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Highly integrated urban energy, water and waste systems

Thomas Ravalde

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Declaration of originality

I declare that this thesis is my own work, and that the work of others is appropriately referenced and acknowledged.

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Abstract

Urbanisation continues to bring socioeconomic well-being to an ever-growing global urban population. Nevertheless, there is an environmental and economic imperative for cities to use resources more sustainably. One way to achieve this is to take advantage of the fact that, in cities, resource management infrastructure from the energy, water and waste sectors is co-located, such that the wastes and by-products from one process can become the inputs to another (for example, sending organic waste to anaerobic digestion to produce biogas for energy generation). This thesis provides planners and policy makers with means to begin realising these intersectoral synergies, through contributions to the field of urban metabolism. First, a conceptual model is developed which can describe how a city's mix of processes affect its metabolism. Second, methods are needed which quantify how well different sectors work together to make an area's metabolism more efficient; to that end, analysis on historic urban resource flows show the usefulness of exergy analysis and ecological network analysis. Third, data is required which shows the possibilities for one process's wastes to become another's inputs; for this, a database is assembled which records the resource consumption and production of 202 types of urban resource management process, and made available under an open-source public license. Fourth, the Processes, Resource and Qualities (PRaQ) model is developed; PRaQ is a mixed-integer linear programme which simultaneously chooses the mix of energy, water and waste management processes an area could use to minimise an objective (emissions, for example), thereby taking into account intersectoral synergies. The formulation is made available as a benchmarking study to facilitate future development of the model. Applying PRaQ to a new urban development in China shows how an area's urban metabolism can be made measurably more efficient according to various metrics. In summary, this work advances the urban metabolism concept for its application to improving urban resource sustainability, by showing how a city's mix of process affects its overall metabolic flows.

Publications arising from this work

Research presented in this thesis has been published in the following papers:

- Ravalde, T. and Keirstead, J. (2015). Integrated Resource Planning for a Chinese Urban Development. In *International Symposium for Next Generation Infrastructure Conference (ISNGI 2014)*, pages 59–62. UCL STEaPP.
- Ravalde, T. and Keirstead, J. (2015a). A database to facilitate a process-oriented approach to urban metabolism. *Journal of Industrial Ecology*, 21(2):282–293.
- Ravalde, T. and Keirstead, J. (2015b). Comparing performance metrics for multi-resource systems: The case of urban metabolism. *Journal of Cleaner Production*, 163:S241–S253.

Work done by the candidate

The work (literature review, analysis, modelling and coding, summarisation of results and discussion) presented in this thesis has been carried out by the candidate unless otherwise stated. Dr Nouri Samsatli shared the GAMS code for the model described in Samsatli et al. and Keirstead (2013), on which the Null model of Chapter 5 was based, and thus Dr Samsatli's code provided inspiration for the encoding and architecture of code written for this thesis, though new code was developed by the candidate for the models. An initial mathematical formulation for attributing 'qualities' to resources in the PRaQ model was proposed by Dr James Keirstead (Section 5.3.2). The published papers were written by the candidate, but benefited from feedback and proof-reading by the co-author, Dr Keirstead.

Resources arising from this work

Where possible, I have made this work publicly available as open-source, in the spirit of helping others use, and build-upon the findings here. The work of this thesis has provided two tools to the urban metabolism research community:

- The first is a database of processes which manage energy, water and waste in urban areas, recording the relative quantities of energy, water and waste resources these processes consume and produce. This is introduced in Chapter 4 and Ravalde and Keirstead (2017a). The database is available at <https://github.com/tomravalde/urban-metabolism-process-database>.
- The second tool is a ‘benchmark problem’, which was used to test various possible formulations of the model this thesis develops. This is introduced in Chapter 5 and is available at <https://github.com/tomravalde/model-development-code>. This enables others to test their own developments of the model on the same test problem which was used to develop the model in this thesis.

For the sake of transparency, I have also made available:

- The code for the case study to which the model was applied in Chapter 6. This can be found at <https://github.com/tomravalde/shann-gu-case-study>.
- The source of the thesis itself. This thesis has been written using R-markdown¹, which means that embedded within the text of the thesis is all the R-code used to manipulate and/or visualise any data which forms part of this thesis. The thesis source is available at <https://github.com/tomravalde/thesis>.

¹An The knitr R-package (Xie, 2018) converts the R-markdown source (i.e. an `*.Rmd` file) into a markdown file (i.e. `*.md`, Gruber (2018)). A programme called pandoc – see MacFarlane (2017) then converts this to a $\text{\TeX}$ file (`*.tex`), which is converted into this PDF via the $\text{\LaTeX}$ document preparation system. Keiran Healy has made a well-argued justification for this type of workflow, as well as a helpful explanation of how to set it up (Healy, 2017).

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Abbreviations, acronyms, symbols, units of measurement, and other notation

Acronyms

DP	Database Process
PC	Process Category
CO ₂	Carbon dioxide
CF	Carbon footprint
CHP	Combined heat and power
CSV	Comma Separated Value
EF	Ecological footprint
EIP	Eco-industrial park
ENA	Ecological network analysis
GA	Genetic Algorithm
GAMS	General Algebraic Modelling System
GDP	Gross domestic product
GHG	Greenhouse gases
GIS	Geographic Information System
HUGO	Human Genome Organisation

IDSA	Industrial Designers Society of America
IE	Industrial ecology
IEA	International Energy Agency
IS	Industrial symbiosis
LB	Lower Bound
LP	Linear programme
MILP	Mixed-integer linear programme
MINLP	Mixed-integer nonlinear programme
MR	Multi-resource
M RTP	Multi-resource trade-off problem
NEI	Nuclear Energy Institute
NL	The Nonlinear model (Chapter 5)
NLP	Nonlinear programme
OECD	Organisation for Economic Co-operation and Development
PRaQ	The Processes, Resources and Qualities model
RTN	Resource-technology network
SPC	Shann Gu Power Company
STN	State-task network
UB	Upper Bound
UM	Urban metabolism
US EPA	United States Environmental Protection Agency
USD	United States Dollar
WF	Water footprint

YAML Yaml Ain't Markup Language

Units of measurement

J Joule

kg Kilogram

MJ Megajoule

MW Megawatt

s Second

Symbols used in Bettencourt et. al's model of urban growth

β An exponent constant which quantifies how a variable in a city (e.g. GDP), $Y(t)$, grows with time

E Resource quantity required to sustain a new inhabitant of a city

$N(t)$ Population of a city at time, t

R Resource quantity required to sustain an individual in a city

t Time (e.g. a year)

t_c The critical time at which the population of a knowledge-based city tends to infinity

$Y(t)$ A quantity in a city (e.g. GDP or length of electrical cables) at time, t

Y_0 A normalisation constant which describes how a quantity in a city (e.g GDP), $Y(t)$, grows with time, t

Symbols used to define black- and grey-box metrics

α Generic term for the absolute measure of a multi-resource system's performance

α_{ex}^{in} The total exergy entering a system

α_{ex}^{prod} The total exergetic products of a system

η Generic term for the efficiency measure of a multi-resource system's performance

η^{ex} The exergy efficiency of a system

η_1	Generic term for the efficiency measure of a multi-resource system's performance, with respect to a single resource type
η_2	Generic term for the efficiency measure of a multi-resource system's performance, as the ratio of two resource types
η_3	Generic term for the efficiency measure of a multi-resource system's performance, as the ratio of a resource type relative to a baseline
Ex^{in}	Exergetic value of inputs to a process
Ex^{irrev}	Exergetic value of a process's irreversibilities
Ex^{prod}	Exergetic value of products of a process
Ex^{waste}	Exergetic value of wastes from a process
i	Indexes a system input resource
j	Indexes a system output resource
k, k'	Generic constant which can be added to the weighted sum of inputs and outputs
N	Number of resources flowing into and out of a system
$p \in P$	Indexes a conversion process (e.g. a power plant)
$r_i \in R$	Resource flow quantity (e.g. coal) into a system
$r'_j \in R'$	Resource flow quantity (e.g. heat) out of a system
w	Weighting applied to an input resource flow (e.g. to quantify the carbon emissions associated with coal)
w'	Weighting applied to an output resource flow

Model sets

$\tau \in \mathcal{T}$	Transport processes
$p \in P$	Conversion processes
$q \in Q$	Qualities attributed to resources (PRaQ model only)

$r \in R$	Resources
$t \in T$	Time periods
$z, z' \in Z$	Zones; the z' is used to denote the destination zone, when a resource is being transported from zone z to zone z'
$zz' \in nb$	Pairs of zones which neighbour one another (and hence can be connected by transport technologies)

Model variables and parameters, defined over the sets

δ_{rz}^E	Binary variable defining whether zone z is allowed to export resource r
δ_{rz}^I	Binary variable defining whether zone z is allowed to import resource r
δ_{prq}^P	Binary variable defining whether quality q is attributed to resource r and can be converted by process p
δ_{rq}^R	Binary variable defining whether quality q is attributed to resource r
$\delta_{\tau zz'}^T$	Binary variable defining whether transport technology τ exists between zones z and z'
$\delta_{\tau rq}^\tau$	Binary variable defining whether quality q is attributed to resource r and can be transported by transport process τ
ϵ_r	Emissions factor for resource r
γ^P	Weighting factor assigned to system conversion process costs
γ^R	Weighting factor assigned to system resource costs
γ^T	Weighting factor assigned to system transport process costs
κ_{pr}^I	Input of resource r to conversion process p
κ_{pr}^O	Output of resource r from conversion process p
$\mathcal{S}_t$	The length of time of period t
S_t	Length of time period t
A_p^P	Spatial footprint (area) of conversion process p

A_z^Z	Area of zone z
C	Overall system cost
C^T	Cost of all transport processes used by a system
C^P	Cost of all conversion processes used by a system
c_p^P	Cost of conversion process p
C^R	Cost of all resources used by a system
c_r^R	Cost of resource r
c_t^T	Cost of transport process t
$D_{rqz}^{(qual)}$	Demand for resource quality q attributed to resource r in zone z
D_{rz}	Demand for resource r in zone z
E_r^{max}	Maximum allowable exports of resource r
E_r^{min}	Minimum allowable exports of resource r
E_{rz}	Exports of resource r out of zone z
F_{pz}^P	Operation rate of conversion process p in zone z
$F_{\tau}^{T,max}$	Maximum allowable operation rate of transport process τ
$F_{\tau}^{T,min}$	Minimum allowable operation rate of transport process τ
$F_{\tau z'z}^T$	Operation rate of transport process τ between zones z and z'
$F_p^{P,max}$	Maximum allowable operation rate of conversion process p
$G_{prz}^{(qty)}$	Net production of resource quantity r in zone z by process technology p
$G_{prqz}^{(qual)}$	Net production of quality q attributed to resource r in zone z by process technology p
G_{prz}	Net production of resource r in zone z by process technology p
I_r^{max}	Maximum allowable imports of resource r
I_r^{min}	Minimum allowable imports of resource r

I_{rz}	Imports of resource r into zone z
$J_{\tau rz}^{(qty)}$	Net transfer of resource quantity r into zone z by transport technology τ
$J_{\tau rz}^{(qual)}$	Net transfer of resource quality q attributed to resource r into zone z by transport technology τ
$J_{\tau r z}$	Net transfer of resource r into zone z by transport technology τ
k_{pr}^P	Net production of quality q attributed to resource r from conversion process p
k_{pr}^P	Net production of resource r from conversion process p
$k_{\tau r}^{\alpha'}$	Quantity of resource r leaving transport technology τ , which does not depend on the length of distance the resource will travel
$k_{\tau r}^{\alpha}$	Quantity of resource r entering transport technology τ , which does not depend on the length of distance the resource will travel
$k_{\tau r}^{\beta'}$	Quantity of resource r leaving transport technology τ , which depends on the length of distance the resource will travel
$k_{\tau r}^{\beta}$	Quantity of resource r entering transport technology τ , which depends on the length of distance the resource will travel
$l_{zz'}$	Distance between zones z and z'
N_r^E	Maximum number of zones which are allowed to export resource r
N_r^I	Maximum number of zones which are allowed to import resource r
N_{pz}^P	Number of conversion processes p allocated to zone z
X_{rq}	Defines the quantities of all qualities q attributed to a unit of resource r

Tat model abbreviations – resources

CO ₂	Carbon dioxide
App. use	Domestic appliance use
BM (med)	Biomass (medium water content)
BM (wet)	Biomass (high water content)

El.	Electricity
F. Feed	Fish feed
Fish	Fish
Fish (c)	Fish (cooked)
G. man.	Green manure
H	Heat (domestic)
HW	Hot water
Man.	Manure
Meat	Meat
Meat (c)	Meat (cooked)
Pet.	Petrol
Veg (c)	Veg (cooked)
Veg.	Vegetables
W	Water (for various uses: in a dam, livestock, domestic use, irrigation, pumping)
WW	Wastewater (for various uses: from livestock cleaning, domestic

Tat model abbreviations – conversion processes

Agric.	Agriculture
Agric. Mach.	Agricultural machinery
App.	Domestic appliances
Aqua	Aquaculture
BMD (med.)	Biomass drying (medium moisture content)
BMD (wet)	Biomass drying (high moisture content)
Cook.	Cooking

Dam	Dam
Heat.	Heating
Irrig.	Irrigation
L/stock	Livestock
Pump	Pump
Stove	Stove
WH	Water heating
WT (dom.)	Water treatment (for domestic use)
WT (l/stock)	Water treatment (for livestock)

Tat model abbreviations – transport processes

Cab.	Cable
P (dom.)	Pipe (for domestic water).
P (irrig.)	Pipe (for irrigation water).
P (l/stock)	Pipe (for livestock water).
V (f/feed)	Vehicle (for fish feed)
V (f/wood.)	Vehicle (for firewood)
V (fish)	Vehicle (for fish)
V (g/man.)	Vehicle (for green manure)
V (man.)	Vehicle (for manure)
V (meat)	Vehicle (for meat)
V (pet.)	Vehicle (for petrol)
V (veg.)	Vehicle (for vegetables)

Other

g Acceleration due to gravity

h Height

M Mass

Chapter 1

Introduction

“Cities are the crucible of human civilization, the drivers towards potential disaster, and the source of the solution to humanity’s problems.”

Bettencourt and West (2010), *Nature*

“**system**, n. An organized or connected group of things ...A group or set of related or associated things perceived or thought of as a unity or complex whole.”

Oxford English Dictionary (2016b)

Urbanisation has brought a high quality of life to billions of people. In cities, labour, business, infrastructure and local government all come together in geographical proximity, to enable the efficient provision of goods and services to their citizens, with the result that while being home to over 50 per cent of the global population, cities generate around 80 per cent of global GDP (The World Bank, 2015). Thus with growth in the global urban population, more and more people can have access to greater wealth, improved healthcare, and other socioeconomic and cultural benefits (The World Bank, 2004). However, cities face many challenges, and questions about how they should be developed, governed, and organised, are increasingly important. In amongst these challenges – providing suitable transport links, preventing the spread of infectious diseases, and reducing air pollution to name just three – this

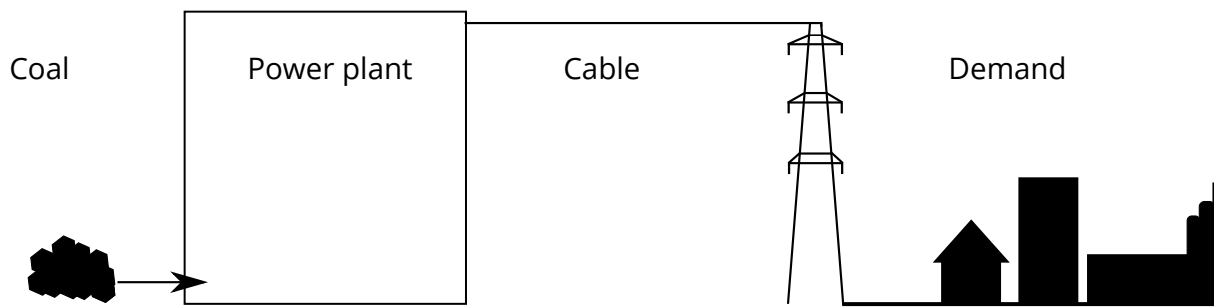


Figure 1.1: Some components of an urban electricity system. The combustion of coal results in heat energy, which heats water and thereby produces steam which rotates a turbine to generate electricity. The electricity is then delivered to the consumer via a cable.

thesis takes up one challenge in particular, namely, how cities could support their populations sustainably with vital resource management services. As will be argued later, this is important in order to address the economic and environmental challenges cities face (Section 1.1).

More specifically, this thesis will focus on how integrating the management of energy, water, and waste sectors can enable cities to support their populations more sustainably. In addressing the challenges of urban resource management, there are many complementary approaches which planners and policy makers might take. Consider a city whose electricity is partly supplied by a coal-fuelled power plant, which is trying to reduce its coal consumption (Figure 1.1). One possible intervention is to encourage consumers to use less electricity. Another option is to increase power plant efficiencies, so as to minimise energy losses within the plant. Alternatively, the power plant could be replaced by technologies which use renewable resources (e.g. solar). While interventions such as these have their place, this thesis will take a broader perspective to examine how resource management works as a whole. Is the overall mix of power plants, water treatment facilities, waste management procedures, and other activities, the most efficient way to manage resources?

In meeting consumer demand for electricity, the coal, power plant, electricity, and power lines are only a few of the components which comprise the network of infrastructure used to manage a city's electricity. This network could include other energy sources (renewable and non-renewable), at various scales (large centralised power plants at one extreme, and small distributed microgeneration units at the other), all of which work in combination to meet electricity demand at the point of need at any moment in time. In other words, a city's electricity supply is an example of a 'system' as defined in the epigraph which opened this chapter. Furthermore, the electricity system is just one part of a larger

system which manages a city's energy, and this system is in turn just one of several systems at work in a city; others include water management, waste management, buildings and transport. The energy, water and waste sectors are connected in various ways (for example, through the use of cooling water in power plants, or the consumption of energy by waste management services). This means that the design and operation of one sector will have impacts on the others¹. This thesis considers how systems for the energy, water and waste sectors – traditionally considered separately – could work together. In other words, how can the design and operation of the 'system-of-systems' in urban areas benefit urban resource management? What is interesting about this work is that it is the very nature of a city which presents this possibility – that fact that infrastructure is geographically co-located means that the different sectors can be managed in an integrated fashion.

1.1 Urbanisation: the challenges

Before considering the economic and environmental challenges of urban resource management, it is important to note that global urbanisation is a trend that expected to continue, and any solutions to these challenges cannot ignore this reality. At present, urban areas are home to just over half of the global population (United Nations Department of Economic and Social Affairs, 2014). By 2030, this figure is expected to grow to 60 per cent, and to over 65 per cent by 2050 (Figure 1.2). This growth has three components: cities absorbing population growth; migration from rural areas; and the reclassification of rural areas as urban (Cohen, 2006).

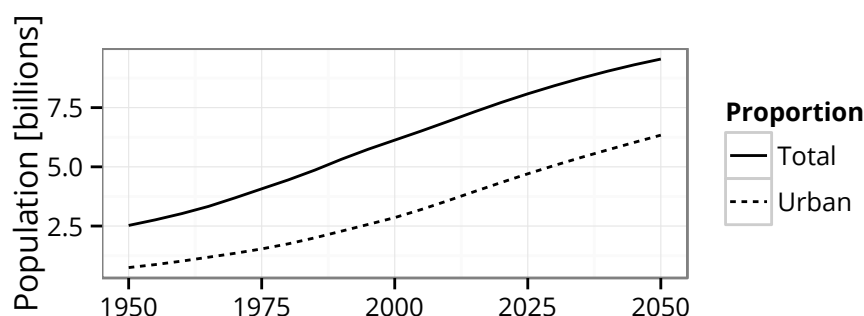


Figure 1.2: Global population between 1950 and 2014, and forecasts up to 2050, according to the United Nations Department of Economic and Social Affairs (2014).

The inevitability of urbanisation derives from its desirability. Urbanisation is the long-term result

¹These ideas are explored more in Sections 1.1.1 and 1.2.1

of humanity's search for the good life, causing people to migrate from the countryside in search of employment, as well as improved access to education, healthcare, and other services. Thus an urban population grows. As it does, firms benefit from economies of scale, and at the same time, cities start to become 'agglomeration economies' (in which different types of firms and industries benefit one another by supplying each other with goods and services, on account of their proximity to one another). With scale and agglomeration, cities can specialise in the goods and services they provide. These goods and services can then be traded with others outside the city; this increases prosperity, which in turn attracts migrants. Thus urbanisation becomes a virtuous cycle in which city size and economic growth feed one another (Figure 1.3) (The World Bank, 2004).

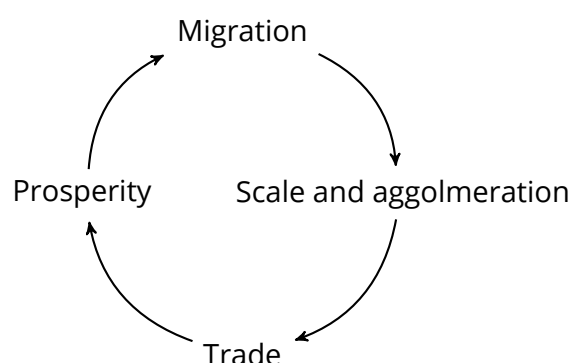


Figure 1.3: Virtuous circle of urban growth and economic prosperity.

Urbanisation is a proven path to prosperity, so it is unsurprising that expert opinion reveals little appetite to oppose it, especially now that the urbanisation patterns seen historically in OECD countries are being replicated in the developing world, where the majority of growth is happening – Africa and Asia will together account for over 85 per cent of the increase in urban dwellers by 2050 (United Nations, 2011). This is not to say that cities provide an immediate solution to all issues of poverty. Cities often have a widespread presence of slums, especially at the beginning of their development. The World Bank describes these as 'growing pains' and notes their historical precedence in cities like London, where slums are no longer to be found (The World Bank, 2004, p.69). All this is to say, that whatever mix of approaches is used to address the challenges of urban resource management (outlined in the following two sections) should assume that urbanisation will continue.

1.1.1 Environmental challenges

The environment is a huge field of study, and to summarise all negative environmental effects arising from the way that cities use resources would be impossible. However, just a few examples build a compelling case that levels of resource use by urban areas is problematic enough to warrant attention from researches, planners, and policy makers. To give some sense of order to the environmental challenges, they will be listed in relation to the resource ‘sectors’ which cause them, first as problems which are manifestations of a specific sector, and second as problems which emerge from the interactions of two or more sectors. This notion of sectors will become an important theme of the thesis².

Sectoral strains

Consider first the **energy** sector. Cities are home to just over 50 per cent of the global population, yet they are responsible for around 60 per cent of primary energy consumption, and over 70 per cent of energy-related greenhouse gas emissions IEA (2014). The disproportionately high energy consumption is driven mainly by the higher quality of life enjoyed by city dwellers relative to their rural counterparts (Grubler, 2009). This fact means cities should be playing a key role in the fight against climate change (C40 Cities, 2018).

In the **waste** sector, the primary issue is the volume of waste generated, which municipal governments need to deal with, even as disposal capacity is decreasing (Lu et al., 2009). With their higher quality of life, urban inhabitants consume more goods, and so produce more waste. Thus per-capita waste generation rates are higher in cities than in rural areas. As urbanisation continues, the World Bank estimates that total municipal solid waste could increase by 70 per cent between 2012 and 2025 (Alford et al., 2014). Waste also contributes to climate change – about five per cent of total greenhouse emissions come from waste, as the combined contributions of methane (from organic waste) and carbon dioxide (from incineration) (Alford et al., 2014). Other waste-related challenges include: flooding due to the blocking of drainage (Lamond et al., 2012), groundwater contamination (Li and Huang, 2006), and public health concerns (Kouamé et al., 2014) (especially from open landfill sites in developing countries) (Eurostat, 2015).

²The energy, waste, and water sectors have been chosen here since they will be considered throughout the rest of this thesis, for reasons given in the definition of ‘energy, water, and waste’ in Section 1.4.1. Other sectors not considered here could include transport and materials.

The **water** sector has also felt the strain of urbanisation: increases in affluence, and business and industrial activity, has increased per-capita rates of water consumption (Fry, 1978). Water stress (where the available water cannot meet all required uses) is commonplace – about half of the world’s cities with populations greater than 100,000 people are unable to replenish their water resources at the rate they use them (Richter et al., 2013). The effects of water stress may not be felt where they are caused, since the infrastructure use to treat and transport water is more easily afforded by the affluent, thus water stress is disproportionately suffered in the developing countries, which is also where most urbanisation is happening. Some large cities use water networks extending up to 200 kilometers into their surrounding area to meet demand, but for many urbanising regions, it is difficult to invest quickly enough to build the infrastructure to meet demand (European Environment Agency, 2016).

The meeting point of the above issues is climate change, which is arguably the greatest environmental threat of all (World Economic Forum, 2016). The energy and waste sectors are large contributors of greenhouse gas emissions, and climate change limits the availability of water in many places (Fry, 1978). However, not only do the energy, water and waste sectoral strains share a point of contact with climate change, they also interact with one another; in other words, demand in one sector can feed the problems of another. These ‘intersectoral interactions’ (introduced below, and summarised in Figure 1.4) exacerbate the environmental challenges of individual sectors.

Intersectoral interactions

First consider the interactions of the **energy and water** sectors. As demand for water increases, so do energy requirements for its treatment and distribution – it is estimated that approximately 35 per cent of the energy used by municipalities in the United States is for water supply and wastewater treatment (Elliott, 2005). In the other direction, these sectors interact through the need for cooling water – the more energy generated by power plants, the more cooling water that is required (McMahon and Price, 2011). Climate change serves only to intensify this energy-water nexus, because it limits the availability of water in many places, thus increasing energy requirements (e.g. to provide water via desalination and other energy-intensive treatment methods). This increased energy use further exacerbates climate change. Thus the energy-water intersectoral interactions create a self-perpetuating challenge. (Webber, 2011).

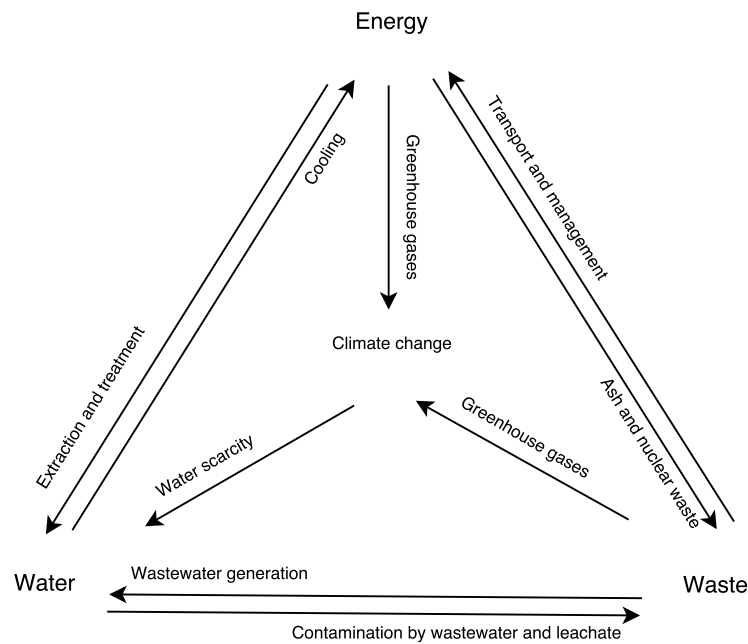


Figure 1.4: Summary of some environmental challenges arising from intersectoral interactions (GHGs = greenhouse gases).

The **energy and waste sectors** interact through the energy consumption needs of waste transportation and management processes (such as sorting, recycling, and crushing) (Institute of Civil Engineers, 2011; Alford et al., 2014). In the other direction, increased energy consumption increases waste output. To take one example: the amount of fly ash produced by coal plants in the United States is over half of the quantity of municipal solid waste³. A more specific challenge is that of dealing with the radioactive waste produced by nuclear power plants (NEI, 2008).

Finally, in the **water and waste** sectors, increased water consumption leads to a corresponding increase in wastewater generation which needs to be managed through either treatment or disposal (McMahon and Price, 2011). In the other direction, wastewater is often discharged into freshwater systems, thus contaminating them. While nature can purify and recycle contaminated water to some extent, contamination happens at a rate that nature cannot keep up with and so expensive (and energy intensive) treatments are required (Fry, 1978). Solid waste is also problematic in this regard as leachate contaminates groundwater and surface water sources (Alford et al., 2014).

³ Annual MSW generation as about 254 millions tons (Center For Sustainable Systems, 2014), and annual fly ash generation is about 130 million tons (Things Worse Than Nuclear Power, 2012).

1.1.2 Economic challenges

In addition to the environmental challenges outlined above, another sustainability challenge brought about by rates of urban resource consumption is that of economic stability. Bettencourt et al. (2007) have demonstrated that a city's socioeconomic attractiveness can cause its population to grow a rate that is impossible to sustain with the available resources. This fact is derived from two equations which model features of urban growth. First, at time t , quantities in cities $Y(t)$ (such as energy consumption or wealth), scale with population, $N(t)$, according to a power law:

$$Y(t) = Y_0 N(t)^\beta \quad (1.1)$$

where Y_0 is a normalisation constant, and β is a constant which corresponds to the measured quantity and city type under consideration. This is a well-known result, and is interesting in and of itself because it shows that cities of different sizes are, in essence, scaled versions of one another, and thus different cities do in fact operate in very similar ways⁴. This feature of cities makes it possible to predict many of its characteristics from just knowing its population.

The values which β take vary for different types of Y quantities (examples are given in Table 1.1. For material quantities (such as the number of petrol stations, or the length of electrical cable), $\beta < 1$; but for socioeconomic quantities (such as GDP, or the number of serious crimes), $\beta > 1$. In the former case, Y exhibits economies of scale, such that bigger cities can serve their cities more efficiently (e.g. the number of gas stations required does not need to increase as quickly as the population). In the latter case, Y exhibits increasing returns to scale (e.g. wealth increases more quickly than that population), because bigger cities benefit from the agglomeration effects of knowledge spillover and other social dynamics.

In a second equation of urban growth, population growth is related to the resources required to sustain it. If each individual requires some quantity of 'resources', R , to maintain them per unit time, and 'extra' resources, E , to accommodate a new member, then a city's total resource requirement, Y , is given by:

⁴In this way, cities are analogous to animals, whose physiological characteristics (e.g. metabolic rate) scale with its mass.

Table 1.1: Example β values taken from Table 1 of Bettencourt et al. (2007).

Y	β	Country-year
GDP	1.15	China 2002
GDP	1.26	EU 1999-2003
GDP	1.13	Germany 2003
Total electrical consumption	1.07	Germany 2002
Household electrical consumption	1.00	Germany 2002
Household electrical consumption	1.05	China 2002
Household water consumption	1.01	China 2002
Length of electrical cables	0.87	Germany 2002

$$Y(t) = RN(t) + E \frac{dN(t)}{dt} \quad (1.2)$$

The economic challenges that some cities face is shown by equating Equations 1.1 and 1.2, and solving for $N(t)$ ⁵. This solution, shows that a city's population can be driven by its socioeconomic properties (i.e. where $\beta > 1$) to grow at greater-than-exponential rates, with $N(t)$ theoretically reaching infinity after critical time, $t = t_c$ ⁶. However, unbounded growth assumes sufficient resources, R and E , to sustain it. In reality, these resources are limited, and thus Bettencourt's model predicts a collapse in population and an economic crash (Ledford, 2007).

The key to economic sustainability of urban economies therefore, is to prevent this collapse through innovation that can sustain this growth. In Bettencourt's model, this corresponds to resetting the values of Equation 1.1's parameters, before t_c is reached. However, t_c for each new cycle of innovation becomes shorter and shorter requiring innovation to take place at increasingly frequently (see Figure 1.5). This need for innovation to happen after ever-decreasing time intervals is consistent with historical movements between the Stone, Bronze, and Iron Ages, and the Computer, and Information and Digital Ages (Bettencourt and West, 2010), has been demonstrated using historical data from New York City (Bettencourt et al., 2007).

⁵This gives $N(t) = \left\{ \frac{Y_0}{R} + \left(N^{1-\beta}(0) - \frac{Y_0}{R} \right) \exp \left[-\frac{R}{E}(1-\beta)t \right] \right\}^{\frac{1}{1-\beta}}$

⁶Critical time is given by $t_c = -\frac{E}{(\beta-1)R} \ln \left[1 - \frac{R}{Y_0} N^{1-\beta}(0) \right] \approx \left[\frac{E}{(\beta-1)R} \right] \frac{1}{N^{\beta-1}(0)}$

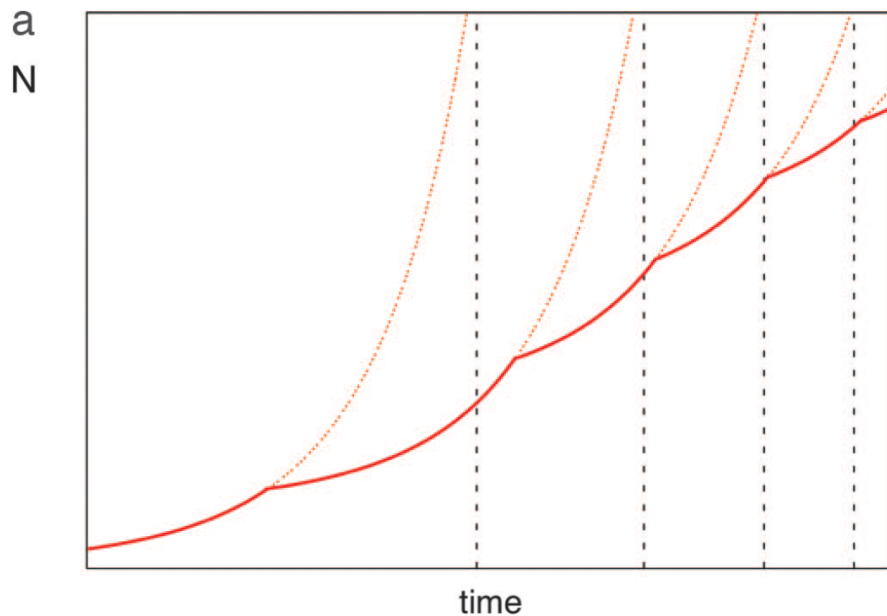


Figure 1.5: Population growth, and the cycles of innovation required to sustain it in agglomeration economies. Note how the critical time t_c reduces for each cycle. Figure copied directly from Bettencourt et al. (2007).

