = \frac{du}{T} = c\frac{dT}{T}. \tag{6.6}$$

with s, u and T being the specific entropy, specific internal energy, and temperature respectively. c is the specific heat capacity of the fluid. The difference in entropy that occurs during a process occurring between a start state 1, and end state 2, is found by integration of this equation, thus

$$s_2 - s_1 = \int_1^2 c\,(T)\,\frac{dT}{T} \tag{6.7}$$

$$s_2 - s_1 = c_{\text{av}} \ln\left(\frac{T_2}{T_1}\right) \tag{6.8}$$

where $c(T)$ is the specific heat capacity of the fluid as a function of temperature and c_{av} is the average specific heat capacity over the temperature range (values for which are tabulated in engineering texts). Setting state 1 to be the dead state (represented by the suffix 0) and noting that $\Xi_0 = h_0 = 0$ by definition,

$$\dot{\Xi} = \dot{m}\big\{h - T_0\, c_{\text{av}} \ln\Big(\frac{T}{T_0}\Big)\big\} \tag{6.9}$$

Equation 6.9 provides an expression for the storable exergy rate of an incompressible fluid stream. Recalling that a convection bond representing this stream is characterised by its pressure, p, its specific enthalpy, h, and its mass flow rate, $\dot{m}$, the stream temperature T must be calculated as a state property; generally the linear relation $T = T_0 + (h/c_{\mathrm{av}})$ can be used.

A numerical example here will help to illustrate the calculation of exergy quantities. Suppose a liquid water stream at 320 K and 1.02 bar (specific enthalpy of $h = 91.77 \times 10^3$ J/kg) is flowing at 1.0 m/s into the exergy store. The dead state is given as $T_0 = 25\,°\mathrm{C}$, $p_0 = 1.02\,\mathrm{bar}$, and $h_0 = 0\,\mathrm{kJ/kg}$. The exergy storage rate is given by Equation 6.9, so

$$\begin{aligned}\dot{\Xi} &= 1.0\left\{91.77 \times 10^3 - 298.15 \times 4.2 \times 10^3 \times \ln\left(\frac{320}{298.15}\right)\right\} \text{ J/s} \\ &= 91.77 \times 10^3 - 88.563 \times 10^3 \text{ J/s} \\ &= 3206 \text{ J/s}, \text{ or } 3.21 \text{ kW}\end{aligned}$$

If the above thermal flow is an energy flow in the form of heat instead, then the Carnot junction model is appropriate. In this case, referring to Figure 6.3a, the high temperature source is at $T_1 = 320$ K, the low temperature source is at $T_2 = 298.15$ K, and the entropy flow from the high temperature source which is equivalent to the convection model is $S_1 = \dot{Q}_1/T_1$.

$$\begin{aligned}\dot{Q}_1 &= \dot{m}_1 h_1 = 91.77 \text{ kJ/s} \\ \dot{S}_1 = \dot{S}_2 = \dot{S}_3 &= \frac{\dot{Q}_1}{T_1} = 286.781 \text{ J/Ks} \\ T_3 &= T_1 - T_2 = 21.85 \text{ K} \\ \dot{\Xi}_3 &= \dot{S}_3 \times T_3 = 6266 \text{ J/s}, \text{ or } 6.27 \text{ kW}\end{aligned}$$

The quantity $\dot{\Xi}_3$ is the reversible work, i.e. exergy, rate for the Carnot engine model; this is the rate that will be transferred into the exergy store, and is the limiting exergy transfer rate that can be attained for the energy stream. Thus, the exergy contained within the convective stream is $\phi = \frac{3206}{6266} = 51.2\%$ of the exergy contained within a conductive source at the same temperature, in this case.

The bond graph model for the exergy store is shown in Figure 6.4. The operation of the multi-vector exergy storage device is controlled by the system operator — in the model this is replicated by choosing the power available for import or export for each energy domain. The behaviour of a particular storage device should be defined with reference to the constraints of the physical device as discussed in Chapter 5 but for the purposes of this demonstration model it is assumed that a multi-vector exergy storage device exists which can charge or discharge both vectors simultaneously. For example, certain classes of molten salt tri-generation devices can approximate this behaviour. The flows into and out of the exergy store are controlled by the power setting on the modulated signal bond to the source elements S_{lb} and S_p — thermal power for thermal streams, and P-Q characteristics for electrical discharge. The use of power sources creates free causality on

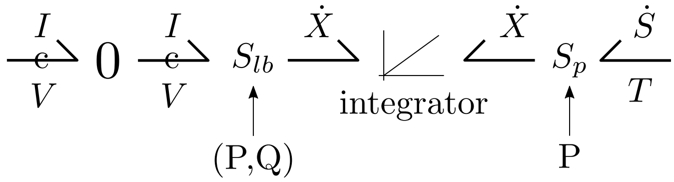


Figure 6.4: Exergy accumulator bond graph model

the bonds connected to the sources, and the resultant effort and flow values (temperature / entropy flow, or complex voltage and current) are computed from the state of the system at the point of connection to the source element, depending on the boundary conditions elsewhere in the model.

Charging and discharging Exergy stream accumulation is computed using an integrator, i.e. $\Xi_{t+1} = \Xi_t + \dot{\Xi}_t\,\delta t$, where Ξ_t is the stored exergy value at time t. $\dot{\Xi}_t$ is positive when charging, and negative when discharging. The connected stream parameters are driven by the modulation signal connections to the bond power source elements that defines the required thermal and electrical powers. Note that because a single power value controls the flow into or out of the accumulator for both domains, it is not possible to simultaneously charge and discharge into the same domain.

6.3.2 Electrical subsystem

The one-line diagram and equivalent bond graph of the electrical subsystem are shown in Figures 6.5 and 6.6. The electrical subsystem consists of an 11kV distribution network to which the CHP unit, exergy accumulator and community electrical demand are connected. The distribution network is also connected to the national grid supply through a transformer. For the sake of simplicity and without loss of generality the community electrical demand is modelled as a single load. The network is specified and solved using per-unit values on a 1MVA base, requiring a power conversion element within the model to convert power flow between the electrical network (per-unit) and the exergy accumulator (in MW).

Grid supply is modelled as a one-port S_{sb} element that implements a slack bus. Power under- or over-supplied by the plant is balanced by grid supply and consumption respectively at this element. **Bus** connections are modelled as 0-junctions, with the label b_i. Redundant 0-junctions are used to connect the source elements to the graph; although redundant they demonstrate more clearly the mapping of the one-line diagram to the bond graph. **Lines**, labelled l_j are modelled as 1-junctions with attached impedance elements. Community electrical demand is modelled as a one-port S_{lb} load bus element. **Plant generation** is modelled as a parameter-controlled one-port S_{lb} load bus element with a negative demand value, while the **exergy accumulator** electrical connection is modelled as a modulated one-port S_{lb} with a secondary power port converted to MW from per-unit values, as described above. The generation and load parameters for all load

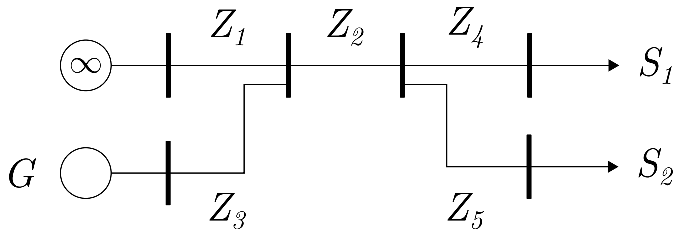


Figure 6.5: Electrical subsystem one-line diagram

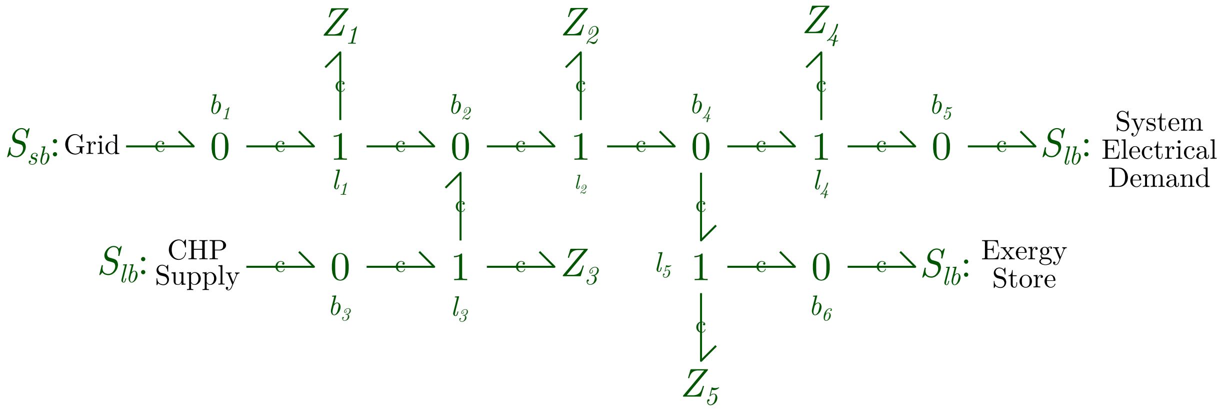


Figure 6.6: Electrical subsystem bond graph

bus components are set by tabulated data elements attached to the modulation port of the source elements.

6.3.3 Boiler subsystem

The boiler transfers heat from the hot gases produced by a combustion reaction to the water which supplies the heating network. A basic model similar to that presented by Lubega and Farid [26] and using concepts from the counterflow heat exchanger described by Brown [166] is shown in Figure 6.7. HS elements representing the convective fluid flow sections (the combustion gases and the water flow) are linked via a heat conduction RS element which represents the thermal transfer between the fluids. An additional RS element is connected to the gas flow section via a 0-junction to represent thermal losses through the boiler housing wall. Note that because of the location of the heat-splitting 0-junction the model is uni-directional, and heat must flow only from the gas to the water stream. Defining sources for the convective flows requires careful consideration of the desired control parameters and boundary conditions. The exhaust gas flow (left hand side of the boiler diagram) has an inlet source which is a modulated power flow source, S_p, and an outlet flow source, S_e, which is a "blank" source which has no defined state information, all of the state information for this source being computed elsewhere in the model. The heat loop section which flows through the boiler has an upstream flow, S_f, source which defines the mass flow rate of the fluid, and a downstream effort, S_e source which defines the outlet temperature. The environmental temperature is defined as an S_e source for conductive heat loss from the boiler. Other combinations of these boundary parameters are possible, depending on the nature of the problem.

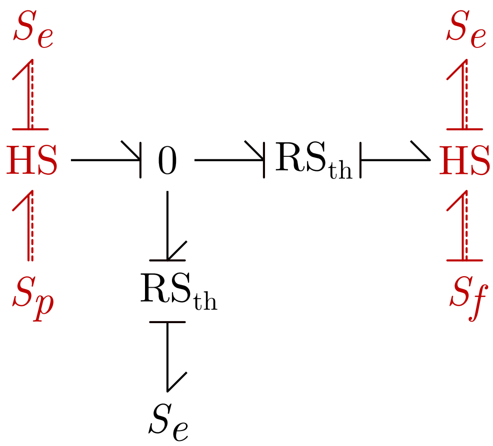


Figure 6.7: Boiler subsystem bond graph

6.3.4 Controllers and sensors

Bondgraphic sensors are represented computationally by signal bonds. Recall that signal bonds transmit either no flow (for an effort signal) or no effort (for a flow sensor) and thus transmit no power and hence have no effect on the system. Signal bonds can either be represented as a non-power conducting port at a 1-junction (for flow sensing) or a 0-junction (for effort sensing), or as a modified power bond with a take-off signal port, which is the approach used here (see e.g. Cellier *et al.* [181]). The advantage of using a signal-port modified power bond is that the power transmitted through the bond can also be reported by a suitable sensor port. The sensor-enabled bonds allow for the monitoring of entropy and power flow for the calculation of system efficiencies.

6.3.5 System model

The full system bond graph corresponding to the schematic diagram shown in Figure 6.1 is shown in Figure 6.8. The system model is completed by the addition of elements representing the heating system loop, and the connections to the exergy accumulator.

Heating loop The heating loop transporting hot water from the heat plant to the local district is approximated by a series of convection bonds. The flow mechanics of the fluid are ignored in this approximation and so no pressure loss elements appear - these could be added in a more developed model. The boiler heat exchanger shown previously and three additional bond graph HS heat exchanger elements complete the loop specification. The first additional HS element occurs before the boiler heat exchanger and is labelled "S_p: CHP Supply". This is a bond graph power source representing the power output of the CHP unit, which is always positive into the heating loop. The second occurs just after the boiler heat exchanger; labelled "S_p: Exergy store", this represents power flow into and out of the exergy store. Finally, the system demand, "S_p: System thermal demand", is located beyond the exergy store and is represented as another bond graph power source.