1.2 Urbanisation: the opportunity

A key principle of urban areas is that they can supply goods and services to their point of need more efficiently than smaller settlement types – this is what drives the urban growth described in Section 1.1, whereby socioeconomic variables (e.g. employment and GDP) increase more quickly than physically-derived variables (e.g. consumption of energy and water). The detailed mathematics which describe the origin of these scaling laws is presented in Bettencourt (2013). The mathematics is rather involved, but the ability of urban areas to provide physical services efficiently can be explained simply, with one word – *proximity*. It is the idea of proximity which is key to this thesis. The geographical co-location of urban resource management infrastructure means cities might be well placed to be the solution to their own problem. Specifically, where management processes are close both to one another, and to consumers (who have a diverse mix of resource management demands), there are various strategies which can be exploited to make more efficient use of resources.

The first strategy is **decentralisation**. This is terminology from energy management, to refer to energy generation that takes place closer to the point of use than traditional centralised generation of large power plants). In electricity networks, this can reduce distribution power losses (Fleten et al., 2007). Of even greater interest, is that decentralisation enables a diverse mix of energy-generation

technologies to play a part in energy supply, including combined heat and power (CHP), photovoltaic systems (PV), small wind turbines, biogas digesters and other devices (Ren and Gao, 2010). These processes can be fed by a variety of local resources including renewables such as wind, solar and biomass, as well as traditional fuels such as coal and gas. Modelling (Webber, 2011) and empirical studies (Carbon Trust, 2013) show environmental and financial benefits to integrating traditional centralised energy management with decentralised processes.

Decentralisation can also be applied to water systems (Stefan Holler, 2016). Rather than using large facilities to treat water and wastewater, distributed infrastructure can harvest rainwater through roof collectors and permeable pavements, and reclaim or reuse waste water at multiple locations around a city (even down to the household scale). This disaggregation of collection, management, and treatment can reduce rates of freshwater withdrawal, as well as water-related energy requirements (Daigger, 2009).

A second strategy to improve the efficiency of resource management is via **cascading**. The classic example is CHP, in which the waste heat from power generation is used to provide useful heat energy (Grubler, 2009). While the water management sector does not tend to use the term cascading, the same principle can still be applied, namely using waste products of one process, as the input to another. Often, this is when wastewater from one purpose is used for another purpose whose quality standards are less stringent. An example at the household level is the separation of potable and non-potable water streams, such that grey water from the washing could be used in toilet flushing or plant watering (Water Corporation, 2013).

1.2.1 Intersectoral synergies

Both decentralisation and cascading are possible because of the proximity of infrastructure to resource feeds, to consumers and to each other. The examples listed above show how cities can extract the most out of a particular infrastructure system. However, these efficiencies are not necessarily the limit of what can be achieved. In cities, infrastructural proximity can also apply to the infrastructure of *different* sectors. In theory, this allows the waste and by-products of one sector to become the inputs to another. In other words, resources can be cascaded between sectors, and this cascading can be facilitated by decentralised processes. So not only are there the intersectoral interactions described

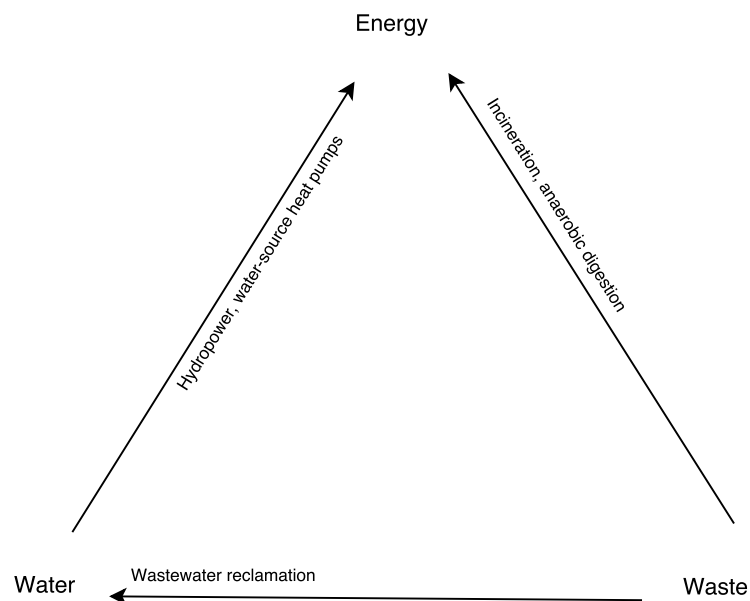


Figure 1.6: Some intersectoral synergies made possible by the co-location of infrastructure.

in Section 1.1.1, but the same sectoral pairings also present opportunities for intersectoral *synergies*.

Between the **energy and water** sectors, synergies include hydroelectric power (which converts water's hydrostatic and dynamic energy into electrical energy); and water source heat pumps (which extract the heat energy stored in water). If energy and water systems are integrated in the right way, it is possible to improve the efficiency of both systems (Makropoulos et al., 2008). Synergies between the **energy and waste** sectors include waste incineration, to generate heat which can be used for power generation or heating (and save on landfill space at the same time), and anaerobic digestion, where waste with organic content (e.g. food waste) is used to generate biogas (which can then be used as a fuel). Finally, synergies between the **water and waste** sectors include various forms of wastewater reclamation, so as to reduce the need for freshwater withdrawal.

Exploiting these (and other) intersectoral synergies (summarised in Figure 1.6) creates opportunities for cities to reduce their consumption and waste. Calls for this type of approach are found in the literature, for example, by Leduc and Kann (2010) who advocate an approach to urban planning they call 'urban harvest'; this takes advantage of infrastructural proximity and connectivity to maximise the reuse of water, waste and other materials within an urban system. This kind of reorganisation of resources flows within a city was also proposed by the Dutch Working Group on Sustainable Urban

Development (Meijer et al., 2011).

1.2.2 Intersectoral synergies in practice – industrial symbiosis

There is precedent for exploiting intersectoral synergies in this way, which comes from the field of ‘industrial symbiosis’ (IS). In IS, firms use each others’ waste outputs as inputs in other processes (IDSa, 2016). Often, this is realised in ‘eco-industrial parks’ (EIPs) in which industries and businesses are co-located with the deliberate intention of practising IS (President’s Council on Sustainable Development, 1996). The classic EIP case study is the town of Kalundborg in Denmark. A key component of Kalundborg’s economy are industrial production facilities and agriculture: these engage in a set of mutually beneficial material and energy exchanges with one another, and with the local energy system (Lewis, 2000). Exchanges include a power plant which provides its waste steam to an oil refinery (which in turn produces gas for the power station); the power plant also sends its waste heat to fish culture, and its waste ash to cement manufacturing; the fish culture provides sludge to local farmers, who also use sludge from a bioplant fed by steam from the power station. These and other exchanges are shown in Figure 1.7.

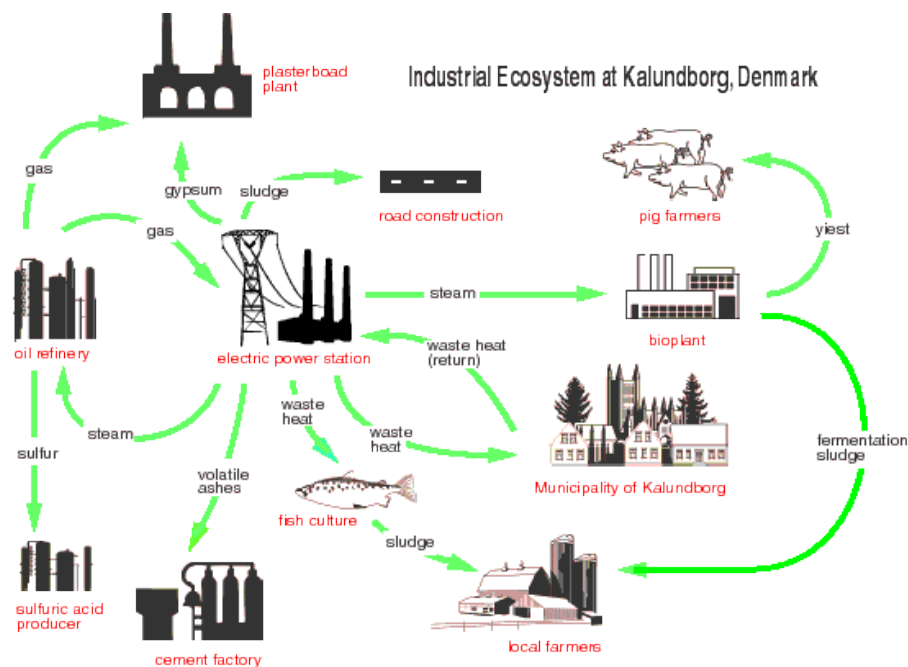


Figure 1.7: Kalundborg’s resource exchanges as of 2000. Figure taken from Lewis (2000).

Researchers have been able to quantify some of the benefits of Kalundborg’s IS. One finding suggests that Kalundborg has avoided extracting four million gallons per day of freshwater, by treating and

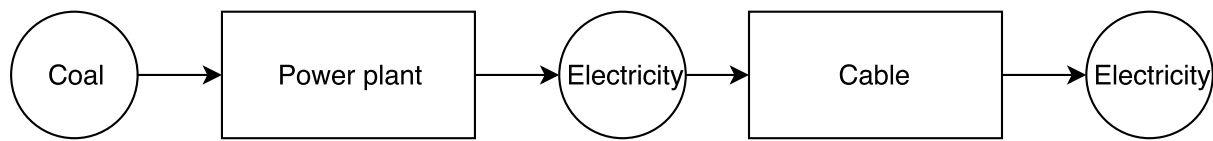


Figure 1.8: A node-link conceptualisation of the urban electricity system of Figure 1.1.

reusing effluent from wastewater treatment (Grimm et al., 2015). What is interesting about Kalundborg is that these intersectoral synergies evolved over time through the initiative of private firms – they were not centrally planned by planners and policy makers (Desrochers, 2001). In contrast, this thesis is concerned with actively helping planners and policy makers realise intersectoral synergies, and not just in a few specific industrial production facilities, but in urban resource management more generally. But just a little reflection reveals the practical challenge of this. If an area contains a large number of resource management processes, located in different places, then what is the best way to adopt resource-saving strategies without breaching any financial, practical or other constraints? In a system as large as that at the urban scale, there are many different decisions to be made: Which management processes should be used? Where should they be located? At what rates of operation should they run (e.g. the power output of a power plant)? How should these rates of operation vary for different time periods (e.g. season, month, week, hour, minute, second)? How should the processes be connected to one another? The number of possible choices which are technically feasible grows rapidly as the problem grows with the size of the area under consideration, the length of time the decisions are being made for, the granularity at which decisions are made, and the number of possible process types which could populate the network of resource-management infrastructure. Out of all the technically feasible options, though, which is to be preferred?

1.2.3 Systems optimisation

To help navigate the complexity of resource management that integrates energy, water and waste, it is time to return to a point noted at the start of this chapter, namely that a network of resources and their associated management infrastructure can be thought of as a ‘system’. A system of this sort can be conceptualised as a network made up of nodes and links, in which the nodes represent processes (such as a power plant, or a cable), and the links represent the transfer of resources between the nodes (such as electricity leaving the power plant to enter the cable). This is visualised in Figure 1.8 which re-presents Figure 1.1 using nodes and links.

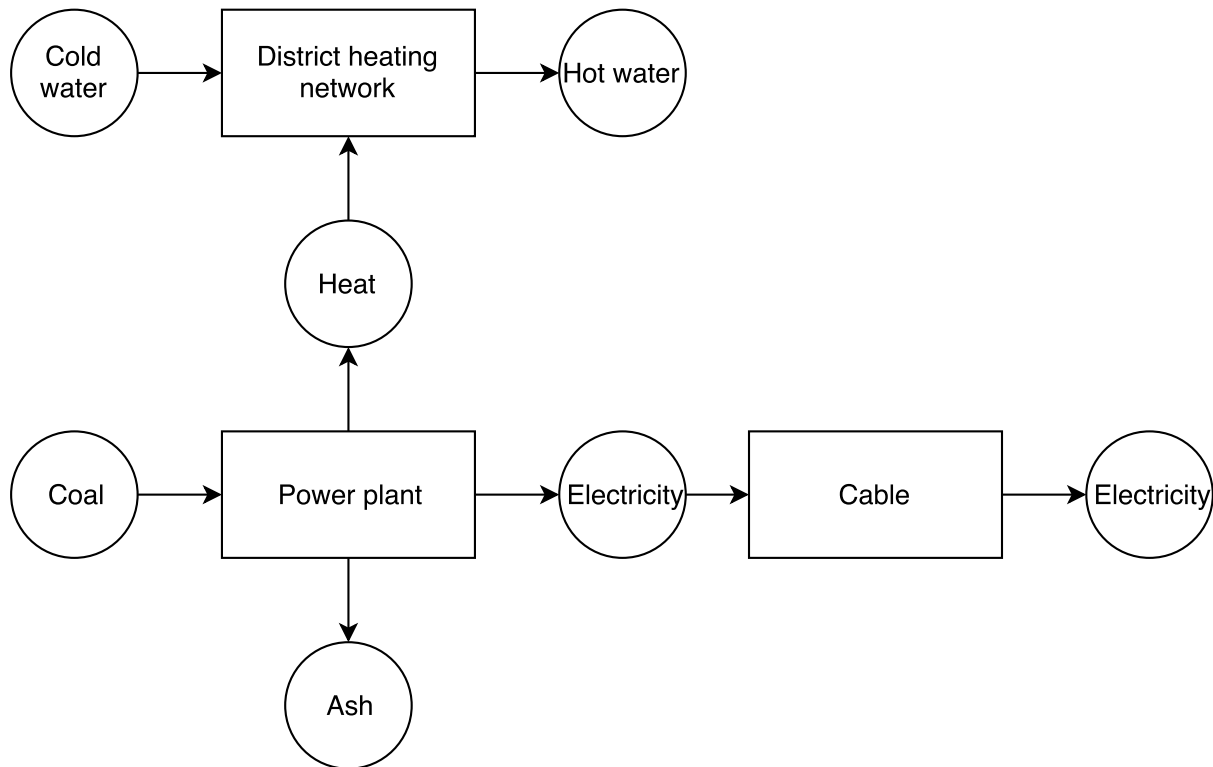


Figure 1.9: A node-link conceptualisation of how an urban electricity system interacts with the water and waste sectors.

From this node-link formalisation, one can formulate a mathematical representation of a system, in which the behaviour of processes (e.g. the quantities of resource they consume and produce), and other system properties are described by equations. In other words, it is possible to mathematically *model* urban resource management. By applying appropriate algorithms to the mathematical model, one can navigate through the choices which need to be made (for example, which processes should be used, where they should be located, their rates of operation, etc., as described above) and compute the optimal mix of processes and the schedule of resource transfers between them, using a technique known as *optimisation modelling*.

This methodology is used extensively in urban resource management, though it tends to be applied to individual sectors such as energy systems, or water distribution. As the literature review in Chapter 2 will show, current models do not consider the different urban resource management systems together in such a way as to either account for intersectoral interactions, or take advantage of intersectoral synergies. Another way to express this existing models do not consider the multi-functionality of nodes: Figure 1.9 shows that a power plant is not just part of the electricity network, but is also part of the water network (because of its need for cooling water). Nevertheless, existing models could provide

a helpful starting point for the development of a model which plans the integrated management of energy, water, and waste in urban areas.

1.3 Urban metabolism – the theoretical framework

Any discussion on the sustainability of urban resource management should engage with the field of ‘urban metabolism’ (UM). UM – whose history and methodology will be considered in more detail in Chapter 2 – proposes that cities and living organisms are in some ways analogous: both entities consume resources, and produce wastes, and in doing so, sustain their activities and growth (Kennedy et al., 2011). This analogy offers a ‘metaphorical framework’ (Pincetl et al., 2012, p.194) which provides the concepts and language to aid understanding of the relationship between a city and its resources. The field is broad and flexible, and patterns of resource use can be related to many aspects of a city, including its form and geography, socioeconomic indicators, political and institutional arrangements, the health of its citizens, and its activities and functions (Hobbes et al., 2007).

Some key findings of UM studies show that in general there is an increasing per capita consumption of water, energy and materials, and output of waste and wastewater (Kennedy et al., 2007), and that this growth of resource flows is coupled to growth in GDP (Schulz, 2007). Nevertheless, for some cities, there are per-capita reductions in energy and water use (through increased efficiency) and reduced per capita waste consumption (following increased recycling rates) (Kennedy et al., 2007). Some UM studies adopt a more wide-angle perspective, for example showing that as human settlements grow (from hunter-gather, to agricultural communities, to industrial centres), they become dependent on an ever-widening surrounding area for their resources (Haberl, 2001, 2002; Barles, 2009). Other studies focus in on the detail: for example, considering exactly how a city becomes water-stressed through the different stages of its development (Kennedy et al., 2007).

The metaphor has proved to carry lots of explanatory power. Indeed, the challenges set out in this thesis have already been expressed by others using the language of UM. For example, many have proposed that cities should move from having a linear metabolism (where resources are consumed and expelled by a city with little or no reuse or recycling within the city) to a circular metabolism (where co-located activities use one-anothers’ wastes and by-products) (Leduc and Kann, 2010, Leduc and Van Kann (2013), and Villarroel Walker et al. (2014)), as represented in Figures 1.10 and 1.11. The

UM concept is increasingly invoked during the design and planning of urban areas, and even finds its way into urban planning policy (Agudelo-Vera et al., 2011, Agudelo-Vera et al. (2012)) and education, with Kennedy et al. (2011) advocating UM thinking to generate “more ecologically sensitive designs” (p.1970) of a city through infrastructure integration, closing loops to minimise overall inputs and outputs of resources. In summary, the UM concept is key to improving resource management by bringing resource sustainability considerations to urban planning.

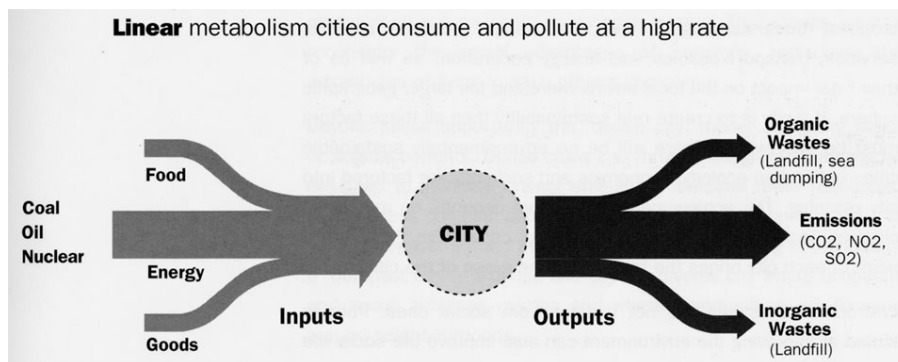


Figure 1.10: Schematic of a linear metabolism. Figure taken from Ecology in Architecture and Design (2016).

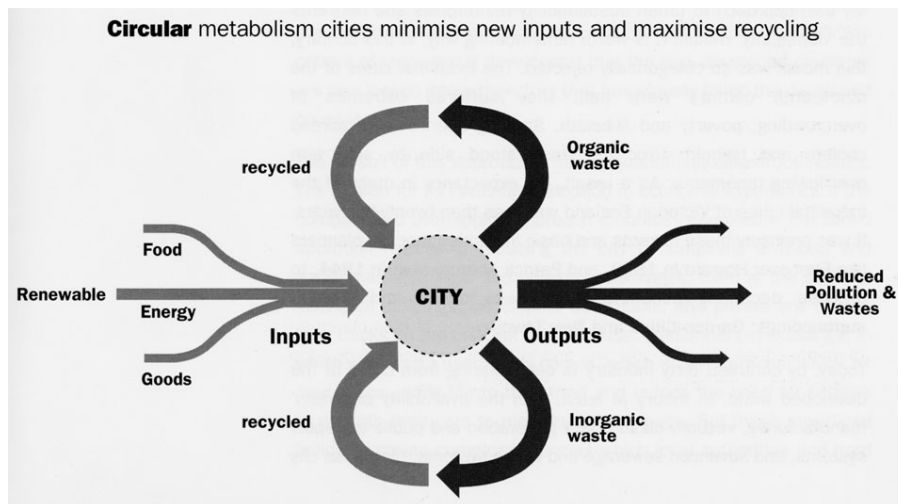


Figure 1.11: Schematic of a circular metabolism. Figure taken from Ecology in Architecture and Design (2016).

1.4 Aims and scope of the study

This thesis is built on the case that the urbanisation seen around the world should be embraced because of the quality of life it brings to more and more people, but this brings with it environmental

and economic sustainability issues. However, due to the co-location of their infrastructure, cities may have inherent to them the ability to partly address these challenges by encouraging synergies between energy, water and waste management sectors. The overall aim of these synergies would be to improve an urban area's metabolism. To realise these benefits in practice is no small challenge – not least because of the difficulty of choosing which mix of processes will result in the overall optimal set of interactions and synergies. However, this type of problem is well-suited to optimisation modelling, in which the urban resource management networks are formalised as a system that can be mathematically represented in such a way that optimisation techniques can find the optimal configuration of energy, water and waste management infrastructure.

1.4.1 Definition of thesis title and research boundaries

Urban resource consumption is connected to many different issues, and so to provide a focussed area of research with clear novel contributions, requires posing a precise research question. One way to arrive at this point is to clearly define the thesis title, to avoid the vague, unbounded meanings which many words can have in everyday use (such as 'resources' and 'sector'):

Highly integrated This term refers to resource management optimisation models that consider the simultaneous optimisation of more than one system (e.g. not just an energy system), in order to take into account interactions and synergies between them. (Section 2.3.2 defines this more thoroughly and provides examples.)

urban There are various ways to define 'urban'. Ramaswami et al. (2011) proposes three, which are adapted by Keirstead et al. (2012a):

- *Pure geographic* defines a city's in terms of its administrative boundaries
- *Geographic-plus* extends the pure geographic definition to include readily traceable upstream flows, such as electricity consumption
- *Pure consumption* attributes resource flows to the economy which generated the demand for a good or service. For example, a service-based city will require products manufactured in an industry-based city (and vice versa). On this definition, consumption is accounted to the service-based city, even though manufacturing took place in the industry-based city.

This approach attempts to even out disparities between cities arising from their different functions.

With its focus on resource management infrastructure, the interest of this thesis is essentially focussed on a city's engineering, rather than its politics, administration or economy; in particular, the way that a set of co-located consumers uses infrastructure to deliver goods and services. Thus the 'geographic-plus' definition is most appropriate. In this way, infrastructure that is located outside a city's administrative boundaries, but is nevertheless responsible for a city's resource management can be considered as part of the urban resource management system.

energy, water, and waste These resources belong to three of the five 'lifeline infrastructures' (Young and Hall, 2013)⁷. Limiting the study to these three sectors means some resource-heavy processes are not considered (such as steel manufacture and chemical industries). Defining this clear boundary makes the thesis manageable; other sectors could be considered in future work.

systems These are the networks of resources and processes (those that convert and transport) within a city.

As well as the research boundaries identified by the title definition, there are a few others worth noting. With respect to the optimisation modelling itself, there will be no discussion on the detailed mathematics of optimisation algorithms, and there will be no attempt here to either soft- or hard-link this model to other tools. In the application of the modelling, there will be little consideration of how modelling results could be implemented within the real-world – these concerns about administration and governance are beyond the scope of this thesis. For the same reason, this work considers how modelling affects urban resource flows, but not its effect on other aspects of UM, such as a city's economy, livability, or governance. In summary, this thesis focuses on the engineering possibilities of urban resource management challenges, in sufficient detail to be useful to researchers, planners and policy makers, but without becoming lost in an unbounded set of political, social, and economic considerations.

⁷The other lifeline structures defined by Young and Hall (2013) are communications and transportation.

1.4.2 Research question

With the research boundaries in place, the following research question is posed, to give a clear focus to the thesis, and which can be used as a benchmark to measure the success of the research:

By how much can an area's metabolism be quantifiably improved by an optimisation model which integrates the planning of energy, water and waste systems?

This end goal is made up of three aims, which combine to answer the overall research question:

1. *Investigate the opportunity and methodology.* This addresses the background necessary to develop and apply the model, including identifying motivations, methods to build the model, data for the model, and the means by which the model can be assessed.
2. *Develop a model which computes the optimal mix of resource management processes to meet demand for goods and services for an urban area.* This model must integrate the energy, water and waste systems, be computationally tractable, and provide insights useful to researchers, planners and policy makers. This will involve developing test models which will be applied to a small-scale application to provide a 'benchmark' case study, which can be used to assess the performance of models (in terms of tractability, ease of writing, etc.)
3. *Assess how well the models improve urban metabolism.* This requires applying the model to a case study to quantify how well the model optimises a mix of technological opportunities to minimise environmental impacts and ensure economic stability for urban areas.

1.4.3 Contributions

The main novel contributions of this thesis are:

1. To advance the UM concept by considering how resource management processes affect an area's overall metabolic flows. The need for this contribution is discussed in Section 2.1.2. This will help those interested in urban sustainability think about it in a new way, as well as providing the concepts behind the mathematical formulation of the systems optimisation model. This is proposed in Chapter 2 and Ravalde and Keirstead (2017a).
2. To offer guidance on the appropriate set of metrics to quantify how well an area's metabolism is performing. These metrics could be used to assess an area's metabolism as well as the results

of the modelling work. This is the subject of Chapter 3 and Ravalde and Keirstead (2017b).

3. Following from the first item, this thesis contributes a new open-source database of resource management processes which records their various features, including the quantities of resources they consume and produce, their rates of operation, and other properties. The work which describes this database in in Chapter 4 and Ravalde and Keirstead (2017a).
4. To formulate a model which simultaneously optimises energy, water and waste management processes at the urban scale (Chapter 5). Traditional siloed optimisation modelling considers neither interactions or synergies between sectors, which is the shortcoming that this thesis addresses. The development of this model will be described in some detail given its novelty to the field. Development will be done in the context of a ‘benchmark study’, which others can use to develop and improve the model presented here. This tool brings together systems optimisation and urban metabolism, to help planners and policy makers incorporate UM thinking into sustainable urban design and planning. An early version of this model was described in Ravalde and Keirstead (2015).

1.4.4 Thesis structure

This chapter has argued that urbanisation is both a socioeconomically desirable phenomenon, and yet also a source of environmental and economic problems stemming from resource overconsumption, but that cities possess the solution to their own problem, if only they were to take full advantage of the resource integration opportunities inherent in them coupled with the possibilities afforded by optimisation modelling. Chapter 2 examines the literature to show how this work advances the urban metabolism concept, and develops existing models which optimise resource management.

Chapters 3-5 contribute the work that is needed to develop and apply the model. Chapter 3 explores the different ways one could quantify the efficiency of urban metabolism. Chapter 4 systematically researches all the processes that can be used to manage energy, water and waste in the short- to mid-term, to provide data for the model (which is also provided in the open-source database). Chapter 5 formulates three possible optimisation models, and applies them to the benchmark study to establish the most suitable mathematical formulation of the highly integrated urban energy, water, and waste management systems optimisation model. Chapter 6 applies the model which proves most suitable in

Chapter 5 to a real-world application case study in China, and Chapter 7 evaluates how successful the work has been at meeting its aim of quantifiably improving UM, considers the broader implications of the thesis, and suggests areas of further work.

A summary of each chapter's objectives and contribution, and how they relate to each other, are given in Table 1.2.

Table 1.2: The relationships between research objectives, thesis chapters and novel contributions.

Chapter	Objective	Contribution to thesis	Contribution to the field
1	Objective 1: Research the links between urbanisation trends, and resource management challenges and opportunities to motivate the thesis.	Define the research question.	
2	Objective 2(a): Research the urban metabolism concept which provides a theoretical framework to assess urban resource consumption. Objective 2(b): Research modelling methods used currently in designing for sustainable resource management.	Locate this research question within the existing literature.	Identify theoretical and methodological opportunities and gaps in the literature and so advance the UM framework providing a new way to conceptualise the way a city relates to its resource flows.
3	Objective 3: Determine metrics to quantify performance of multi-resource systems, appropriate to measure the success at meeting environmental and economic challenges.	Propose the theory which can be used to assess an area's metabolism (and so assess the results of modelling).	Determine metrics appropriate to quantify the performance of an area's metabolism (work published in Ravalde and Keirstead (2017b)).
4	Objective 4: Systematically research the processes likely to influence urban metabolism between now and 2030 (to provide model inputs).	Assemble data for use in the model.	Assemble an open-source database of the resource management processes over the coming years (work published in Ravalde and Keirstead (2017a)).
5	Objective 5: Develop the mathematical formulation and the computational implementation of the model.	Formulate the modelling method.	Development of the model using a benchmark test case which others can use as a starting point to further develop the model.
6	Objective 6: Apply the model to a case study to demonstrate resource integration.	Apply the model to a case study.	Demonstration of model to show how it might be employed by decision makers. (Early version of this work published in Ravalde and Keirstead (2015).)
7	Objective 7: Evaluate the success and implications of the model.	Answer the research question, and propose an agenda for future research.	

Chapter 2

Urban metabolism and systems optimisation

Assistant 1 “So minister, we’ve run every viable model through the computer and it looks there are just no easy solutions to this recession.”

Assistant 2 “Yeah, raising VAT, cutting VAT, raising interest rates...”

Assistant 1 “... raising interest rates and VAT, lowering income tax and raising VAT...”

Assistant 2 “None of it seems to really help.”

Minister “Have your tried kill all the poor?” ... “I’m not saying do it, I’m just saying run it through the computer, see if it would work.”

Extracts taken from a sketch of *That Mitchell and Webb Look* (BBC Television, series 4, episode 4)

Section 2.1 has been adapted from Ravalde and Keirstead (2017b) (Section 2, entitled ‘Urban metabolism and sustainability’), and Ravalde and Keirstead (2017a) (Section entitled ‘Approaches to Urban Metabolism’).

This chapter reviews two key bodies of research to investigate the gaps in the literature which this thesis will address. The first subject of exploration shows how the UM field has developed to better understand issues of urban resource management, and identifies how UM concepts should be further developed in order that the field becomes equipped to consider how different sectors work together to affect an area’s metabolism. The second subject of exploration introduces the various ways modelling has been used to optimise the performance of resource management systems, in order to show the need for the model which will be developed in this thesis. The work described in this chapter feeds into the first aim of the research question.

2.1 The past, present and future of urban metabolism research

UM was introduced in 1965 by the American engineer Abel Wolman. He recognised that resource consumption was necessary to sustain urban living, but wanted to make a close study of this dependency because of concerns that as cities grew, their rising material and energy inputs and outputs presented challenges for public management of water supply, sewage disposal and air pollution. In that cause, he coined the phrase ‘urban metabolism’, defining the metabolic requirements of a city as “all the materials and commodities needed to sustain the city’s inhabitants at home, at work and at play” (Wolman, 1965, p.156, *Scientific American*). To explain the issues, Wolman quantified the material and energy inputs and outputs of a hypothetical city of one million inhabitants. This kind of accounting exercise – known as material flow analysis, and energy flow analysis – is often the starting point of UM studies. In this seminal work are the two elements typical of UM studies: first, the quantification of urban resource flows; and second, some assessment of how these flows relate to other aspects of the city – in Wolman’s case, this was to highlight the environmental factors which should inform the ways cities make decision on how to provide public services.

Since Wolman, the UM framework has cultivated a whole field of studies which seek to understand the scale and origins of urban consumption and waste, and its relationship to an area’s form, geography,

and other characteristics. A more recent definition of UM which encapsulates the current breadth and depth of the field is given by Kennedy et al. (2007), who defines UM as “the sum total of the technical and socioeconomic processes that occur in cities, resulting in growth, production of energy and elimination of waste” (p.44). Since initial steady growth in UM studies, there has been a recent rise in research facilitated by conferences, journals, and research collaborations (Zhang et al., 2015).

The field has grown such that ‘urban metabolism’ is fast becoming a buzzword in urban research literature, perhaps enjoying the benefits of increased data availability in conjunction with “an explosion of research on cities and on sustainability in recent years” (Next City, 2014). Kennedy and Hoornweg (2012) write of the “substantial momentum” (p.781) to its study and highlight its usefulness to “address concerns over the magnitudes of global resource flows” as well as the “analysis of specific policy issues” (p.780). Thanks to UM’s close association with ‘sustainability’, the UM concept is helping planners and policy makers understand and address urban sustainability issues, and is even employed by governments seeking approaches to urban sustainability (for example, in the United Kingdom, by Clift et al. (2015)).

2.1.1 Methods

Typically, the methodology to conduct a UM study begins by defining a boundary around an urban area, and then quantifying the *flows* of material, energy, water and other resources into and out of a city (i.e. crossing the urban boundary) over a given time period, and/or the *stocks* of these resources held within the boundary (Kennedy et al., 2014). These quantities can be found either by consulting data sources, or using estimations and calculations¹. A recent important example is the UM study which quantified the energy and material flows of 27 megacities (Kennedy et al., 2015). Once stocks and/or flows have been quantified, there are then at least four types of study (identified from a survey of the literature):

- *To provide inputs to other types of analysis.* Useful information can be calculated when inventories of resource flows are coupled to other data for further analysis. For example, by combining metabolic flows with carbon emissions factors, a city’s greenhouse gas emissions can be calculated (with examples in Kennedy et al. (2009) and Kennedy et al. (2010)). The ‘ecological foot-

¹More details on these methods are given in Section 2.1.2.

print' (EF) is another quantity that can be calculated from UM data (Chambers et al., 2002). Zucaro et al. (2014) use UM data to calculate 'urban sustainability indicators' for Rome, including emissions, acidification and energy flows.

- *To make comparisons of resource consumption.* This type of study identifies trends or differences in resource flows, either over time, or between cities. For example, Kennedy et al. (2007) studies the metabolism of eight metropolitan regions around the world since 1965, and, amongst other findings, shows that in general, there is an increase in per capita energy and consumption, and waste output (with some exceptions, such as Toronto's water use, whose reduction would be in part traced to a change in industrial behaviour). Alternatively, resource flows could be compared for cities at different stages of their development – for example, Krausmann et al. (2008) compare the metabolism of agrarian, developing and industrialised societies. Comparison studies might focus on just a single city, and compare the resource flows between its different sectors (such as construction or commercial services), for example to determine which sectors produce the most waste (Browne et al., 2009).
- *To relate consumption/output to other dependent variables.* Wolman's 1965 study is an example of this type of study, in which he relates resource flows with challenges of water supply, sewage disposal, and air pollution. Other studies highlight studying the relationship between flows and challenges include Browne et al. (2009), who consider impacts of waste generation; and Kennedy et al. (2007), who addresses issues of water stress and contamination. Another type of relationship is studied by Schulz (2007) who relates economic growth to material consumption.
- *To understand or model relationships in the urban environment.* At a fairly simple level, this could mean finding relationships between the use of different resources, for example the examination of the links between urban energy and water consumption (Kenway, 2013). Geographical dependencies can also be studied; for example Barles (2009) reveals Paris' reliance on surrounding regions for material provisions and waste management. Bristow and Kennedy (2013) identifies the relationship between Toronto's energy consumption (i.e. a flow) and its energy stocks (with the purposes of assessing the city's ability to cope with supply failure or other shocks to the energy stocks). Moving to a greater level of sophistication, a number of studies – including Zhang and Chen (2010) and Liu et al. (2011) – have studied how resources flow between a city's different economic sectors, and thus determine the extent to which sectors are interdependent;

studies of this sort could enable planners to decide how sectors could best work together to use a city's resources more efficiently.

This overview of the literature shows that UM is an important idea, which provides a framework to examine resource consumption alongside issues of urban sustainability (Next City, 2014). Specifically, UM studies enable comparisons of resource consumption and output; facilitate the calculation of greenhouse gas emissions and similar important measures; identify relationships between patterns of resources use, challenges, and socioeconomic indicators; and explore relationships at work within urban boundaries. In these ways, UM studies can provide insight on how to maintain of urbanisation's socioeconomic benefits while limiting environmental harm.

2.1.2 The place of processes in urban metabolism modelling

UM has contributed many useful insights, but of most interest to this thesis is the fourth type of study listed above – the understanding and modelling of relationships in the urban environment – since this work is concerned with how different mixes of resource management processes (i.e. activities occurring within an urban boundary) can affect overall metabolic flows. A key question then, is to what extent have UM studies sought to understand the role of resource management processes on an area's metabolic flows? This section considers this by taking a closer look at how resource management processes fit within urban resource management as a whole, and considering how the UM literature has understood this.

Analysis of a city can focus on the different parts of an urban metabolic system, each of which work together in a hierarchical framework defined especially for this thesis (Figure 2.1). At the 'bottom' lie end the consumers, namely the homes, business, industry and transport that exert demands for final energy and water consumption, as well as generating wastes. At the 'top' are the aggregate exchanges between a city and the surrounding environment: both the import of natural resources required to meet consumer demand, and the export of a city's wastes and effluents. In the 'middle' is a network of processes that link the top and the bottom, converting natural resources to demands, as well as treating and managing locally generated wastes. Typically, urban metabolism studies seek to quantify the overall metabolic flows at the top, and to locate the origins of these flows at their point of demand at the bottom.

This section extends published arguments that advocate giving greater attention to the middle of the system, in order to show how the mix of processes used to meet demand at the bottom will affect overall metabolic inputs and outputs at the top.

“Top-down”

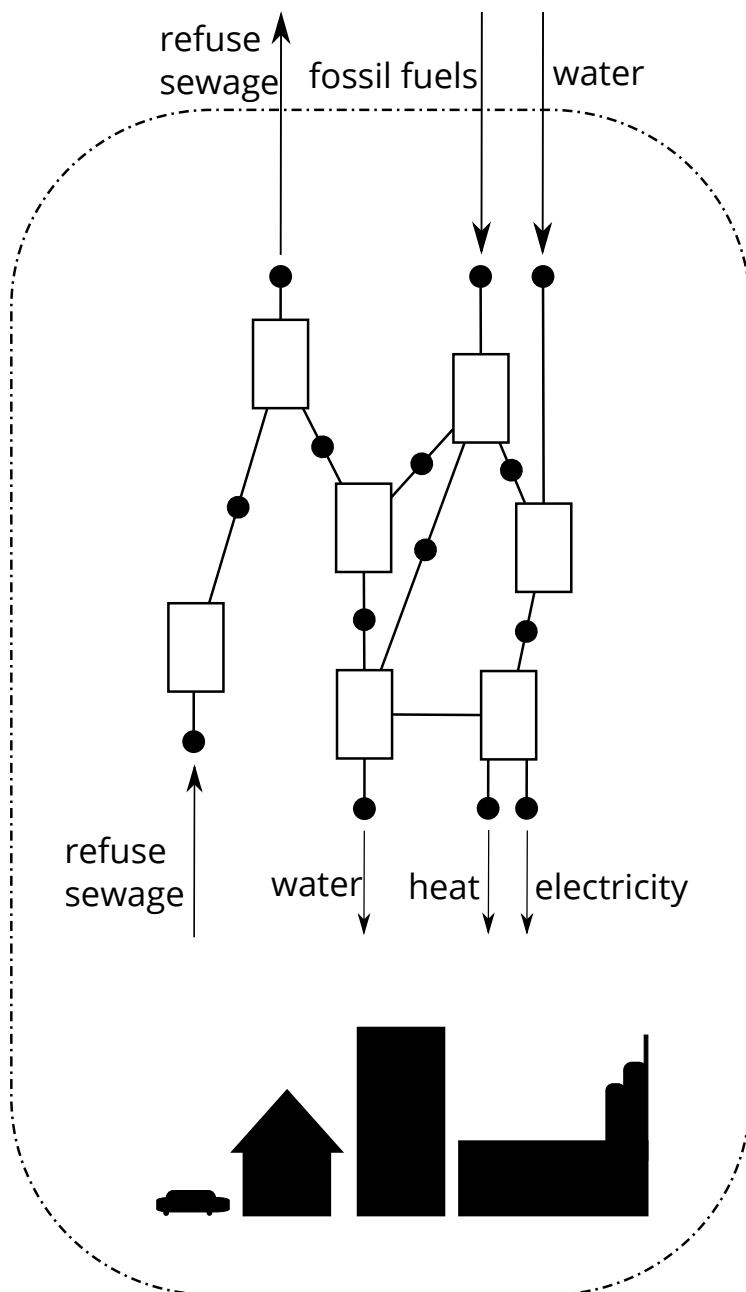
According to Chrysoulakis et al. (2015), most urban metabolism studies take a top-down approach. Their aim is to quantify the impacts of an entire urban area’s consumption and waste generation (Sahely et al., 2003). Typically studies do this using data aggregated at the city scale (i.e. it cannot be traced back to particular locations or activities) (Chrysoulakis et al., 2015). Several methods are described in Sahely et al. (2003). One example is Wolman’s seminal study which derived a hypothetical city’s resource flows from national rates of consumption (water, food and fuel) and generation (sewage, waste and air pollutants).

A more sophisticated approach might adjust these values; for example, a city’s food intake could be calculated by adjusting the national average food consumption according to a city’s grocery bill expenditure (as suggested by Sahely et al.). Ideally though, data would be supplied directly from appropriate organisations: water consumption data from the public or private providers; electricity consumption data from market operators; and waste data from municipal authorities. Once collected, the data can be used to analyse trends and make inter-city comparisons, to reveal how variables (such as climate, urban form, economic activity etc.) correlate with overall metabolic flows, as exemplified by Kennedy et al. (2015)’s study of megacities.

Top-down studies can inform policy, as seen in Liang and Zhang (2011) who use government statistics in a top-down metabolism study of Suzhou, China. Their findings lead to precise proposals to achieve decarbonization (in this case focussing CO₂ mitigation strategies on vehicle pollution because trends indicate that the city is on course for low-carbon development in other sectors).

“Bottom-up”

An alternative approach is to build up a picture of a city’s metabolism from the bottom up, by quantifying resource flows at small scales and then aggregating these over the region of study (Chrysoulakis et al., 2009). For example, Kellett et al. (2013) describe a method to quantify a neighbourhood’s CO₂



(A) Top

The top represents the flow of resources into and out of a city.

(B) Middle

The middle represents the network of resource management processes (boxes) through which resources (circles) flow, in order to meet demand for goods and services at the bottom.

(C) Bottom

The bottom represents user demands for electricity, heating and water, and the generation of solid waste and wastewater.

Figure 2.1: Three components to an urban metabolism system with example resource flows adapted from the hypothetical city in Wolman (1965).

emissions by modelling the CO₂ flows in the neighbourhood's buildings, transport, humans, and vegetation components. For instance, to calculate the total emissions attributable to buildings, first building types are determined from architectural features (found from fieldwork, databases, and LiDAR information), enabling researchers to know the number of each building type of building in the neighbourhood; next the emissions for each type of building (such as an apartment) are estimated using a model which takes into account a building's occupancy, age and HVAC equipment. Finally, emissions for each building type can be multiplied by the prevalence of each building type to calculate total emissions.

Another bottom-up approach comes out of the Vulcan Project which measures CO₂ emissions at fine spatial and temporal resolutions, using networks of ground and air remote sensing technologies (Rayner et al., 2014). Gurney et al. (2012) present results for the city of Indianapolis to understand the origins of its emissions, enabling decision makers to implement mitigation strategies, which are both effective and low cost.

Bottom-up methods often depend on high-tech tools including: sensor technology to measure energy, water, and pollutant fluxes; Geographic Information Systems (GIS) and remote sensing devices to collect information on land-use, thermal radiance and rainfall; and advanced numerical modelling to simulate resource fluxes (Chrysoulakis et al., 2009). An alternative low-tech approach is to survey residents of a city about their resource use habits; for instance, deriving information on urban water flows by asking householders about their typical dishwasher loads and shower durations (Eberlein, 2014).

Merits, limitations, and a complementary approach

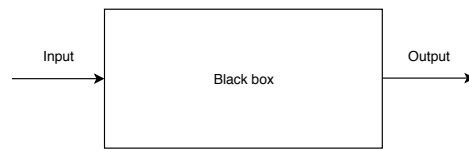
Top-down approaches are methodologically simple, but they do not easily nurture an appreciation of the ultimate causes of emissions or other environmental impacts (Kellett et al., 2013), and are thus unsuited to predicting how metabolic flows might change under different scenarios, hence the power of bottom-up methods which can be used to test scenarios and policies. Kellett et al. exemplify this in their neighbourhood emissions model by altering land-use, building efficiency, transport fuels, and consumer behaviour to observe how overall emissions change.

Zhang (2013) traces the evolution of the UM concept and concludes that more attention should be paid to the *middle* of a system (figure 2.2). Starting with Wolman's seminal study, UM understood a city to be a linear system into and out of which resources flowed. On this view, sustainability efforts are focussed on minimising the inputs and outputs. This understanding was refined by Girardet (1990), who suggested that in addition to minimising resource inputs (e.g. by using solar energy and more efficient energy processes such as CHP), cities should be adopting circular metabolisms, whereby outputs could be reused as inputs through waste recycling (as discussed in Section 1.3). Both of these understandings are 'black-box' representations. As Zhang (2013) notes, both bottom-up and top-down approaches fail to consider the mechanisms within the urban system which determine its behaviour – or as this thesis denotes it – the *middle* of the system. The top-down approaches are well suited to identifying the scale of metabolic problems, and the bottom-up approaches contribute understanding on the ultimate causes of metabolic flows, but appreciation of the middle will add to the insights of bottom-up studies by revealing the role of activities which take place between the top and the bottom of an urban system.

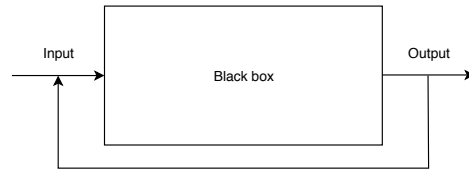
To address this gap in the UM literature, Zhang et al. (2009b) proposed research into how resources move around inside the UM system. Specifically Zhang et al.'s work (and its offspring, such as Liu et al. (2011)) considers the economic sectors (nodes) within a system, and the degree to which they are dependent upon one another by resource flows (links). Such information is useful to help identify potential problems for an urban system (e.g. identifying where sectors are competing for a limited resource). Thus Zhang argues research should prioritise quantitative analysis of an urban system's components, which models urban systems as a network of linked nodes. This representation of a system provides a framework to understand how fluxes circulate, thus enabling researchers to test how management interventions and other scenarios will change the distribution of resources between economic sectors.

A comprehensive understanding of the 'middle'

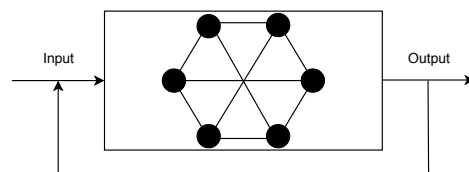
If these recommendations are to be realised, the urban metabolism field should seek a comprehensive understanding of what constitutes the middle to enable modelling to take place; i.e. identifying and describing the nodes and the links within metabolic networks. In Zhang's work, the middle of the system is understood to be a set of economic sectors (represented by nodes), which consume and produce resources that transfer to between sectors (along links), as well as importing and exporting



(a) The linear process of Wolman (1965).



(b) The cyclical process of Girardet (1990).



(c) The network process of Zhang et al. (2009a).

Figure 2.2: Developments in ways to think about urban metabolism. Figure reproduced from Zhang (2013).

them across the urban boundary. This conceptual model has led Zhang and others to conduct UM studies which investigate the effect of the ‘middle’ of the system, using ecological network analysis (ENA) to investigate the extent to which different economic sectors are dependent on each other, and the implications for a city’s overall metabolic flows (e.g. Zhang and Chen (2010) and Liu et al. (2011))².

However, to Zhang’s *economic sector* perspective of a UM system’s middle, this thesis will propose an *engineered-system* perspective. On this view, the nodes and links would correspond to resource management processes (e.g. power plants, water treatment units, and pipe networks) and resource flows, respectively (as per part (B) of Figure 2.1). Studying nodes and links could suggest how a city’s mix of processes could meet resource demand in cheaper and greener ways. As a case in point, consider how a city meets domestic heating demand: bottom-up studies could explore how measures such as thermal insulation and lower thermostat settings reduce fuel requirements at the top (i.e., demand-side management). But studying the middle would explore how investment in processes could reduce fuel usage, for example showing how heat demand could be met by waste heat from power generation rather than gas boilers (supply-side management). This approach can be extended to study how a city’s whole process mix, layout and scheduling can be optimised to maximise synergies, and thereby

²These studies are discussed in more detail in Section 3.1.2.

minimise a city's overall resource consumption and waste generation. Indeed, informing optimisation strategies to improve UM is highlighted by Zhang (2013) as an area of future UM research.

2.1.3 Summary

In summary, UM can be considered as the study of how a cities flows, forms and functions relate. While there is work to be done to study each of these areas (both individually, and how they work together), the arguments of Zhang (2013) should be extended to argue for research into how a city's processes work together as an engineered system. This conceptualisation then becomes the basis for this thesis, from which it becomes possible to formulate an optimisation model which can take advantage of synergies between different resource management infrastructure), and so help answer the research question of this thesis.

2.2 The role of modelling in urban metabolism

The literature review above surveyed UM research to outline the different ways UM contributed to understanding resource flows in cities. In doing so, it highlighted the need for better understanding of the 'inside' of a UM system generally, and the engineered system specifically. i.e. the role of resource management processes in affecting the overall flows of energy, water, and waste into and out of a city. This section seeks to move this idea forward by considering the role that modelling can play in UM by systematically researching the current state of affairs of UM modelling. Before this however, this section introduces the idea of modelling generally.

2.2.1 An introduction to modelling

Whenever models are used, it is important to justify their use, but it is especially important here specifically, when introducing a new model to the urban metabolism field. A model can be defined as:

“A simplified or idealized description of conception of a particular system, situation, or process, often in mathematical terms, that is put forward as a basis for theoretical or empirical understanding, or for calculations, predictions, etc...”

(Oxford English Dictionary (2016a), definition 8a)

Note in this definition, the explicit reference to a ‘system’. It is precisely the complexity of a system (a concept introduced back in Chapter 1) – with its various interactions and moving parts – which warrants simplified, formalised descriptions in the form of models to aid understanding, calculation, and prediction. The specific benefits of modelling are highlighted by Williams (1990):

1. The act of model building itself will reveal relationships that were previously unapparent;
2. The results may reveal courses of action which were otherwise uninvestigated;
3. One can experiment on a model in a way that may be impractical or unethical for a real system³.

(For these situations, it is important to note that models are very difficult to validate – because it is impractical or unethical to build the real-world system, it is hard to compare the behaviour of the model results with the behaviour of the real system.)

However, modelling is not without its critics, and it is right to address their objections if this thesis is to propose, formulate and apply a new model. Some only see crude reductionism in the way that mathematical programming seeks to quantify something, basing decisions on the numerical value of an equation. Williams (1990) points out that in fact all decisions will make quantitative evaluations implicitly, if not explicitly, and suggests modelling is at least an honest and scientific way to formalise the quantitative component of decision making. (Note that this benefit of modelling is still true, even when models cannot easily be validated, as described above). Others point out that inaccuracies in a model’s coefficient values will propagate to inaccurate results. Williams responds by showing how models can be tested for a range of parameter values (to reflect uncertainty), for example establishing the ranges for which parameters can change with predictable effects on the values of model outputs. Models are therefore not a ‘magic bullet’, but nonetheless they are still important as “one of a number of tools for decision making” (Williams, 1990, p5) to understand systems, test their performance, and identify ways to improve the system.

2.2.2 Types of models

Some of the different types of models that exist are summarised in Figure 2.3 (based on Williams (1990)). The first categorisation divides models into those that are *concrete* or *abstract*. The former

³This idea is the premise of the sketch from *That Mitchell and Webb Look* quoted at the beginning of the chapter.

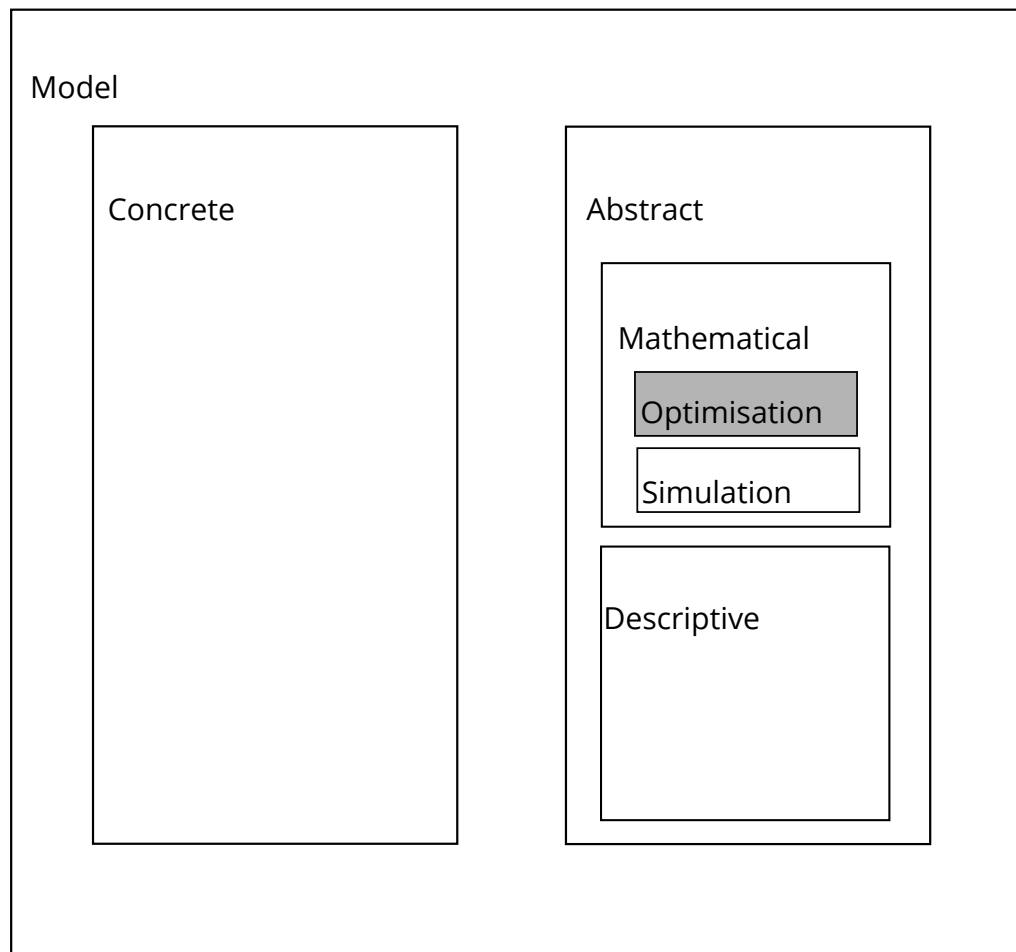


Figure 2.3: A summary of different types of models, based on Chapter 1 of Williams (1990).

type exist physically, for example, a scaled-down construction of an aeroplane or laboratory-scale version of some resource management process). The latter type exist as conceptualised representations of a system. Abstract models can be *purely conceptual* (sometimes called ‘descriptive’). These models graphically, visually or diagrammatically represent a system so as to provide an explanatory which helps people understand the workings of the real system. A classic example is the nitrogen cycle diagram that many learn in school, which uses arrows to show how nitrogen transfers between the atmosphere, ground, and plants (Figure 2.4). This representation of the cycle does not include any mathematical content, but it does visualise how plants, bacteria, the atmosphere, and other components convert nitrogen (Killpack and Buchholz, 2014).

Abstract models can also be *mathematical*. These use mathematical relationships to describe a system. One particular type of mathematical models are statistical models. In these, the statistical properties of a set of sample data (for example, the relationships between the height and weight of 50 children

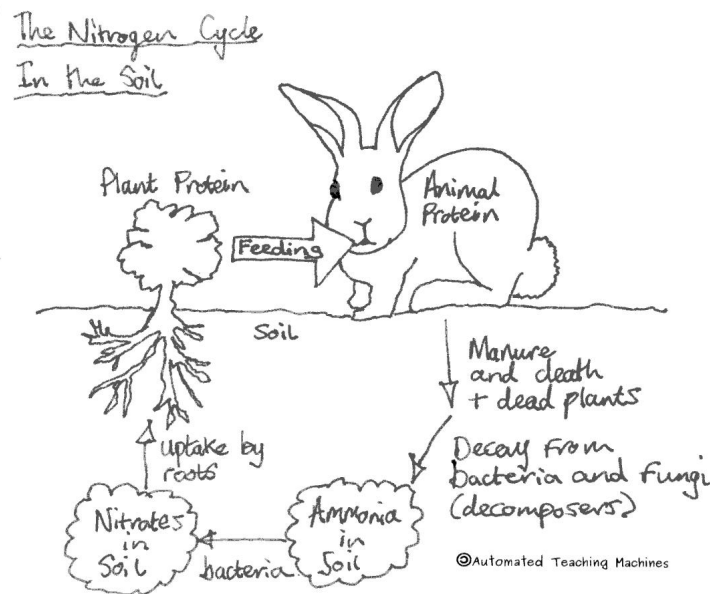


Figure 2.4: The nitrogen cycle represented as a conceptual model (Automated Teaching Machines, 2018).

selected randomly from a school) are used to predict the characteristics of a larger group (for example, the weight of any student in the school, given their height). Other types of mathematical models include simulation models, and optimisation models (the latter is also known as mathematical programming, and was briefly introduced in Section 1.2.3). Both of these use equations, inequalities and logical dependencies to represent the workings of a system. Simulation models predict how a system will perform under a given set of conditions. An example could be the length of a traffic queue given a particular system of traffic signals (Grether et al., 2012). Optimization models compute the conditions under which a system will perform achieve the objective defined by the modeller). An example would be to compute when traffic signal changes should be timed in order to minimise traffic congestion (Osorio and Bierlaire, 2008).

The equations of simulation and optimisation models are formed of parameters, which are fixed values representing unchanging conditions of the system (such as the length of a given road); and variables, which are at liberty to to change (such as the length of time for a signal to display a green light). In simulation models, the variable values are selected by the modeller, who wants to investigate the effect of their changes; whereas for optimisation models, the reverse is true – the desired outcome is specified first, and the variables to achieve this are chosen by mathematical algorithms. Normally, the formulation of a mathematical model (i.e. the equations, parameters, and variables) is based on

a conceptual model: what the conceptual model visualises, the mathematical model can formalise in equations and inequalities. A conceptual model has already in fact been proposed in this chapter, namely the hierarchical framework of Figure 2.1.

2.2.3 An overview of models in urban metabolism

Each of the model types above can be found in the UM literature. Indeed, the idea of urban metabolism is itself a descriptive model, i.e. the concept of ‘metabolism’ has inherent to it the fact that resource flows relate to an entity’s form and function. To show where this thesis can fit within the UM modelling landscape, this section systematically reviews the literature found by exploring the Scopus database⁴ using the search term `urban metabolism AND model OR modelling` (excluding irrelevant subject areas such as medicine). This search returned 239 results which were manually reduced to 108 after removing articles which were inaccessible, not published in English, only tangentially related to UM, or did not satisfy the definitions of ‘model’ as described above. Looking further at the remaining results, each paper was classified according to three categories: the **type** of model (according to the definitions given in Section 2.2.2, above); the model’s **focus**, which refers to the component(s) of urban metabolism studied by the model; and **level** of detail to which a system is modelled. The following three subsections summarise the variety of models to be found in UM.

Type As explained above, the idea of UM itself is a **conceptual** model, which appropriates the language and ideas of real biological systems to describe urban resource flows. The concept has grown from Wolman’s first study which considered simply the flows of resources, and the challenges of their public management. One such development of the concept is that of Newman (1999), who proposed the ‘Extended Metabolism Model of the City’ (p.220), which adds ‘livability’. Newman’s intention was to encourage researchers to consider how resource flows relate health, incomes, housing stock, and other aspects of urban living. Other extensions of the UM conceptual model were introduced in Section 2.1.2 and include the work of Girardet (1990), who incorporates the recycling of resource outputs as inputs, and Zhang et al. (2009a), who asks modellers to consider how resources flow between sectors within the urban boundary 2.1.2.

Moving beyond conceptual models, various types of mathematical models have been developed

⁴<https://www.scopus.com/>

to understand urban metabolism. An example of a **statistical** model is that of Liang et al. (2014) who find a relationship between the level of a city's night-time lighting (as measured by satellite observations) and the city's steel stock, making it possible to predict the latter from the former. Kellett et al. (2013) provide an example of a **simulation** model, in which a city's emissions are quantified from equations which calculate the contributions from building, transport, human, and vegetation sources. Finally, an **optimisation** model is put forward by Pedersen and Vanmater (2013) who 'evolve' optimised city designs by using heuristics to choose new building envelopes, road networks, public spaces etc. according to an area's metabolic capabilities and limitations.

Focus UM models have different foci, which are considered here under two sub-characteristics: models that try to understand more about the resource flows of a city, and models which study non-resource components of UM. Resource-focussed models can study just a **single resource**, as in the case of Zeng et al. (2014), who formulate mathematical models of water treatment technologies and end-uses to simulate the quantity of water and wastewater flows between them. Other models focus on **multiple resources**, such as Liang and Zhang (2011), who evaluate how various energy and material flows (including coal, water, biomass and pollutants) change under proposed policies. Sometimes, these models consider multiple resources but **umbrella** them under a single type of measurement; examples include Huang and Chen (2005) who quantify various flows including solar energy, rain and fossil fuels in units of energy⁵. Non-resource-focussed models might look at **urban form**, such as the steel-stock accounting model of Liang et al. (2014); **socioeconomics**, such as Newman (1999); and the **environment**, such as Huang and Chen (2005) who predicts an area's greenhouse gas emissions based on the construction characteristics of houses in an area.

Level The third way UM models are classified here is according to the level at which they represent components of an urban system (either conceptually or mathematically), which this thesis defines from low to high. **Low-level** models capture the most detail, considering those models which quantify resource flows occurring among an urban area's resource management processes and/or its points of demand. One example is the model of Zeng et al. (2014) who quantify the water flows between different sectors (domestic, industrial etc.) and systems (supply, treat-

⁵Energy is outlined in greater detail in Section 3.1.1.

ment etc.). Alternatively, low-level models could include those which use equations to create bottom-up mathematical descriptions of system components (e.g. Kellett et al. (2013), described earlier).

At the next level of detail, **medium-level** models include those in which conceptual or mathematical relationships are defined for a UM system's organisational sectors and/or socioeconomic functions. For example, Zhang et al. (2010) use ecological network analysis⁶ to model the resource-interdependence of 17 economic sectors to each other. In other medium-level models, Fung and Kennedy (2005) relate an area's institutional activities to its sustainability, and Huang and Chen (2005) relate an area's energy flows to its level of urban development. Finally, **high-level** models capture system dynamics in their broadest sense. For example, using simple ratios to relate the size of a society to its transport volumes (Fischer-Kowalski et al., 2004), or to relate long-term trends of energy demand to an area's upstream energy consumption (Baynes and Bai, 2012).

Each of the 108 papers captured in the search and filtering of the UM modelling literature are plotted as a point on Figure 2.5. The location of the point represents a model's focus and level, while its colour represents the type of model. The models cited above are labelled on the figure. Examining the plot, it is possible to note features and gaps in the UM modelling landscape, such as the dominance of simulation models and models which focus on how an area uses resources. However, when it comes to optimisation models, there is only one (which considers urban form). This reveals a gap for the contribution of this thesis, namely a model whose purpose is to consider the optimisation of energy, water and waste flows (i.e. multiple resources) between resource management processes (i.e. low level).

2.3 Review of resource management optimisation modelling

So far, this chapter has introduced UM as a research area that can support studies of urban sustainability, and has shown that modelling is one means by which this can happen. This thesis will add to UM modelling capabilities, a model which can optimise the simultaneous design of urban energy, water, and waste systems, so as to account for intersectoral interactions and synergies, and thus improve an area's metabolism. As discussed in Section 1.2.2, there are so many choices to be made (i.e. variables

⁶Ecological network analysis (ENA) is described in detail in Section 3.1.1.

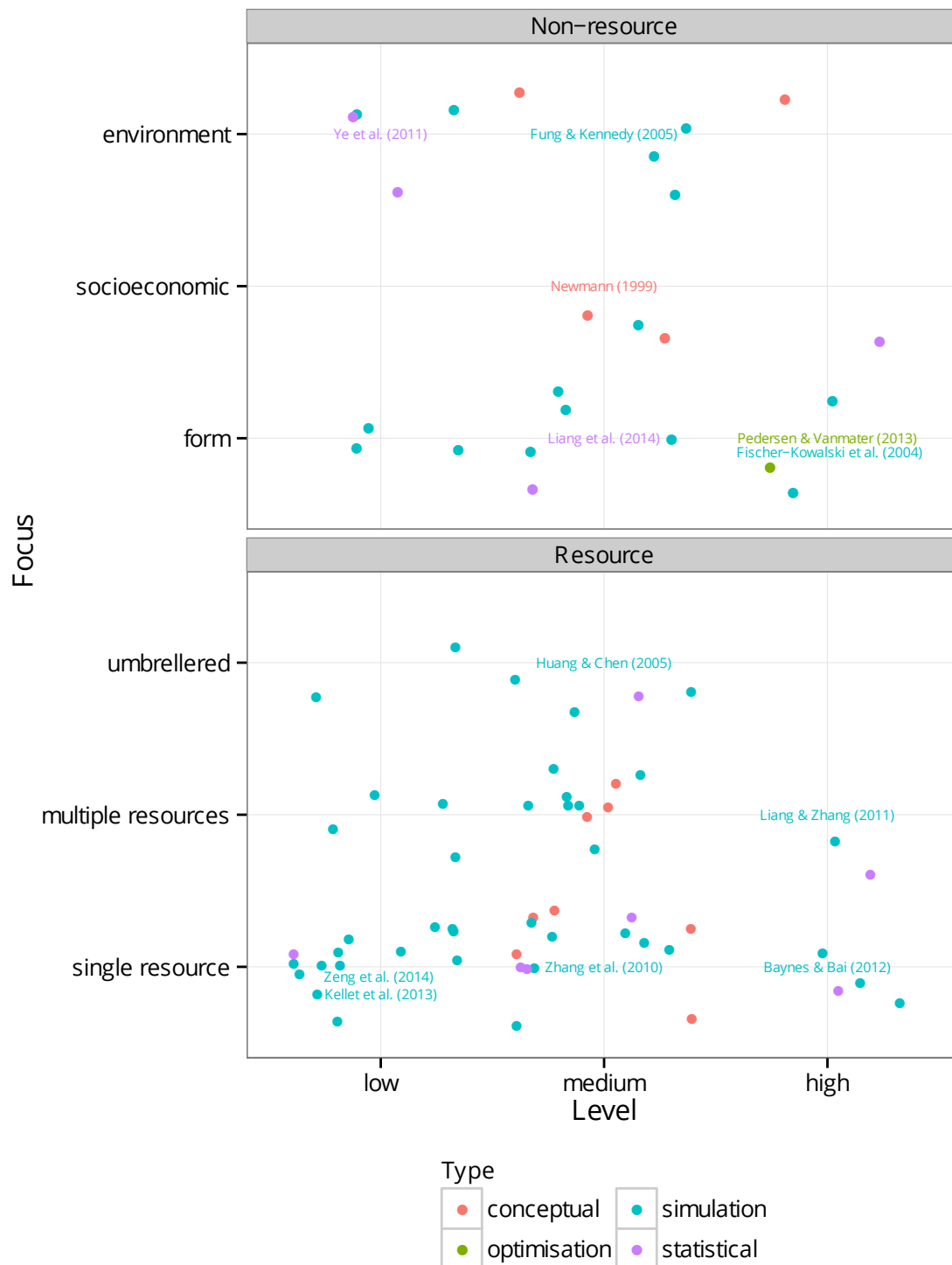


Figure 2.5: An overview of the UM modelling literature. Jitter (normally distributed random noise) has been applied to the points to prevent them plotting over one another. Models cited above have been labelled on the plot.

whose values are to be chosen) when it comes to resource management networks (which processes should be used, where should they be located, and at what rates should they operate, to name just three), that optimisation modelling should be considered a suitable approach to support the design of highly integrated urban resource management systems. In view of this need, this section reviews a number of ‘resource management optimisation models’⁷. This has two purposes: first, to confirm the need for a model which can simultaneously optimise multiple resource management systems at the urban scale (thus complementing the findings above that the UM modelling literature includes no such models); and second, to suggest possible methodologies which can be adapted for this thesis.

Each of the model types introduced in Section 2.2.2 can be found in resource optimisation modelling. Concrete models are often used to find the optimal parameters and conditions for running some process (e.g. anaerobic digestion) – these are in the form of laboratory experiments or scaled-down versions of a plant. (Often, these concrete models are coupled with statistical techniques to help find the most optimal conditions under which to operate a process.) At other times, the processes under study are represented mathematically. In simulations, variables can be changed, to investigate the effect on resource yield or some other objective related to resource management. In optimisation modelling, planners and policy makers are helped to determine the design and operation of the infrastructure which extracts, refines, converts, and transports resources. Often these optimisation models take the form of a ‘minimum cost network flow’ problem, in which a set of equations are solved to select a mix, layout, and operation schedule for resource management infrastructure to meet some objective, e.g. to maximise profit or minimise emissions (Williams, 1990, p81).