The two ends of the thermal loop, a flow source "S_f: Return" and "S_e: Out" are in

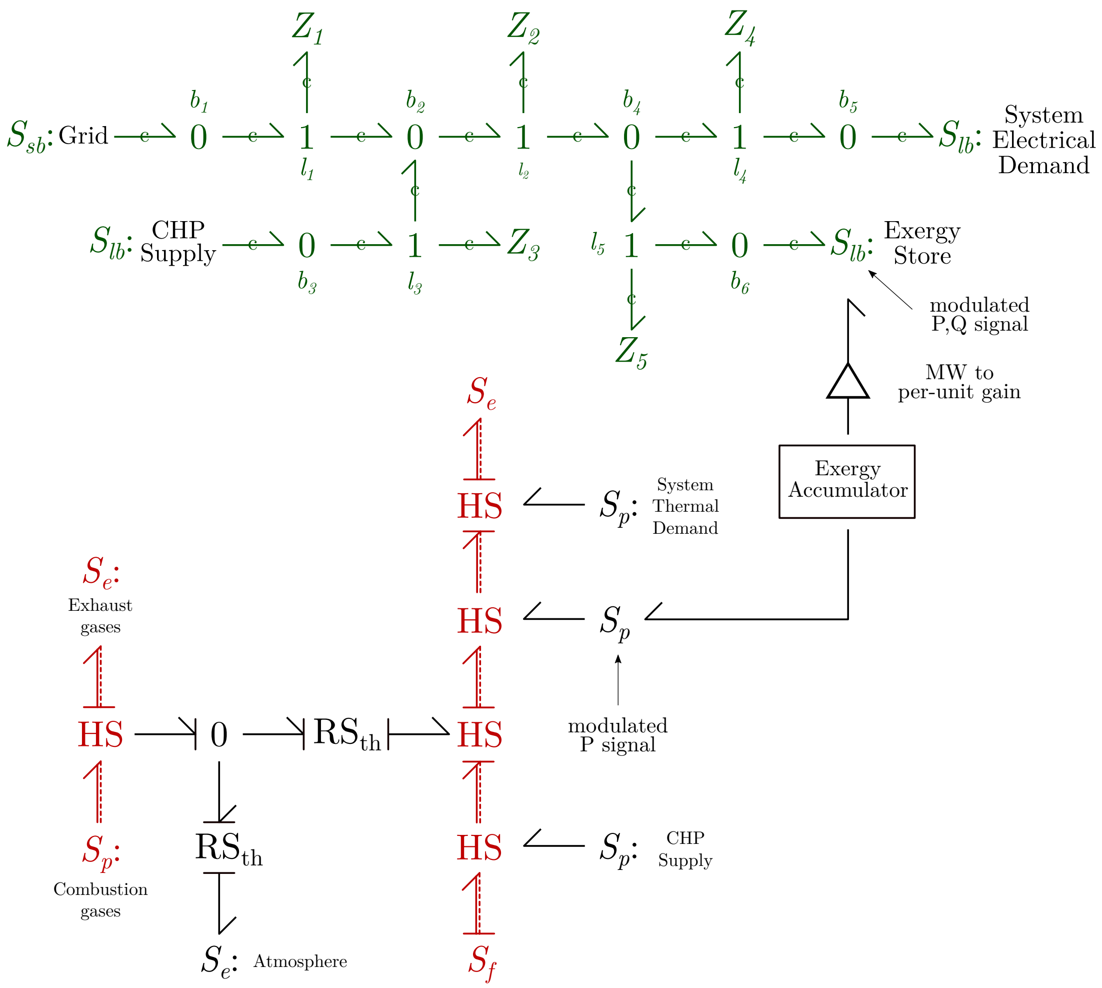


Figure 6.8: Complete demonstrator system bond graph model

fact the same effective point in the real heat network; following the connection to the load, the heat loop reconnects to the plant, transporting the lower-temperature fluid back for reheating. These two points are not connected because the presence of power source elements in the model — as a result of the supply and demand boundaries being specified as power (see next section) — has created an unusual type of bond graph. Ordinarily, bond graphs are effort- or flow-driven, and the resultant computational causality can be traced effectively through an examination of the types of terminal element present in the graph. Power-based bond graphs are defined by sources which are the product of effort and flow, and computational causality becomes ambiguous. Similar to power-based electrical load flow analysis, the system then requires a *slack* power source which can balance the supplies and losses in the system. This is not explicitly modelled here, and so the ends of the loop cannot be joined; they are at different states, with the "S_f: Return" source effectively providing this power-balancing mechanism. This modelling anomaly will be returned to in Section 7.2.5 .

6.4 Software implementation

The model was implemented in OpenModelica, an open-source application implementing the Modelica language. Modelica is an object-oriented declarative language designed "for modelling of large, complex and heterogeneous systems" [182]. The OpenModelica tool implements algorithms which handle the large number of model equations, creating 3$^{\text{rd}}$-language code, typically using the C language, which can be complied and executed. Compiled model code conforms to functional mock-up interface (FMI) standards, with an individual model representing a functional mock-up unit (FMU). The domain-neutral and algorithmic-independent nature of Modelica makes it ideal for implementing multi-domain systems such as integrated energy systems.

Bond graph elements were implemented in a similar fashion to that presented by Cellier and Nebot [181]. The library developed by Cellier and Nebot for [181] was used to implement the basic bond graph elements in the demonstrator model, while the convective flow and complex electrical bond elements used in the model were implemented in a new Modelica library that uses the same Modelica architectural principles as the Cellier and Nebot library and is compatible with it. General Modelica elements such as time series inputs, logic and signal connectors, and other fundamental types were used to construct the model.

6.5 Operational test case

6.5.1 Simulation data and system properties

The operation of the demonstrator over a 24-hour period forms the basis of the simulation. The following data were collected to create representative electrical and heat demand inputs to the system, which are shown in Figure 6.9.

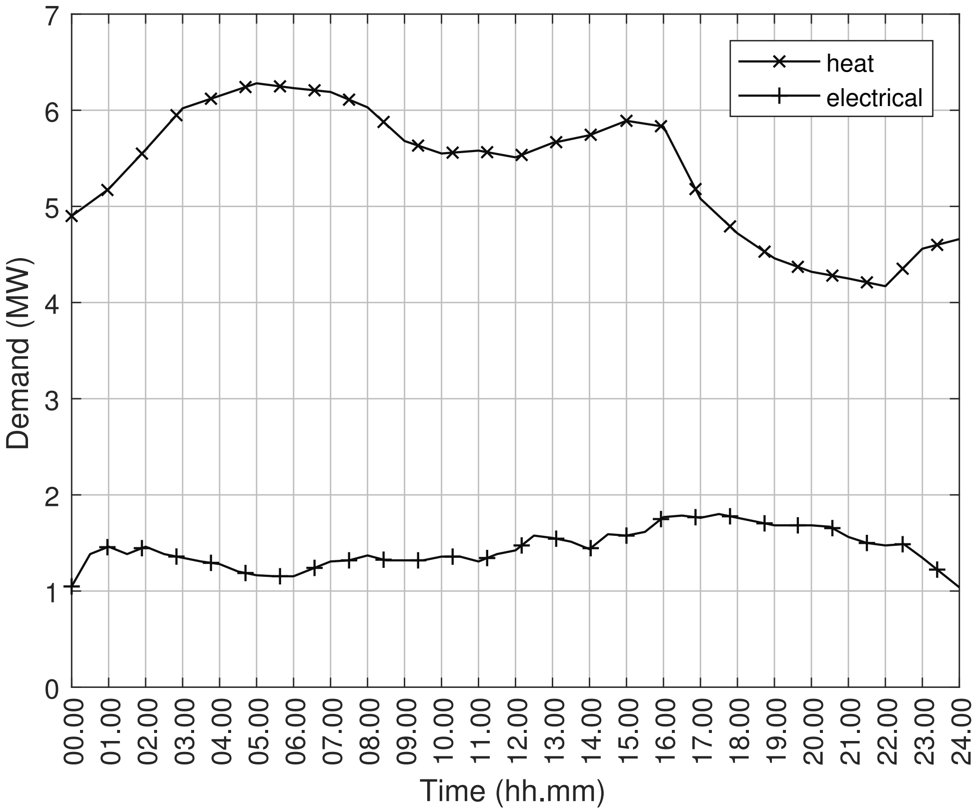


Figure 6.9: Demonstrator system electrical and heat demands

Electrical demand data Data for the feeder network connected to the Byker CHP plant and supplying the connected estate was supplied by the regional distribution network operator (DNO) Northern Powergrid. Half-hourly per-unit power values with a base of 1 MVA were calculated from measurements from the relevant feeder way of 3-phase current in amps and a corresponding voltage (nominal 11 kV). Demand was assumed to have no reactive component, which is a reasonable assumption below 11 kV for a region consisting mostly of residential loads with some municipal and light commercial properties. Data were available from 01/11/2013 to 09/01/2016, but an approximate 1 MW dip in supply at the 11 kV transformer from 06/12/2013 during the period 7 a.m. to 7 p.m., Monday to Friday, was observed. This is presumed to be the commissioning date of the Byker CHP unit and thus the next earliest full day of weekday data — Tuesday 03/12/2013 — was chosen to be representative of the underlying electrical demand for the purposes of the demonstrator.

Thermal demand data Heat data were supplied by the Byker Heat Network monitoring centre. The data consist of a cumulative MWh record for 17 heat substations on the heat network, collected hourly for the year between 13/07/2017 and 13/07/2018 inclusive. The day 05/12/2017 was chosen as being "close" (a Tuesday, early in December) to the electrical demand day. Half-hourly demand data in MW were produced by subtracting successive hourly measurements and then linearly interpolating. No other processing was conducted. The demand for the network as a whole was created by summing the readings from the heat stations. Two heat stations presented no monitoring data for the date selected, and these were filled by duplicating data from another heat station which, through visual inspection of annual graphs of daily demand (supplied by the Byker Heat Network), most closely matched the rest of the data from the absent data heat station. This approximation is adequate for the purposes of simulating the demonstrator system.

CHP operation As described elsewhere in Section 4.2.1, the CHP unit at the Byker heat plant operates Monday to Friday, 7 a.m. to 7 p.m., primarily as a supplement to the base-load gas boiler and in line with feed-in-tariff and maintenance cost considerations. This is simulated in the demonstrator by a scheduled power input to both the electrical and heat networks of 1 MW. A 30 minute ramp-up to and from the operating power is presumed, to prevent "cliff-edge" loading jumps during simulation. Although some variation in output would be expected in reality, evidence from the heat plant monitoring displays (see Appendix A) suggested that the actual electrical output was stable and very close to 1 MW. No empirical evidence is available for any variation in heat output, so a stable 1 MW is also assumed in this case.

Networks No information describing the network conductor properties was available, so generic properties as used by Hosseini *et al.* [183] of $(0.3 + j0.3)\Omega$ per-unit were used for each conductor[1]. The pressure properties of the thermal network were not modelled in the demonstrator, thus no pipework details were required.

Boiler operation Two heat transfer terms are included in the boiler model — one representing gas-to-water conduction and one representing the conduction of heat through the boiler wall to the environment. These parameters were approximated by a trial-and-error approach which produced a boiler thermal efficiency of ∼90%. The boiler model itself only represents the post-combustion process during which heat is transferred to the pressurised water in the heat network from the combustion gases. The states of the combustion gases are fixed and are taken from the calculations in Appendix A.

Exergy accumulator For the purposes of the demonstrator, the accumulator was constrained to operate a daily net-zero energy storage schedule. While this is not strictly required for real finite storages, it is required on average and represents a reasonable working constraint on the operation. Otherwise, no capacity constraints (energy or power) were imposed; it is presumed that the store is operating at its mean storage point and is large enough to support the energy stored and discharged, and the powers involved in doing so. In fact, the simulation trials investigate the effect of these parameters on the operation of the system, and thus the storage capacities and powers are regarded as parameters to the problem.

[1] Values obtained through personal communication with the authors

Source type	Title	Description	Specified parameters
S_e	Combustion gases	Post-combustion supply of heat	Gas temperature, T Gas pressure, p Heat power, P_h
S_e	Exhaust gases	Boiler flue exhaust to atmosphere	None
S_e	Atmosphere	Heat rejection to atmosphere	Ambient temperature, e
S_e	Heat return (A)	Heat flow into the heat plant	Water mass flow rate, $\dot{m}$
S_f	Heat return (A)	Heat flow into the heat plant	Water temperature, T Water pressure, p
S_p	System thermal demand	Heat flow out at thermal substations	Heat power, P_h
S_p	CHP heat supply	Heat supplied by the CHP unit	Heat power, P_{CHP}
S_ϕ	Exergy supply & demand	Connection to the exergy storage device	Exergy rate, $\dot{E}$

Table 6.2: System sources (boundary flows)

6.5.2 Boundary conditions

The system sources represent the system boundary. Table 6.2 summarises the information supplied at each source.

6.5.3 Simulation trials

Six trial cases were carried out on the model to illustrate the joint operation of the thermal (convective and conductive) and electrical networks, supply and demand, and the operation of the exergy accumulator.

1. Baseline operation. The accumulator is deactivated, and the two networks operate independently.
2. Net transfer from the electrical to the heat network. The schedule is the same as in trial 2, but with the directions of the charging and discharging reversed.
3. Net transfer from the heat to the electrical network. Transfers to the accumulator from the heat network, and from the accumulator to the electrical network, are separated in time.
4. A synchronised transfer of energy from the electrical to the heat network, at a period of low electrical and high thermal demand (2am to 8am).
5. A synchronised transfer of energy from the heat to the electrical network, at a period of high electrical and low thermal demand (4pm to 9pm).
6. The same as Case 4, but for varying amounts of transfer power. Because of physical constraints connected to electrical losses and thermal capacities, the amount of power that can be transferred to the heat network from the accumulator has an upper limit (about 1.1 MW).

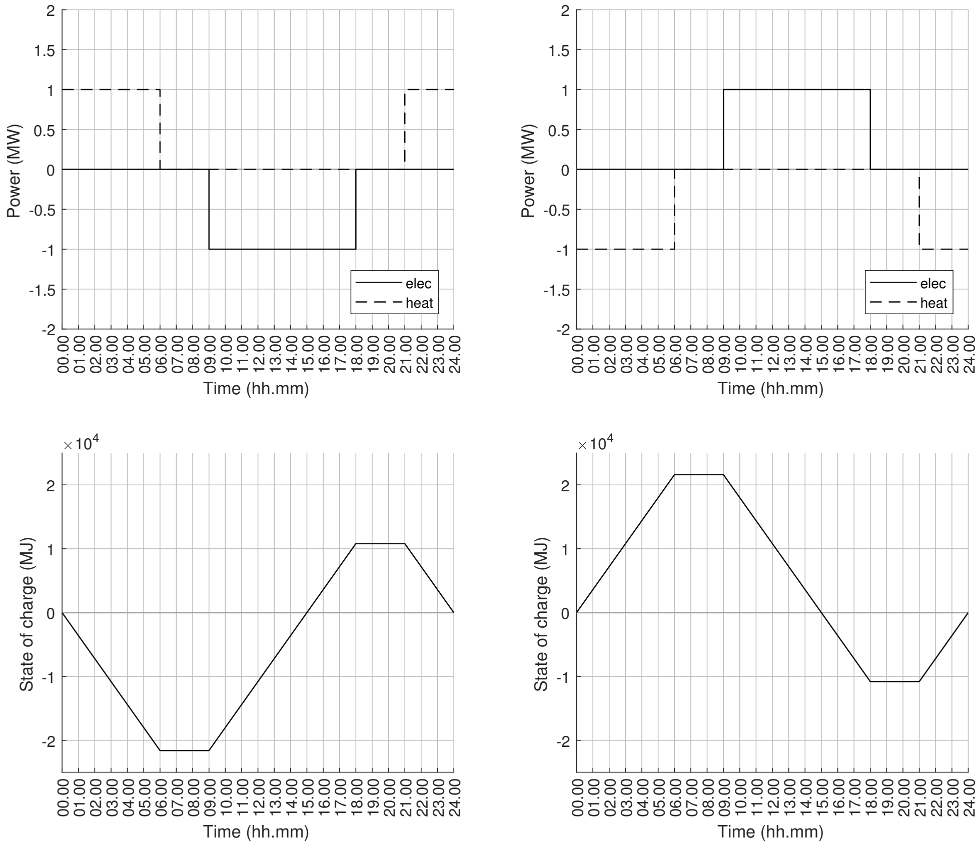


Figure 6.10: Cases 2 (left) and 3 accumulator operation

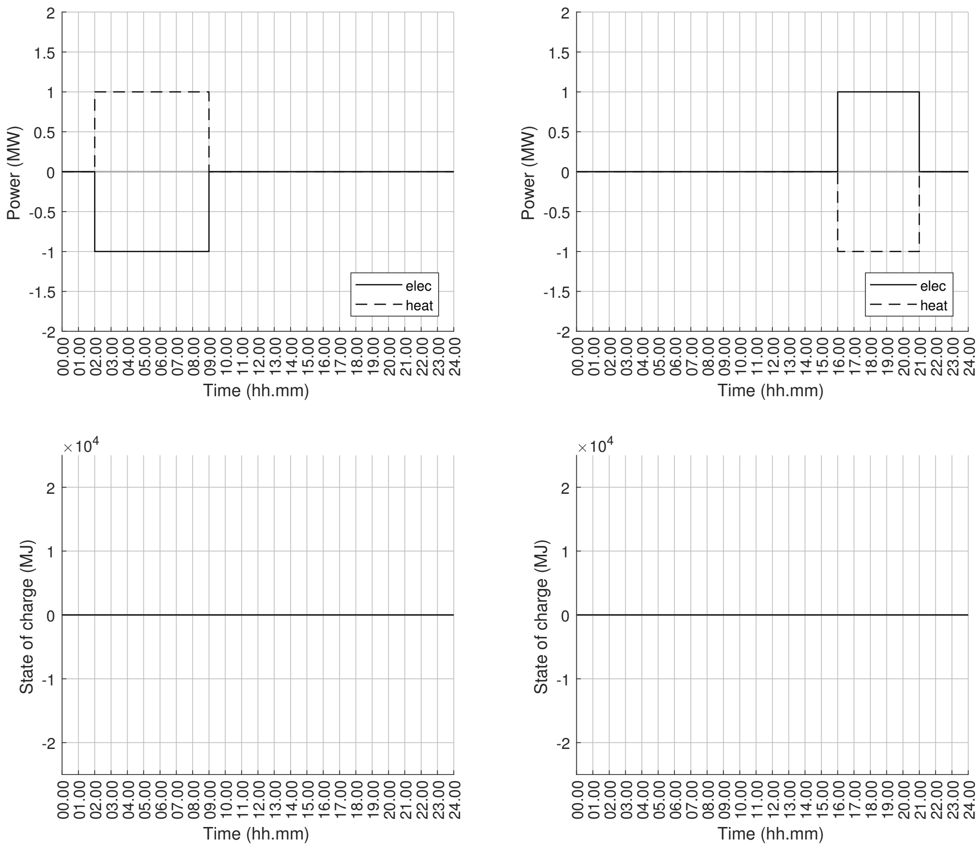


Figure 6.11: Cases 4 (left) and 5 accumulator operation

Figures 6.10 and 6.11 show the operational schedule for the exergy accumulator for cases 2, 3, 4 and 5. The operational schedules for case 6 are the same as for case 4, but at intermediate values of 0.2 MW, 0.4 MW, 0.6 MW and 0.8 MW peak charge and discharge. In all cases, as described in the previous section, the accumulator operates at a net zero stored energy capacity over the course of the day. Positive power flow is out of the accumulator.

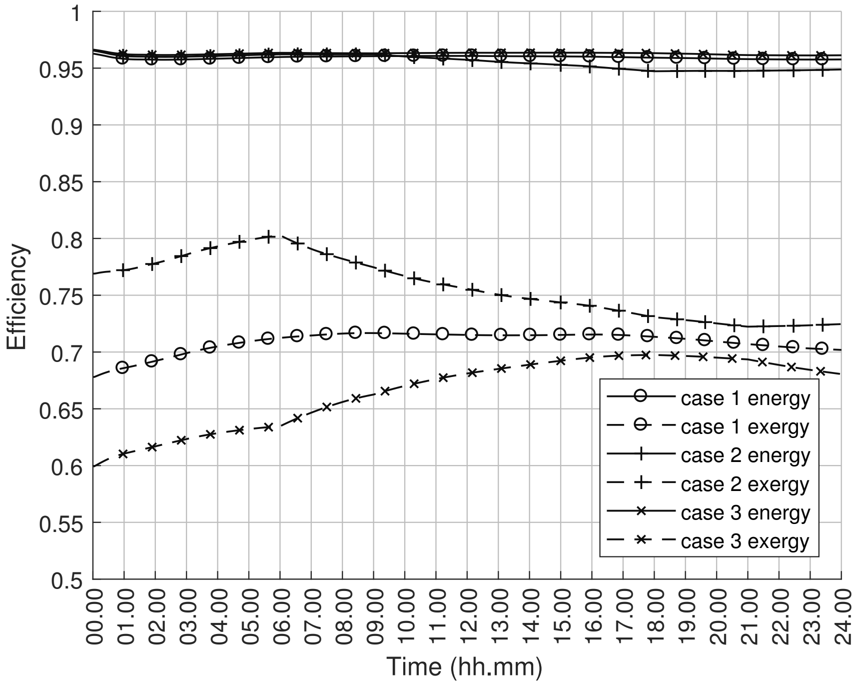


Figure 6.12: Cases 1, 2 and 3 cumulative energy and exergy efficiencies

Figure 6.12 shows a plot of the system's cumulative energy and exergy efficiencies over the course of the day for cases 1, 2 and 3. The cumulative respective energy and exergy efficiencies are calculated as

$$\eta,\ \psi = \frac{\text{net removed from system between time 0 and time } t}{\text{total supplied to system between time 0 and time } t} \tag{6.10}$$

where the net removed excludes component losses.

This efficiency measure incorporates all system inputs and outputs and is designed to be a measure of the system as a whole.

Recall that case 1 is the baseline system, with no interaction between the two energy domains. Two major observations can be made from these charts. First, the system energy and exergy efficiencies work in opposition to each other. Case 2, in which energy is net transferred to the thermal system, has a lower energy but a higher exergy efficiency than the base case, while in case 3 the opposite is the case. When energy is being transferred to the thermal system, less energy is available overall but there is more available exergy; and vice versa for energy transfer to the electrical system. It is worth considering why this is the case.

There are three sources of exergy entry to the thermal system, and four sources of exergy departure. Exergy enters as hot gas from the combustion process; hot water from the heat network return boundary; and the CHP plant. It leaves the system as hot boiler exhaust gases (unreclaimed heat entering the atmosphere); the heat network supply boundary; the heat customer load; and thermal losses during heat transfer from the boiler gases to the heat network water. The exergy accumulator provides a further source and sink for heat energy. When energy is supplied to the thermal system — between midnight and 06.00, and then again from 21.00 to midnight — the influx of heat from the exergy accumulator means that less heat is required from the boiler (which runs continually), and so more of the boiler hot gases are vented to the atmosphere. At the same time, the water inlet to the system is at a lower temperature relative to that of the demand, because the influx of heat energy from the store raises the temperature of the water. For case 2, this results in more exergy removed from the system as boiler hot gases, and less exergy supplied as hot water, compared to the baseline system. The hot gas exergy differential is lower than the hot water exergy differential (by an order of magnitude), and thus the exergy efficiency of the system as given by Equation 6.10 rises. The opposite effect happens for test case 3.

During the accumulator charging period 09.00-18.00 in test case 2 the electrical conductor losses are also higher, which contributes to the declining exergy efficiency during this period. As noted in Subsection 6.5.1, the impedances used in the demonstrator network were taken from [183] and are quite high. For the base case 1, with no operation of the exergy accumulator, the highest electrical loss occurs at 17.30. At this time the grid current is 116 A per phase from a nominal 11 kV grid supply, the total power into the system from the grid and CHP connections is 4.01 MW, the total demand is 2.80 MW, and the resulting system loss is 1.29 MW. This would be a very high loss for a real system, and more accurate projections for a real system would need to take more consideration of the actual system impedances of the electrical network cabling. These energy losses are offset by the conversion of electrical energy to thermal through the (ideal) exergy storage, which effectively operates as an ideal heat pump. The opposite effect occurs when heat is being transferred from the thermal to the electrical system, where the exergy store effectively operates as an ideal heat engine.

Noticeable inflection points occur in the efficiency curves at 7 a.m. and 9 p.m., corresponding to the end and start points of accumulator energy transfer to the heat network. Of particular note is the inflection at 9 p.m. As the efficiencies are calculated cumulatively, one might expect them to regress to a constant value in time. The noticeable increase (respective decrease) in efficiencies at the start of energy transfer respectively to (from) the heat network at this moment indicates the strength of the efficiency boost (reduction). Longer-scale simulations would be required to understand the amount of permanent increase or decrease of system efficiency caused by the operation of the accumulator.

Overall, the energy and exergy efficiencies of the system are quite high. Thermal storage losses are not modelled, nor are transport losses. More accurate modelling of the boiler heat transfer to the environment would give a more accurate picture of losses, as would accurate modelling of the electrical network conductor impedances.

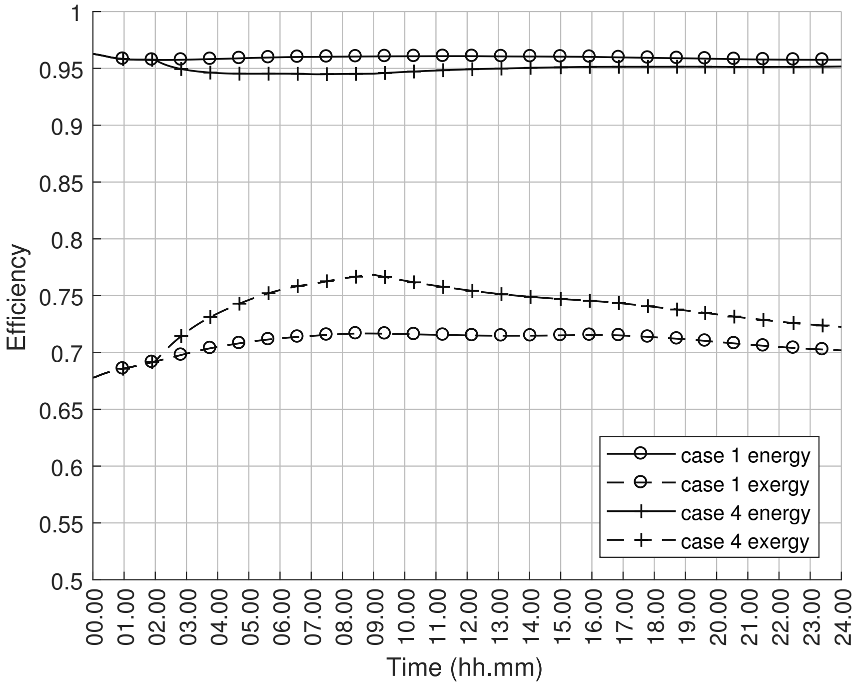


Figure 6.13: Case 4 cumulative energy and exergy efficiencies

Figure 6.13 shows the effect of a synchronised transfer of energy to the heat network from the electrical network. In this operating mode, the accumulator is doing no time shifting of energy. The decrease of energy efficiency, and the increase in exergy efficiency is noticeable in this situation, as the accumulator is operating as a heat pump. If this cycle were to be repeated daily, the overall exergy efficiency of the system would be seen to improve over time. This would suggest that for the asynchronous case (case 2), depending on the network conditions, an overall long-term increase in exergy efficiency would be seen. The opposite observations apply to case 5, as illustrated in 6.14, although the efficiency decrease is smaller than case 4's increase. The exact value of the increase depends on the stream temperature at the outlet of the accumulator heat exchanger, which in turn is governed by the thermal demand in this simulation.