2.3.1 An introduction to the literature

The most famous resource management models are arguably the models used to help design energy systems at the national scale, such as MARKAL which attempts to plan an energy system by taking into account resource availability, infrastructural capabilities, technological possibilities, and taxation and policy regimes (UCL, 2015). It is used by governments, non-governmental organisations, and researchers around the world to help propose and plan national energy strategies (US EPA, 2015).

⁷Note that ‘resource management optimisation modelling’ is not a subject area which has a formal definition (unlike say, ‘urban energy systems modelling’ (which is formally defined in Keirstead et al. (2012a)), rather it is used here to refer generally to optimisation models which are used to assist planners and policy makers improve the management of an energy or material resource for which they are responsible. It can incorporate everything from the efficient production of a single resource in some component of a plant, up to global strategies to manage.

Of most interest to this thesis however, are optimisation models formulated at the urban scale, and in particular, those that consider energy, water, and waste systems. One example of an urban-scale resource management optimisation model is the urban energy systems model of Keirstead and Shah (2013). In one application, the model evaluates energy supply for a UK eco-town, focussing on the potential benefits of biomass-based systems (Keirstead et al., 2012b). A set of linear equations represent the resource quantities (e.g. biomass, heat, electricity, etc.) supplied to and removed from zones within the town at any given time. Parameters represent the zonal resource demands, resource availability, and technology behaviour. Variables represent whether a technology is present in a given zone, and at what rate it operates, as well as a schedule of resource movements within and without the city.

Optimisation models also are used to help plan urban water supply networks. For example Samani and Zanganeh (2010)'s model optimises the performance of an area's existing water network, choosing reservoir heights and pump sizes. Lejano (2006) applies optimisation modelling to a network design, starting with the spatial distribution of customer demands, it selects appropriate locations for the pipes. Some water optimisation models also seek to minimise a system's freshwater consumption through employing water reclamation processes and water saving technologies – examples of these can be found in Lim et al. (2010) and Makropoulos et al. (2008). Finally, there are a number of municipal waste management planning models such as Li and Huang (2006). These models allocate waste flows from their point of generation to various management facilities, to inform long-term decisions. (i.e. investment choices and capacity requirements).

2.3.2 An overview of the literature

The energy, water and waste models introduced above vary in their formulations, according to their different purposes. Moving from these specific examples, to consider the resource optimisation models more generally, a quasi-systematic literature review can help to identify trends and patterns in how model formulations vary according to purpose. This will reveal gaps in the literature which will be met by this thesis, as well as precedent methods which can inspire the formulation of the model in this thesis. The first stage of the review used the Scopus tool to search for relevant literature, using the search term `energy AND water AND waste AND optimization model` (excluding irrelevant

subject areas such as psychology).

This step returned 6,840 results which were filtered using R code to automatically remove titles not containing words related to ‘optimization’, and titles unrelated to resource management⁸; before other irrelevant titles were removed manually. This left 135 documents, which describe optimisation models at various scales, from optimising some component in a power plant, to planning strategies at a regional level. The results include both concrete models (usually in the form of laboratory-based experiments which find the operating conditions which resulted in optimal resource production), and abstract models.

This review could consider many different ways to categorise models (e.g. spatial and temporal resolution, time horizon, incorporation of endogenous resource demands, integration capabilities with other models, etc.), but will focus on three characteristics most relevant to this thesis, namely: the **scale** for which the model optimises resources; the **level** at which models make infrastructure planning decisions; and the extent to which models integrate different resource management systems in order to take advantage of synergies (**integration**). Note that this reviews the way the system has been conceptualised, rather than the technical detail of the model (which will be discussed in Chapter 5)⁹.

Scale There are various scales at which resource management is optimised, ranging from a component in a plant (e.g. Wu et al. (2015)) to thinking about how resources should be managed at the global level (e.g. Liu and Papageorgiou (2013)). The majority of the literature concerns how to optimally use resources within a plant such as a power plant (e.g. Prasertsan et al. (2001)), or a chemical refinery (e.g. Rizwan et al. (2015)). However, there are still a significant presence of models which consider multiple facilities, within EIPs (e.g. Taskhiri et al. (2014)) and cities (e.g. Newman et al. (2014)).

Level Some optimisation models are used in research, or the early exploratory stages of a system design, whereas other models are used to generate the precision required to design and operate a real-world system. These models tend to differ in terms of the detail to which they design a

⁸This filtering began by removing common words (e.g. ‘the’) using the functionality of the text mining package `tm` in R, before identifying 11,967 unique words. Then, from this automatically generated list, words which did not refer to resources (e.g. ‘network’) were removed manually, leaving 366 unique words. Only titles containing words from this list remained in the review.

⁹The review methodology used here has similarities with those used elsewhere – see for example the review of urban energy systems models in Keirstead et al. (2012a).

model. (Note: this is not the same as spatial or temporal scale, though it might be more likely for models which consider smaller geographical areas and/or shorter time horizons to be more detailed.) The most detailed models make **low-level** decisions, optimising variables such as the concentration of chemicals used in the production of lithium hydroxide (Grágeda et al., 2015), and the moisture content of biomass in a gasification plant (Morandin et al., 2013).

At the **high-level**, models consider a system's superstructure, representing it as a network of resource sinks and sources, and the connections between them. Often, their job is to identify optimal quantities and timings of resource transfers between these sinks and sources. They may optimise a spatial layout (the location of, and distance between sinks and sources), but they do not go into the precision of detailed design. Examples include Keirstead et al. (2012a)'s urban energy system model, the urban water system models of Lim et al. (2010) and Makropoulos et al. (2008), whose models maximise opportunities for wastewater reuse, by identifying urban sinks and sources of waters of various different contamination levels, and optimising how they might be connected.

Between the high- and low-level models are those that make decisions at the **medium-level**. These models have as their main focus a system's superstructure, yet there are still some low-level variables considered by the model. An example is Newman et al. (2014) which not only models the relationships between sinks and sources of an urban water distribution system, but also design features such as pump sizing.

Integration Thirdly, resource management optimisation models can vary in the extent to which they integrate different resource management systems. Here, three levels of integration are defined, each of which indicates to what extent a model considers intersectoral interactions and synergies as part of the optimisation. These levels of integration are diagrammatically represented in Figure 2.6.

Some models are **non-integrated**. These models optimise just one resource system, such as the urban energy systems model of Keirstead et al. (2012b), or the urban water network model of Keedwell and Khu (2006). **Integrated** models on the other hand will optimise for one resource, but while describing other systems, such as Deng et al. (2013), which considers a chemical plant, but optimises its water network (i.e. the quantity of chemical production is mathematically

modelled, but the model's objective is to minimise freshwater use). These integrated models will explicitly model the interactions between systems. Finally, **highly integrated** models try to simultaneously meet the demands for more than one resource management system. These highly integrated models will explicitly model not only the interactions between systems, but also the synergies. Examples include Moon et al. (2009) which simultaneously optimises treatment of waste water and the provision of heat (via heat exchange networks) in process industries.

The resource management optimisation models in the filtered list have been plotted as points on Figure 2.7. The points are coloured according to the modelling type, while its scale, level of integration, and level are represented by its location. The models cited above are labelled on the plot. The figure shows that, in general, smaller-scale systems are more interested in just a single resource, and their systems are modelled in greater detail. These models are also more likely to be experimental. Larger systems are more likely to consider multiple resources in an integrated or highly integrated fashion, but none of these models go into design detail (all are either medium- or high-level). For these models, mathematical optimisation is the most commonly used method.

Highly-integrated models (the focus of this thesis) are still the least common type, and especially so at the city scale where models tend to only consider one resource sector in isolation (e.g. an urban energy system), or the integration of energy or water systems into other systems. The two highly-integrated models at the city scale consider how water and wastewater systems can work together to minimise freshwater consumption (Newman et al., 2014, Lim et al. (2010)). This lack of urban-scale highly-integrated models means there is little to help the decision maker to take advantage of the infrastructure co-location to realise intersectoral synergies in the urban environment. By neglecting these synergies, current optimisation models used to help plan urban resource management systems impose a ceiling on potential material and energy savings.

This thesis will begin to meet this gap by formulating a city-scale, highly-integrated optimisation model. An additional insight this literature overview gives is that the model should be high-level. This is intuitive when considering multiple resource system types: it is prudent to start with a simple representation of the various systems, before delving into the intricacies of design detail and system operation, which require specialist expertise about the systems being modelled.

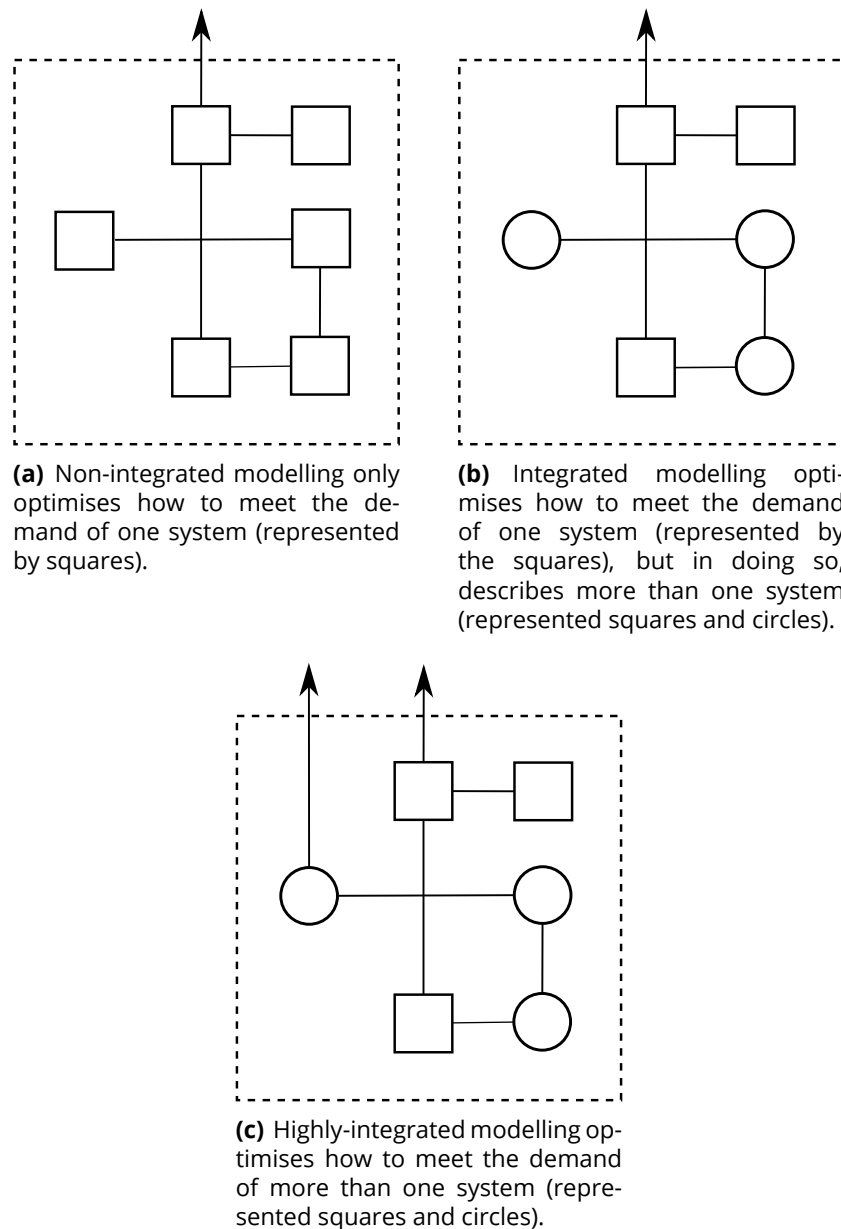


Figure 2.6: Different levels of modelling integration of resource management systems. The dotted line represents the boundary of a system; the arrows represent demands for which the system is optimising.

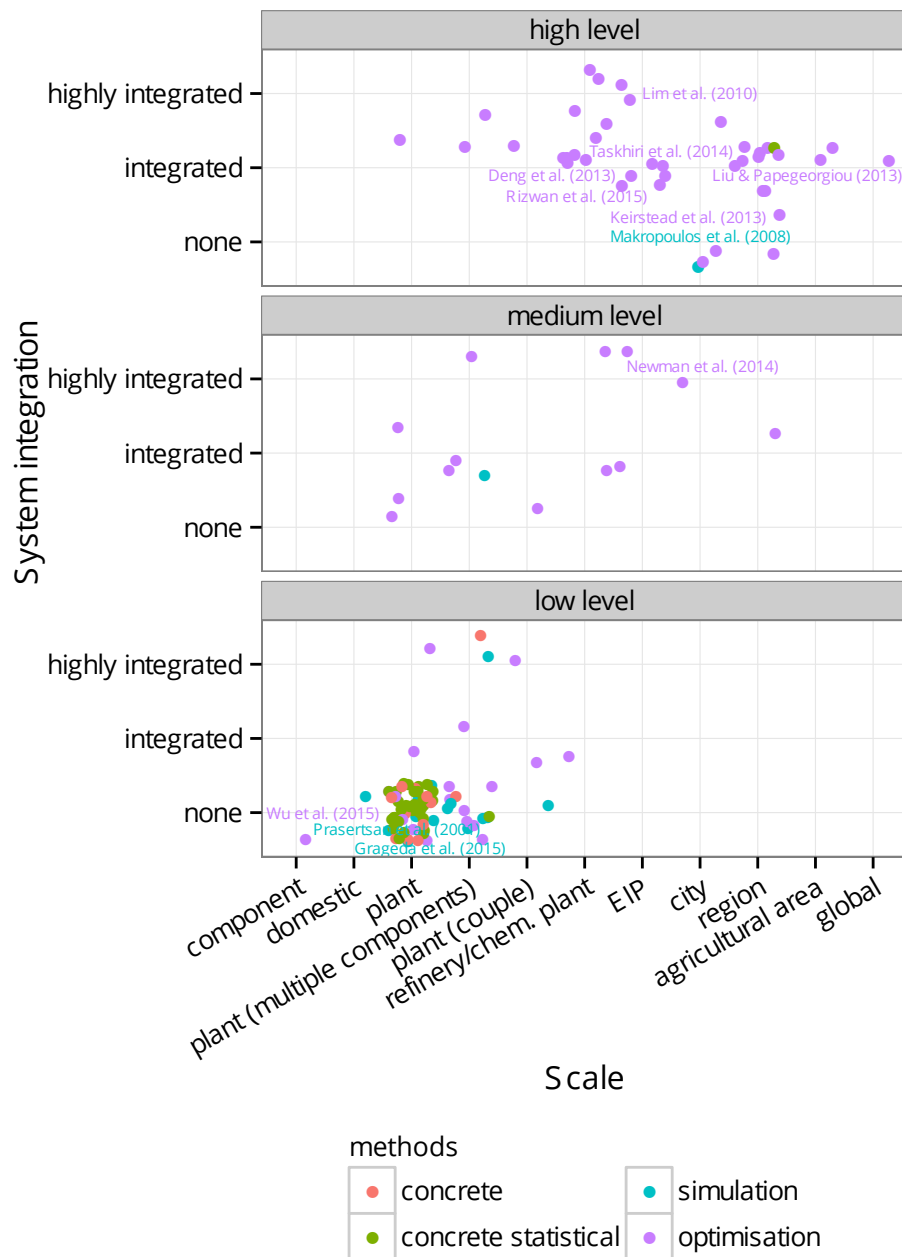


Figure 2.7: An overview of the resource management optimisation literature, with each point representing a reference. Jitter has been applied to the points to prevent them overlapping one another.

2.4 Conclusion

This chapter has revealed two gaps in the literature which motivate and inform the rest of this thesis. First, as a framework which examines how cities manage resources, the urban metabolism concept does not sufficiently account for how an area's network of processes affects its aggregate metabolic flows. Second, while modelling is often used to aid understanding of urban metabolism, there is space for a model which considers the integrated planning of energy, water and waste management processes at the urban scale, to optimise how an area meets resource management demand in view of the impossibility of evaluating all the possible choices which can be made to make up an urban resource management network. The rest of this thesis brings these two research needs together. Representing a city's network of resource management processes in a conceptual model which describes its metabolism (Figure 2.1) will become the foundation for building an optimisation model which can consider interactions and synergies between the energy, water and waste sectors.

Chapter 3

Performance metrics for urban metabolism

“This article, certain to become the classic in the field, clearly demonstrates that apples and oranges are not only comparable; indeed they are quite similar. The admonition ‘Let’s not compare apples with oranges’ should be replaced immediately with a more appropriate expression such as ‘Let’s not compare walnuts with elephants’ or ‘Let’s not compare tumour necrosis factor with linguini.’”

Barone (2000), *The British Medical Journal*

A version of this chapter was published as: Ravalde, T. and Keirstead, J. (2015b). Comparing performance metrics for multi-resource systems: The case of urban metabolism. *Journal of Cleaner Production*, 163:S241–S253. The ‘Urban metabolism and sustainability’ section of the paper was reworked into Section 2.1 of the literature review.

Chapter 1 argued that there is untapped potential for cities to improve their metabolism by getting

their energy, water, and waste management sectors to work together; Chapter 2 showed that the UM and resource management optimisation fields lack the modelling capability to realise this possibility. However, before developing a model to support the integrated management of urban resource systems, it is important to consider how to measure the performance of such an integrated system – i.e. which metrics could (or should) quantify the metabolic performance of a system which is made up of many different resources and processes? It is this question which is the concern of this chapter.

The conceptual model described in Section 2.1.2, shows that for a city to meet demand for products and services, a mix of resources must pass through a chain of processes. Systems such as these are hereafter referred to as *multi-resource* (MR) systems. Examples of MR systems include: agriculture, which converts nutrients, water, and solar energy into various forms of plant and animal matter; a factory producing products from inputs of capital, labour, and raw materials; or indeed entire economies which generate wealth and well-being from diverse inputs. Although the definition of a resource can thus be very broad,¹ a common feature of these resource-process networks is that the system operators normally face a choice about how best to allocate resources and processes for a desired set of outputs. Consider a manufacturer who requires a certain metal for a production process. This metal could be acquired from virgin sources or it could be reclaimed through recycling. However the latter option would require additional energy and chemical inputs to achieve the desired quality (Amini et al., 2007; Ignatenko et al., 2007), and so the final choice of virgin or recycled metal will depend on the manufacture's priorities, for example, minimising cost, maximising supply chain reliability or improving environmental performance. This decision-making process whereby system operators evaluate a range of alternative options to produce required products and services, each with different impacts, can be described as the *multi-resource trade-off problem* (MRTP).

If cities (the important subset of MR systems relevant to this thesis) are to shift from linear to circular metabolic patterns, there need to be effective measures of system performance to assess whether one conversion pathway is more benign than another; in this way, the MRTP manifests itself in urban areas. The aim of this chapter is to evaluate how UM flows (energy and material) can be used to calculate performance measures of urban resource use in view of the MRTP. This makes a general novel contribution to UM research (for example, to guide policy or investment decisions), but also makes a

¹This chapter considers GDP, population and land as resources, since these are examples of the socioeconomic services provided by urban areas.

specific contribution to this thesis, namely to to meet Aim 1 of the research question (to “Assess how well models improve urban metabolism”, Section 1.4.2). The next section proposes a general framework for assessing the resource performance of an MR system, thus unifying previously published metrics. Recognizing that the MRTP can be shaped by a number of subjective criteria, this review focusses primarily on physical measures of performance (but the framework is general and could be used for other objectives as well). The metrics are then applied to a global set of UM data (Section 3.2) and this is followed by discussion on what the results mean for decision makers seeking to measure and improve urban resource performance, the limitations of these measures, and how the UM field might develop to overcome these obstacles (Section 3.3).

3.1 Measuring the resource performance of MR systems

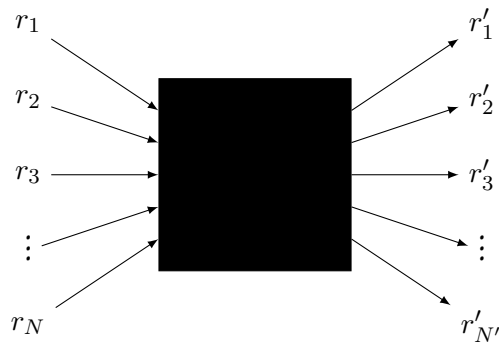
This section considers MR systems, providing a formal definition of resource performance measures and identifying how they have been applied in the literature to date. This begins by introducing a general framework which distinguishes between ‘black-box’ and ‘grey-box’ representations of an MR system (illustrated in Figure 3.1).

3.1.1 ‘Black-box’ metrics

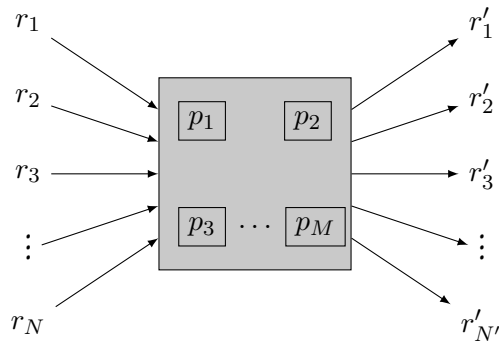
In this representation, there is no knowledge of the processes within the MR system; one only observes the resource flows in and out, as is the case with typical UM accounts. This is also the standard representation of a system within systems engineering and it allows one to define two broad categories of performance metric: absolute measures (α) and efficiency ratios (η), which are outlined below, with their properties summarised in Table 3.1. This understanding is consistent with most conceptual models of urban metabolism, in which a city is essentially a black box, into and out of which resources flow.

Absolute measures

Absolute measures are simply a linearly weighted sum of inputs and outputs (3.1):



(a) 'Black-box' representation, with no knowledge of internal system processes.



(b) 'Grey-box' representation, with internal processes $p \in P$, for $|P| = M$. These could include energy conversion, water supply and waste management.

Figure 3.1: Representations of MR systems with resources $r_i \in R$ and $r'_j \in R'$ for $i = 1, 2, 3, \dots, N'$ and $j = 1, 2, 3, \dots, N'$, where R is the set of input resources, and R' is the set of output resources.

$$\alpha = \sum_{i=1}^N w_i r_i + \sum_{j=1}^{N'} w'_j r'_j + k \quad (3.1)$$

where R and R' are the set of input and output resources, respectively, and are populated by input resource quantities r_i , and output resource quantities r'_j , with w_i and w'_j denoting weights which can be applied to these resource flow quantities. For completeness, a constant k may also be added, although the discussion below assumes that $k = 0$. The simplest theoretical case is where $N = N' = w_i = w'_j = 1$, such that just one resource is considered in a performance metric. However by applying weights, multiple resources can be resolved into a common measure of value, often corresponding to some environmental or other impact. Three such approaches include ‘footprints’, other sustainability measures and more subjectively weighted sums, considered below. (The categories are not definitive but have been selected here for convenience.)

Footprint measures are usually associated with specific environmental impacts, and a common example is the carbon footprint (CF). CFs are often used to measure the contribution of a system to global warming and are calculated using weights which correspond to the carbon emissions produced in the production of system input resources r_i , thus quantifying the total emissions associated with a system as it meets demand for goods and services. The CF is widely used, with examples found in MR systems of all scales, from cement production (Amato, 2013) and biodiesel production (Batan et al., 2010), to urban energy systems (Bhatt et al., 2010), and to cities as a whole (Ramaswami et al., 2011). Alternatively, the water footprint (WF) of a system represents the total freshwater required to produce and supply goods and services to consumers (Water Footprint Network, 2015). Examples include fuel production processes (Okadera et al., 2014), or entire cities such as Vienna (Vanham and Bidoglio, 2014) and Macao (Chen and Li, 2015). CF and WF evaluations differ in formulation, since the CF is calculated from resource inputs (such as fuels and materials) only, such that $w_i \neq 0$ for at least one i , but $w_j = 0$ for all j ; but the WF sums water embodied in non-water resource inputs together with the system’s water outputs (e.g. domestic drinking water), so $w_i \neq 0$ and $w_j \neq 0$ for some cases of both r_i and r_j . A more complicated footprint measure is the ‘ecological footprint’ (EF) which converts resource consumption and waste outputs into the equivalent land area required to sustain a system (for example, by meeting food and fossil fuel demands and absorbing emissions (Rees, 1992)), with example city EF

evaluations including London (Chambers et al., 2002), Shenyang and Kawasaki (Geng et al., 2014).

Other weighted sums can be found within the sustainability literature. The sustainable development concept seeks to meet the “needs of the present without compromising the ability of future generations to meet their own needs” (Brundtland et al., 1987, Chapter 2), and much effort has been devoted to measuring the sustainability performance of an industry, business or economy. This concept has environmental, economic and social aspects and thus the literature covers biophysical measures (which quantify environmental impacts, by explaining “the relationships within complex systems through a natural science perspective” (Gasparatos et al., 2008, p.299)), and monetary measures (which quantify the economic dimension). These can then be combined into integrated sustainability assessments (Gasparatos et al., 2008). One biophysical measure is energy, which is a “thermodynamical measure of the energy used to produce a resource” (Siche et al., 2008, p.630). The single measure under which system performance is quantified is the solar energy required to sustain it, with weights corresponding to the solar energy required to produce input energy and material resources (Odum, 1983). Emergy analysis generally finds application in larger systems, such as cities (Zhang et al., 2009c,b) or countries (Gasparatos et al., 2009a). For an economic evaluation, financial cost offers another possible weighted sum. This need not be limited to the purchase price of individual inputs; environmental effects can be incorporated by costing wastes and emissions as taxes or purchase credits (Sirikitputtisak et al., 2009). Another environmentally informed financial costing method is the ‘genuine savings’ index (which is typically applied at the national level); this adjusts the GDP of an economy by employing a formula which assesses natural resource depletion and pollution damage in economic terms (Nourry, 2008).

However many sustainability problems are highly subjective. Multi-criteria decision analysis (MCDA) weights resource flows according to a stakeholder’s priorities, which are then summed to give an overall score which can be used to assess system performance. For example the food production model of Mehdizadeh et al. (2011) combines energy consumption and cost in this way, weighting these terms using coefficients which reflect the relative importance of energy and monetary expense to the system operator (rather than the physical units as above). MCDA can provide methods to carry out life-cycle assessment (LCA), which associates a system with various impacts (each of which might be the result of weighted sums). Impacts could include greenhouse gas emissions, ozone depletion and eutrophication amongst others. These impacts are then combined using subjectively defined weights, resulting in a weighted sum of weighted sums. LCA methods are applied at all scales: from sewage sludge-to-

energy conversion (Mills et al., 2014), to waste management more generally (Eriksson et al., 2002), and to urban areas as a whole (Chester et al., 2012).

Efficiency ratios

Often it is the efficiency, rather than absolute performance of an MR system which is of interest. This is commonly understood to be the ratio of outputs to inputs and therefore a general linear representation of efficiency can be defined as in (3.2).

$$\eta = \frac{\sum_{j=1}^{N'} w'_j r'_j + k'_j}{\sum_{i=1}^N w_i r_i + k_i} \quad (3.2)$$

The literature contains at least three specific configurations of system efficiency. This thesis denotes the first class of efficiency metrics as η_1 ; these are where only one resource type is considered as both an input and an output. (A ‘resource’ and a ‘resource type’ are distinct: electricity and coal are different resources, but they are both ‘types’ of energy resource). For example, first law energy efficiency is given as $\eta_{\text{energy}} = \text{final energy} / \text{energy source inputs}$, and is used to evaluate the performance of electrical power systems (Rosen and Bulucea, 2009), or urban energy systems as a whole (Rosen et al., 2005). Water efficiency can also be considered in this way, where the final demand for water from a system is measured with respect to the water entering the system; examples can be found in Makropoulos et al. (2008) (who use this ratio for an urban water usage indicator), and Lim et al. (2010) (whose urban water model has the objective of meeting demand whilst minimising freshwater consumption). The equivalent η_1 metric within the urban waste sector is the waste diversion rate: the ratio (by mass) of recycled waste to total waste (Zaman and Lehmann, 2013).

η_2 metrics on the other hand take the ratio of two different resources types: Keirstead (2013) calculates alternative urban energy efficiencies as the ratio of total final energy consumption relative to the area’s economic output, population or geographical area. Similarly, Zhang and Yang (2007) interprets the ratio of an area’s GDP or population to its material consumption as its ‘resource efficiency’. Browne et al. (2009) evaluate urban performance of an area from the ratio of waste disposal to product consumption. Sanders and Webber (2012) apply an efficiency metric of this type at the national level,

quantifying the energy consumption that can be attributed to water use in the United States. The final type of efficiency metric, η_3 , is where resource consumption is measured relative to a baseline, perhaps representing some environmental condition or constraint, such as urban energy consumption per unit of solar radiation (Santamouris et al., 2001). (Efficiency ratios can take other forms, but these are the main examples found in the literature.)

Table 3.1: Black-box resource performance metric classes.

Class	N	$w_{i,j}^{(l)}$	$r_{i,j}^{(l)}$	$k_{i,j}^{(l)}$	Example
α	> 1	1	≥ 0	0	Carbon footprint
η_1	≥ 1	1	i, j of same type, $r_{i \vee j}^{(l)} \geq 0$	0	Final energy / energy source inputs
η_2	> 1	1	i, j of different type, $r_{i \vee j}^{(l)} \geq 0$	0	Final energy / GDP
η_3	≥ 1	≥ 0	$r_{i \vee j}^{(l)} \geq 0$	$k_{i \vee j} > 0$	Final energy / solar radiation

3.1.2 Grey-box metrics

Black-box metrics are widely used and understood but they provide very little information about the processes at work within the urban boundaries, which is a key consideration of the new conceptual model which seeks to understand the middle of an urban metabolic system. In the grey-box representation (Figure 3.1(b)), analysts have information about the conversion processes occurring within the city, which would allow them to identify industrial symbioses that could not be discovered simply by examining overall system inputs and outputs. This is in line with the process-oriented conceptual model proposed in Chapter 2. This section considers two methods that can be used to derive metrics from knowledge of the resource-management processes at work within a city: exergy analysis and ecological network analysis.

Exergy analysis

Exergy is the “maximum useful energy we can extract from some source of energy” (Allwood et al., 2012, p. 119). To obtain ‘maximum’ energy requires that the resource is brought into equilibrium with its surroundings, which means that exergy is defined relative to a reference environment. For example heat energy is more ‘valuable’ (or is said to be of better ‘quality’) at higher temperatures, since it is more readily transformed into other energy types (such as movement). When taking all energy types

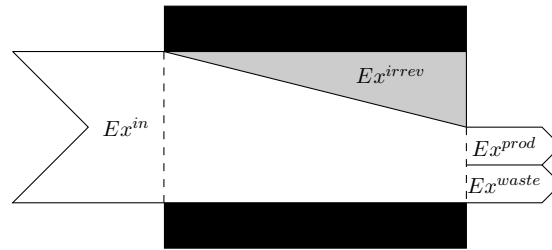


Figure 3.2: Exergy flows Ex^* for a process p .

into consideration, the exergy of a system is a sum of the temperature, pressure and chemical potential of material and energy flows relative to the reference environment (Rosen and Dincer, 2001).

As a resource is brought into equilibrium with its surrounding environment, chemical reactions, as well as mass and energy transfers, occur which reduce the useful energy that can be extracted. For example during combustion, heat is transferred from hotter oxidised molecules to cooler unoxidised molecules (Som and Datta, 2008). Energy has not been lost, but it has been devalued into a form that cannot be recovered. Thus while a system conserves mass and energy, it destroys exergy in proportion to the system's increase in entropy (or disorder) (Rosen and Dincer, 2001). This dissipation of mass and energy throughout a system is impossible to reverse without an input of energy, and thus exergy destruction is said to arise from 'irreversibilities'. Therefore any process p which produces outputs from a set of inputs, exergy flows (Ex^*) can be related as in (3.3):

$$Ex_p^{in} = Ex_p^{prod} + Ex_p^{waste} + Ex_p^{irrev} \quad (3.3)$$

where each term (reading left to right) corresponds to the exergetic value of inputs, desired products, wastes and irreversibilities. This exergy balance is visualised for a generic process in Figure 3.2.

These terms can be used to define absolute and efficiency metrics for each process p within a system, and for the system as a whole. A process's exergy depletion, α_{ex} , is equivalent to Ex_p^{in} , whilst its efficiency is given as $\eta_{ex} = Ex_p^{prod} / Ex_p^{in}$. The exergy efficiency of an area as a whole can be found by combining each process to evaluate the sum of the parts (3.4):

$$\eta_{ex} = \frac{\alpha_{ex}^{prod}}{\alpha_{ex}^{in}} \quad (3.4)$$

where,

$$\alpha_{ex}^{in} = \sum_{p \in P} \sum_{i \in R^i} Ex_{p,i}^{in} \quad (3.5a)$$

$$\alpha_{ex}^{prod} = \sum_{p \in P} \sum_{j \in R^j} Ex_{p,j}^{prod} \quad (3.5b)$$

Equations (3.5a) and (3.5b) limit the consideration of energy to only those flows which cross the grey-box boundary. Other process inputs and outputs which remain inside the boundary are ignored, since efficiency is assessed at the whole-system level, not the process level.

Exergy analyses are commonly applied to energy conversion processes, such as district heating (Çomakli et al., 2004; Rosen et al., 2005; Ozgener et al., 2005), space heating (Rosen et al., 2008) and power plants (Kaushik et al., 2011). Because exergy efficiency analysis takes into consideration the “different nature and quality” of energy forms (such as electricity and heat), it “pinpoints the locations and causes of inefficiencies more accurately” than energy efficiency analysis (Rosen et al., 2005, p.158), and thus will inform a system operator where optimal efficiency improvements can be made.

In energy conversion processes, Ex^{in} typically originates from a fuel source (such as coal), whose exergy is quantified from its chemical composition relative to a reference environment. This principle allows the exergy concept to extend beyond energy resources, and provide a common measure of resource quantity and thereby enable the comparison of “apples with oranges” (Ayres et al., 1998b, p.361). Thus the exergetic value of water is not just dependent on its temperature, but also on the chemical composition of pollutants it contains (Huang et al., 2007). Therefore, by using reference environments based on water treatment standards (for drinking or other uses), exergy analysis has found application in measuring the performance of water resource systems (Chen et al., 2009a,b; Huang et al., 2007). This includes quantifying the benefits of water reclamation in urban water management (Wang et al., 2011); assessing the environmental performance of wastewater treatment plants (Mora

and de Oliveira, 2006; Khosravi et al., 2013), and comparing water supply and treatment technologies (Martínez, Amaya; Uche, Javier; Rubio, Carlos; Carrasquer, 2010). More generally, exergy analysis is applied at many different scales, from lower-level processes such as cement production (Koroneos et al., 2005; Madloul et al., 2012; Renó et al., 2013), biofuel production (Sciubba and Ulgiati, 2005), chlorine production (Ayres et al., 1998b) and car recycling (Amini et al., 2007; Ignatenko et al., 2007); up to the highest level, where studies quantify exergy flows for the whole of the United Kingdom (Hammond et al., 2001; Gasparatos et al., 2009b) and China (Zhang and Chen, 2010).