The effect of varying the power transfer between the electrical and thermal networks (case 6) is shown in Figure 6.15. The range of increase is relatively narrow; the effect can be seen to be non-linear in power, which is a consequence of the relationship between exergy and temperature. Simulations were not conducted above 1.0 MW — above this point the system inlet temperature becomes unrealistic, and above 1.1 MW no solutions are possible for the system as the system's physical constraints (temperature) are exceeded. This demonstrates that there are hard limits to the amount of power transferable between domains in an integrated energy system. No similar computational limits exist for power transfer from the thermal to the electrical domain, however in this case again the inlet temperatures become unrealistically high and so there is a practical limit that must be observed. More general energy-hub type models in themselves would not detect these

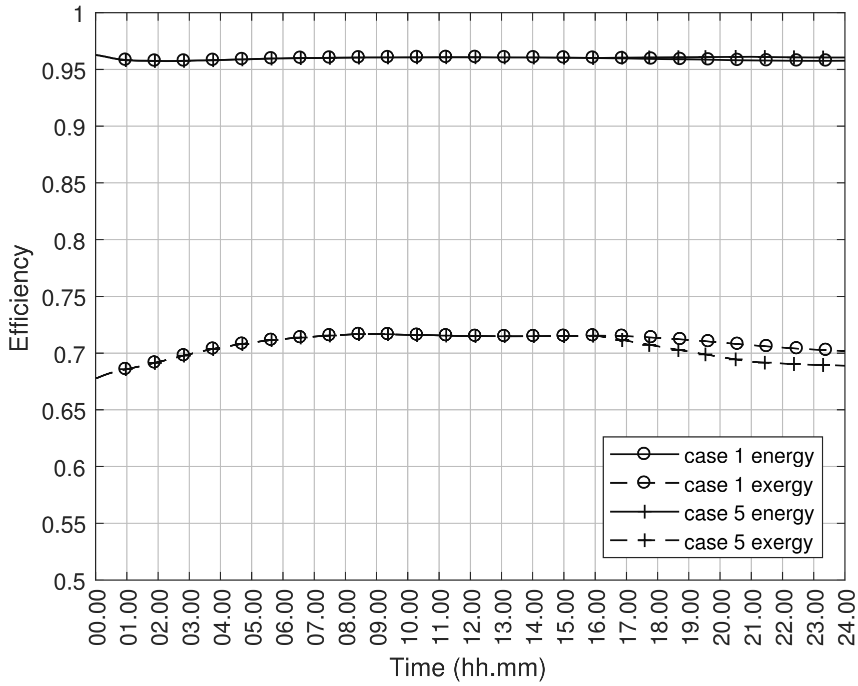


Figure 6.14: Case 5 cumulative energy and exergy efficiencies

kinds of violations of physical behaviour.

The final set of charts, Figure 6.16, show the effect of the simulation cases on the electrical grid connection. Of particular interest is case 4. While this case shows a marked improvement in system exergy efficiency, and reduction of energy efficiency, this is somewhat at the expense of a notable increase in demand at the 11kV transformer connected to the wider transmission network. Whether or not this increased power throughput is acceptable would of course be dependent on the transformer rating. However, this case demonstrates that the model is able to illustrate the wider system effect on one domain of energy caused by a potential wish (improved system exergy performance) originating from another domain. While temperatures and voltage levels are not explored in this demonstrator, these quantities are readily available from the model outputs and could form part of a system assessment or controller design.

Cases 3 and 5 are of interest as these illustrate a strategy for controlling the maximum power at the 11kV transformer supply. However, as has already been seen, this is at the expense of an overall reduction in system exergy efficiency (although an improvement in energy efficiency). In this way, the consequences for the integrated energy system of a control strategy which primarily benefits one energy domain can be determined from the integrated model.

6.6 Conclusions

6.6.1 Model principles

This chapter has presented a demonstrator model designed to illustrate a set of modelling principles regarded as important for the representation of integrated energy systems. The

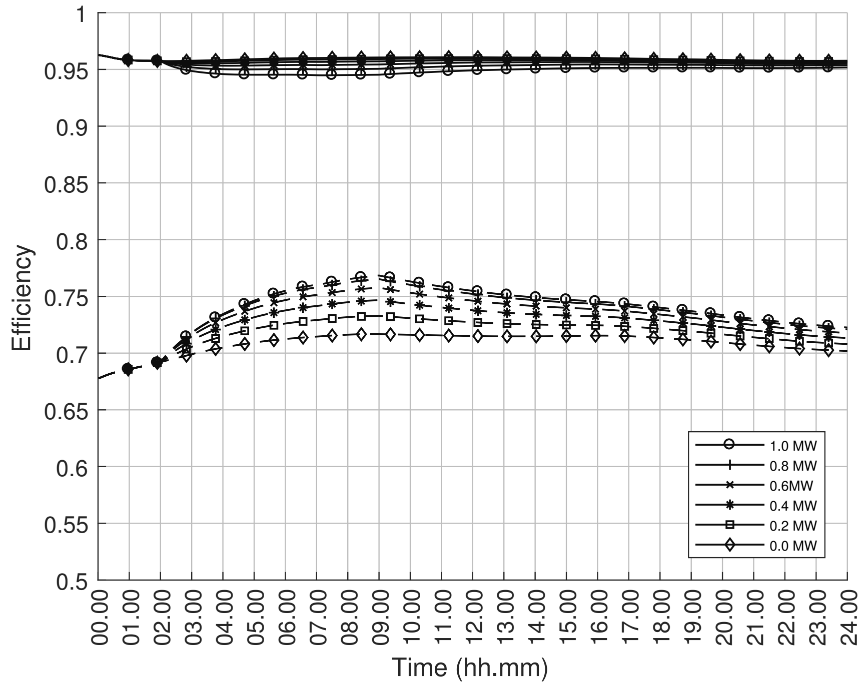
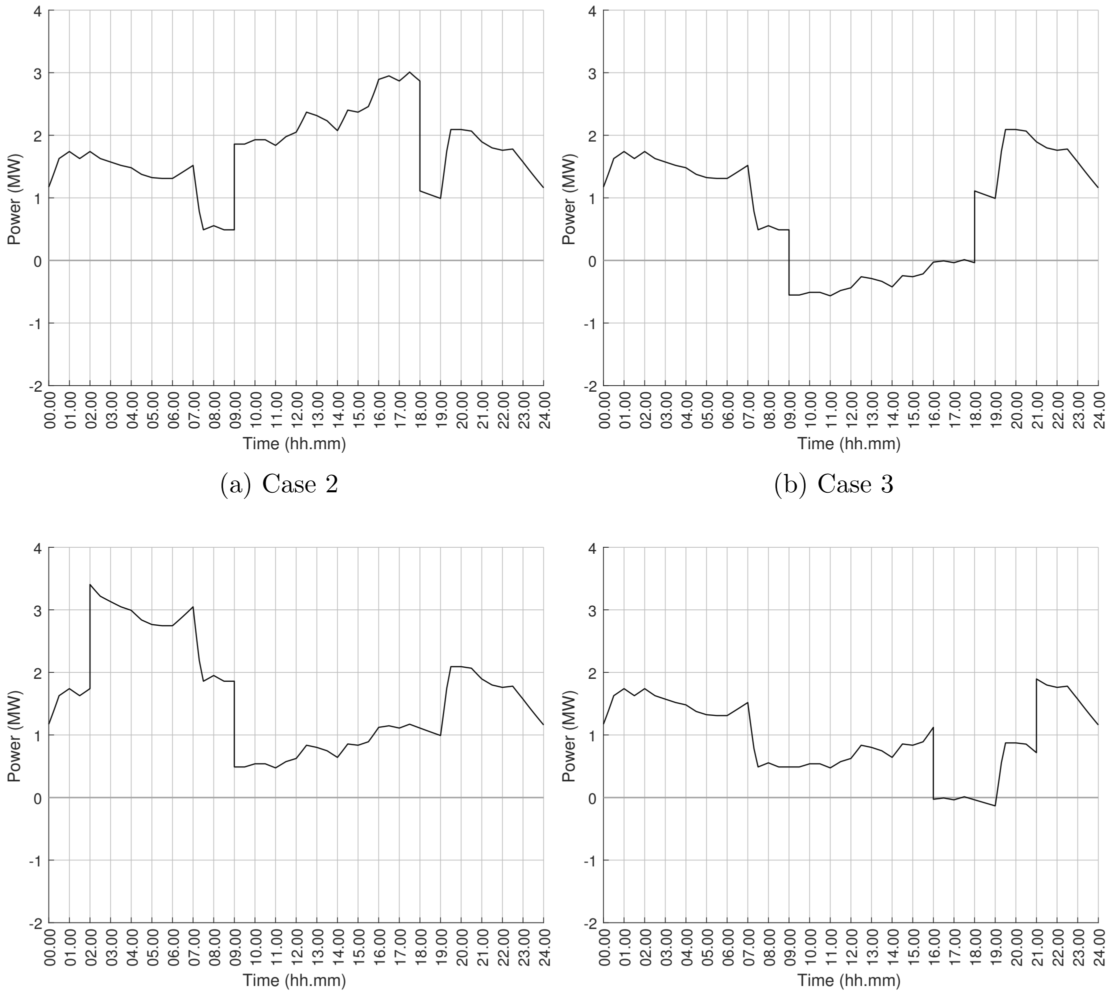


Figure 6.15: Case 6 cumulative energy and exergy efficiencies

logic for the inclusion of these principles stems from the development of subjects in the earlier chapters of this thesis. The three modelling strategies presented in Chapter 5 were evaluated and their ability to meet all the outlined principles were tabulated, with the bond graph approach seen to be the only method that could meet all nine of the stated principles.

A demonstrator model was constructed to illustrate how an integrated energy system model can be built using the bond graph method which meets all of the modelling principles. The model integrates electrical, thermal convective and thermal conductive networks, which satisfies principle 1. Each energy domain is represented using power bonds and bond elements, with all such bonds and elements having a primary representation that is physically valid and without recourse to analogies, which satisfies principle 2. Principle 3 is met with the addition of an ideal accumulator element which can interact with both thermal and electrical domains. The system is inherently a lumped-parameter model, which is "baked in" to the use of bond graph energy system representation, satisfying principle 4. Although not explicitly demonstrated within this model, the use of Modelica and the bond graph representation to construct the model is implicitly an "object-oriented" approach; each sub-network, including the entire demonstrator network itself, can be treated as a black box or a FMU. This is a system-of-systems approach using lumped parameter representations of the system components and enables the demonstrator model to meet the requirement of principle 5.

Figure 6.2 showed a SysML representation of the demonstrator network using the methods developed in Chapter 4, highlighting the means to defining a system boundary and meeting principle 6. In fact, an examination of the boundary of the demonstrator network shows where two boundary points ought to be the same state in the model and



(a) Case 2 (b) Case 3

(c) Case 4 (d) Case 5

Figure 6.16: Grid supply power for trial cases 2–5

suggests how this should be amended (by inclusion of thermal storage or a "slack" input). Principle 7 is satisfied by the ability of the bond graph representation to compute exergy values of the system energy flows. The system operates in pseudo-steady state, mainly as a consequence of system loads being supplied as constant half-hour values, which meets principle 8. Nevertheless, the dynamics of the accumulator, which requires an integration of its input signal, are able to be computed within this structure. Finally, principle 9 is satisfied by the presence of accumulative storage is present within the model; while capacitive storage is not shown in this model it would be accommodated by the bond graph framework. A shunt device controlling reactive power at the electrical supply transformer would demonstrate this.

6.6.2 Demonstrator system

The demonstrator system model represented a moderately-sized community supplied by electrical and thermal energy supply devices operating through their attached networks, with an accumulative storage device, abstracted as an exergy storage unit, mediating energy flow between the energy domains. This demonstrator system shows how an integrated energy system model satisfying the principles described above can be built and operated in practice.

Six simulation trials were conducted on the model to show some possible ways of operating the exergy accumulator unit. The main measure of the effect of the accumulator was through the energy and exergy efficiencies of the whole system, rather than for each energy domain independently. It was seen that for net transfers of energy to the heat network from the electrical network, the energy efficiency of the system fell slightly, while the exergy efficiency rose. This was reversed when the system operated with a net flow of energy from the heat network to the electrical system. Of particular importance was the observation that certain regimes that benefited either one domain or the whole system exergy or energy efficiency led to the violation of operational or physical limits. In the heat case, the energy transferred led to invalid or unrealistic temperatures, while the electrical network suffered high power flow through its supply transformer. Losses (reflected in efficiency measures) increased with the operation of the accumulator. The model therefore demonstrates that a holistic, and detailed, view of an integrated energy system which includes the values of physical variables can be obtained using the method shown.

Some deficiencies were noted in the model. Some of the devices in the system, notably the accumulator, had an ideal energy conversion efficiency of 100%. A real device would be less efficient. Thermal storage was not present in the model, which created an unrealistic boundary condition that could be ignored for the purposes of calculating system efficiencies but which nevertheless leads to an unresolved discrepancy. The use of power source elements in the thermal network creates an unusual type of bond graph which requires a "slack" source element, in a similar fashion to how the power-based electrical network requires a slack bus. The addition of this would resolve the thermal system boundary discrepancy. The convective heat network also omits any pipe frictional elements, and thus pressure losses are not represented in this system. Finally, a number of the parameters of the model are estimated from data or literature, and a more comprehensive model would aim to determine these values more accurately.

A final limitation of the model concerns the ability of it to contribute to an economic assessment of the system configuration and operating schedules under currently-existing market pricing. Exergy is not as-yet accounted for in the market price of energy, and a meaningful treatment of the subject would likely require an evaluation of the grid exergy content and the value of that exergy, taking into account traditional and renewable sources. While the market value of energy is the main method for evaluating a resource, this does not fit within the method and analysis of the demonstrator system as presented. The treatment of exergy and energy pricing separately, or in a unified fashion, would form the basis of a productive study that would extend the usefulness of the model framework presented here.

6.6.3 Proposed methodology advantages and limitations

As noted in Section 6.6.1, the proposed methodology fulfils the requirements of the suggested modelling principles developed in Section 6.1. This section will evaluate in more detail the specific features of the proposed methodology that make it suited to modelling integrated energy systems, as well as pointing out some drawbacks.

Bond graph methods, through element constitutive equations and bond expressions (which also include boundary conditions), produce a non-causal set of equations describing the system, for which a solution state is required. The equation sets created from the models used in this thesis are described using the generalised systems modelling language Modelica. Modelica on its own is not a numerical solution environment. The software application OpenModelica, which implements Modelica as a systems description language, was used to construct the equation sets and solve the system state. OpenModelica accomplishes this using the numerical solver DASSL, which includes a Newton-Raphson stage for step-wise convergence.

An advantage of using a generalised system description language and equation solver for implementing bond graphs is that any bond elements from any energy domain can be included in the system definition, and that a genuine multi-domain problem can be analysed. This can be seen in the demonstrator model where thermal and electrical systems, along with a generalised exergy accumulator, are present in the same model. The disadvantage of the approach is that specific problem domain properties are not used to advantage. For example, electrical power system load flow problems are usually solved using fast decoupled load flow methods, which take advantage of specific known properties of actual electrical power systems to reduce the problem dimensionality. A generic numerical solution algorithm does not take advantage of this domain knowledge and as a result is likely to execute slower than dedicated electrical power flow algorithms, possibly significantly so. However, domain-specific solution tools create solution 'silos' and the different tools must be joined somehow. Section 3.5.1 addressed these differences between philosophies, with the bond graph approach representing an 'integrated' approach, and a discrete approach resulting from domain-specialised tools requiring a 'co-simulated' or 'sequential' approach. The selection of one approach over another is likely to be determined by non-functional requirements, some of which are described below, and may even be a matter of taste.

A benefit of using bond graph methods is the ability to produce graphical displays of the power flow topology in an energy system. The bond graph topology in general tends to match the physical topology — not necessarily the engineering topology, but certainly the base physical processes — and thus is highly expressive as a tool for understanding energy flows in systems. While, therefore, a generalised bond graph tool might not necessarily provide a more efficient numerical solution environment than a dedicated domain-specific tool, it excels at providing physical insight into detailed energy movements through systems. This is perhaps most appealing in mixed energy domain systems, as exemplified in the demonstrator model, where the interactions between domain energy flows are of interest and the domains may be connected at multiple points. Bond graphs are thus a promising tool for education, insight and learning intricate details about how energy flows might behave in integrated energy systems.

The implementation of bond graph models in an object-oriented language such a Modelica creates a situation where system element libraries can be extended without disturbing the underlying design logic and existing system components. “System of system” approaches are possible under this modelling philosophy. The demonstrator system could, for example, be extended with a cooling system component with suitable elements. The cold-system elements can be designed and implemented in isolation and “plugged in” to the existing system. Bond graphs are not just a block diagram replacement however - the non-causal physical description of bonds and elements describes system components at a fundamental physical level rather than as input-output blocks.

In summary, using the demonstrator system as an example, the bond graph method of representing integrated energy systems is at its most useful when developing a fully-integrated model using a unified modelling structure within a single solution environment — possibly using a system-of-systems structure — is desired, and understanding the precise structure energy and exergy flows for all energy domains is an important objective. Existing, domain-specific solutions using application-targeted algorithms are potentially more appealing when computational speed is critical and a co-simulated approach to joining simulation outputs is possible.

Chapter 7. Discussion, Conclusions and Recommendations

7.1 Objectives

This thesis set out to examine how integrated energy systems should function, and in particular how the multiple domains of an integrated energy system can be brought together through a mediating storage mechanism. It not being possible to experiment on real integrated energy systems, a way of modelling them was sought instead. This led to a method using bond graphs to build these systems in a unified, integrated, domain-independent way. The requirement to be able to equivalence the energy in multiple domains suggested the introduction of exergy into integrated energy systems as a base "standard" for domain-independent energy quality. Recognising the growing importance of district energy storage from government incentives and the literature, the idea of using an exergy accumulator to mediate between energy domains has been proposed. The exergy accumulator as described here, having multiple lossless connections to supply and receive energy from different energy domains, is an ideal approximation, but the concept is based on the existence of some real devices such as adsorption machines. A demonstrator integrated energy system, based on the district heat and power system at Byker, Newcastle upon Tyne, UK, which incorporated thermal conductive, thermal convective and electrical systems in a unified bond graph diagram with an exergy accumulator mediating between the domains, has been developed and presented. A series of system use cases explored the operation of the model and the practical performance of the demonstrator system, and showed how the energy and exergy efficiencies of the whole network changed as a result of the operational schedule, and the consequences or side-effects such operations have on system constraints such as thermal or electrical limits.

7.2 Discussion

7.2.1 Integrated energy systems

Despite what is recognised as energy system infrastructure — the cables, pipes, energy generation and transformation technologies, and so on that make up the engineering hardware supplying energy in a usable form to the civic population — having underpinned modern society for decades, energy is increasingly becoming perceived as a service, rather than a commodity or an engineering activity. This focus on the end use rather than the transport mechanism is leading to a call for tighter coupling between energy domains, in which the energy medium is less important than the effect desired by the end-user. The rapid increase in renewable energy generation, particularly distributed and local generation, is also modifying the requirements of energy infrastructure, from a centralised to a scattered model of energy production. This thesis has discovered that methods for modelling and assessing these new forms of energy systems are still relatively in their infancy, and that a number of open questions exist as to how energy domains or vectors ought to be combined, what kind of boundaries are required to determine whether a system can be described as integrated, and how such systems should be designed and controlled.

The work in this thesis has concentrated primarily on systems which integrate heat, electricity and cooling as energy domains being supplied from generation plant to end-users. However, the partnership between these domains in an unequal one. Although heat is described by UK governmental and professional institutions as an energy domain crucial to the success of future integrated energy systems, it is still considered by some to be very much a "Cinderella" domain. Where heat features in integrated energy systems it is often only through the electrification of heat using heat pumps or other means. This is particularly noticeable in comparison with other European countries, which have a more mature heat network culture. Case studies of three integrated energy systems in the UK were used along with a broader literature study and a series of semi-formal interviews with industry practitioners to explain the prejudices, inconsistent management and lack of standards, along with the pre-eminence of North Sea gas supplies, that have historically stifled growth of district heat networks in the UK as a major contributor to local energy provision.

One of the case studies — a heat network in Byker, Newcastle upon Tyne, UK — was taken to a deeper level than the others in an investigation of the substantive motives behind the management objectives. Taking this case study to at least represent "typical" heat networks in the UK[1], it was found that the goals of local heat networks management aligned with more prosaic objectives — obtaining subsidised capital investment, reducing residential bills, and creating insulation from future energy price volatility — than commonly-stated reasons for encouraging integrated energy systems (see e.g. [9, 10]) of reducing emissions or using fossil fuel reserves efficiently. Naturally, the manager of a local energy network is behaving correctly in basing their operational strategy on the economics of costs and subsidies that actually exist, rather than exergy. The literature on thermo-economics, covered in Section 2.5, makes a case for costing exergy, or some derivative value of exergy, as a principal measure in the assessment and operation of energy systems; but in order for this to be realised and for exergy to form this measure of a system's "goodness" with respect to national and international de-carbonisation objectives — assuming that the arguments from the literature hold — a governmental-level push through incentives, pricing and subsidies based on the reduction of exergy destruction in energy provision would need to occur. Only in this way would a local energy systems manager's objectives be directly aligned with a principal aim of reducing exergy waste.

[1] Personal correspondence with the heat network management team. Their communications with other UK heat network management groups suggest that the case study network is not an outlier.

7.2.2 Systems analysis

The development of novel methods for understanding and assessing integrated energy systems required some definitions. Literature and the three case studies were used to develop a structure that could be used to meaningfully talk about what an integrated energy system is. A systems approach was chosen as a natural way of discussing integrated energy systems. Systems approaches specify three elements that are required for a system to qualify for development and analysis: components; a boundary; and component connections. Additionally, "systems-of-systems" approaches create a natural hierarchy which is necessary for analysis tractability.

The three integrated energy system case studies were used as a basis for creating a template or reference model for a general integrated energy system. Other studies were found in the literature that had mapped systems to reference models but these had not used case study references. A method was developed to identify and extract the principal system components and connections from the case studies, the extracted elements forming a stock set of generic system components for use in subsequent modelling. While this thesis was limited to three case studies, a bigger exercise involving a broader range of integrated energy systems would yield a more complete set of components. System boundaries are often very difficult to define but a suitable pragmatic definition was provided by [25] as "an open thermodynamic boundary". Although this seems oddly vague, this definition leads to a system specification that focuses on which components of the system ought to be included and which are not, and how the system interacts with the rest of the world at the boundary, avoiding the definitional problems that arise when a geographic definition is attempted. Thus a working definition of the composition of an integrated energy system along with a potential reference system were able to be specified, which are necessary to enable a meaningful approach to modelling.

The creation of a reference system, a set of components, and component connections for an integrated energy system enables the system to be viewed through an engineering design lens. An application of Axiomatic Design principles to the reference system reveals the structural connection between the customer needs that are to be satisfied by the system, and the design elements (system components) that make up the system. This powerful method allows the system analyst to understand which elements of the systems are coupled, and thus not amenable to independent control. An illustration of the technique has been presented in this thesis, but the application to the control of an actual system would be the subject of future work.

The development of the integrated energy system model does not include an economic evaluation of the system — this was out-of-scope for this project. However the ready availability of exergy and efficiency values calculated in the simulation environment would permit the integration of a method such as SPECO (Lazzaretto and Tsatsaronis [82], which is described in Chapter 2. This method, which uses the exergy in- and out-flows from system elements along with exergy efficiencies, would extend the capabilities of the integrated energy system simulation environment into the economic domain to enable thermo-economic evaluations.

7.2.3 Systems integration

The incorporation of renewable energy into energy systems at a regional or local level, which has mainly been driven by carbon emission reduction strategies, has been shown to result in “wrong-time” and “wrong-type” energy supplies. That is, the uncontrollable nature of renewable sources leads to a supply-led system rather than one which follows the end-user demand. The literature surveyed for this thesis, particularly including governmental and professional bodies publications showed that the inclusion of energy storage is of particular interest in managing the energy flows. While it was noted that much has been written in the literature about dealing with “wrong-time” energy using storage, the nature of “wrong-type” energy management is less well-developed. A survey of the different types of energy storage principles and practical realisations was presented with these aims in mind.

The idea of exchanging energy between energy vectors through an intermediate device which may store the energy in the interim emerged as an important conceptual element of an integrated energy system, wherein energy from different domains can be converted at will. However, what is apparent is that all energy types are not equal. Thermal energy cannot be converted in its entirety into an equivalent amount of electrical energy; this is a consequence of the second law of thermodynamics. A survey of literature and thermodynamic theory shows that the quantity exergy, rather than energy, can be used to equivalence different domains of energy, enabling correct modelling of the cross-vector conversion of energy. Extending this concept it has been proposed that energy storage in integrated (multi-vector) energy systems models be instead regarded as exergy storage. The exergy storage concept is independent of any underlying technology and conversion process and can thus be used in studies of general integrated energy system performance. A hierarchy of exergy storage systems, from the theoretical limiting case of an ideal system, to something which would more practically represent a real element, has also been proposed.

7.2.4 Systems modelling

The development of energy infrastructure systems is different to many other engineering enterprises. Any particular system is unique, and can only be built once. Prototypes and real-world models are not possible, and knowledge transfer from similar systems is limited, not least because an energy infrastructure system is an active, live realisation and experimental or disruptive activities cannot be conducted except in very narrow cases. This thesis argues that this leaves building computer models as the primary means by which integrated energy systems can be designed and evaluated before construction or extension.

In order to be able to model integrated energy systems, a solution is looked-for that allows multiple energy domains to be represented in one model, and which can incorporate exergetic quantities to allow cross-domain energy exchanges to be properly accounted for. Sola *et al.* describe three main modelling paradigms used in modelling energy systems: *sequential*, whereby sub-models feed their outputs into other sub-models as inputs; *co-simulated*, in which sub-models exchange information in step with each other to converge to a solution simultaneously; and *integrated*, where all sub-models are fully-integrated into a unified representation and solution method [184]. While the other approaches have advantages — for example, the sequential model type allows for discrete model development, while the co-simulation type can take advantage of specialist domain solution techniques — the work outlined in this thesis has pursued the integrated approach. By incorporating all energy domains as well as the means to exchange energy across domains within a single model format, the integrated model provides a means of capturing the clarity of energy flow and complex interactions within the system.

Many different forms of integrated model types exist and this thesis examines three; energy hubs, circuit equivalent, and bond graphs. Ultimately, bond graphs are seen to best meet the modelling selection criteria, particularly with regards to physical energy flow and the interchangeability of energy domains. Despite being the only method that satisfied the modelling principles as laid out in Chapter 6, bond graphs will be an unfamiliar method to many energy systems modelling practitioners. This might be a practical factor in using the method to develop an integrated energy systems model that can be used and understood by a wide audience, despite the more transparent nature of the modelling notation and applicability.