In summary, exergy analysis provides appropriate metrics for grey-box analysis (i.e. looking at the middle of an urban metabolic system) because it is performed at the process level, providing information about resource flows inside a region. Further to this, it does not disqualify any resource type or process from study (unlike energy or mass flow analysis), being able to umbrella energy, water and waste resources into a common measure of value.

Ecological network analysis

Thus far, this chapter has considered system performance metrics which quantify the resource flows, but an alternative approach is to calculate the degree to which system processes are dependent on each other. This can reveal if there is scope to increase the symbiotic links between processes (using a waste from one process as an input to another); or conversely, if process dependencies should be minimised to reduce the risk of overall system failure in the event that one component fails. Such a method is provided by ‘ecological network analysis’ (ENA). ENA finds its origins in evaluating how species interact in ecological networks (Finn, 1976) by quantifying their interdependencies, to see how species persistence or extinction might develop through mutually beneficial or exploitative relationships. ENA is based on work by Leibovich (1978) who adapted the economic input-output analysis of Leontief (1986) to quantify the interdependence of species within an ecosystem, and can be derived from the representation of interactions within the environment formalised by Patten (1978). Figure 3.3 presents an example where a bee and a plant both mutually benefit from their interactions, but the plant is exploited (i.e. eaten) by a butterfly (this example is adapted from Bascompte (2010)). This case shows only ‘direct’ dependencies (which are usually empirically measured, and must be valued with some common unit of ‘currency’, such as mass or energy). In order to appreciate fully the system interdependencies, ‘indirect’ relationships must be incorporated; for example, the butterfly is indirectly

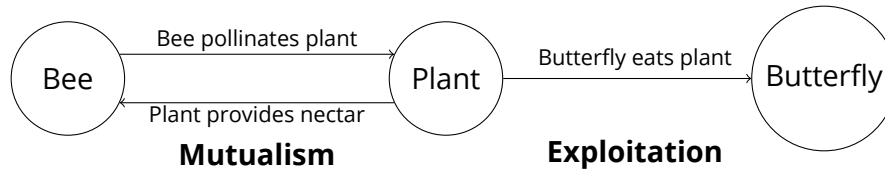


Figure 3.3: Direct dependencies in the bee-plant-butterfly ecological network. Arrows going in both directions between nodes indicate a mutual relationship, whereas an arrow in one direction indicates an exploitative relationship.

dependent on the bee, by virtue of the plant's direct dependence on the bee. To quantify interdependencies in a system that take indirect relationships into account, direct flows between species (more generally referred to as 'compartments') undergo matrix-based mathematical operations (for these see Zhang et al. (2009a)). These results are then interpreted to reveal whether pairs of compartments possess mutually beneficial or exploitative relationships.

ENA methods have been applied to urban systems (Bodini and Bondavalli, 2002), since they are analogous to natural eco-systems, in the way that compartments interrelate. Furthermore (as mentioned earlier in Section 2.1.2), they have been used in UM studies, for studies which view the middle of a UM system as a set of economic sectors (rather than engineering-process view proposed in this thesis). A simple example of the ENA-type dependencies in cities is energy conversion, which requires cooling water, whilst water supply requires energy (for treatment and transportation); thus these sectors are in a mutual relationship.

In the ENA of urban areas, the system compartments are determined by the analyst; for example Zhang et al. (2009a) studies the relationships between five compartments (the domestic sector, agriculture, industry, the internal environment and the external environment) using energy as the common unit of flow. Liu et al. (2011) apply the same methods to Beijing (but with compartments of extraction, agriculture, industry, energy conversion, transportation, and domestic and tertiary services), and use exergy to value the intercompartmental flows (which include fuels, ores and agricultural products). Liu et al. (2011) show how decision-making support can emanate from ENA, by revealing that relationships between most of Beijing's inter-sectoral pairings are exploitative, and thus arguing that there is greater scope to encourage symbiotic relationships between compartments, and thereby reduce the overall dependence of Beijing on its surrounding environment.

3.2 Applying the methods

Having described the variety of ways in which the performance of an MR system might be assessed, with examples from the UM literature, this section goes on to apply these methods in order to illustrate the utility of the black-box and grey-box approaches. The analysis uses the dataset from Kennedy et al. (2014) which includes urban metabolic flows and other data (such as GDP, population, land area etc.) for 27 megacities for 2001, 2006 and 2011.² The aim here is not to identify the best performing city, as measured by one or more metrics. Rather, it is to assess the relative merits of the two approaches calculated from UM data in aiding decision makers faced with the MRTTP.

3.2.1 Black-box metrics

Selecting metrics and cities

In selecting the metrics to be calculated, there were three criteria: firstly, the metrics must have been introduced in Sections 3.1.1 and 3.1.2 and be based on physical units (thus ruling out monetary measures and MCDA, which contain subjective elements); secondly the dataset must have the required fields to make their calculation possible; and thirdly, the fields must not have any missing entries. This third criteria is applied because the next step will correlate how well cities perform according to each pair of metrics. It would be unfair to do this when some observations had missing metric values. This filtering achieves a balance between having sufficient observations to make their comparison meaningful, and having a range of metrics that reflect the different types of metric (Table 3.1). This process results in evaluations of eight metrics for 29 observations (five cities for 2001, nine cities for 2006, and fifteen cities for 2011). The metrics are summarised in Table 3.2, and the performance of each city in 2011 according to each metric is displayed in Figure 3.4. Each city is scored relative to the best performing city for the metric. (This score reflects whether superior performance is indicated by a high or low value (for example, for carbon footprint, superior performance is considered a low value, but for GDP/waste, it would be a high value).)

²Thus, in theory, the metrics could be calculated for 81 city-year observations. As discussed below however, incomplete data meant that only 29 observations were used in the calculations.

Table 3.2: Summary of the black-box metrics applied to UM data.

Metric	Units	Class	Notes and references
CF	kg CO ₂	α	Ramaswami et al. (2011). This is calculated both with and without cement flows included, to observe the effect of isolating cities which have large cement production industries (such as Manila), which results in very poor performance.
WF	Litres	α	Vanham and Bidoglio (2014)
Final energy / energy sources	per cent	$\eta_{1j/i}$	Rosen et al. (2005)
Water out / water in	per cent	$\eta_{1j/i}$	Makropoulos et al. (2008)
Final energy / GDP	J/USD	$\eta_{2j/i}$	Keirstead (2013)
Final energy / capita	J/person	$\eta_{2j/i}$	Keirstead (2013)
GDP / waste	USD/kg	$\eta_{2i/j}$	Zhang and Yang (2007)
Final energy / solar radiation	-	$\eta_{3i/k}$	Santamouris et al. (2001). Both terms normalised per unit area of urban land.

Correlating the metrics

Having calculated the eight metrics for each city, and ranked city performance as described above, the performance of each city according to one metric is correlated with its performance according to another, for all pairs of metrics, using Spearman's ρ rank method. The correlations between pairs of metrics are presented as a heat map in Figure 3.5, each tile indicating the ρ value between a pair of metrics. The distributions of correlations are summarised by boxplots in Figure 3.6. Note that larger samples are more likely to reflect the statistical properties of a population (since extreme values will have a greater impact on a smaller sample). This is reflected in the confidence interval whose width is proportional to $(n - 3)^{-1/2}$ for a sample of n observations (Bonett and Wright, 2000); thus confidence in a ρ value is proportional to $(n - 3)^{1/2}$. One therefore has less confidence in the increased presence of stronger correlations in the 2001 data due to its smaller sample size. With this qualification considered, the results show that in general, the correlation of metric values is weak. In other words, there are no cities that are consistently ranked top or bottom (or any other position) across the metrics (which can be seen intuitively in Figure 3.4). This suggests that a city's resource performance depends on features

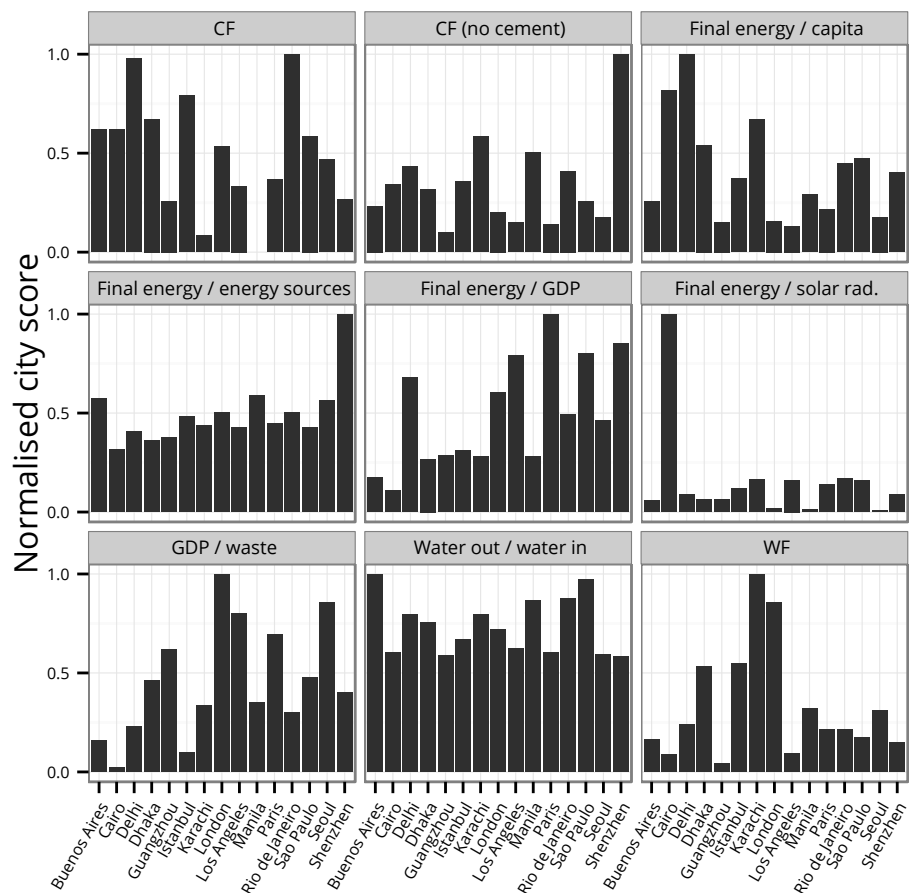


Figure 3.4: City performance score in 2011 for each metric normalised with respect to the best performing city. Best performing cities have a score of 1. CF = carbon footprint, WF = water footprint.

that are invisible to black-box metrics.



Figure 3.5: The correlation of urban resource performance according to Spearman's ρ rank.

3.2.2 Grey-box metrics

As additional data are required to calculate the grey-box metrics, they have only been applied to three cities: Beijing, London and Sao Paulo (for 2006). In addition to the energy, water and waste related flows common to most cities, the dataset records steel and cement manufacturing flows for Beijing and Sao Paulo, but not for London. Thus discussion of how grey-box analysis relates to the MRTTP (Section 5) can take place in the context of both comparable and contrasting cities. Apart from seeking areas with similarities and differences, the selection of these cities was otherwise arbitrary for the sake of convenience.

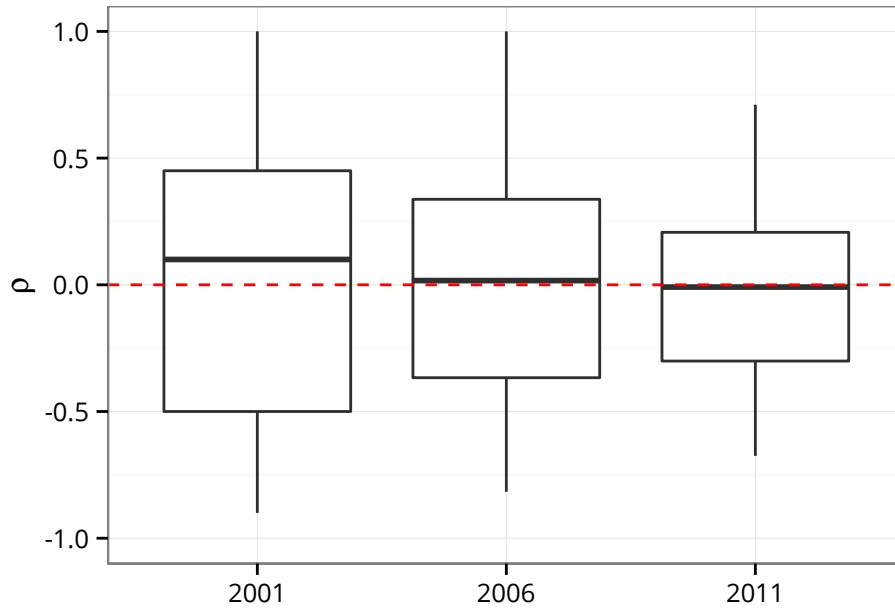


Figure 3.6: Boxplots summarising the distribution of ρ values for each year. (The dashed line indicates $\rho = 0$.)

Exergy analysis

The exergy analysis follows the procedure of Sciubba and Ulgiati (2005). Firstly, a grey box (the ‘control volume’) is defined around the M processes, using a geographic-plus definition of ‘urban’³. Secondly, from a city’s metabolic flow data the flows of materials and energy are distributed between processes inside the control volume and across its boundaries. For instance, coal may be imported from outside of the system, for use as an input to a power plant inside the urban boundary. The power plant would produce electricity, which then might be used in other processes. When flows have been distributed for all processes, the analyst should be able to draw a directed graph (where nodes represent processes, and vertices represent resource flows) in which the control volume’s inputs and outputs (energy and mass) are conserved, and all the resources can be tracked through it, with nothing unaccounted for. Thirdly, each of the flows into and out of each process p are assigned identities as exergetic inputs, products, or wastes (Equation 3.3). For example, for a coal-fuelled power plant, Ex^{in} , Ex^{prod} and Ex^{waste} are defined from quantities of coal, electricity and heat, respectively. (Irreversibilities, Ex^{irrev} , arise through heat transfer and chemical reactions during combustion.) Finally, using values from the literature (such as chemical exergies of materials, and process exergy efficien-

³Recall that this was defined in Section 1.4.1.

cies), values are assigned to Ex_p^* for $p = 1, 2, 3, \dots, M$. The flux assignments and information sources for exergy values are given for each process in Table 3.3, along with any assumptions made.

From this point, exergy depletion and efficiency are calculated for the urban system as a whole using, Equations (3.4) to (3.5b). These results are summarised in Table 3.4, revealing that Sao Paulo has a much higher exergy efficiency than the other cities. This can be explained with reference to the visualisation of the flows as Sankey diagrams in Figure 3.7(a). These display Ex^* for each process, and the system as a whole, illustrating the unification of energy and material flows under one measure, and therefore highlighting the relative exergetic impacts of a city's internal processes. The results show the dominance of exergy flows in power generation and steel production, with Sao Paulo using a much higher proportion of hydropower in the energy mix, which is a more exergetically efficient process than fossil fuel based generation.

Table 3.3: Summary of Ex_p^* flows, information sources and assumptions for exergy analysis calculations.

P	Ex^{in}	Ex^{prod}	Ex^{waste}	Notes and references
Power plant	Fuel	Electricity	Heat	Coal plant (Szargut et al., 1998); oil plant (Koroneos et al., 2004).
Hydro power	Water	Electricity		Rosen and Bulucea (2009)
Wind power	Wind	Electricity		Koroneos et al. (2003)
Heating	Fuel, electricity	Heat		Ozgener et al. (2005)
Cement production	Fuel	Cement	Heat, effluents	Madloul et al. (2012)
Steel production	Fuel	Steel	Heat, effluents	Allwood et al. (2012)
Groundwater abstraction	Electricity	Water		Rosen and Bulucea (2009). Adapting hydropower exergy methods to ground water abstraction.
Water treatments	Water, contaminants	Treated water	Effluent	Wang et al. (2011)
Wastewater treatment	Wastewater, electricity, chemicals	Treated wastewater	Effluent	Wang et al. (2011) gives thermodynamics of BOD calculations; Khosravi et al. (2013) provides quantities of process input and output flows.
Landfill	Domestic, commercial and industrial wastes		Organics, paper, plastic, glass, metal and others	Assume waste composition given by Alford et al. (2014); material exergy values from de Oliveira (2013) and Ayres et al. (1998a).

Table 3.4: Results for exergy analysis for Beijing, London and Sao Paulo. All quantities are at an annual level.

City	Depletion $\alpha_{ex}^{in} [\times 10^{12} \text{ MJ}]$	Efficiency η_{ex} [per cent]	$\alpha_{ex}^{in}/\text{GDP} [\text{MJ}/\text{USD}]$
Beijing	1.5	20	6.3
London	0.42	29	1.1
Sao Paulo	0.45	44	1.7

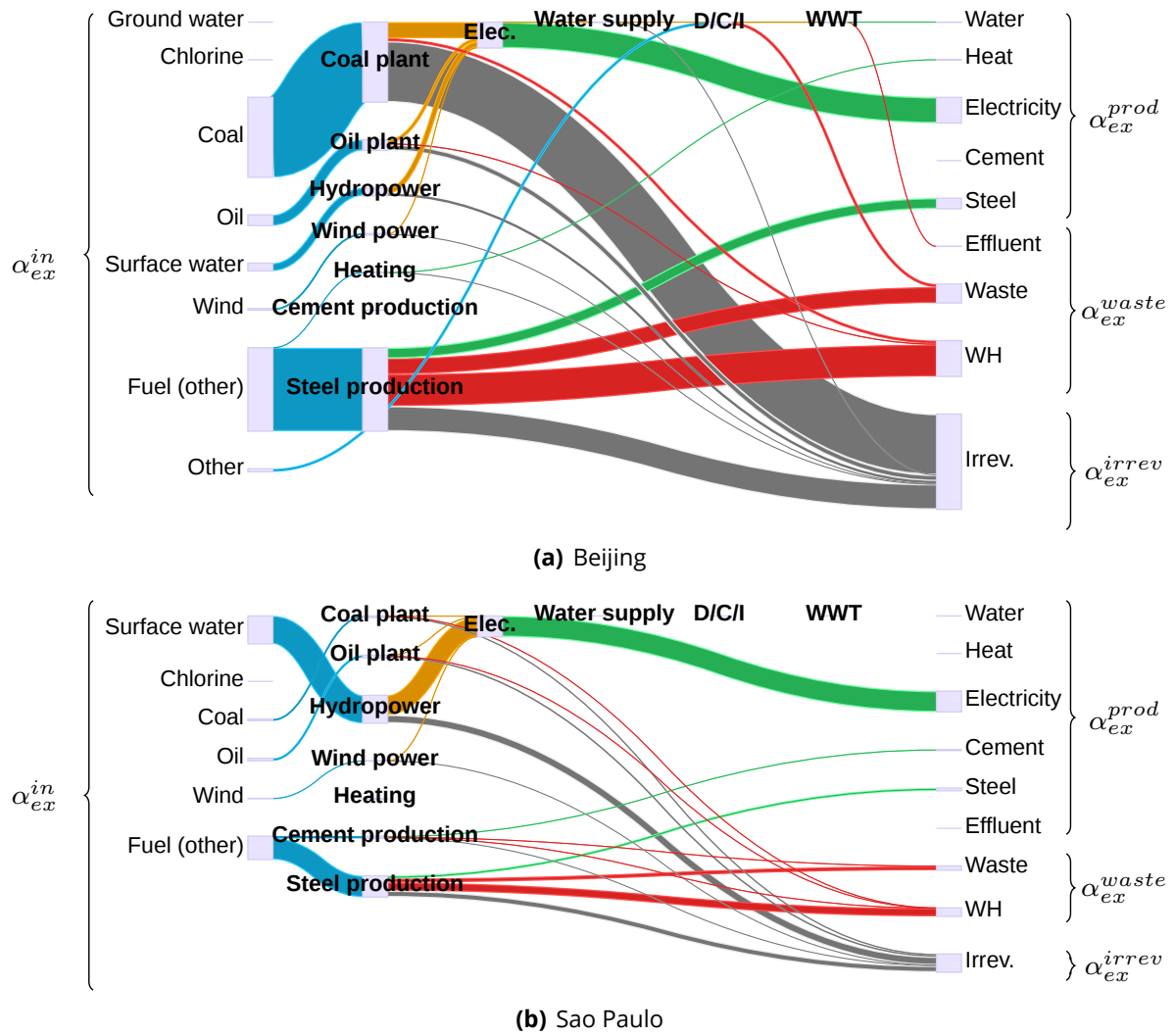


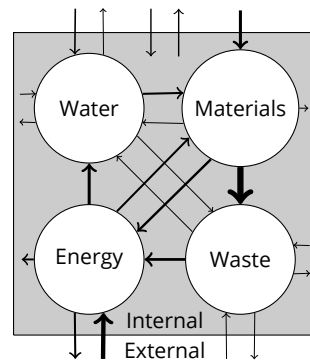
Figure 3.7: Exergy flows represented as a Sankey diagram, drawn using the tool built by Counsell (2014). **Key:** 'Elec.' = electricity used in other processes, 'D/C/I' = Domestic, commercial and industrial water use, 'WH' = waste heat, 'Irrev.' = irreversibilities. Note: 'Fuel (other)' includes natural gas, and other fuels accounted for but not identified by name in the UM dataset of Kennedy et al. (2014).

Ecological network analysis

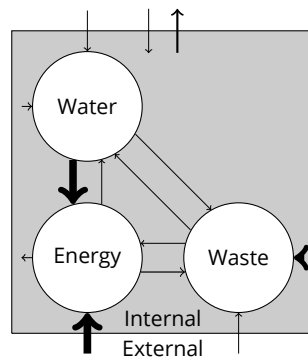
ENA requires a ‘common currency’ to unify resource flows, and the following analysis uses exergy given (i) the precedent provided by Liu et al. (2011), and (ii) the exergy flow quantities are known from the analysis above. The method follows a simplified version of the methodology in Liu et al. (2011), which starts by defining the same control volume around the resource flows and processes as for the exergy analysis. Appropriate organisational compartments into and out of which all exergy fluxes will transfer, are defined; there are six sectors, broadly based on those used by Zhang et al. (2009a):

- a. External environment (everything outside the grey box)
- b. Internal environment (everything inside the grey box, which contains the remaining four compartments)
- c. Energy management (the conversion of renewables and fossil fuels into final energy)
- d. Water management (the treatment and supply of water for industrial, commercial and domestic use)
- e. Waste management (landfill and incineration)
- f. Materials management (cement and steel production)

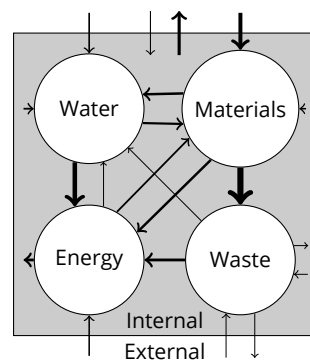
Using the exergy analysis results, exergy flows are assigned between compartments. For example, electricity from a coal-fuelled power plant comes from the energy compartment (c) some of which is used for final consumption in the internal environment (b), and so would be recorded as flow f_{cb} . All the flows are combined into a matrix, on which operations are performed which enable the identification of mutualism and exploitation between each pair of compartments (specifically Equations (12) and (13) in Liu et al. (2011)). These operations return an ‘integral utility matrix’ whose elements give a non-dimensional quantification of the combined direct and indirect exergy contributions to each compartment. The results are displayed as directed graphs in Figure 3.8; these show similarities and differences between the three cities. For example, each city exhibits mutualistic exergy transfers between the internal and external environments, but when comparing the water-energy relationships, London and Sao Paulo exhibit mutualism, while in Beijing the water sector exploits the energy sector (due to groundwater pumping requirements).



(a) Beijing



(b) London



(c) Sao Paulo

Figure 3.8: Exergetic dependencies for the three cities. The sum total of direct and indirect exergy flows are quantified between four resource management sectors as well as the city's internal and external environments (note that the Kennedy et al. (2014) dataset does not record material flows for London). Arrow directions indicate mutualism and exploitation as per Figure 3.3; arrow thickness is proportional to the element value in the integral utility matrix.

3.2.3 Summary

This section has applied black-box and grey-box analysis to UM data, so that those faced with various options to meet demand for products and services in urban areas (the MRTP) can appreciate the relative benefits of different performance metrics. Analysis showed that any single black-box metric cannot be indicative of the resource consumption performance of a city more generally (owing to the weak rank correlations). This variability in metric rankings must be due to features that are invisible to metric calculations. Specifically, these differences are identified as the characteristics of the processes used in cities, and the way they are organised. Variations in process and organisation detail, and their associated resource flows, mean that the overall system-level performance metrics will also vary. Therefore, to understand how an MR system such as a city affects resource flows requires analyses which are sensitive to such variations; an advantage which belongs to grey-box methods, which consider the resource flows at the individual process level (exergy analysis) and the organisational level (ENA).

3.3 Discussion

The aim of this chapter is to show how one can evaluate the resource performance of an urban area, specifically with regard to decision makers who are faced with a number of pathways (chains of resource management processes) to convert resource inputs r_i into products and services r_j . This is important, because foundational to this thesis is a conceptual model of UM in which a mixture of resource management processes are organised to operate in a way which has a particular impact on an area's metabolism. There are various possible configurations in which these processes realise intersectoral synergies, and these will have different impacts on the overall metabolic flows of a city. The analysis here shows that a process-oriented conceptualisation of UM cannot be fully appreciated by black-box metrics. This leads to the conclusion that grey-box metrics are preferable to black-box metrics, because of the need to understand the effect on resource flows of variations in process organisation and detail. This section discusses some of the ways in which grey-box analysis could provide useful information to stakeholders, before highlighting its limitations.

3.3.1 Applications for grey-box metrics

By looking inside an urban resource management system, this chapter has shown that exergy analysis and ENA make it possible to observe the interactions of resource conversion processes and their associated management sectors. These can be used by stakeholders to bring about real-world benefits. For example, exergy analysis brings a process-based ‘engineering’ perspective to the MRTP, meaning a decision maker can:

- *Understand resource efficiency at the process level.* Exergy analysis highlights the presence of inefficient processes (those with large irreversibilities) in an urban system (such as the coal plant in Beijing), and hence where investment could be used to upgrade or replace technologies in order to reduce Ex_p^{irrev} ; thus increasing $Ex_p^{prod} + Ex_p^{waste}$. This will reduce the Ex_p^{in} requirements and/or increase availability of wastes for use in other processes (see the next item); both of these interventions will increase an area’s overall exergy efficiency.
- *Understand the deployment of resources amongst the process.* By unifying energy and material flows under a common measure, a decision maker can see the ‘value’ of different resources in relation to each other, which can inform decisions on how resources might be redeployed so that a system can meet demand, and simultaneously increase exergy efficiency. For example, Figure 3.7(a) shows that if Beijing’s waste heat exergy from power generation was recovered, it would be sufficient to meet heating demand and provide the energy required for wastewater treatment. Similarly, urban waste has a high exergetic worth, which might provide an energy source for other processes.
- *Understand the need for contextual allowances.* The analysis showed that the exergy depletion α_{ex}^{in} caused by Beijing is an order of magnitude larger than that caused by London; but it is also known that Beijing is meeting a demand for steel and cement, and London is not. This additional knowledge shows where higher α_{ex}^{in} or α_{ex}^{in}/GDP might be justified when comparing city performance.

To complement the engineering perspective of exergy analysis, ENA offers an organisational or management view of an MR system, providing an objective measure of compartmental interdependencies from the point of view of a system’s ‘organisational actors’ (such as government authorities, utility service companies, and industrial and commercial services). The interventions will vary according to

the value judgements made by the system operator. One benefit is to identify where actors from different management sectors might work together to promote symbiotic relationships in order to reduce exergy depletion and increase exergy efficiency. For example, in both Beijing and Sao Paulo, the waste sector ‘exploits’ the materials sector, by failing to contribute any exergetic value to it (Figures 3.8(a) and 3.8(c)). This relationship could be made mutual via indirect flows, for example through manufacturing refuse derived fuel (RDF) from solid waste, and using energy obtained from its incineration for material production processes.⁴ A change in the system like this would require the operators of the waste and energy sectors to collaborate. An alternative application would identify where compartmental interdependencies might put the system at risk of failure. For example, rather than a benefit, it might be considered problematic to rely on energy from waste for the materials industry, if increased recycling rates were to reduce waste output. Another application arises from the city’s contrasting dependencies between the water and energy sectors: in London and Sao Paulo, there is a mutual relationship, but in Beijing the water sector exploits the energy sector. This is because Beijing’s water supply energy requirements are higher due to energy consumption by groundwater abstraction. Decision makers should therefore be aware that Beijing’s water supply is particularly sensitive to energy production, and therefore ensure that energy stocks are sufficient to guarantee the long-term stability of water supply.

3.3.2 The limitations of grey-box metrics

The above discussion has laid a strong theoretical foundation for decision makers to adopt grey-box metrics, but if they are to use these methods to assist investment or policy decisions, they must be aware of their limitations. Two types of limitation are outlined here, along with suggestions of how they might be overcome. The first limitation is the sensitivity of the exergy analysis (and hence the ENA analysis which is based on the exergy analysis) to the quality of metabolism data. The UM dataset used here identifies only the flows into and out of the urban system, and therefore the exergy analysis procedure of Section 3.2.2 relies on two key assumptions. Firstly, since the UM dataset contains very little information about the types of processes in the conversion chain between r_i and r_j , these must

⁴The terms ‘mutual’ and ‘exploit’ should not necessarily be laden with the respective positive and negative sentiments that the words may carry in everyday usage. For example, it might be considered that an exergetic contribution from the internal environment to the external environment is undesirable (if this is due to wastes, for example), despite the ‘mutual’ relationship signified in each case of Figure 3.8.

be assumed. Identifying the larger-scale processes is less questionable – knowing total electricity demand and the proportion derived from certain fuels (from information provided in the dataset) allows one to ascertain which power conversion processes exist – but smaller, intermediate processes (such as pre-processing of fuels) are harder to determine, which could leave some Ex_p^* terms unaccounted for, affecting the results of exergy efficiency calculations. Secondly, correctly assigning values to the Ex_p^* terms is problematic, due to unknowns about the ‘quality’ of resources and reference environments. These include the temperatures of final energy forms and the areas with heating demands; the chemical composition of fuels; the contaminant content of an area’s water resources, and water treatment standards; and the depths and elevations of groundwater and surface water. Similarly, assumptions pose problems for ENA. This analysis has made assumptions about the way processes are distributed amongst management compartments (for example, that different actors are responsible for water and energy); in reality the assumptions may be incorrect.

The second limitation applies even if the above assumptions are unnecessary, namely that grey-box metrics are arguably harder to comprehend, calculate and communicate than the black-box metrics. The latter can each be defined with a single formula and are easily evaluated from UM data. The former however require multiple-step procedures to calculate, and rely upon potentially unfamiliar concepts like exergy, mutualism, and exploitation. Therefore, the significantly increased knowledge required to use and apply grey-box metrics might inhibit their uptake, especially where non-specialists are involved in policy and investment decisions.

With regards to the first limitation, to reduce the need for assumptions regarding processes and resource flow quality, UM datasets could be made more comprehensive through the inclusion of an additional three layers of information. Firstly, to address the lack of process information in UM data, accounting should include the processes contained within the urban boundary, such that anyone reading the data could intuitively draw the directed graph described in the exergy analysis method (Section 3.2.2). In practice, it would clearly be difficult to include all resource conversion process; however the analysis here suggests that thermal processes (e.g. electricity generation from fossil fuels) dominate exergy flows for an urban area and these should therefore be the focus of early work. Secondly, to correctly value Ex_p^* terms, resource quality values (thermal, chemical and physical properties, as described above) should be recorded. Thirdly, to support ENA, information about resource governance (authorities and companies managing the various resources) should be collected. To address the sec-

and limitation of grey-box metrics – the comprehension, calculation, and communication difficulties – efforts should focus on how exergy analysis and ENA principles are best taught and communicated to the relevant decision makers, perhaps through user-friendly computational tools and informative visualisation techniques.

3.4 Conclusions

This chapter set out to provide ways to evaluate the performance and efficiency of urban resource consumption. More specifically, the goal was to understand how such metrics might assist decision makers for urban areas (which are MR systems) who are faced with a number of options about how to meet demand for products and services r_j (due to the existence of different combinations of processes in an urban area which can convert resource inputs). A theoretical framework to describe how resource performance metrics can be formulated for MR systems was proposed, and then these measures were applied to urban metabolic flow data. In summary, grey-box metrics are useful to those who are seeking to understand how a network of resource management processes affects overall metabolic flows. This is important to this thesis, because it is exploring how processes from different sectors might work together to realise synergies which improve an area's metabolism. Quantifying black-box metrics (e.g. carbon footprints or system energy efficiency) are important, but they are only of limited use, since they cannot account for variations in process and organisational detail, which is important to this thesis's considerations of how processes work together. Hence exergy analysis and ENA has been demonstrated to be useful to researchers, planners and policy makers wanting to understand the middle of a UM system. These findings can be carried forward to the modelling work (Chapter 6), and so help to meet Aim 3 of the research question.

As well as contributing to the specific purposes of this thesis, this chapter's work highlights work for the UM field more generally; namely that UM accounts should be extended to include the necessary data on major urban resource conversion processes (in order to minimise the need for assumptions in exergy and ENA calculations); and that efforts should be made to support decision makers who want to use these methods. In addition to these two recommendations, further work can develop the findings in four ways. Firstly, the conclusions are based on the new empirical result that black-box metrics of urban resource performance show no significant rank correlation with each other; this finding

should be confirmed using other datasets. Secondly, higher resolution grey-box analysis (using more internal processes and compartments) should be conducted to quantify the trade-off between insights obtained and data required. Thirdly, additional metrics might be explored which provide further insights to decision makers (for example, decomposition analysis (Zucaro et al., 2014)). Fourthly, work could demonstrate how these methods apply to other types of MR systems (from the production of a single resource, to the management of entire economies). The urban systems studied here are just one example of this larger category of production systems, whose improved performance are vital for wider sustainability goals.

Chapter 4

A database of urban resource management processes

“It is a capital mistake to theorize before one has data.”

Sherlock Holmes in *A Study in Scarlet*

(Arthur Conan Doyle)

A version of this chapter was published as: Ravalde, T. and Keirstead, J. (2015a). A database to facilitate a process-oriented approach to urban metabolism. *Journal of Industrial Ecology*, 21(2):282–293. The ‘Approaches to urban metabolism’ section of the paper was reworked into the literature review as Section 2.1).

To date, little attention has been paid to how the mix of resource management processes in the middle of a UM system affects the aggregate exchanges of material and energy with the external environment (Section 2.1.2). This thesis hopes to address this gap by contributing a model which can optimise the mix and operation schedule of resource management processes in cities such that they can work together to realise synergies which improve the metabolism of an area. However, to do this requires understanding the behaviour of the processes themselves, in order to define inputs to the model. This chapter identifies the resource conversion processes that can shape UM both now and in the future, and quantifies the resource consumption and production of each individual process, assembling this

(and other) information into a database. The chapter then discusses applications of the database, including its main contribution to this thesis (which is to provide data for use in the optimisation model, thus forming part of Aim 1 of the research question), as well as other uses, all of which are facilitated by the model's public availability under an open-source licence.

4.1 Supporting fields of research

This background section introduces two research areas important to the assembly and use of the database: first, it takes a look at databases that currently exist which are similar to the one built here, as well as identifying a method to research the contents of such a database. After this, the subject of 'open data' is introduced – particularly in relation to industrial ecology – to show the benefits of making the database publicly available.

4.1.1 Existing databases and technology scanning

There are a number of precedents for the proposed database; this section considers three of them in order to locate it within the existing landscape of tools. The first example comprises the 'technology roadmaps' published by the International Energy Agency (IEA, 2015). These constitute comprehensive reports which outline important energy management technologies in view of climate change targets. For example, the technology roadmap for hydrogen and fuel cells outlines various hydrogen-using systems (e.g. fuel cell vehicles) and hydrogen-generating technologies (e.g. electrolyzers), and includes prose-based descriptions of how the technologies work; tables of numerical values such as process capacity, efficiency, capital cost, and life expectancy; and the results of modelling which indicate the role hydrogen technologies could play in achieving targets (Körner, 2015).

Second, and also from the energy sector, is the Enipedia wiki, which is a collaborative environment that collects information about energy technologies, infrastructure, resources and other related issues (Davis et al., 2015). For example one section of Enipedia assembles a database of energy storage technologies, which notes their maturity, possible applications, operating efficiency, and lifetime expectancy, alongside descriptions of how they work. A third example covers a broader range of technologies, namely the ecoinvent life cycle inventory database which specifies the material and energy

inputs and outputs for processes within energy supply, transport, packaging, electronics and other areas. The database is usually used to assess the environmental impact of supply chains to produce a good or service (Weidema et al., 2013).

These examples have many useful applications, but none of them are geared towards the UM analysis of this thesis, which is attempting to optimise intersectoral synergies. For example, the IEA roadmaps and Enipedia are limited to energy management processes, and furthermore they do not record the non-energy flows associated with these processes, such as water and waste. The ecoinvent database is more comprehensive, in both the processes and flows recorded, but its focus is on product manufacturing supply chains, and thus it ignores processes important to urban metabolism such as drinking water treatment and HVAC systems. To facilitate process-oriented approaches to UM modelling, a new database is needed.

The building of the database will draw on the principles of technology scanning, which can be defined as “a way of taking a creative look at the world of technological developments and the cultural, regulatory, and business environments in which they emerge” (Electric Minds, 2006). In general, it is used to support corporate strategy, by enabling industry to keep up-to-date with the current technology landscape, or to scan the horizon to identify emerging technologies (Van Wyk, 1997) (though the specific aims and methods vary on a case-by-case basis). As an example, in healthcare, researchers identified technologies which would improve clinical care in the most financially viable way through searching literature, databases and digital libraries, as well as consulting industrial experts (U.S. Department of Health & Human Services, 2015). In another case study from the railroad industry, technology scanning was used to sift through many possible technologies to identify those which reduce costs or improve services, in order to direct research and investment efforts (Martland et al., 2002). Martland et al.’s method involves first a “general search” to identify technologies, and second “technology mapping” which researches the performance and cost of each technology, and goes on to classify technologies according to maturity, functionality and other variables. Their scanning proved valuable as it uncovered technologies (such as nanotechnology) which had never before been identified in railroad technology strategies.

4.1.2 Open data

Open data is “data that can be freely used, re-used and redistributed by anyone – subject only, at most, to the requirement to attribute and sharealike” (Open Knowledge, 2013), and is increasingly prevalent in academic research (Figure 4.1). A high profile example is the Human Genome Project which placed all their human genomic sequence information in the public domain, so research would be of maximum societal benefit (HUGO, 1997). The term ‘open data’ first appeared in 1995, and was formally clarified in 2007 to incorporate three principles: “openness, participation and collaboration” (Chignard, 2013). Open data brings many benefits, including: opening up scientific enquiry, promoting new research, allowing verification of published results, and enabling research to go in directions not envisaged by the initial investigators (Uhlir and Schröder, 2007). Added to this, making data open protects it from loss due to hardware malfunction, and also makes it useful as a teaching tool (Roche et al., 2014).

When it comes to open data within Industrial Ecology (IE) specifically, Davis et al. (2010) argues that the community needs to improve its data management between sub-disciplines, so that research findings can more effectively contribute to the sum total of IE knowledge. Nevertheless, there are a few examples, such as Zhu et al. (2014) who provide an open data set from the European Pollutant Release and Transfer Register (E-PRTR) (Environmental Protection Agency, 2015), to identify the type and location of pollutant releases from over 30,000 industrial facilities. They propose that this information be coupled with a dataset of industrial process inputs for European facilities, to matchmake facilities, so that the waste outputs of one facility meet the input requirements of another. Several open-source IE and UM datasets (in addition to this one) are listed on open-source repositories such as the Industrial Ecology dashboard (<https://github.com/IndEcol/Dashboard>) and the Metabolism of Cities website (<https://metabolismofcities.org/page/about>).

4.2 Assembling a database of resource conversion processes

The database will include as many processes as feasibly possible which could be defined as a node in the middle of an urban system (Figure 2.1). To assemble the database, this chapter will adopt principles from technology scanning, however for these purposes, this procedure will be renamed to ‘process

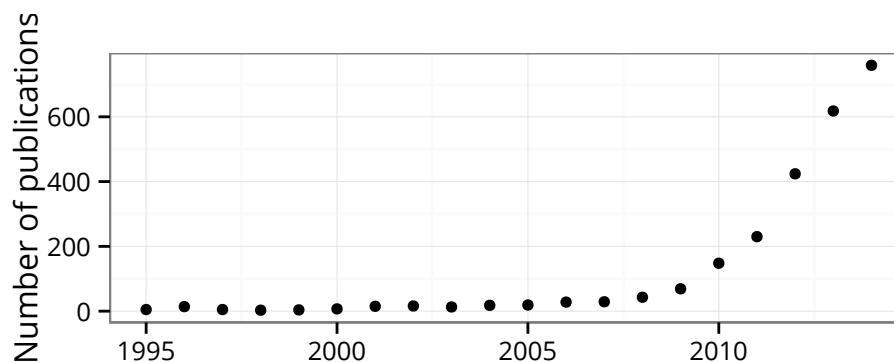


Figure 4.1: The growing research interest in open data since its first occurrence in 1995 until 2014. Data from the Scopus analysis tool, from searching titles, abstracts and key-words for 'open data' or 'open-data'.

scanning' which is more appropriate for the larger-scale activities (which may involve more than one technology) that provide energy, water and waste management services in cities (such as a wastewater treatment plant). The methodology is inspired by Martland et al. (2002)'s two-stage approach: first, the general search stage systematically searches academic literature to identify the processes; second, the process mapping stage gathers data on each process to assemble the database.

4.2.1 Systematic literature search (the general search)

This systematic literature search uses online search engines, together with the Bash and R programming languages to identify relevant processes from the literature available online, following the procedure below:

1. *Assemble the titles of relevant journals.* The titles of all the journals listed with the Thomson Reuters Master Journal List¹ were downloaded (at the time of download there were 17,614 journals). This list was then reduced to a list of relevant journals, using an automated search to remove journal titles which contained no words that matched words from a list of keywords². The list of journal titles was subsequently reduced to 379 by manually removing the rest of the irrelevant content.
2. *Filter journals by impact.* This step reduced the literature to a manageable volume, which represents the highest quality research. First any journals with impact factors less than 0.5 were removed. From the remaining journals, top 75 percent of the 'impact' was retained by ranking

¹<http://science.thomsonreuters.com/cgi-bin/jrnlst/jlresults.cgi?PC=MASTER>

²The keywords are available at <https://github.com/tomravalde/metabolism-database/tree/master/literature-search/keywords-journals.txt>

the journals from highest to lowest according to their impact factor, and calculating a cumulative sum of their impact factors, and then removing all journals in the bottom 25 percent. This left 168 journals remaining.

3. *Find relevant journal articles.* Using the Web of Science search facility, the list of journals were searched for articles containing specified combinations of keywords³ which indicate they could include content related to urban resource management processes. This searched found 9,929 paper titles which were reduced to 7,681 titles after manual filtering.
4. *Article categorisation and further filtering by impact.* The article titles were then searched for keywords that enabled reorganisation of the articles into categories representing either a process or a resource. Each category was then divided into sub-categories. For example, the effluent category (a resource) contained sub-categories on agriculture, fermentation, hydrogen and wastewater amongst others. Each sub-category is therefore a list of journal articles whose titles contain both the word 'effluent' and the sub-category heading. This resulted in 65 main categories with a combined total of 955 sub-categories. Finally, the lowest impact categories were removed, by calculating each category's mean article impact factor (totaling the impact factors of each article in a category before dividing by the number of articles in the category), then ranking the categories from highest to lowest mean impact, and removing categories in the bottom 33 percent. This filtering left 4,747 unique article titles, thus making the process mapping stage more manageable.

4.2.2 Data collection and database assembly (process mapping)

Having categorised the processes and resources, each category was manually searched for articles which refer to processes that manage energy, water or waste. For example, if an article referred to a fuel cell which treats landfill leachate, this would lead to a search for information to describe the leachate treatment process, first studying the original article, and then if necessary other literature. Information on each process was recorded using the YAML⁴ format. YAML uses mappings to relate a value to a key. Mappings can be nested like sub-points and sub-sub points (and so on) in a bullet-point list by using a mapping-of-mappings, thus multiple layers of information can be attributed to

³The keywords are available at <https://github.com/tomravalde/metabolism-database/tree/master/literature-search/keywords-articles.txt>

⁴YAML Ain't Markup Language': yaml.org

any mapping. Moreover, YAML uses very lightweight syntax and is therefore human-readable when compared to other similarly structured data storage formats (such as JSON and XML). Furthermore, YAML data can easily be converted into other formats. The main keys making up a process's YAML file are as follows:

process identifies the process name. For some processes, there exist a few variants, with different capacity values (see below); thus this key distinguishes these variants from one another by specifying both the process name (e.g. `anaerobic-digestion-wastewater`) and its capacity (e.g. `557 kg/s`).

flow contains a list of mappings which specify the quantities of energy, water and waste consumed and produced by the process. Data on resource flow quantities come from process descriptions, inventories, and process mass and energy balances in the literature. Each flow contains another list of mappings comprising three items: the numerical quantity of the flow (which is negative for a process input and positive for a process output), the units (MW for energy quantities, and kg/s for everything else), and a reference to the information source.

trl defines the 'technology readiness level' (TRL) which is used to assess a technology's maturity, from the initial stages of scientific research to its implementation in the real world (National Aeronautics and Space Administration (NASA), 2012). TRLs were initially developed by NASA as a nine-point scale, but other organisations such as the U.S. Department of Defense use different scales (Mankins, 2009). This thesis uses its own simplified TRL definitions which define a process as 'current' (9 on NASA's scale, for processes found commonly); 'rare' (also 9 on NASA's scale, where processes exist in only a few places); 'mid-term' (5–8 on NASA's scale, for processes which might have working pilots); or 'long-term' (1–4 on NASA's scale, for those processes which only exist in the literature or the laboratory). For each process, this information was found by searching the literature and other online content. Sub-mappings record a justification of the TRL value attributed to a process, and a reference to the source of the justification.

main specifies which resource is considered the main input or output. For a power plant, this would be the electricity output; for a wastewater treatment plant, this would be the wastewater input. All the resource flow quantities are normalised with respect to this value, such that its magnitude equals 1.

capacity specifies the maximum rate at which the process can consume or produce the main resource. For example, for a 350 MW power plant, capacity would take a value of 350. Due to the normalisation of the flows with respect to the main resource, any process's resource flow multiplied by its capacity will provide the maximum rate of consumption or production of any resource for the process. This item contains two mappings specifying both a value and a reference.

The database is available as a GitHub repository at <https://github.com/tomravalde/metabolism-database>. An example database record is given in Figure 4.2.

4.3 Database overview and possible applications

As of November 2018, the database currently contains 202 unique processes (or 334 when the different capacities are counted). These processes all manage energy, water and waste, encompassing 63 resource types, of which 25 are main resources. Processes where energy resources are the main output include fossil fuel- and renewable-based generation technologies (such as power plants and concentrating solar power), as well as methods to produce biofuels and hydrogen. Where water resources are the main output, processes include the delivery and treatment of groundwater and surface water for potable and non-potable purposes. The waste management processes include treatment and energy extraction methods for many waste types including wastewaters, agricultural wastes, municipal solid waste and landfill leachate. Of the 202 unique processes, 148 are current, although 12 of these have been identified as having low levels of market penetration (rare). The remaining 54 are still in the research and development stage.

A central claim of this thesis is that a process-oriented perspective on UM could offer insight on how changing a system's mix of processes could meet demand for energy, water and waste management, but with reduced negative impacts. This database facilitates this a few ways, as described in the following three subsections.

```
process: power-plant-coal
flow:
  coal:
    value: -0.101
    unit: kg
    reference: http://www.sciencedirect.com/science/article/pii/S0301421508007301
  electricity:
    value: 1
    unit: MJ
    reference: http://www.sciencedirect.com/science/article/pii/S0301421508007301
  heat:
    value: 1.570
    unit: MJ
    reference: http://www.sciencedirect.com/science/article/pii/S0301421508007301
  water:
    value: -0.867
    unit: kg
    reference: http://iopscience.iop.org/1748-9326/7/4/045802/pdf/1748-9326\_7\_4\_045802.pdf (a review of water consumption for electricity generating technologies)
  CO2:
    value: 0.234
    unit: kg
    reference: https://www.ipcc.ch/pdf/special-reports/sroc/Tables/t0305.pdf (International Energy Agency's values for carbon dioxide intensities of fuels)
  ash:
    value: 0.010
    unit: kg
    reference: http://www2.epa.gov/radiation
capacity:
  value: 5400
  reference: Maximum capacity plant from those listed at https://en.wikipedia.org/wiki/List\_of\_coal\_power\_stations
trl:
  level: current
  reference: https://en.wikipedia.org/wiki/List\_of\_coal\_power\_stations
  justification: "Large list of coal power stations at Wikipedia list"
main: electricity
```

Figure 4.2: An example YAML record for a coal-fuelled power plant.

4.3.1 Process comparison

First, consider how processes meet demand for a single resource, using the subset of processes whose main output is methane as an example. Figure 4.3 visualises the resource inputs and outputs for six processes to produce 1 kg of methane. At a glance, the proximity of points to the Quantity = 0 intercept makes evident which production methods have the smallest of the various input and output flows. Coupling these flow values with the impact categories used in life cycle analysis and/or the constraints associated with a specific area would identify the most desirable process choice under certain circumstances. For example, a city which uses the very water-reliant ‘Biogas upgrading – AWR’ method may like to consider lower water alternatives. Alternatively, another city may have a ready supply of biomass (perhaps from agricultural waste), which would otherwise go to waste, but could instead feed the gasification process. This latter example is one of the ‘medium-term’ processes, and therefore would require research and investment if it was to be implemented.

4.3.2 Synergies in process networks

The methane production example above demonstrates the resource transfers which can take place between the energy, water, waste and other sectors. Figure 4.3 shows how methane production (an energy resource) can result in energy flows (such as electricity or heat requirements), water flows (such as water inputs) and waste flows (such as vegetable waste inputs and digestate outputs). Inter-sectoral links such as these occur frequently in the database, and are summarised in Figure 4.4, which reveals numerous processes that link the energy, water, waste and other sectors. These links are central to this thesis, because these are what the model will later consider when performing the optimisation; namely, the use of one process’s wastes and by-products as inputs to another. Consider the simple example of the material flows in an Indian village reported by Kestemont and Kerkhove (2010). A material flow analysis of the village indicates it has both biomass waste outputs and electricity imports. Searching the database revealed 22 processes which have biomass inputs and electricity outputs (including biomass-fuelled CHP plants, straightforward combustion or biomass-to-ethanol conversion processes and in the medium term, fuel-cells). The village could invest in one of these processes, to reduce their expenditure on electricity imports. Some options could even produce other resources, such as methane or heat which can be used elsewhere in the village or sold. However, these bene-

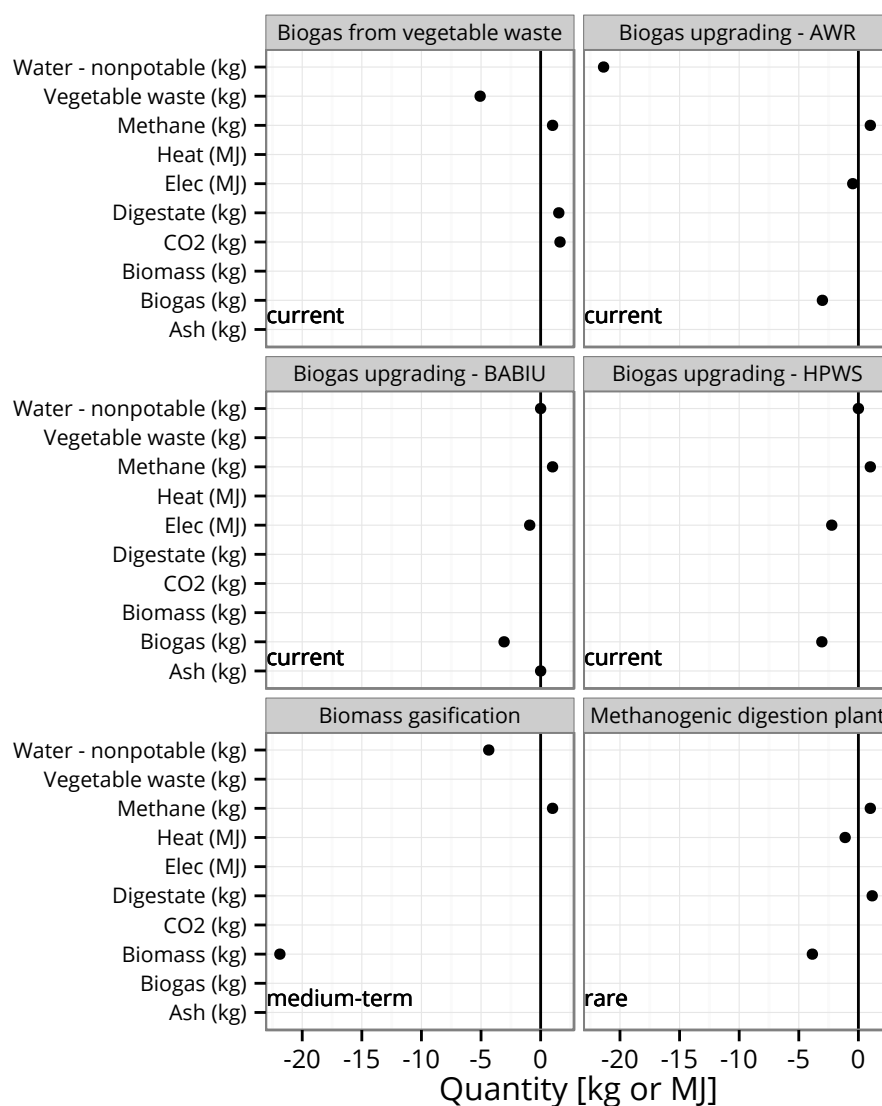


Figure 4.3: Resource consumption (negative values) and production (positive values) for different processes producing 1 kg of methane. Key: AWR = alkaline with regeneration, BABIU = bottom ash upgrading, HPWS = high pressure water scrubbing; text labels indicate the TRL for each process.

fits must be traded off against the resource input requirements (e.g. for coal or water) and economic decisions (e.g. payback time).

Another way to identify synergies is inspired by Zhu et al. (2014)'s matchmaking proposal using the publicly available E-PRTR dataset introduced in Section 4.1.2. Searching this dataset reveals that methane and CO₂ are both common pollutants (produced by 1,623 and 2,153 European industrial facilities respectively, from a total of 32,368 facilities). The database here lists 13 processes which require methane or CO₂ inputs, and thus could be used to redirect harmful emissions towards beneficial purposes such as electricity production, algae cultivation and wastewater treatment.

4.3.3 Optimisation of networks

Considering the possibilities for inter-sectoral synergies in the ad-hoc manner above is impossible when expanding to the city scale. Chapter 1 therefore argued for the need for systems thinking, in which the processes and resources are represented formally, such that mathematical techniques can find the optimal system configuration (Section 1.2.3). This modelling approach will be more fully realised through the optimisation model developed and applied in the next two chapters. However, as a preview, an early version of the model (described in Ravalde and Keirstead (2015)) will provide a simple demonstration of how the database could be used in a simple optimisation. In this model, the user specifies the time and location of resource demands and waste generation rates, and a mathematical optimisation routine identifies the mix of processes that meets a city's demands whilst minimising an objective (such as cost, carbon footprint, water footprint, waste generation etc.).

The example is based on the hypothetical city of Wolman (1965), using his data to derive bottom-up demands for electricity, heating⁵ and water (motor fuel and food from his paper are ignored), and generation rates for refuse and wastewater. Making all the technologies in the database available, the city's choice of processes was optimised to minimise CO₂ emissions. Figure 4.5 shows the city's resource flows at the top, both before and after optimisation. The model was able to cut emissions to zero, by choosing gas-fuelled CHP to meet energy demands (which requires a slight increase in gas imports, but eliminates coal and oil imports). The model also chooses algae cultivation to absorb any

⁵It is assumed that the fossil fuels (coal, natural gas and oil) meet all electricity and heating demand, and that electricity consumption is 1.12 times the heat consumption (this value is calculated from the mean ratio of electricity-to-heat consumption for all cities in the UM database from Kennedy et al. (2014)).

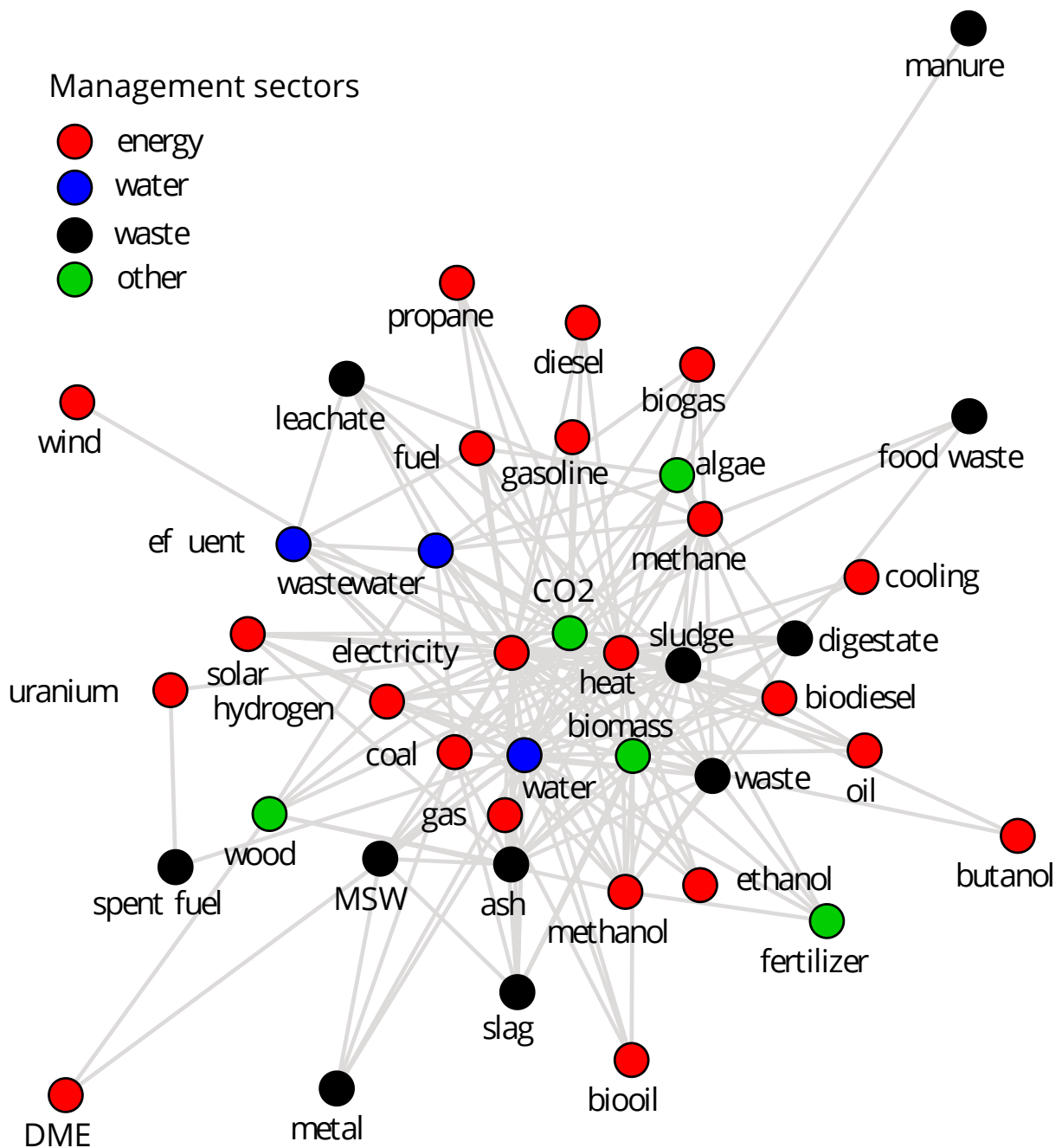


Figure 4.4: The interactions of resources in the database. The proximity of any pair of connected resources is proportional to the number of processes for which one resource of the pair is an input, and the other is an output. This graph is plotted using the R package from Butts (2013).

remaining emissions. Sewage flows are also reduced while refuse and water flows remain unchanged. These system changes are unlikely in reality because of constraints on land-use (e.g. for algae production) and cost, nevertheless this example demonstrates the potential benefits of process-oriented optimisation modelling.

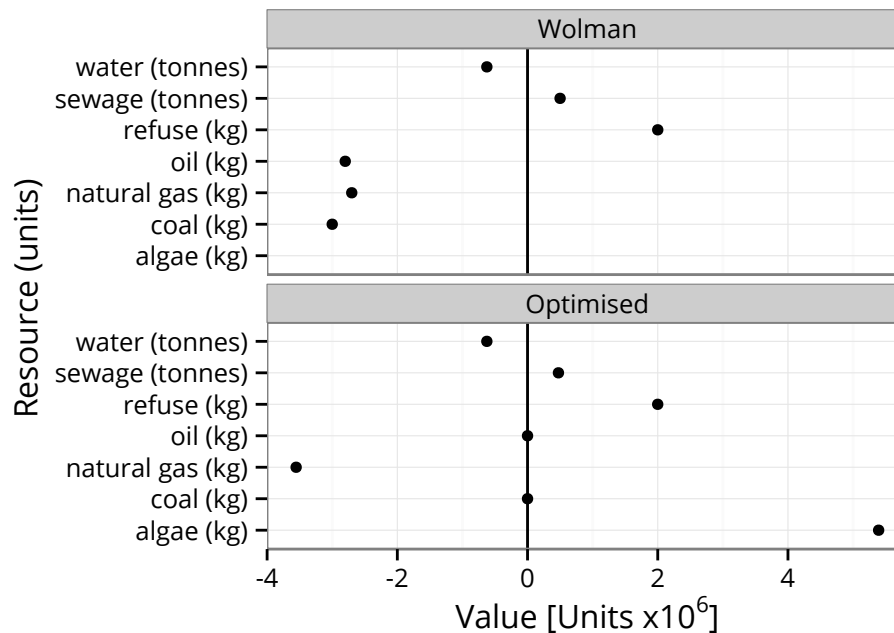


Figure 4.5: Aggregate metabolic flows at the top of Wolman's hypothetical city before and after optimisation modelling proposes an optimal network for the system's middle. Negative values represent inputs crossing the city boundary, while positive values represent outputs.

An optimisation model for a city can explore different aspects to process-oriented planning and policy agendas. For example, it can inform urban planning by considering whether decentralised systems (which use more smaller capacity processes close to the point of resource use or generation) manage resources more efficiently than centralised systems. Modelling could also inform how a system's middle should adapt to changes at the bottom, by altering resource demands to simulate behavioural changes and efficiency measures. Finally, in conjunction with this database, the model can help prioritise research and investment efforts, by identifying which processes with medium- and long-term TRLs would most help an urban area achieve some particular objective.

4.3.4 Reflections: interacting with other datasets

The three applications above each depend on the availability of other data: process comparisons require knowledge of resource inputs and outputs in an existing process; searching for synergies requires knowledge of inputs and outputs to multiple processes; and optimisation modelling needs to know the resource demands and waste generation rates at the bottom of an entire system.

Thus a potential obstacle to using the database is the availability of other data. Davis et al. (2010) argue that within IE, data is often “unavailable, inaccessible, incomplete, incompatible, or unreliable” (p.708), and believes that IE can best overcome these obstacles through increased collaboration. Here, the use of other open-source datasets has been limited to the E-PRTR, but it would be profitable to reach beyond this source and use data more associated with UM to identify synergies between energy conversion, water treatment and waste management processes in existing cities. Similarly, a dataset of demands for electricity, heating, potable and non-potable water, and waste and wastewater management could be established for domestic, commercial and industrial sectors, for real urban areas of different types (such as size, maturity and climate). It would also be beneficial to have some means of linking databases together. Davis et al. (2010) elucidate this by recapitulating the arguments of Bush (1945) concerning the most useful ways to store scientific knowledge. Rather than traditional hierarchical storage (e.g alphabetical order or the Dewey Decimal System) which forces all information into a single location, Bush (1945) argued that information should be located according to associative trails, i.e. paths “where facts are connected to other associated facts” (Davis et al., 2010, p.711), as exemplified by Wikipedia’s use of hyperlinks. Davis et al. (2010) take on board Bush’s concept, and note that it can be facilitated within IE by using Semantic wikis (of which Enipedia is an example), which store information in both structured and unstructured formats. Unstructured information uses prose (such as the history of a particular process); structured information records machine-readable quantitative information (such as a resource flow value, a capacity or a TRL). Information can contain hyperlinks that point to other relevant pages.

The Semantic Web (of which Semantic wikis are a part) has attracted some scepticism, largely due to pragmatic concerns. Any machine readable information needs to be encoded according to some standard, which may not be agreed upon by the different parts of a community, and conforming to multiple different standards would incur a high financial and resource cost (Marshall and Shipman

III, 2003). However, Herman (2008) has observed that the Semantic Web has been successful within specialised communities (such as financial services and health care); thus there is promise for it within IE. Furthermore, to minimise the efforts required by contributors, machine learning has the potential to automate the searching of information to discover structure within it, and then to formally encode this structure with the appropriate Semantic Web code (Lukasiewicz, 2017).

Davis et al. (2010) illustrate how a Semantic wiki could assist a hypothetical life cycle analysis researcher. Inspired by their example, consider the following illustration of how UM research might benefit from the database assembled here. Imagine that the ‘Biogas upgrading – AWR’ processes information (Figure 4.3) was part of a Semantic Wiki. Its wiki page could use unstructured data to describe how it works (perhaps including details on the process chemistry), and use structured data to record the resource inputs and outputs. The text of the resource flow of `Water -- non-potable` would be a hyperlink to a page about non-potable water. This page could then link to another page which lists the all processes which produce `Water -- non-potable` (both from the database, and other sources), which could then link to a page which lists all the cities which currently use such processes. Thus a researcher can navigate through several datasets (including that of this chapter) to find possible applications of technologies in the database.

4.4 Summary and further work

As the thesis has earlier argued, there is a need for models which can improve an area’s metabolism by optimising the network of processes which convert and transport energy, water, and waste. Such a model provides a process-oriented view of UM, and requires data on the properties and performance of resource management processes. This is provided by the database assembled here, which comprises 202 unique processes that manage energy, water and waste, both currently operational and those still in research and development. A few example applications of the database have shown ways to inform decision makers how best to plan and invest in processes which improve a city’s metabolism. This can be to choose the best of several alternatives to manage a single resource (in the case of a single utility service provider); to choose processes which take advantage of potential synergies in an area (in the case of a cooperative of organisations), or to optimise a city’s whole network of processes (which is the main objective of this thesis).

This database is a novel contribution to the UM and IE field, and the information it provides to decision makers will improve as the research community takes advantage of database's open data format to continually improve it, in the following ways:

1. Adding new processes
2. Broadening the type of information each process records, to include process costs (for capital, operation and maintenance), and other pollutants (such as SO₂), and other data.
3. Extending the database beyond energy, water and waste management processes, to consider other processes which affect the metabolism of an area, such as steel and concrete manufacturing.

Another area of future work is to support not just the evolution of the database, but of the whole ecosystem in which it lives. This is because process-oriented approaches to UM study are not isolated from other approaches, but rather are most useful when using information from them, such as demand data from the bottom of a UM system. The UM data ecosystem could flourish in the Semantic Web, which can link together structured and unstructured information in a vast network, through which researchers can navigate, finding innovative and as yet unknown applications for the data. The database is publicly available under an open-source licence and so it is hoped that it will become part of an evolving ecosystem of linked UM data.

In summary, the database can facilitate process-oriented approaches to UM, especially if it becomes part of an information ecosystem in which data from the top, middle and bottom of urban system are considered together in more holistic UM assessments. Ultimately, this will help cities meet their inhabitants' needs more sustainability, in response to the environmental and economic challenges challenges presented by urbanisation and its associated patterns of resource consumption.

Chapter 5

Model development

“Everything must be made as simple as possible. But not simpler.”

Attributed to Albert Einstein (though there is no proof he ever said this).

The systems of urban resource management can be conceptualised as a network of processes which operate to meet consumer demand for goods and services. Upstream and downstream of these networks are the aggregate flows of inputs into and wastes out of a city. Understanding what drives these aggregate flows is a key component of UM research, but – as Chapter 2 argued – the field has not yet produced a formal representation of how the network of processes relates to the overall flows. This is of particular interest to this thesis because of the intersectoral interactions and synergies which present challenges to, and opportunities for, efficient resource provision (Section 1.2). A model that seeks to optimise the management of resources at this systems-of-systems level could be considered a *highly integrated urban energy, water, and waste systems* optimisation model. This chapter takes this idea from a concept to a formalised mathematical model.