7.2.5 Demonstrator model

The bond graph approach was applied to a demonstrator energy systems network model, which brings together the elements discussed throughout this thesis into a single demonstration piece. The need for local integrated energy systems models in itself was argued, because it is otherwise generally not possible to experiment on active energy networks, nor construct experimental ones. The demonstrator model uses, in bond graphs, an energy system model form that can accommodate any energy domain in a standard way, leading to a true integrated system model, in this case of convective, conductive and electrical energy transport, generation and use. Based upon a real energy system, the demonstrator model incorporates real energy demand and supply data. The use of Modelica as a model description language enabled a "system-of-systems" approach whereby elements of the model such as heat exchangers and electrical cables can be parametrised and re-used. A new type of model element, the exergy accumulator, was developed to represent a device which can buffer energy between domains and exchange it fairly, based on its exergetic content.

Integrated energy systems require an approach to efficiency calculations which considers the system as a whole rather than the atomic efficiencies of its constituent parts. The demonstrator model has been used to show how the whole system energy and exergy efficiencies of the demonstrator system can be calculated, using a series of trial cases. The trial cases covered six situations: a base case with the two sub-networks — electrical and thermal — operating independently; two cases where there was a net energy transfer to one of the sub-networks; two cases of synchronised energy transfer which corresponded to potential system constraint alleviation; and a final case examining the relationship between the magnitude of power transfer between the networks and the resulting system efficiency. These cases showed an inverse relationship between energy and exergy efficiency, and that transferring energy from the electrical to the thermal system improved the overall system exergy efficiency. The synchronous energy transfer cases also showed these results, and additionally illustrated how a system designed to alleviate network constraints on one sub-network by transferring energy to or from another could nevertheless fall foul of other network constraints such as temperature or power limits, either physical or equipment.

Some limitations to the model can be observed. The heat network has been simplified by omitting some components such as pipe friction. These simplifications do not affect the results obtained nor the demonstration of the system model, but other models might require the additional detail. The modular bond graph approach permits this without otherwise disturbing the rest of the model. A discrepancy in the boundary conditions is present in the model, whereby the heat loop "outlet" is fixed at what would be the temperature of the water returning from the heat loop. The condition here should match the "inlet", which is physically the same point in the loop; however because these two points are not joined, the temperature at the inlet is a free variable. This nevertheless does not affect the system efficiency calculations. The use of power-based energy sources and sinks in the thermal sub-network, a formulation that is not usually encountered in physically-based formulations of thermal systems (it is commonplace in electrical system analysis however), contributes to this discrepancy. A slack element such as an additional thermal store, could be included to resolve this discrepancy in much the same way as is done in electrical networks power flow analysis.

The boiler operates at a fixed point based on calculations taken from the real boiler in the Byker heat network, and is only able to represent this particular case. A more general model would expand upon this component. Under the fixed-production model it is possible to create a demand-side situation where an unrealistic amount of energy must enter or leave the thermal network, which causes unrealistic boundary temperature variations. This is also a consequence of the use of power boundary conditions in the thermal network, as described above. As further solution to this problem, as well as or instead of using a slack element to account for power discrepancies, would be to add a method of controlling the primary heat production in the boiler. Large-scale discrepancies in the energy balance across the system would be met by increased or reduced thermal production with such additional control. This could potentially also have the effect of expanding the scope of the model to include gas supply as an energy domain, if desired.

7.3 Conclusions

7.3.1 Integrated energy systems as a solution

Much has been written about integrated local energy systems forming an important role in the future of energy production and delivery in the UK. Some important barriers to their development and adoption seem to remain at present however. Firstly, the precise role of the local energy system is often unclear. Ford *et al.* [185] have highlighted the general lack of clear objectives for local energy systems in their study of industry practitioners. The literature review and expert interviews in this thesis show that despite an intuitive inclination towards integrated energy systems, particularly ones which combine heat and electrical systems, the patchy legacy of historical district schemes together with the UK's political and energy reserves landscape are creating resistance to large-scale local energy scheme construction. Two of the biggest obstacles to integrated energy system growth are to what degree government incentives correctly direct investment, and the scale, cost and disruption of the creation of new infrastructure.

Nevertheless, three case studies examined for this thesis demonstrate that where local conditions are favourable, local energy schemes which incorporate multiple energy domains are feasible. The case studies still fall short of being true integrated schemes however, in that their energy domains are largely operated independently. Domain-connecting technologies tend to be devices such as combined heat and power (CHP) or adsorption devices which run under constant schedules, and, while important to the effective use of primary energy, do not create much additional flexibility for the system to meet its varying demands. The demonstrator model presented in this thesis as a synthetic version of one of the case studies shows how system flexibility can be improved through the use of an exergy-based storage device which allows the transfer of energy between domains. Net energy transfer from one domain to another can be accomplished to achieve either under- or over-supply correction for one domain, or to move supply energy in time. These energy transfers are not without substantial system constraints and the model form chosen also allows these constraints to be evaluated.

In Chapter 4 this thesis considered the use of a systematic design method and design representation language to be important for the organisation and clarification of the design elements of integrated energy systems. Axiomatic design and SysML are proposed as a way to accomplish this, particularly in the construction of reference model elements and systems. The case studies investigated in this thesis were used to construct a set of standard reference elements that could be found in integrated energy systems; these reference elements were used to guide the subsequent development of model elements for use in the integrated demonstrator system model. It is envisaged that a reference model set will be important in general integrated energy system studies, particularly for comparing study results, and will facilitate collaborative model exchange either in fully-integrated model structures (as in this thesis, using Modelica), or in systems using functional mock-up interface types of specifications.

7.3.2 The use of exergy in integrated energy system studies

One of the hurdles of analysing multi-domain energy systems is in ensuring equivalence of the energy domains in question. This thesis has taken the approach of equating different energy domains through the use of exergy. Converting energy quantities, whether electrical, heat, cold, chemical, etc. into the common base of exergy permits true equivalencing of energy in integrated systems. The emphasis in this thesis has been on using a convenient device called an exergy accumulator to act as an intermediate store, from which each separate domain can be supplied. This has allowed correct attribution and accountability of system losses caused by different operational schedules. However, exergy could and perhaps should be used as an intermediate value when examining any conversion device in integrated systems. Often, quantities such as device energy efficiencies or coefficients of performance are used in modelling environments. A conversion to intermediate exergy would show more clearly the use and loss of energy quality in multi-domain systems, as exemplified by the exergy cascade diagrams presented in Chapter 2.

Emphasising exergy in integrated systems does come with some overhead. Energy- and economy-centric modelling environments such as energy hubs cannot be used directly, because the direct physical states of the energy flows such as temperature, voltage, chemical potential and so on are needed to calculate exergy values. Additionally, with being defined relative to a baseline (the dead state) exergy is not an absolute value, and care must be taken in comparing studies or models defined on different baselines. Thus unless clear pre-determined exergy flows are known, a physically-based simulation or modelling tool is required. The possibility of creating an exergy hub equivalent of the energy hub model formulation was raised in Chapter 5, but exploration of this concept would need to be pursued in another work. A non-computational obstacle to the widespread use of exergy analysis in integrated energy systems is simply its lack of visibility outside the fields of engineering and chemical thermodynamics. The idea of energy availability emerges from the study of the second law of thermodynamics and Carnot's theorem, which are advanced degree-level subjects that students usually find quite difficult conceptually. Unfortunately there doesn't appear to be an easy way to broaden the communication of this tricky subject, which may limit its use in integrated energy systems, at least in the near future.

Along with the use of exergy in equivalencing energy, the other main expression of exergy has been in the calculation of efficiencies in the demonstrator model presented in Chapter 6. For a combined-domain system, exergy efficiency is a more useful measure of the real performance than energy efficiency. In all of the example trial cases of the demonstrator network the exergy efficiency is much less than the energy efficiency, despite the lossless nature of the exergy accumulator, indicating a genuine loss of energy quality somewhere in the system. As another example, the case study system upon which the demonstrator is built — the heat and power network in Byker — uses heat exchangers in the heat loop which transform heat from around 130 °C to a much lower 60 °C for transport to residential properties. There is little energy loss in this process, but a huge exergy loss, which would be revealed in an extension to the demonstrator model that included these heat exchangers. Therefore it can be concluded that calculation of exergy efficiencies is of critical importance for integrated energy systems analysis.

7.3.3 Modelling of integrated energy systems

In contrast to many engineering systems, integrated energy systems infrastructure is a socio-technical construct that cannot easily be modified or experimented on. It is not possible to build full prototypes of integrated energy systems, and while limited laboratory and field experiments are possible these cannot support extreme loading cases, alternative designs, speculative architectures, or destructive testing. This leaves computer modelling as the only method of exploring much of the operational range of proposed integrated energy systems. In fact, integrated energy systems, by their very nature as speculative and experimental solutions to renewable energy integration and tackling carbon production, even moreso require modelling approaches that can explore radical design and operational proposals.

This study has examined three different ways of constructing models of integrated energy systems models. A series of modelling principles (see Chapter 6) were used to evaluate these methods, with bond graphs emerging as the only method satisfying all of the principles. Perhaps the most important principles proposed were the ability of a modelling scheme to build a genuine multi-domain model without compromise or unnecessary analogy, and to be able to incorporate exergy as an equalising element for the system energy domains. With bond graphs providing an energy domain-independent representation of physical systems, an outline of a series of system reference elements matching the system reference elements developed in Chapter 4 has been proposed. A smaller number of these were developed in full to form a demonstrator model of one of the case study networks also explored in Chapter 4, illustrating how a unified bond graph with thermally conductive, convective and electrical elements along with an exergy accumulator element could be created.

Aside from demonstrating the bond graph modelling approach, the demonstrator model was used to derive some operational performance indicators of the integrated system. It was clear that transferring energy from the electrical to the thermal system through the accumulator (used to shift energy in time in this instance) raised the exergy performance while simultaneously reducing the energy efficiency slightly — this would appear to be caused by increased electrical losses occurring as a result of a higher demand for electrical energy to be transferred into the thermal system. Thus, the importance of examining exergy efficiency and not just energy efficiency in integrated systems can be seen. A further two trial cases involving a synchronised energy transfer centred around network constraint removal (peak shaving) show the same effect, but also here the physically-based nature of the bond graph model was able to show that other constraints, i.e. temperature and electrical transformer power flow, were at risk of being contravened as a result. Again, the truly integrated model demonstrates the interconnected nature of the model domains and how the varying competing objectives for the system can be clearly evaluated.

7.4 Recommendations for further work

7.4.1 Demonstrator model

The demonstrator model was able to show the promise of the integrated system approach and demonstrated some results, but the following improvements are suggested.

A more general boiler model would incorporate the combustion calculations similar to those used in Appendix A (see Kotas [48]). This iterative calculation, required because of the mutual dependence of two unknowns — the gas specific heat capacity over the temperature range, and the temperature of combustion — means that fixed-state sources and sinks as used in the demonstrator model are unsuitable for general work. An even more general approach would be to incorporate Arrhenius' equation into a bond graph model of combustion as presented by Couenne *et al.* [175].

The heat network should be joined properly and a stratified thermal accumulator should sit between the boiler and the heat loop, to provide decoupling of the system and to act as a source of slack power. The accumulator would act as a fixed temperature power supply, albeit with a dropping temperature over time, which is a different behaviour to the boiler's. The physical pipe network itself is also missing entirely in the demonstrator model. A more complete model would feature a resistive element type in the convective system, the element having an appropriate fluid resistance model form, such as provided by the Darcy-Weisbach equation. Work by Strand *et al.* in describing one-dimensional modelling of fluid flow using bond graphs [186] is one possible starting point for such models.

7.4.2 System reference models

More development of the system reference models would provide an anchoring point for systematic modelling of integrated energy systems. Having a common set of system elements and a way of defining system boundaries would enable more straightforward communication of integrated energy system designs. While the principles of axiomatic design and their relationship to real system components and SysML representations were examined in this thesis, they have not been used to analyse the resultant systems designs to any degree. An axiomatic design-based analysis of common integrated energy system topologies with a view to understanding how these systems are coupled, or otherwise, and therefore how they should be controlled, would provide a solid basis for understanding new integrated energy system designs. Such an analysis could be conducted by examining the generic integrated energy system design matrices outlined in Chapter 3.

7.4.3 Bond graphs

Many more bond graph elements for integrated energy systems can be developed. Table 4.1 lists the generic elements found in integrated energy systems. Bond graph elements of all of these could be developed to form a more comprehensive library of modelling elements for integrated energy systems. In particular, models for the cooling domain have not been addressed in this thesis. Many types of bond graph element models have been developed over the years for modelling various physical behaviours (see Borutzky [125], and Brown [166] for an overview), but a rational collection of elements and approaches suitable for modelling integrated energy systems would be of benefit.

7.4.4 Industry perspectives

Further study of the industry perspective on heat networks in the UK could be conducted. This thesis only sampled a small number of practitioners in a semi-formal expert elicitation exercise. A more formal study, similar in form to the work by Ford *et al.* [185] which conducted a more expansive and rigorous survey of industry practitioners regarding their understanding of a smart local energy system (SLES), would serve to produce a more concrete and up-to-date understanding of the industry view of the value of heat networks and how they contribute to integrated energy systems.