Since modelling is a simplification of the real-world (Section 2.2.1), there will inevitably be compromises in the performance of a model. This chapter explores these through three formulations (given in Section 5.3). The formulations are then applied to a case study which is followed by a discussion on their performance in view of the compromises in performance, to determine which formulation should be taken forward to Chapter 6. Given the novelty of this work, the case study in this chapter

is proposed as a ‘benchmark’ problem, i.e. a problem in which others can apply their own solution methods, so that the performance of different approaches can be compared using a single problem (Section 5.1.3). To aid this, the formulations and data are made publicly available. The main contribution of this chapter is to propose a novel model (showing how it develops existing models), being explicit about what the model can and cannot do, and to justify its formulation in view of the aims of this thesis.

5.1 Model performance and formulation

When introducing modelling in the literature review, Section 2.2.1 took care not to overstate the capabilities of a model. Rather, it was noted that modelling provides an honest, scientific tool to help decision makers explore complex problems. Recognising that simplifications are inevitable leads to the understanding that there will be compromises with respect to a model’s performance features. This section discusses some of these performance features, and how they relate to a model’s formulation.

5.1.1 Features of models

Four features of models this chapter will consider are *fidelity*, *generality*, *tractability*, and *usability*. Fidelity and generality are both functions of a model’s representation of the real world. The former measures how well a model describes reality, and the latter corresponds to the number of real world systems a model can be applied to (Matthewson and Weisberg, 2009). In relation to modelling undertaken here, fidelity would be a measure of how accurately the behaviour of a resource management process – for example, a water pipe – is represented by the model’s mathematics¹. Generality would measure to what extent the model’s equations can be applied to multiple process types, for example, can the same equation represent both a water pipe, and an electrical cable? Tractability and usability refer to the practicality of applying a model: the former is the amenability of the model to optimization techniques; the latter measures the ease of applying a model’s formulation to a particular problem (McIntosh et al., 2012).

¹The example of pipe flow is developed in Section 5.3.4.

These four features usually trade off against one another, which is the source of a model's compromise. Models that are more general will be lower fidelity, because they are not tailored to the specific details of a real-world situation (McIntosh et al., 2012). Models of higher fidelity tend to be both less tractable and less usable because they encode real-world system in greater detail, using more equations (to capture the detail), with more advanced mathematics; such models therefore are more difficult to formalise, use, and solve.

5.1.2 Mathematics of models

Moving to consider an optimisation model's mathematics in greater depth, recall from Chapter 2 that the equations of optimisation models are comprised of parameters and variables, where the values of parameters are fixed, and the values of the variables are chosen during the optimisation procedure. There are different forms of equations, and these different forms require their own methods to solve. There are two broad categories of formulation: *linear* and *nonlinear*.

Linear programmes (LP) include many of the energy systems models described earlier (such as Keirstead and Shah (2013)). In these models, variables are never multiplied or divided by one-another. A specific class of linear programmes are those where some variables must adopt integer values (which might be necessary to specify a the number of resource management processes, for example); these are mixed-integer linear programmes (MILP). Their simple mathematics means that linear models are often low fidelity. Indeed, they are formulated with the express purpose of simplifying nonlinear realities.

Nonlinear programmes (NLP) have equations in which variables are multiplied by, divided by, or raised to the power of one another. Again, these models can also have integer variables and are known as *mixed-integer non-linear programmes* (MINLP). NLPs are often used to model water management problems, because hydraulic equations often include the product of two or more variables². Nonlinearity may also exist in water management problems in order to model water contamination levels³ (for example, Moon et al. (2009)). These problems can be solved using nonlinear programming methods, but these are computationally expensive, so heuristics are sometimes used to obtain near-optimal so-

²To take one example (which is considered in more detail in Section 5.3.4), the potential energy of a mass of water due to its elevation is given by $\text{mass} \times \text{gravity} \times \text{elevation}$, where both mass and elevation might be variables.

³Consider two bodies of water, x and y , with volumes V_x and V_y (L) respectively, and contamination levels of c_x and c_y (mg/L) respectively. If these two bodies mix, the new contaminant concentration is given by $(V_x c_x + V_y c_y) / (V_x + V_y)$. If both volume and contaminant concentration are variables, then this model is nonlinear.

lutions with less effort. These heuristics often start with a possible set of variable values, and then imitate processes in nature to modify these solutions until a near-optimal solution is found. Examples include genetic algorithms, which follow evolutionary procedures (Keedwell and Khu, 2005); and particle swarm optimisation, which mimic the flocking of birds (Khor et al., 2012). Such heuristic approaches are an attempt to get around issues of tractability, without sacrificing fidelity (though they do not tend to make models more usable).

5.1.3 Benchmark problems

There are many different ways to model urban resource management systems, and the above considerations of performance features and (non)linearity suggest that there might well be different outcomes to such models, each with their own set of advantages and disadvantages. Because of this, this chapter will propose three different formulations (two linear, and one nonlinear) which vary in their fidelity, generality, tractability and usability. These three formulations will be applied to the same case study to provide a fair test by which to compare the different approaches. This case study will therefore provide a ‘benchmark’ problem. In computing, a benchmark is defined as a “program or set of programs used as a standard against which the performance of other programs (or computer systems running them) is compared or evaluated ...” (Oxford English Dictionary, 2017, Draft Additions October 2001). Benchmarking assesses a model’s quality by providing “a systematic mechanism for comparing computational tools” (Maksimovic et al., 2003, p.250) through the use of a test case, on which all computational tools can be applied.

Benchmarking problems exist in fields related to this thesis. In the energy sector, there are benchmarking problems for energy storage problems (Salas and Powell, 2013), plant location problems (Sabolev Institute of Mathematics, 2013), and plant operation problems (The Institute of Electrical Engineers of Japan, 2015). This third example compared different ways to approximate process behaviour using equations – a task not too dissimilar that undertaken in this chapter. In the water sector, there are benchmark problems to test the different algorithms applied to the optimisation of distribution networks (Wang et al., 2015, Maksimovic et al. (2003), Wu and Simpson (2001))) and the quality of managed water (Piratla et al., 2015). However, the benchmarking study in this chapter will be the first to model the highly integrated management of energy, water and waste systems. This novelty warrants that

the formulations and data can be made available to the wider research community, who can work to improve upon the models developed here, perhaps by modifying the mathematics, in order to achieve a greater performance in terms of fidelity, generality, tractability and usability.

5.2 Tat Hamlet case study

The case study chosen for the benchmarking problem is that of Tat Hamlet, a village in Vietnam. Fieldwork conducted in 2001 led to reports on the village's material and energy flows and socioeconomic characteristics (Schandl and Hobbes, 2006, Heezen (2003)). Following this fieldwork, researchers have explored features of Tat's metabolism, including analysis of the village's livestock development strategies (Thanh Lam and Duc Vien, 2010), and the socioeconomic organization and origins of the material flows (Rambo and Vien, 2001, Hobbes et al. (2007)), making Tat Hamlet a known case study within the UM literature. In this chapter, Tat will be used as a benchmarking study to test the three model formulations, using data from the material flow and energy flow studies.

Tat has 105 households of an average size of 4.4 people, covering 69 acres of farmland. The village has small shops and education functions, but its main activities are agricultural, with rice cultivation (where paddy fields are irrigated by a small river), swidden cultivation, and biomass (timber, bamboo shoots, cassava roots) collection from a forest. Some agricultural products are sold to external traders, though most remain in the village. About 80 of the households own their own livestock (including chickens, dogs, buffalo, and cows), and most households have their own ponds for aquaculture, such that the village produces most of its own meat, dairy products, animal manure and green manure. Water can be piped to homes for drinking, household use, and for washing livestock. Aggregate metabolic flows into the village comprise rainfall, electricity from the grid, construction materials, fossil fuels (such as gasoline for motorbikes, and petroleum lighting), and a small amount of vegetable and meat imports. Metabolic flows out of the village include household and agricultural wastes, incineration products, fossil-fuel emissions, and biomass which is sold. All this is summarised in Figure 5.1.

The small size of Tat serves to make the benchmark problem user-friendly because the problem can be conceptualised in a diagram on a single page of A4. The village's features described above will be used to define the village's demands for goods and services, and the network of resources and processes which will meet this demand. The models will compute how Tat can meet demands for goods and



Figure 5.1: A summary of the resources and processes in Tat's metabolism. The dotted line represents the boundary across which Tat imports and exports resources which are managed internally.

services at the lowest cost, using the village's resource management processes. Goods and services include food, water and energy, and resource management processes include everything from small domestic stoves to agricultural activities.

To construct the problem, data from the literature will be used to derive resource demands, and to select and define the behaviour of the resource management processes. However, to define a benchmark problem that is both user-friendly, and at the same complicated enough to test the different formulations, various adjustments are made, in the form of simplifications, assumptions, and additions (outlined in Appendix A); these are justified on the basis that this the end-goal of the benchmarking is to identify the best formulation, rather than to improve Tat's metabolism. The adjustments achieve a simplicity in understanding the model, and yet retain enough complexity in order to suitably test the formulations. Given that this chapter is developing a benchmarking problem, it would have been possible to entirely invent the problem and its associated data. However, basing the benchmarking problem on Tat Hamlet demonstrates how one can formulate a problem from real world data.

5.2.1 Conceptualising Tat Hamlet's resource management

The information from the literature and the adjustments provide a starting point to conceptualise Tat's means of resource management. This is partly visualised in Figure 5.2, which shows 27 resources

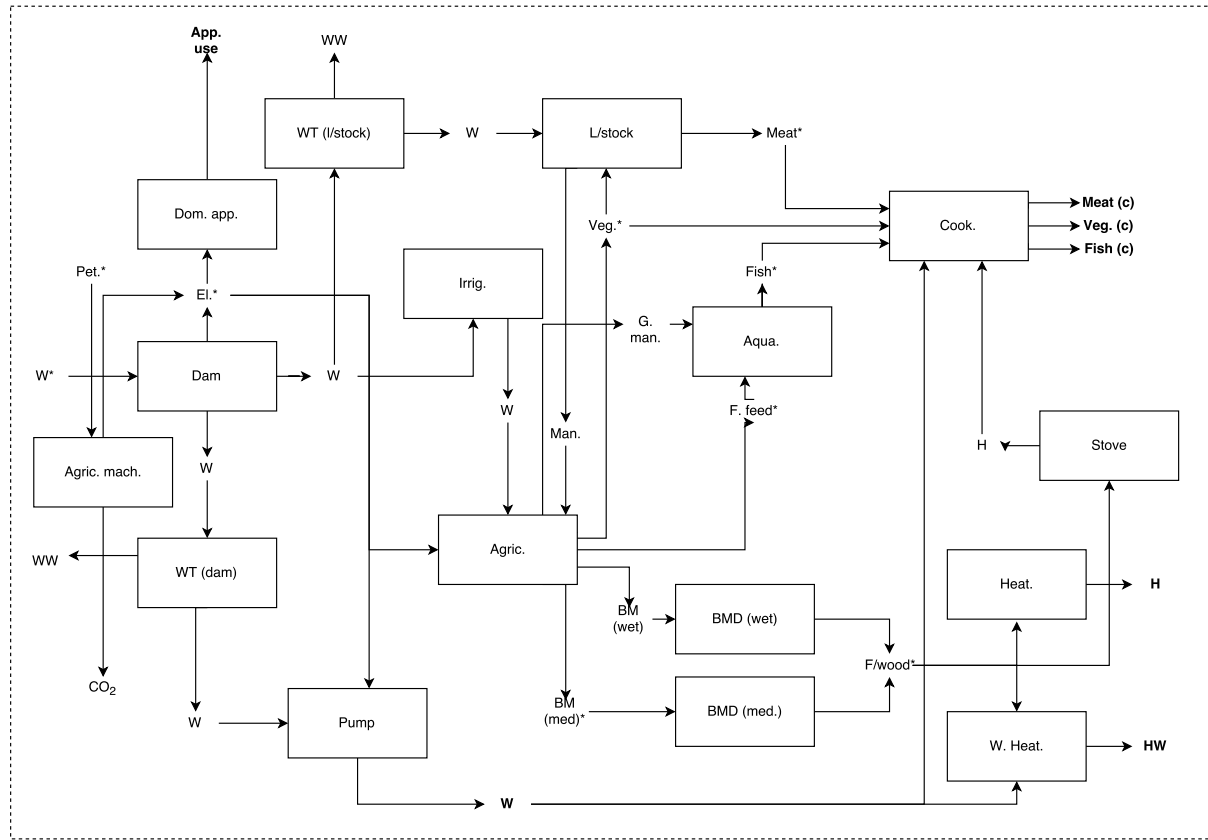


Figure 5.2: Complete network of the resources and sixteen conversion processes in the Tat Hamlet case study. Resource demands are shown in **bold**, while resources which can be imported from outside of the system are indicated by a *****.

managed by 16 conversion processes. The figure also indicates which resources are demands, and which resources can be imported into the village. (It is assumed any resource can be exported from the village.) Not represented here are the four zones into which Tat is split (arbitrarily for the purposes of this chapter, in order to test how the formulations deal with spatial disaggregation), between which resource demands are equally split – the models will be free to locate processes in any of them, but there will be limits imposed as to which zones can import resources, thus to meet demand, there must be the transport of resources from one zone to another (via transport processes, also unrepresented on this diagram).

Figure 5.2 shows seven resource demands for goods and services: water, hot water, electrical appliance use, space heating, cooked meat, cooked fish and cooked vegetables. Demands for water depend upon treatment and pumping processes. Within a household, hot water space heating, and food demands are met by combustion and cooking processes, with food also depending on processes ‘upstream’ of a house, namely: aquaculture, agriculture and livestock, water treatment, irrigation, and the operation

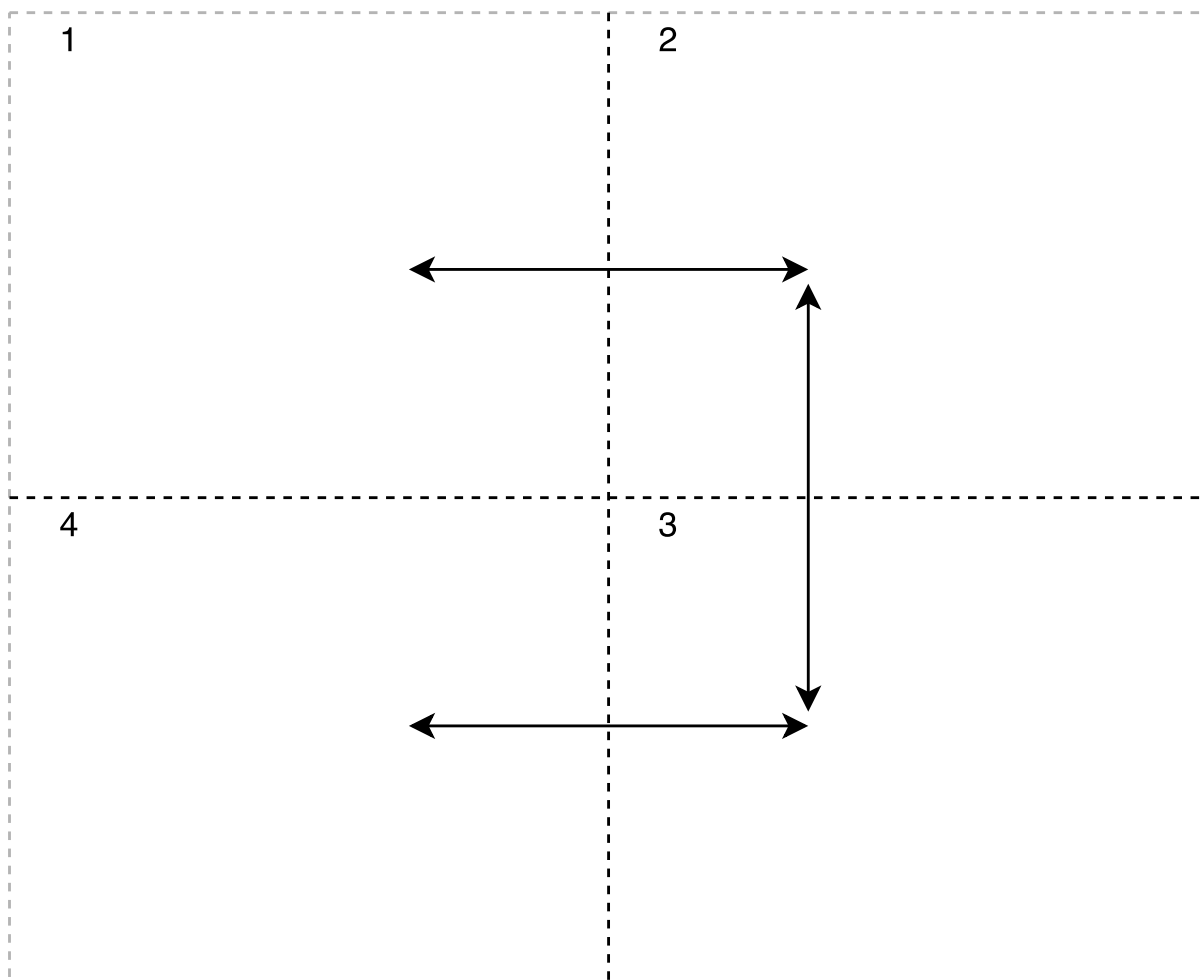


Figure 5.3: A representation of the four zones for the Tat Hamlet problem, and the transport connections that join them (indicated by arrows). More details regarding the transport processes (such as roads, cables and pipes) are provided in Table 5.2.

of agricultural machinery. Figure 5.3 represents the fact that this conceptualisation splits Tat into four zones. Regarding imports, water can be imported from the grid into only one zone, however electricity, food, petrol, biomass and firewood can be imported into any of the four zones; the figure shows the zones are connected such that resources can be transported between zones 1 and 2, and between 2 and 3, and between 3 and 4. The means of transport include vehicles (to transport biomass, manure, food and petrol), pipes (for water), and a cable (for electricity).

5.3 Deriving three optimisation models

As the conceptualisation above indicates, the highly integrated resource management model should be able to consider an area as comprised of a number of zones, for which can be specified resource demands, and which contain the conversion processes which manage resources. These zones can be connected to one another via transport processes. The model should also be able to consider that resources will need to be imported into the village (either to meet a demand directly, or to feed a process), and resources which neither meet a demand nor feed a process (excess waste heat, perhaps), can be exported from the area. Added to this, one might add a temporal component, such that resource demands can vary with time, along with the schedule of resource imports and exports, and process operations; however, for the sake of simplicity, there will be no temporal variation with time in this case study, however, Appendix B does include a time component, t .

An existing model which can accomplish these things – specifically for the energy sector – has been developed by Samsatli et al.⁴ and applied in Keirstead and Shah (2013). This is a MILP which chooses the optimal mix of processes, and schedule of process operation and resource imports and exports, to meet spatially and temporally defined demands for heating, cooling and electricity. Using the terminology of Section 2.3.2, this is a city-scale model, but it is not integrated (because it only optimises the energy sector); it is high-level (because it does not compute detailed design of the optimised energy system, but rather focusses on allocating resources to the right place, at the right time, in their right quantities).

To model the processes which convert resources, Samsatli et al. is based upon the engineering State-

⁴Note that this reference contains the most comprehensive description of the urban energy systems optimisation model, but it is at present unpublished. However, modelling based on this formulation has been published, for example in Keirstead and Shah (2013), though this paper doesn't include as much detail regarding the model's equations.

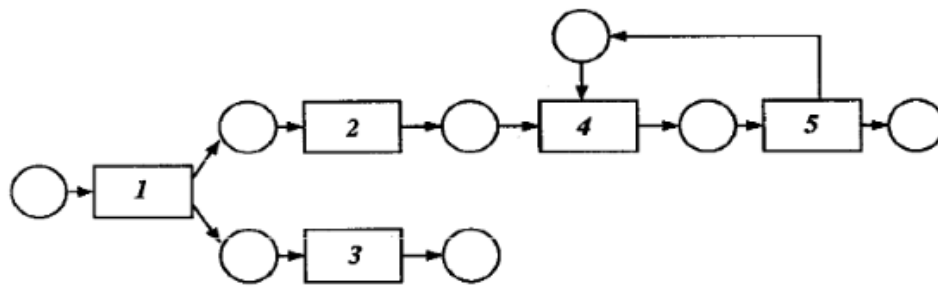


Figure 5.4: A diagram of an STN representation of a chemical engineering system, taken from Kondili et al. (1993, p.241, Figure 1b). The circles represent resources ('states'), while the rectangles represent the 'tasks' which convert a resource from one state to another. The paper then goes on to turn this conceptualisation into a MILP which can compute an optimal operation schedule for a chemical plant which maximises profits.

Task Network (STN) model of Kondili et al. (1993), in which processes ('tasks') convert materials from one 'state' to another (Figure 5.4). Keirstead's model applies this model's principles to urban energy systems using what they term a Resource-Technology Network (RTN), developing a model which chooses the mix of processes using available resources to meet demand for heat and electricity – an example is given in Figure 5.5. While, on this thesis' definitions, Samsatli et al.'s model is categorised as having no system integration (see Section 2.3.2), the STN representation is highly generalised (i.e. all conversion processes are represented by the same type of equation); this makes the formulation extendable to other types of resources and processes. The urban energy systems model has two types of processes: those that convert resources (such as a wastewater treatment plant), and those that transport them (such as a pipe).

A feature of Samsatli et al.'s model is that it is spatially and temporally disaggregated. The urban area is divided up into zones which can each have their own energy demands and set of technologies. Moreover, these demands can be different for each timestep (perhaps representing broad differences such as seasonality, or smaller differences on an hour-by-hour basis). Demand in a zone can be met by a combination of three means: (i) being imported from outside the urban area; (ii) being produced in the zone by a conversion process; (iii) being transported into the zone from another by a transport process. Note that demands can also be negative, for example to represent the demand for a certain quantity of waste to be removed from a zone. These are brought together in the model's main equation, which is a balance of resources in each zone at any moment in time:

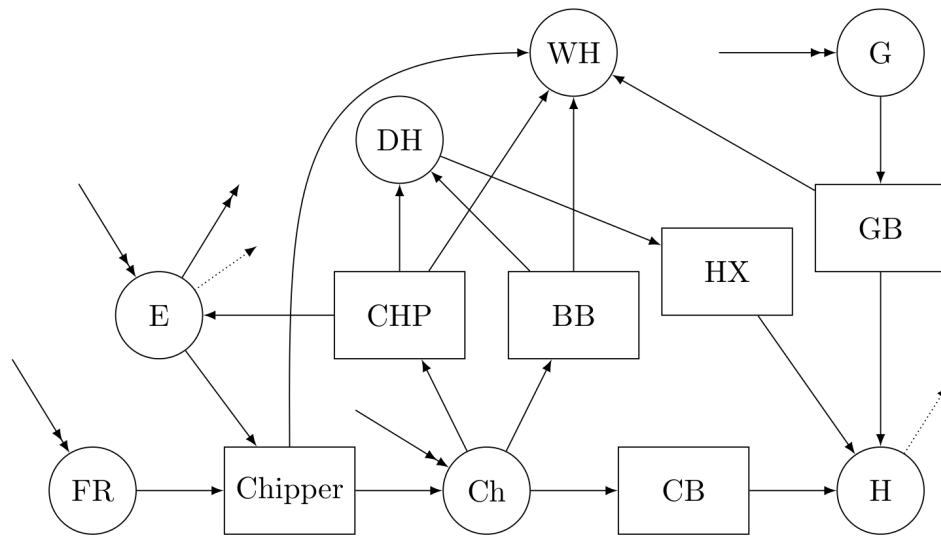


Figure 5.5: Example of an urban energy system optimised by the MILP model of Samsatli et al., which shows resources (circles) and conversion processes (rectangles) – note this diagram does not show transport processes.

$$\begin{aligned} & \text{Imports} + \text{Net inflow from other zones} + \text{Net production of resource by processes} \\ & = \text{Demand} + \text{Exports} \end{aligned} \quad (5.1)$$

This resource balance is visualised for electricity in Figure 5.6. Demand (for each resource, in each zone and each time period) is a parameter given to the model, with the other terms being variables whose values are selected by the optimisation procedures. The import and export variables can be limited using constraints, while the net inflow and net production variables are computed using equations which model the behaviour of conversion and transport technologies. The overall goal of the programme is then to choose variable values which minimise some objective (such as cost or emissions) – this objective is formulated from the programme’s parameters and variables.

The next three subsections specify three different model formulations built around this resource balance equation. The models differ in the way that they model the conversion and transport processes (in other words, how the second and third terms of Equation 5.1 are defined), varying in their fidelity, generality, tractability, and usability:

Null model This formulation is very similar to the MILP urban energy systems model, only it is applied to a broader set of resources and processes, to incorporate the water and waste sectors. The

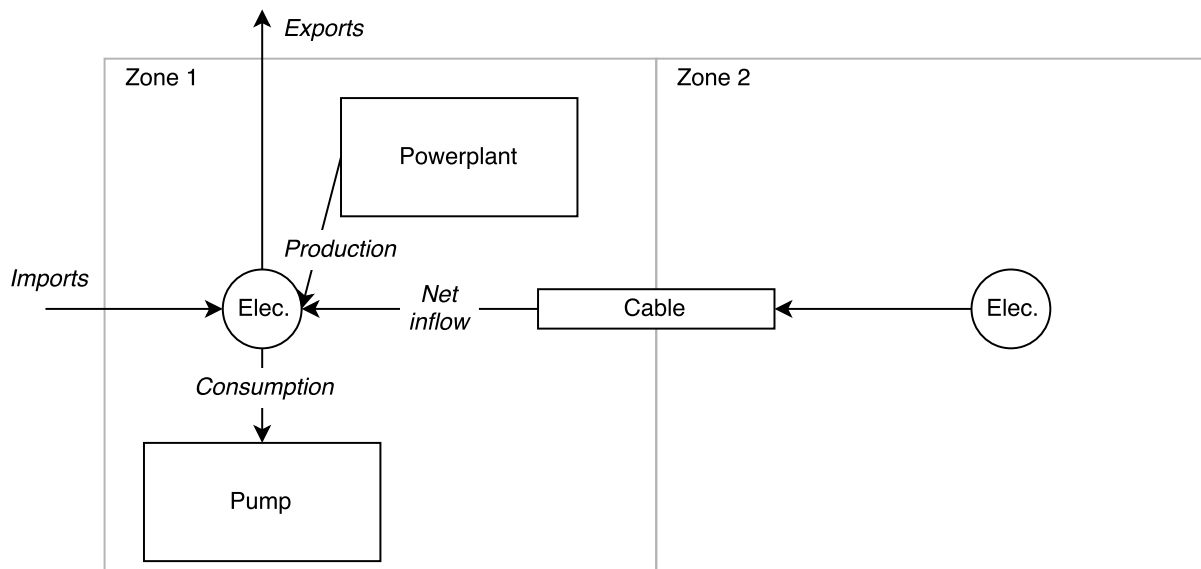


Figure 5.6: An example of how Equation (5.1) might apply to electricity ('Elec.'). Italicised terms correspond to the terms of the equation. In words: the electricity imported into Zone 1 from outside the system + the electricity produced by the power plant + electricity arriving from Zone 2 = the electricity being exported outside the system and the electricity being consumed by the pump.

purpose of this model is to investigate what can be achieved for as little computational effort as possible.

Processes resources and qualities model (PRaQ) This formulation is also linear, and is in many ways similar to the null model, but it develops it to use a more sophisticated definition of resources, in which a resource can have multiple properties ('qualities') attributed to it. For example, water can have both a mass and an energy head. This means that processes can be defined to require (and produce) resources of particular qualities. For example, a dam needs not just a sufficient mass of water, but a sufficient mass of water at a required energy head. This more detailed representation of resources can more precisely characterise the properties of a system's resource, and the transformations it undergoes during a process (e.g. as water passes through a dam, its mass remains the same, but its quantity changes). In practice, this requires defining extra parameters and variables in the model, and inserting some additional equations.

Nonlinear (NL) This formulation allows nonlinear relationships between the resource flows into or out of a process.

Figure 5.7 shows how the three formulations are related both to the original urban energy systems model, and each other. Each formulation, in theory, increases its fidelity relative to the preceeding

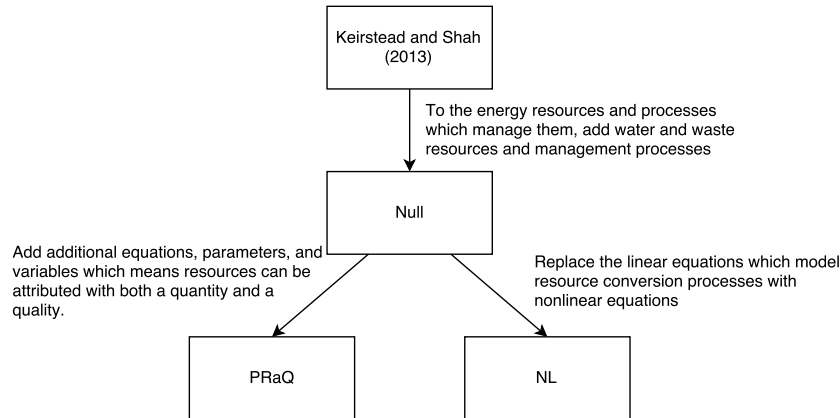


Figure 5.7: The relationship of this chapter’s formulations to each other and the urban energy systems model of Samsatli et al..

model: PRaQ increases in fidelity with respect to resources; and NL increases it with respect to processes too. However, this comes at a cost to generality because the PRaQ and NL formulations require more customisation of the data and equations (this is discussed further in Section 5.5.2). The differences between the formulations can be illustrated with reference to an example of the pipe, pump and dam system in Appendix 5.3.4. The constraints for the three formulations are given in Sections 5.3.1, 5.3.2 and 5.3.3, respectively. Examples of objective functions are given separately in Section 5.3.5.

5.3.1 Null formulation

The null model can be defined using similar base equations as for the Keirstead and Shah (2013) model, having as its main constraint, the balance for each resource r , in each zone z :

$$I_{rz} + \sum_{\tau} J_{\tau rz} + \sum_p G_{prz} = D_{rz} + E_{rz} \quad (5.2)$$

G and J denote the variables of resource production and transport by conversion and transport processes p and τ , respectively (their equations are defined in Equations 5.9 and 5.11, below). D denotes the demand parameter. I and E denote the import and export variables respectively, and these are limited by constraints which specify which zones are allowed to import/export each resource and the maximum they are allowed to import/export:

$$I_{rz} \geq \delta_{rz}^I I_r^{min} \quad (5.3)$$

$$I_{rz} \leq \delta_{rz}^I I_r^{max} \quad (5.4)$$

$$E_{rz} \geq \delta_{rz}^E E_r^{min} \quad (5.5)$$

$$E_{rz} \leq \delta_{rz}^E E_r^{max} \quad (5.6)$$

where I_r^{min} , I_r^{max} , E_r^{min} and E_r^{max} are parameters which limit the quantity of how much of any resource can be imported or exported. δ^I and δ^E are binary variables which equal 1 if a zone is allowed to import or export a resource, respectively, or 0 if it is not; the values of these binary variables are subject to limits on the total number of zones that are allowed to import or export a particular resource, defined by the parameters N_r^I or N_r^E , and must satisfy:

$$\sum_z^Z \delta_{rz}^I \leq N_r^I \quad (5.7)$$

$$\sum_z^Z \delta_{rz}^E \leq N_r^E \quad (5.8)$$

Conversion processes

To calculate the production of a resource by a particular process p in a zone z , the null formulation models processes as black boxes. The relative quantities of resource inputs to and outputs from these black boxes are denoted by the coefficient k_{pr}^P , which means the production quantity of a resource G can be modelled thus:

$$G_{prz} = k_{pr}^P F_{pz}^P \quad (5.9)$$

where the F variable defines the operation rate of a technology (for example, a dam may operate with a generating capacity of 3 MW). Carrying forward the principles of Section 4.2.2, the output resource

always has a coefficient value $k_{pr}^P = 1$ (in the dam example this would be electricity). The value of the F_{pz}^P variable is defined from the number N of any type of process in a zone, and their individual maximum operating capacities, F^{max} :

$$F_{pz}^P \leq N_{pz}^P F_p^{P,max} \quad (5.10)$$

Transport processes

The net resource inflow variable J is calculated from the difference between the resource quantity entering a zone via a transport technology, and the resource quantity leaving a zone via a transport technology.

$$J_{\tau rz} = \sum_{\tau z'} (k_{\tau r}^{\alpha} + k_{\tau r}^{\beta} l_{zz'}) F_{\tau zz'}^T + \sum_{\tau z'} (k_{\tau r}^{\alpha'} + k_{\tau r}^{\beta'} l_{z'z}) F_{\tau z'z}^T \quad (5.11)$$

The calculation of J is somewhat analogous to the calculation of G , in that it constitutes a resource coefficient multiplied by a rate, but it is developed in three ways. First, it is defined for a transport technology τ between two zones, z and z' , and thus considers each zone both as a source from which resources leave, and as a destination (denoted by a ') into which resources arrive, and thus resource flows arriving in zone z must be summed over all flows coming from all other zones z' , and resource flows leaving zone z must be summed over all flows travelling to all other zones z' . Second, the amount of resource arriving in/leaving from a zone is a function both of the technology itself and the distance spanned by the technology. For example, the amount of petrol required to transport goods depends on the distance l the goods will travel. This quantity is represented in the bracketed term, which is the multiplier of the transport technology's rate of operation $F_{\tau zz'}^T$'s variable. Thirdly, it is possible (though not necessary) that several transport technologies can carry the same resource (for example biomass can be transported by both lorries or vans: these would have different rates, and require different amounts of petrol etc.), hence the summation over transport technologies τ . Table 6.2 below

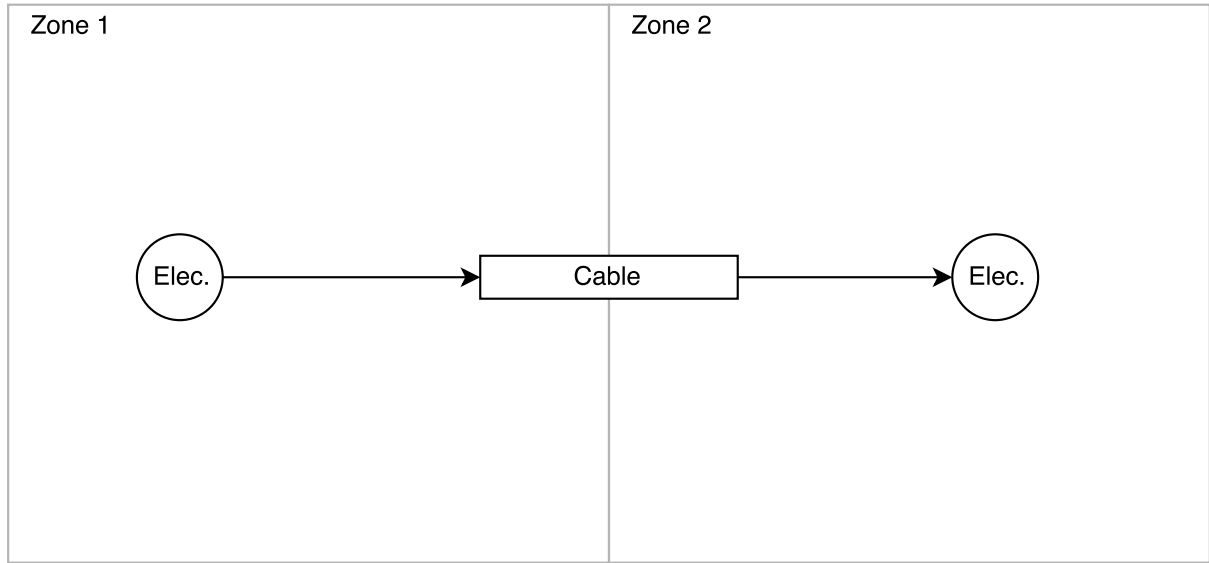


Figure 5.8: Representation of how electricity ("Elec.") transport is modelled. The quantity of electricity arriving in Zone 2 is the same as that leaving Zone 1 (this assumes negligible energy losses along the cable).