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Appendices

Appendix A. Byker heat network CHP analysis

A.1 The Byker CHP plant

The Byker District Heating system is located in Byker, Newcastle upon Tyne, and supplies approximately 2000 residential properties (mostly social housing) alongside a small number of municipal buildings. The system is discussed in detail in Chapter ?? but the basics are recapped here. The district heating system was originally constructed between 1968 and 1982 as part of the Ralph Erskine-conceived Byker estate, now a Grade II* listed building, with the intention of supplying "cost free" heat from the incineration of municipal waste. Despite the energy from the plant being anything but "free", and difficulties with the use of refuse-derived ash being used inappropriately in landfill, the plant today continues to supply the estate residents with heat and electrical power. The original boilers were replaced in the mid-2000s with three 6MW natural gas boilers, with a 1MW biomass boiler and a 1 MWe / 1 MWt combined heat and power (CHP) unit being added in 2011/2012. The site continues to be upgraded in 2018/2019 with enhanced plant and residential controls having been added in 2017/2018 and with a proposed additional 4 MWt CHP plant at the planning stage.

The nature of the Byker plant makes it an ideal study vehicle, as it supplies a large community while being actively upgraded and expanded. The solid pipe and substation infrastructure also makes it an ideal candidate for study of potential additions and "what-if" scenarios. Three site visits and a number of other discussions with the plant operators have enabled a catalogue the architecture of the plant, the equipment, and its general operating conditions to be constructed, along with some basic heat operational data.

One method of studying the plant is as an energy hub approximation as discussed in Section 5.2 and shown in Figure 5.3. In this basic configuration the biomass boiler is ignored and only one of the gas boilers is considered to be operational. The plant component energy and exergy efficiencies are derived here.

A.1.1 Plant overview

Figure A.1 shows the overall layout of the plant. The main heat production base load comes from the biomass boiler, backed up by the CHP plant which serves to pre-heat the water returning from the heating loop. The 6MW natural gas boilers are a legacy installation and are mainly used for top-up winter heat and for additional supply during maintenance. It is not common for all three gas boilers to be in operation simultaneously. Figure A.2 shows a simplified plant layout used in the following analysis. Simplified CHP circuits are shown and only a single gas boiler is used in order to reduce the fuel supply

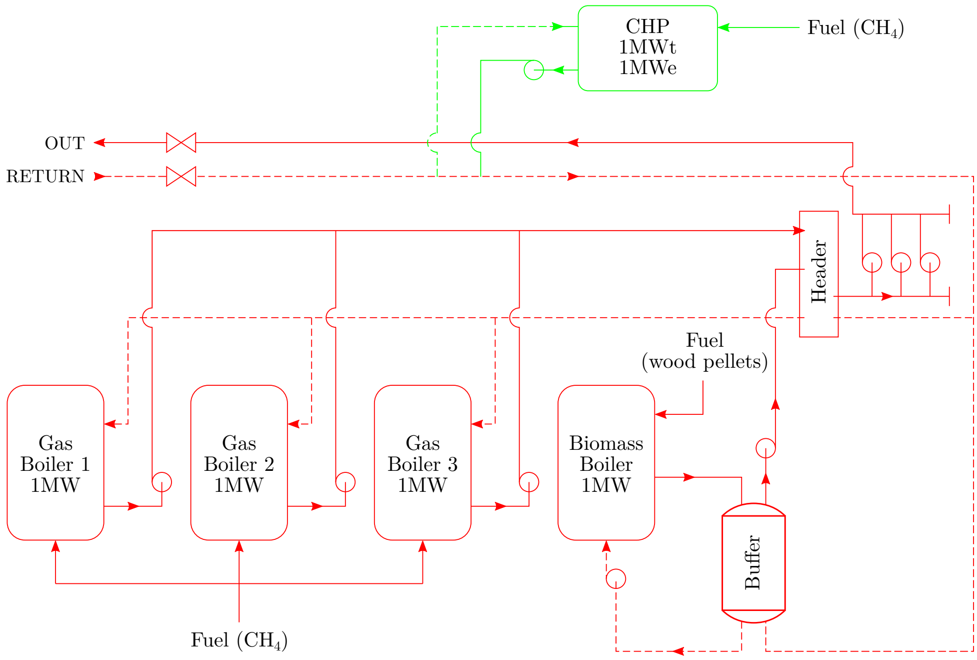

Figure A.1: Byker heat plant

to one of pipe-fed natural gas. The district heating loop supplies hot water at 130 °C and returns it to the heat station at 80 °C.

The following assumptions and observations are made for the analysis.

- The standard reference state when calculating exergy values is defined as $T_0 = 25\,°C$ and $p_0 = 1\,\text{bar}$.
- The combustion plant burns natural gas in air. For the purposes of this analysis, natural gas is taken to be pure methane (CH_4), while air is assumed to be a mixture of 21% oxygen (O_2) and 79% nitrogen (N_2).
- All heat exchangers are adiabatic (100% heat transfer efficiency).
- Pressure and heat losses in the distribution pipework are ignored.
- Pump work is negligible and is ignored.
- All fluid is water under pressure above the saturation pressure. This is approximately 5 bar in the CHP cooling circuit, and 10 bar in the heating loop.
- All water properties are calculated using data from IAPWS IF97 steam tables[1].

[1]Specifically, X STEAM FOR MATLAB by Magnus Holmgren, www.x-eng.com Date: 2006-01-20

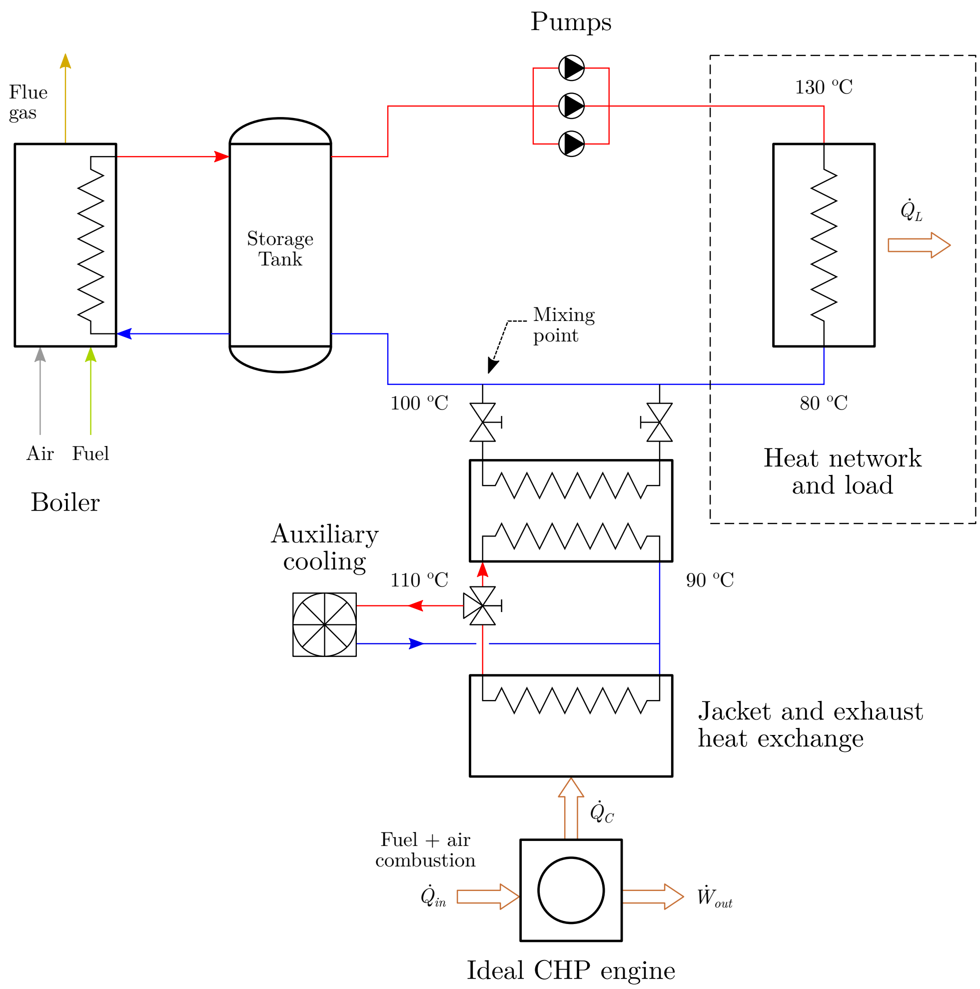

Figure A.2: Byker heat plant CHP and boiler circuits

Figure A.3: Byker heat station Thermax boilers

Figure A.4: Byker heat station Kara biomass boiler

A.1.2 Boiler

Boiler Configuration and Assumptions

The plant boilers are Cochran Thermax models with a reported nominal heat output of 6MW. Referencing the manufacturer's fact sheets for these boiler designs, the closest match is a 6,400 kW model which has a value for 'F&A @ 100 °C' of 10210 kg/h. F&A is a boiler industry term describing the mass of steam produced by the boiler "from and at" the specified saturation temperature. This figure needs to be adjusted using the actual temperature and pressure of the produced steam. Figure A.3 shows the boilers *in situ*. As previously stated, only one boiler is considered to contribute to the plant operation.

The exergy performance of the boiler can be modelled in systematic fashion as in e.g. Kotas, p158 [48] as a three stage process consisting of I) adiabatic combustion from fuel and air at atmospheric conditions, II) transfer of heat from the combustion products to

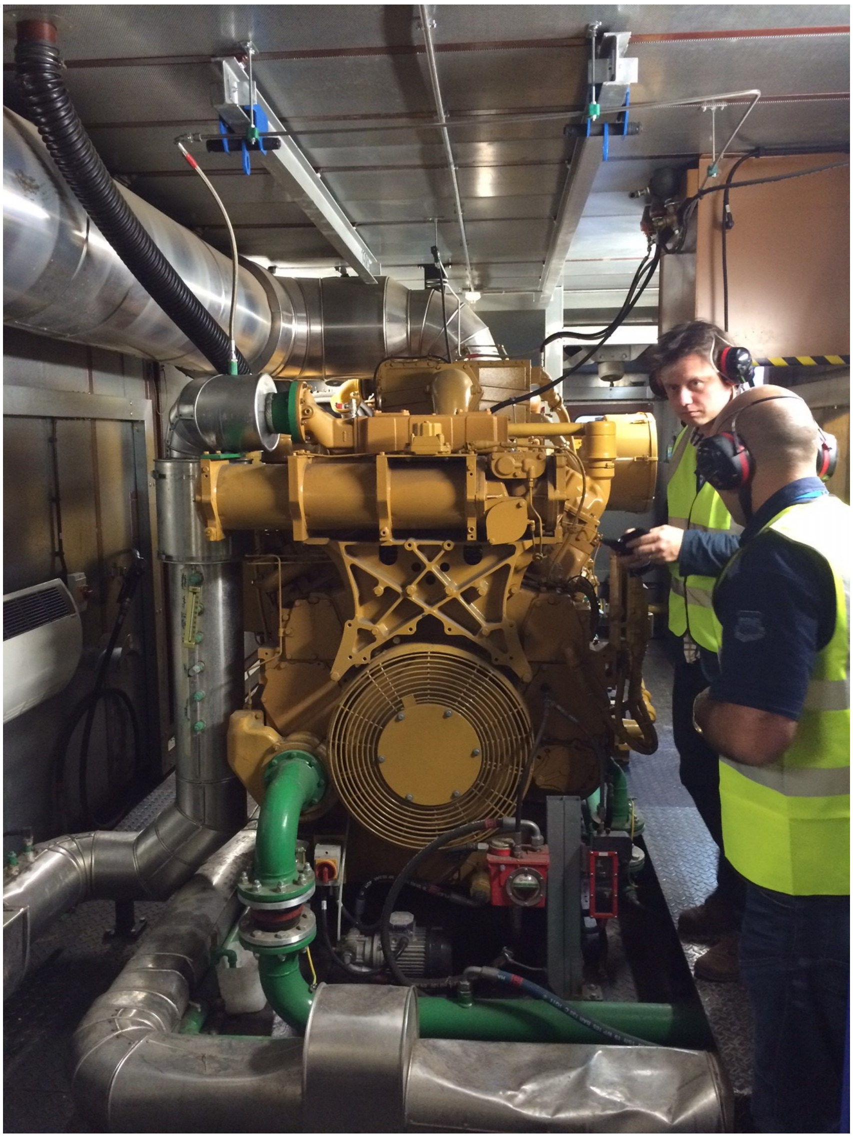

Figure A.5: Byker heat station Caterpillar CHP engine water, and III) mixing of combustion products with the environment.

Part I — Combustion

The reference condition for the analysis is defined as 100 kg of methane gas entering the boiler along with an amount of air required for complete combustion, and an unknown amount of excess air. The excess air amount used in the Byker plant boiler is unknown and thus must be estimated. The precise value for excess air present in the real boiler depends on its application, design, age and loading, but case studies by Pedersen [187] and Carpenter *et al.* [188] give values of anything from 16% to 115% excess air, while other literature by Biarnes [189] and Che *et al.* [190] suggest that the ideal amount of excess air should be 5% to 10%. In this study a low-realistic excess air value of 30% will be assumed. Using the terminology in [48], the temperature of the combustion products is found from the energy balance

$$m_f(\mathrm{NCV})^0 = (\theta_2 - \theta^0)\sum_k n_k \tilde{c}^h_{p,k} \tag{A.1}$$

where m_f is the mass of methane, $(\mathrm{NCV})^0$ is the per-kg lower heating value of methane, θ_2 is the temperature of the combustion products, θ^0 is the initial temperature of the fuel and air, n_k is the number of moles of product k, and $\tilde{c}^h_{p,k}$ is the mean (molar) specific heat for enthalpy of product k.

The combustion equation for the boiler assuming stoichiometric combustion with 30% excess air is

$$\mathrm{CH_4} + 2.6\,(\mathrm{O_2} + 3.76\,\mathrm{N_2}) \longrightarrow \mathrm{CO_2} + 2\,\mathrm{H_2O} + 0.6\,\mathrm{O_2} + 9.776\,\mathrm{N_2}$$

or

$$\mathrm{CH_4} + 2\,\mathrm{O_2} + 0.6\,\mathrm{O_2} + 9.776\,\mathrm{N_2} \longrightarrow \mathrm{CO_2} + 2\,\mathrm{H_2O} + 0.6\,\mathrm{O_2} + 9.776\,\mathrm{N_2} \tag{A.2}$$

which results in a molar and mass breakdown of the reaction as shown in Table A.1. Because the mean specific heat and the final temperature of the combustion products are

Substance	CH_4	O_2	N_2	$\longrightarrow$	CO_2	H_2O	O_2	N_2
Moles in reaction	1	2.6	9.776		1	2	0.6	9.776
Molar mass	16	32	28		44	18	32	28
kmol / 100 kg fuel	6.25	16.25	61.1		6.25	12.5	3.75	61.1
Mass (kg) in reaction	100	520	1710.8		275	225	120	1710.8

Table A.1: Byker gas boiler combustion reaction

both unknown and depend on each other, they can be found from the energy balance equation Equation A.1 using an iterative method. From an initial guess of $\theta_2^0 = 2000\,°\mathrm{C}$ the iteration shown in Table A.2 is obtained. Values for $\tilde{c}^h_{p,k}$ are taken from Table D.1

given by Kotas [48]. After four iterations the temperature of the combustion products has converged to an acceptable tolerance, and thus $\theta_2 = 1694\,°\mathrm{C}$.

Part II — Heat transfer

During the heat transfer process, the combustion products cool, transferring their heat to the water. The exact temperature of the products is unknown therefore it will be assumed to be $150\,°\mathrm{C} = \theta_3$; this is an average flue gas temperature suggested in [191] for industrial boilers without condensation heat recovery, which we assume applied to this particular boiler. Table A.3 gives the properties of the combustion products from which the energy transferred can be calculated. There are two cases to be considered:

Case A: The heating loop water is pre-heated to 100 °C by the CHP engine, and is then subsequently heated from 100 °C to 130 °C by the gas boiler. The water enthalpies at these temperatures are

$$h_{f@100\,°\mathrm{C}} = 419.10\,\mathrm{kJ/kg}$$
$$h_{f@130\,°\mathrm{C}} = 546.34\,\mathrm{kJ/kg}$$

The total enthalpy of the products at the start of the heat transfer process, H_2 is

$$\begin{aligned} H_2 &= \tilde{c}_p^h(\theta_2 - \theta_1) = 2966.57(1694 - 25) \\ &= 4,951,199\,\mathrm{kJ} \end{aligned}$$

and thus the mass of water that can be heated from 100 °C to 130 °C using 100 kg of methane is

$$\begin{aligned} m_w &= \frac{4,951,199 - 322,677}{546.34 - 419.10} \\ &= 36,376\,\mathrm{kg} \end{aligned}$$

Iteration 1				
$\theta_2 = 2000\,°C$	Products			
	CO_2	H_2O	O_2	N_2
$\tilde{c}_p^h$ (kJ / kmol K)	54.89	42.67	34.88	33.46
n (kmol)	6.25	12.5	3.75	61.1
$n\tilde{c}_p^h$ (kJ / K)	343.1	533.4	130.8	2044.4
$\sum_k n_k \tilde{c}_{p,k}^h = 3051.66$ kJ/K				
$\theta_2' = 25 + \frac{100\times50\times10^3}{3051.66} = 1663.50\,°C$				

Iteration 2				
$\theta_2 = 1663.50\ \ °C$	Products			
	CO_2	H_2O	O_2	N_2
$\tilde{c}_p^h$ (kJ / kmol K)	53.70	41.28	34.50	32.90
n (kmol)	6.25	12.5	3.75	61.1
$n\tilde{c}_p^h$ (kJ / K)	335.65	515.99	129.36	2010.00
$\sum_k n_k \tilde{c}_{p,k}^h = 2991.00$ kJ/K				
$\theta_2' = 25 + \frac{100\times50\times10^3}{2991.00} = 1696.68\,°C$				

Iteration 3				
$\theta_2 = 1696.68\,°C$	Products			
	CO_2	H_2O	O_2	N_2
$\tilde{c}_p^h$ (kJ / kmol K)	53.83	41.42	34.54	32.96
n (kmol)	6.25	12.5	3.75	61.1
$n\tilde{c}_p^h$ (kJ / K)	336.4	517.7	129.5	2013.6
$\sum_k n_k \tilde{c}_{p,k}^h = 2997.20$ kJ/K				
$\theta_2' = 25 + \frac{100\times50\times10^3}{2997.20} = 1693.2\,°C$				

Iteration 4				
$\theta_2 = 1693.2\,°C$	Products			
	CO_2	H_2O	O_2	N_2
$\tilde{c}_p^h$ (kJ / kmol K)	53.82	41.40	34.53	32.95
n (kmol)	6.25	12.5	3.75	61.1
$n\tilde{c}_p^h$ (kJ / K)	336.4	517.5	129.5	2013.2
$\sum_k n_k \tilde{c}_{p,k}^h = 2996.57$ kJ/K				
$\theta_2' = 25 + \frac{100\times50\times10^3}{2996.57} = 1693.6\,°C$				

Table A.2: Calculation of combustion temperature

$\theta_3 = 150\,°C$	CO_2	H_2O	O_2	N_2
$\tilde{c}_p^h$ (kJ / kmol K)	40.46	33.64	28.81	29.46
n (kmol)	6.25	12.5	3.75	61.1
$\sum_k n_k \tilde{c}_{p,k}^h = 2581.42$ kJ/K				
$H_3 = (\theta_3 - \theta^0) \sum_k n_k \tilde{c}_{p,k}^h$				
$= (150 - 25) \cdot 2581.42 = 322,677\,\text{kJ}$				

Table A.3: Boiler combustion products

Using the system efficiency equations, the energy and exergy efficiencies can be calculated as

$$
\begin{aligned}
\eta_{comb} &= \frac{m_w(h_2 - h_1)}{m_f(\text{NCV})^0} \\
&= \frac{36,376 \cdot (546.34 - 419.10)}{100 \cdot 50 \times 10^3} \\
&= 0.926 \\
\psi &= \frac{\eta_{comb}}{\phi}\left[1 - \frac{T_0(s_2 - s_1)}{h_2 - h_1}\right] \\
&= \frac{0.926}{1.04}\left[1 - \frac{298(1.635 - 1.307)}{546.34 - 419.10}\right] \\
&= 0.206
\end{aligned}
$$

Case B: The CHP plant is switched off and the boiler heats the loop water from 80 °C to 130 °C. The water enthalpies at these temperatures are

$$
\begin{aligned}
h_{f@80\,^{\circ}\text{C}} &= 334.95\,\text{kJ/kg} \\
h_{f@130\,^{\circ}\text{C}} &= 546.34\,\text{kJ/kg}
\end{aligned}
$$

The total enthalpy of the products at the start of the heat transfer process, H_2 is the same as above, i.e. $H_2 = 4,951,199$kJ. Thus the mass of water that can be heated from 80 °C to 130 °C using 100 kg of methane is

$$
\begin{aligned}
m_w &= \frac{4,951,199 - 322,677}{546.34 - 334.95} \\
&= 21,896\,\text{kg}
\end{aligned}
$$

Again using the system efficiency equations, the energy and exergy efficiency values are found to be

$$
\begin{aligned}
\eta_{comb} &= \frac{21,896 \cdot (546.34 - 334.95)}{100 \cdot 50 \times 10^3} \\
&= 0.926 \\
\psi &= \frac{0.926}{1.04}\left[1 - \frac{298(1.635 - 1.075)}{546.34 - 334.95}\right] \\
&= 0.187
\end{aligned}
$$

The energy efficiency is the same in both cases — this is evident because for adiabatic combustion and heat transfer no energy is lost except to the boiler flue. However there a slight (approximately 2%) decline in the rational (exergy) efficiency of the boiler can be observed as the temperature differential between the heating loop inlet and outlet

LOAD	100%	75%	50%
Power In (LHV fuel) (kW)	3333	2569	1817
Electrical Power Out (kW)	1090.7	817.6	545.3
Thermal Power Out (kW)	1623	1305	1001
Electrical Efficiency η_e	32.7	31.8	30.0
Thermal Efficiency η_h	48.7	50.8	55.1

Table A.4: G3516 power input and output vs loading

increases by 20 °C.

A.1.3 CHP unit

The plant uses a CHP unit to co-produce electrical power and heat for the estate. The CHP unit is a Caterpillar G3516A, which is a 16-cylinder 4-stroke spark ignition engine burning natural gas and co-producing 1 MWe and 1 MWt (see Figure A.5[2]). The engine has a compression ratio of 11:1 and a per-cylinder displacement of 69 litres. The attached generator is driven at 1500 rpm (geared to a 50 Hz generator output) and connects to the external electrical network at 3-phase 400 V. Heat generation comes from water circulated under pressure through the engine jacket and also through a heat exchanger surrounding the engine exhaust; the primary function of the cooling circuit is to dissipate heat from the engine and thus the cooling circuit also features a thermal dump load in the shape of an outside-air fan-cooled heat exchanger.

No measured performance data were available for the device, but accessible manufacturer's technical data for a similar engine, the G3516LE, were used to model the engine's performance under various loads, which is shown in Table A.4 [192]. The values in Table A.4 can be used to estimate the exergy efficiency of the CHP engine for the three load cases. Using data taken from plant control system readings, the CHP cooling loop water cools from approximately 110 °C to 90 °C, while heating the incoming heating loop water from 80 °C to 100 °C (corresponding to Case A in the previous section). It is assumed that no heat is otherwise lost from the heat exchanger. In the following, the subscript CW refers to the CHP cooling water, and the subscript LW to the district heating loop water.

100% Load During heat exchange 1623 kW of heat transfers from the CHP cooling loop to the district heating loop.

$$\dot{E}_{\mathrm{LW}} = \dot{m}_{\mathrm{LW}} \left[\left(h_{@100\,^\circ\mathrm{C}} - h_{@80\,^\circ\mathrm{C}} \right) - T^0 \left(s_{@100\,^\circ\mathrm{C}} - s_{@80\,^\circ\mathrm{C}} \right) \right]$$
$$\dot{E}_{\mathrm{LW}} = \dot{m}_{\mathrm{LW}} \times 15.014\,\mathrm{kJ/kg}$$

but also

$$\dot{m}_{\mathrm{CW}} \left(h_{\mathrm{CW}_2} - h_{\mathrm{CW}_1} \right) = -\dot{m}_{\mathrm{LW}} \left(h_{\mathrm{LW}_2} - h_{\mathrm{LW}_1} \right),$$

[2]Photograph courtesy and by permission of Geoff Wallman

so

$$\frac{\dot{m}_{\text{LW}}}{\dot{m}_{\text{CW}}} = -\frac{(h_{@90\,^\circ\text{C}} - h_{@110\,^\circ\text{C}})}{(h_{@100\,^\circ\text{C}} - h_{@80\,^\circ\text{C}})} = 1.003$$

But also $-\dot{Q} = (h_{\text{CW}_2} - h_{\text{CW}_1})\,\dot{m}_{\text{CW}}$, so

$$\dot{m}_{\text{CW}} = \frac{-1.623 \times 10^6}{(376.97 - 461.36) \times 10^3} = 19.23\,\text{kg/s}$$
$$\dot{m}_{\text{LW}} = 19.17\,\text{kg/s}$$

The overall system exergy input is 3466 kW, and the exergy output from the engine is

$$\dot{E}_{\text{LW}} = 19.17\,\text{kg/s} \times 15.014\,\text{kJ/kg}$$
$$= 287.9\,\text{kW}$$

Hence the rational (exergetic) efficiency at 100% load is

$$\psi_h = 287.9/3466 = 0.083$$
$$\psi_e = 1090/3466 = 0.314$$

75% Load Similarly to before,

$$\dot{m}_{\text{CW}} = \frac{-1.305 \times 10^6}{(376.97 - 461.36) \times 10^3} = 15.46\,\text{kg/s}$$
$$\dot{m}_{\text{LW}} = 15.41\,\text{kg/s}$$

And so

$$\dot{E}_{\text{LW}} = 15.41\,\text{kg/s} \times 15.014\,\text{kJ/kg}$$
$$= 231.36\,\text{kW}$$

Hence the rational (exergetic) efficiency at 75% load (2672 kW exergy input) is

$$\psi_h = 231.36/2672 = 0.087$$
$$\psi_e = 817/2672 = 0.306$$

50% Load Finally,

$$\dot{m}_{\text{CW}} = \frac{-1.001 \times 10^6}{(376.97 - 461.36) \times 10^3} = 11.86\,\text{kg/s}$$
$$\dot{m}_{\text{LW}} = 11.83\,\text{kg/s}$$

And so

$$\begin{aligned}\dot{E}_{\mathrm{LW}} &= 11.83\,\mathrm{kg/s} \times 15.014\,\mathrm{kJ/kg} \\ &= 177.56\,\mathrm{kW}\end{aligned}$$

Hence the rational (exergetic) efficiency at 50% load (1890 kW exergy input) is

$$\begin{aligned}\psi_h &= 177.56/1890 = 0.094 \\ \psi_e &= 545/1890 = 0.288\end{aligned}$$