Table 5.1: Example parameter values to model transport processes represented by Figures 5.8 and 5.9.

τ	r	Source		Destination		Comment
		$k_{\tau r}^{\alpha}$	$k_{\tau r}^{\beta}$	$k_{\tau r}^{\alpha'}$	$k_{\tau r}^{\beta'}$	
Cable	Electricity	-1	0	1	<0	Small electricity losses
	Biomass	-1	0	1	0	No losses
Road	Petrol	0	<0	0	0	Petrol is supplied in source zone with the amount depending on distance
	CO2	0	>0	0	>0	Emissions depend on distance and are split between zones

gives examples of the parameter values for the examples of electricity and biomass transport in Figures 5.8 and 5.9, respectively.

As for conversion processes, $F_{\tau z'/z}^T$ is contingent upon a binary variable which specifies if transport technology τ exists between zones z and z' , and must lie between minimum and maximum rates of operation:

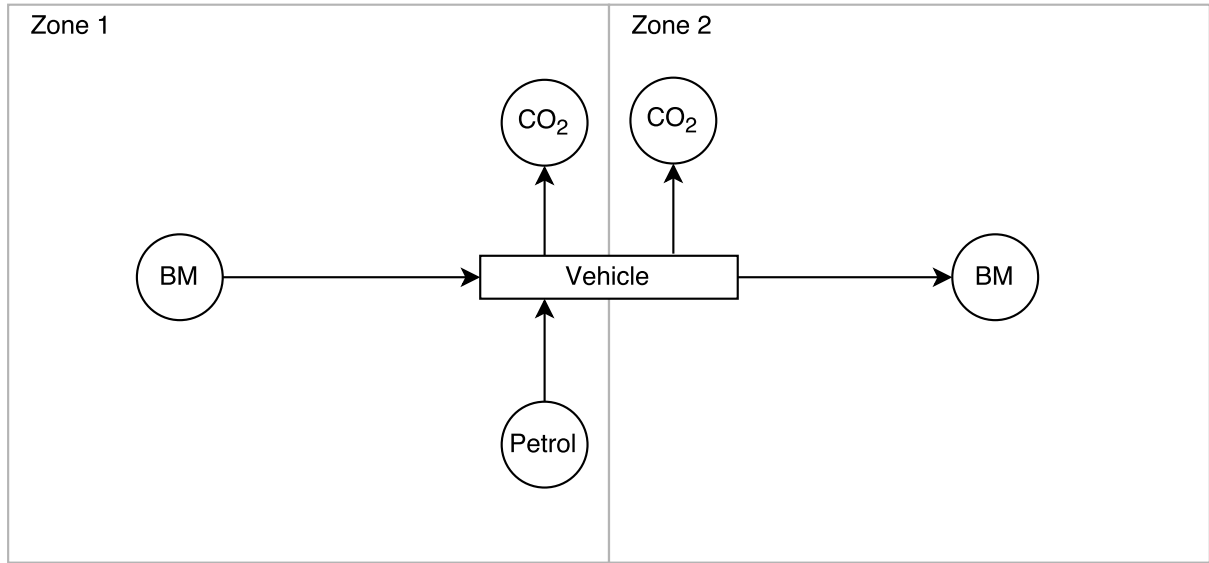


Figure 5.9: Representation of how biomass ('BM') transport is modelled. The quantity of biomass arriving in Zone 2 is the same as that leaving Zone 1. Transporting biomass by road requires petrol to be supplied in Zone 1 (the quantity of which is a function of the distance between the zones); the carbon dioxide emissions due to road transport are also dependent on distance, and are shared between Zones 1 and 2.

$$F_{\tau zz'}^T \geq \delta_{\tau zz'}^T F_{\tau}^{T,min} \quad (5.12)$$

$$F_{\tau zz'}^T \leq \delta_{\tau zz'}^T F_{\tau}^{T,max} \quad (5.13)$$

and transport technologies can only exist between zones which are defined as being neighbours:

$$\delta_{\tau zz'}^T = 0, \quad \forall (z, z') \notin nb \quad (5.14)$$

where nb defines a set of neighbouring pairs of zones. Finally, equation (5.15) allows resources to be transported in both directions along a connection:

$$\delta_{\tau zz'}^T = \delta_{\tau z'z}^T \quad (5.15)$$

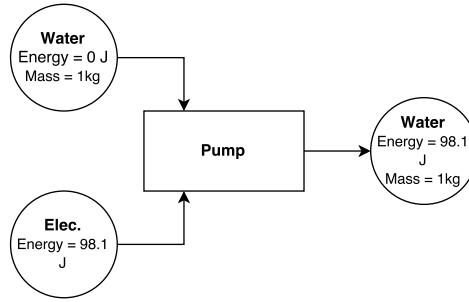


Figure 5.10: Example of PRaQ's resource-quality balance for a water pump which is bringing a kilogram of water to an elevation of 10 m. In this example, there are two input resources (water, and electricity). The water has two qualities attributed to it (mass and energy), and the electricity has just energy associated with it. Both mass and energy balance across the pump.

5.3.2 Processes, resources and qualities (PRaQ) formulation

The PRaQ model is based on the same equations as the null model, also following a black-box approach to modelling the conversion processes and transport technologies, and so as before, there is an equation which balances the resource quantities in each zone (Equation 5.16):

$$I_{rz} + \sum_{\tau} J_{\tau rz}^{(qty)} + \sum_p G_{prz}^{(qty)} = D_{rz} + E_{rz} \quad (5.16)$$

In addition, PRaQ develops Samsatli et al.'s formulation, to incorporate a more sophisticated definition of a resource, in which it possesses not just a quantity, but also the qualities, mentioned earlier. This is useful when considering the interaction between different sectors. Consider a body of water: this can supply (for example) both cooling for industrial processes, and hydroelectric electricity – this means the PRaQ model needs to know both its mass, and its energy head due to elevation. To model this, PRaQ uses an equation analogous to the quantity balance, which balances the resource qualities, q , within each zone z . The PRaQ formulation relates a resource's quantity to its quality by way of the parameter X_{rq} : this is multiplied by a resource quantity value to separate a quantity into its qualities⁵.

⁵For example, 1 kg of water at a 10 m elevation would have an energy head of 98.1 J, thus, X_{rq} would be defined as $X_{\text{water, mass}} = 1$, $X_{\text{water, energy}} = 98.1$. Therefore, if this body of water were being imported into zone z , $X_{\text{water}, q} I_{\text{water}, z} = 1 \text{ kg}$ and 98.1 J , for $q = \text{mass}$ and energy , respectively.

$$X_{rq}I_{rz} + \sum_{\tau} J_{\tau rz}^{(qual)} + \sum_p G_{prqz}^{(qual)} = D_{rqz}^{(qual)} + X_{rq}E_{rz} \quad (5.17)$$

The limits on imports and exports are defined in the same way as for the Null model:

$$I_{rz} \geq \delta_{rz}^I I_r^{min} \quad (5.18)$$

$$I_{rz} \leq \delta_{rz}^I I_r^{max} \quad (5.19)$$

$$E_{rz} \geq \delta_{rz}^E E_r^{min} \quad (5.20)$$

$$E_{rz} \leq \delta_{rz}^E E_r^{max} \quad (5.21)$$

Conversion processes

The modelling of conversion processes is similar to the black-box formulation of the null model, but again, two equations are used. The first defines the net resource quality, $G_{prqz}^{(qual)}$, generated by a conversion process in a zone at a particular time, for a process with variable operation rate F_{pz}^P , and parameters to define the relative ratio of resource inputs and outputs, k_{prq}^P :

$$G_{prqz}^{(qual)} = k_{prq}^P F_{pz}^P \quad (5.22)$$

The second equation is required so that resource quantities also balance. This constraint is effectively the same balance of quality as above, but is defined using the quantity variable ($G_{prq}^{(qty)}$), by using the X_{rq} parameter to split a resource's quantity into its quality attributes:

$$X_{rq}G_{prz}^{(qty)} = k_{prq}^P F_{pz}^P \delta_{rq}^R, \quad \forall \delta_{prq}^P = 1 \quad (5.23)$$

This equation uses two binary parameters to ensure the balance only applies to qualities when they

are attributed to a resource: therefore $\delta_{rq}^R = 1$ for all resource-quality pairings which exist, otherwise it takes a value of zero⁶. There is then a process equivalent parameter, δ_{prq}^P , which takes a value for 1 for all resource-quality pairings which exist (i.e. $\delta_{prq}^P \forall p$ when $\delta_{rq}^R = 1$).

The constraint on the number of allowable processes is defined as for the Null model:

$$F_{pz}^P \leq N_{pz}^P F_p^{P,max} \quad (5.24)$$

Transport processes

The transport processes are defined similarly, following the same logic as the Null model formulation to quantify the net inflow of resource quality, $J_{\tau rz}^{(qual)}$, into a zone, according to the rate at which the transport technologies can operate, and losses, and other resources involved:

$$J_{\tau rz}^{(qual)} = \sum_{z'} (k_{\tau rq}^{\alpha} + k_{\tau rq}^{\beta} l_{zz'}) F_{\tau zz'}^{\mathcal{T}} \quad (5.25)$$

$$+ \sum_{z'} (k_{\tau rq}^{\alpha'} + k_{\tau rq}^{\beta'} l_{z'z}) F_{\tau z'z}^{\mathcal{T}} \quad (5.26)$$

Again, this balance is also defined in terms of net inflow of quantities, $J_{\tau rz}^{(qty)}$, by using the X_{rq} parameter, and the binary parameter, $\delta_{rq}^R = 1$, where $\delta_{\tau rq}^{\mathcal{T}} = 1$ (these parameters are defined according to a similar logic to that used for the conversion processes⁷):

$$X_{rq} V_{\tau rz}^{(qty)} = \left[\sum_{z'} (k_{\tau rq}^{\alpha} + k_{\tau rq}^{\beta} l_{zz'}) F_{\tau zz'}^{\mathcal{T}} \right. \quad (5.27)$$

$$\left. + \sum_{z'} (k_{\tau rq}^{\alpha'} + k_{\tau rq}^{\beta'} l_{z'z}) F_{\tau z'z}^{\mathcal{T}} \right] \delta_{rq}^R \quad \forall \delta_{\tau rq}^{\mathcal{T}} = 1 \quad (5.28)$$

⁶For example, $\delta_{rq} = 1$ when $r = \text{water}$ and $q = \text{mass or energy}$, and when $r = \text{electricity}$ and $q = \text{energy}$; but when $r = \text{electricity}$ and $q = \text{mass}$, $\delta_{rq} = 0$.

⁷As for the conversion processes, $\delta_{\tau rq}^{\mathcal{T}}$ takes a value for 1 for all resource-quality pairings which exist (i.e. $\delta_{\tau rq}^{\mathcal{T}} \forall p$ when $\delta_{rq}^R = 1$).

The existence of transport processes between zones are defined using the same equations as for the Null model:

$$F_{\tau zz'}^T \geq \delta_{\tau zz'}^T F_{\tau}^{T,min} \quad (5.29)$$

$$F_{\tau zz'}^T \leq \delta_{\tau zz'}^T F_{\tau}^{T,max} \quad (5.30)$$

$$\delta_{\tau zz'}^T = 0, \quad \forall (z, z') \notin nb \quad (5.31)$$

$$\delta_{\tau zz'}^T = \delta_{\tau z'z}^T \quad (5.32)$$

5.3.3 Nonlinear (NL) formulation

The two model formulations derived thus far (null and PRaQ) are both as generic as it is possible to be. That is to say that all resources, conversion processes and transport technologies can be defined using the same equations – for example, Equation 5.22 will apply to every conversion process in the PRaQ model. The earlier discussion of model generality and fidelity noted that greater fidelity could be achieved with a less general model. This derivation will show how a nonlinear formulation can achieve closer correspondence between the model and reality for conversion and transport processes. The equations of this model are largely based on those of the Null model, with the main balance equation, and the imports and exports defined in the same way (Equations 5.33 to 5.37):

$$I_{rz} + \sum_{\tau} J_{\tau rz} + \sum_p G_{prz} = D_{rz} + E_{rz} \quad \forall r, z \quad (5.33)$$

$$I_{rz} \geq \delta_{rz}^I I_r^{min} \quad (5.34)$$

$$I_{rz} \leq \delta_{rz}^I I_r^{max} \quad (5.35)$$

$$E_{rz} \geq \delta_{rz}^E E_r^{min} \quad (5.36)$$

$$E_{rz} \leq \delta_{rz}^E E_r^{max} \quad (5.37)$$

Conversion processes

The change that the NL model makes is in the way conversion processes are modelled – these can be characterised as having either linear or nonlinear behaviour, by way of an adaptation to the conversion process equation (5.9):

$$G_{prz} = (\kappa_{pr}^O - \kappa_{pr}^I) F_{pz}^P \quad (5.38)$$

In Equation (5.38), the κ_{pr}^P parameter has been replaced by an expression which calculates the net output of a resource from process p , in which κ_{pr}^O and κ_{pr}^I represent the output and input of quantities of resource r , respectively. These variables can then be defined in a bespoke way. For a linear process, κ_{pr}^* is defined by a number, which essentially reduces Equation (5.38) to the null formulation Equation (5.9). However, for a nonlinear process, these values can be defined by equations. For example, for a dam's management of resources could be defined by two equations – an energy balance (5.39) and a mass balance (5.40), based on the formula for potential energy, 'energy = mass $\times$ gravity $\times$ height of water elevation' (and assuming a dam of 100 per cent efficiency):

$$\kappa_{p,r=\text{water}}^I g H_I = \kappa_{p,r=\text{water}}^O g H_O + \kappa_{p,r=\text{elec}}^O \quad (5.39)$$

$$\kappa_{p,r=\text{water}}^I = \kappa_{p,r=\text{water}}^O \quad (5.40)$$

where H_I and H_O are heights of the water on the input and output sides of the dam, respectively. In this dam example, the variables are $\kappa_{p,r=\text{water}}^I$, $\kappa_{p,r=\text{water}}^O$, $\kappa_{p,r=\text{elec}}^O$, H_I , and H_O – notice that variables can be multiplied by each other (i.e. the mass of water and its height).

The number of processes is defined in the same way as the Null model:

$$F_{pz}^P \leq N_{pz}^P F_p^{P,max} \quad (5.41)$$

Note that as in the Null model, F_{pz} is defined with respect to the resource that is considered the ‘main output’ which by definition has a magnitude of 1 – this needs to be fixed in the NL formulation. In the case of the dam, the main output is electricity, thus $\kappa_{p,\text{elec}}^O = 1$

Transport processes

In theory, these could be formulated in a similar way to the conversion processes, to allow for non-linear behaviour, however, they have been defined using the same set of equations as for the Null model:

$$J_{\tau rz} = \sum_{tz'} (k_{\tau r}^{\alpha} + k_{\tau r}^{\beta} l_{zz'}) F_{\tau zz'}^{\mathcal{T}} + \sum_{tz'} (k_{\tau r}^{\alpha'} + k_{\tau r}^{\beta'} l_{z'z}) F_{\tau z'z}^{\mathcal{T}} \quad (5.42)$$

$$F_{\tau zz'}^{\mathcal{T}} \geq \delta_{\tau zz'}^{\mathcal{T}} F_{\tau}^{\mathcal{T}, \min} \quad (5.43)$$

$$F_{\tau zz'}^{\mathcal{T}} \leq \delta_{\tau zz'}^{\mathcal{T}} F_{\tau}^{\mathcal{T}, \max} \quad (5.44)$$

$$\delta_{\tau zz'}^{\mathcal{T}} = 0, \quad \forall (z, z') \notin nb \quad (5.45)$$

$$\delta_{\tau zz'}^{\mathcal{T}} = \delta_{\tau z'z}^{\mathcal{T}} \quad (5.46)$$

5.3.4 Explaining the difference between the linear and nonlinear models

This chapter has developed both linear and nonlinear models to consider the integrated management of energy, water and waste systems. Section 5.3.3 used the example of a dam to show the implications of nonlinearity on a model. This section further explains the difference between linear and nonlinear formulations, using the example pipe-pump-dam system of Figures 5.11 and 5.12. In this example, an optimisation programme calculates the pumping energy and water volumes required at point A to raise the water to a sufficient height at point B, that will allow the dam to generate enough electricity to meet demand at point C. The relevance of this example to the Tat Hamlet benchmarking problem is that there has been a dam incorporated into the model of the village in order to give an oppor-

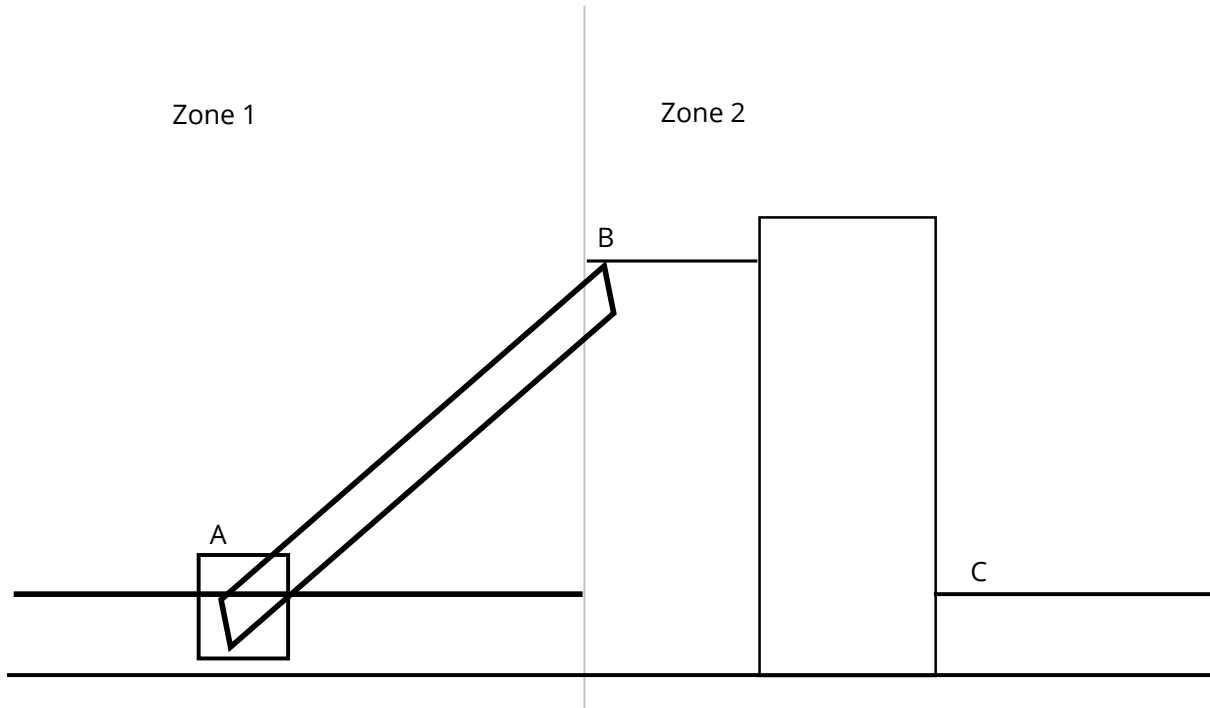


Figure 5.11: An example to illustrate the difference between model formulations. There are two zones. Zone 2 has an electricity demand which can be met by a dam (a conversion process), also in zone 1. However, the water must first be pumped (via the pump – a conversion process in zone 1) and transported to zone 2 via a pipe (transport process).

tunity to test how linear and nonlinear formulations compare. The following description expresses this problem using equations of fluid mechanics, discussing how it would be modelled by the three formulations.

The Bernoulli equation states that energy is conserved along a streamline of a fluid of density ρ :

$$\frac{P}{\rho g} + z + \frac{v^2}{2g} = \text{constant} \quad (5.47)$$

where at a given point along the streamline, P is the water's pressure, z is its elevation with respect to a reference, and v is its velocity (and g is the constant of acceleration due to gravity).

First, consider the water flow from A (zone 1) to B (zone two) via the combination of a pump and a pipe. The pump provides the energy to raise the water's elevation and has an electrical efficiency of η^{pump} . This energy includes that which is required to overcome the energy loss due to friction. Typically this friction loss is defined as a function of the pipe's length l and diameter D , and the water's velocity

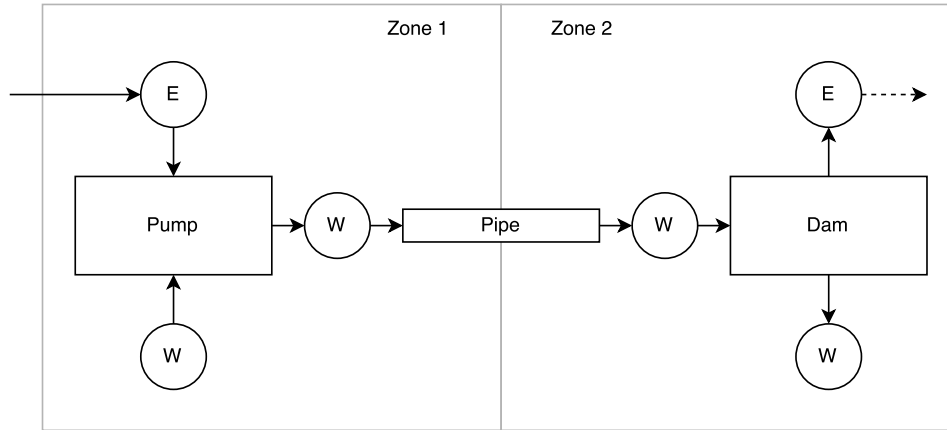


Figure 5.12: An RTN representation of Figure 5.11. The electricity (E) required by the pump can be imported from outside the system; the amount required depends on the mass of water (W) to be pumped, and the elevation to which it needs pumping. The dashed arrow indicates that the electricity in Zone 2 is a demand.

v , with friction loss being given as $f_D(l/D)(v^2/2g)$, where f_D is the Darcy Friction Factor. It is also assumed that $P_1 = P_2$ and that $v_1 = v_2 = v$, and that the datum is measured from A and C (which are at equal height), thus $z_A = z_B = 0$. Finally, given that the model equations are defined formulated in terms of mass and energy balances, it is helpful to multiply each term by mg . The resulting equation gives the water's energy at points A and B expressed in terms of its mass, velocity and elevation:

$$\eta^{pump} \cdot (\text{pump energy}) = m \left(gz_B + f_D \frac{l}{D} \frac{v^2}{2} \right) \quad (5.48)$$

Second, consider the flow across the dam, between B and C . Using the same assumptions as above, and defining the dam with an electrical generation efficiency, η^{dam} , and again multiplying through by mg , the relationship of input water attributes with the dam's electrical output is given by:

$$mgz_B = \eta^{dam} \cdot (\text{electricity generated}) \quad (5.49)$$

In this problem, a model needs to calculate the value of variables which enable the system to meet demand for electricity generated by the dam, which in this example will be 1 megajoule. With the electrical output already defined, the required mass m and dam height z_B can be calculated using

Equation (5.49). Given that the quantity of water required to generate a given amount of electricity (m) is always a variable, for a model to remain linear, the water's elevation head (i.e. the dam height, z_B) cannot be considered a variable, and must be a fixed parameter. Therefore, both the null and the PRaQ models require a dam to be defined with fixed height. Thus, assuming a dam of height $z_B = 11$ metres and efficiency $\eta^{dam} = 80$ percent, the mass of water required to produce a megajoule of electricity is 12,742 kg. In contrast to this, however, the nonlinear model does not need to fix the height of the dam, and can achieve the required 1 megajoule of electricity through any suitable combination of m and z_B ⁸.

Similar principles apply to the pump and pipe, whereby a model needs to calculate how much pumping energy is required, based on Equation (5.48). In the Null and PRaQ models, only m is a variable, and hence l , D and v must all be fixed; however, the nonlinear model would be able to consider these as variables.

5.3.5 Model objectives

The three models derived in Sections 5.3.1–5.3.3 will minimise some objective. There are numerous possibilities. A common objective for these models is to minimise the cost of a system, i.e. the summed costs of the resources, conversion processes, and transport processes, (C^R), (C^P), and (C^T), respectively:

$$C^R = \sum_{rz} c_r I_{rz} \quad (5.50)$$

$$C^P = \sum_{pz} c_p N_{pz} \quad (5.51)$$

$$C^T = \sum_{\tau zz'} c_\tau \delta_{\tau zz'}^T l_{zz'} \quad (5.52)$$

where the parameters c_r , c_p , c_τ defines the cost of an item per unit (e.g. a kilogram of water, a joule of energy, or a single process). These costs can be combined into a single objective function:

⁸For example, if z_B is doubles to 22 metres, then m can be halved to 6,371 kg.

$$C = \gamma^R C^R + \gamma^P C^P + \gamma^\tau C^\tau \quad (5.53)$$

where coefficients γ^* could weight the costs appropriately: for example, annualising system cost by multiplying the resource imports up to a yearly level, and dividing the capital costs over its expected lifetime.

Other types of objective function could include the carbon footprint of an area, defining this using the emissions factor of a resource, ϵ_r :

$$\text{Carbon Footprint} = \sum_{rz} \epsilon_r I_{rz} \quad (5.54)$$

Multiple objectives can be used, and traded-off against one other, in so-called ‘Pareto optimisation’ (Chiandussi et al., 2012). In this method, one objective is used as the objective function (such as cost), while another is defined as an inequality constraint (such as emissions):

$$\sum_{rz} \epsilon_r I_{rz} \leq \text{Emissions limit} \quad (5.55)$$

The model is then run multiple times, changing the value of the emissions limit each time, enabling the plotting of a curve of the system’s emissions against its cost.

5.3.6 Summary

The Null model is built around the resource balance (5.33), for which resource imports and exports are constrained by (5.34)–(5.37). The conversion processes operate according to (5.9) and the number of them which exist is constrained by (5.10). Similarly, transport processes operate at rates governed by (5.11), with their existence between zones defined by (5.12)–(5.15).

The PRaQ model is formed using a similar set of constraints to the Null model (Equations (5.16)–(5.32)),

namely resource balances, import and export limits, and black-box models of conversion processes and transport processes. In order to incorporate resource qualities, the formulation introduces additional equations, which use new parameters and variables whose purpose is to map resource qualities onto quantities. Finally, the NL model is formulated in the same way as the Null model, apart from for the conversion process equation, which is formulated to allow processes to be modelled using nonlinear mathematics.

The three formulations use continuous variables (e.g. resource quantities and process rates), integer variables (e.g. the number of conversion processes in a zone), and binary variables (e.g. to define the existence of a transport process between two zones). The Null and PRaQ models are linear, and so form mixed-integer linear programmes (MILPs), whilst the nonlinear model forms a mixed-integer nonlinear programme (MINLP). In each case, the models require users to specify zonal demands for the resources available to an area, as well as the parameters which describe the behaviour of available conversion process and transport technologies. The constraints are solved in order to minimise an objective function.

5.4 Implementation

The models have been encoded using the specialist GAMS language⁹, and uses IBM's CPLEX¹⁰ solver to solve the linear models, and the BARON solver to solve the nonlinear model. Each model has two components, namely the *formulation*, which includes the mathematics (i.e. the equations, abstracted from the data), and the *data*, i.e. the parameter values which will populate the equations (site layout, resource demands, process behaviour, etc.).

The data are separated into two types. *Library* data defines the properties of resources (i.e. their quality attributes) and processes (i.e. their k_* coefficients and maximum processes rates F_*); this data is defined in YAML format. *Site* data defines everything else, including the site's spatial layout, the resource demands, and restrictions on imports and exports; this is all defined in comma-separated value (CSV) format. Both CSV and YAML data formats are chosen for their human-readability, their ease of editing, their ability to be understood by programming languages, and the fact that as plain-text, they

⁹General Algebraic Modelling System: <https://www.gams.com/>

¹⁰<https://www-01.ibm.com/software/commerce/optimization/cplex-optimizer/>

can be version-controlled[[^]version-control]. [[^]version-control]: Version control is a way to track any changes made to a set of files (Ernst, 2018). This facilitates the development of the project over time, by enabling multiple collaborators to work on parts of a project without interfering with one another's work, and to enable easy reversion to previous versions of a project.

These two components of data and formulation are kept strictly separate. To build a model, the requisite sets of data needs to be combined with the correct aspects of the formulation in the correct order. For example, a case study may consider just a limited set of conversion technologies, and might choose a minimum cost objective (rather than a minimum emissions objective, for example – thus only requiring a subset of the library data). Combining the data and formulation, is performed by a script (written using the R programming language), which assembles the GAMS code for a particular model run. This architecture is visualised in Figure 5.13.

This approach to implementation means its easy to build versions of a network for each formulation. For example, one might want to change the set of processes available to the network – the user just needs to change the CSV and YAML data, and then run the R-script, which will then build the model for each of the three formulations. This 'modular' implementation also makes it easy to modify or extend the formulation, and apply to multiple cases. Structuring the code in this ways serves not just the practical convenience for a modeller, but helps to establish this model as a benchmarking study by reducing the effort required to compare formulations on the same case study. All the data and code to run these models, as well as the results of the Tat Hamlet study (below) are freely available online at <https://github.com/tomravalde/model-development-code>.

5.5 Applying the formulations to Tat Hamlet

Each formulation is applied to the Tat Hamlet case study, to compare how each model performs in relation to the tradeoffs in generality, fidelity, usability and tractability (Section 5.1). The approach taken is to build up the Tat network one conversion process at a time (beginning with the just the dam, as shown in 5.14) – introducing resources necessary for each set of processes, and transport processes used by these resources – until the complete network of Figure 5.2 is realised. Each network is modelled using all three formulations, in each case recording data on the model's properties and performance (such as number of variables and runtime). The order in which the network is built up

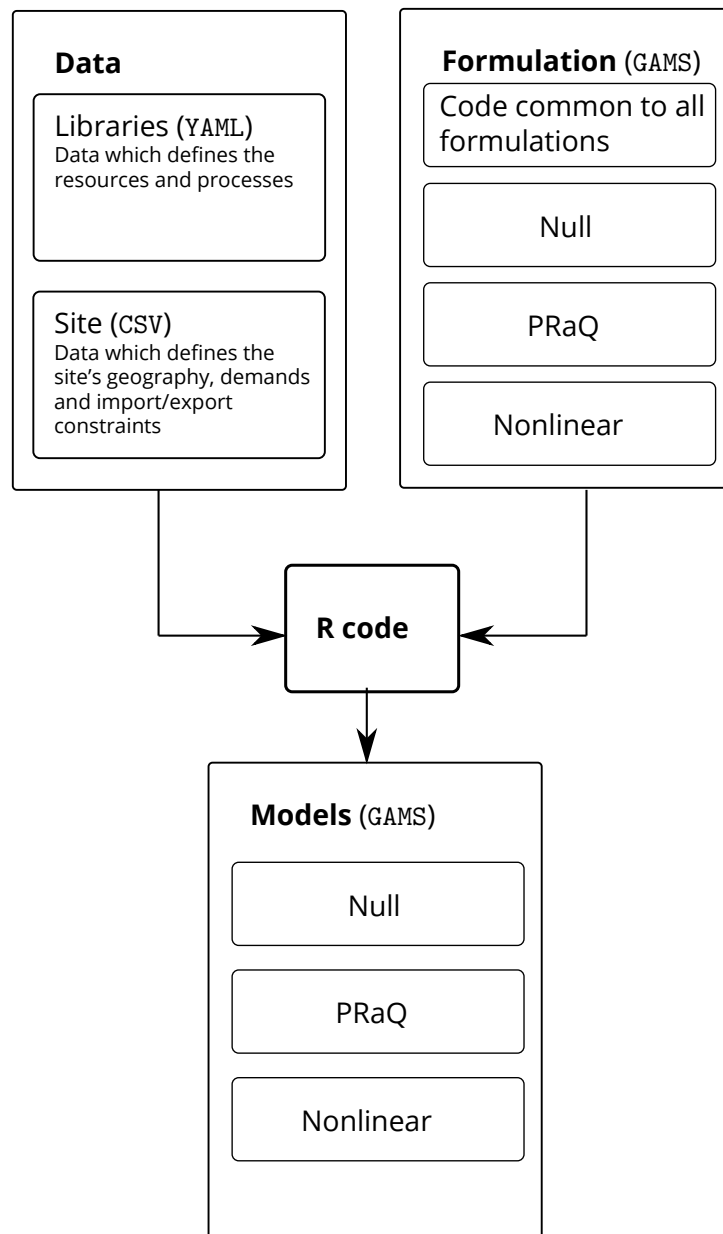


Figure 5.13: Code architecture and workflow for assembling the benchmark models for the Tat Hamlet case study.

is given in Table 5.2, along with the resources, conversion processes and transport processes used at each stage of building up the Tat network.

Table 5.2: The resources, conversion processes, and transport processes used in each stage of building up the Tat network between Figures 5.14 and Figures 5.2. The model is applied to the first network (Figure 5.14), and then processes are added one by one, with the model being run for each system, until the final network has been assembled (Figure 5.2). The table also indicates the abbreviations used in network diagrams.

Conversion processes			Resources			Transport processes		
No.	Added	Abbrev.	No.	Added	Abbrev.	No.	Added	Abbrev.
1	Dam	Dam	3	Water, Water (dam), Electricity	W, W, El.	1	Cable	Cab.
2	Water treatment (for livestock)	WT (l/stock)	5	Water (livestock), Wastewater (livestock)	W, WW	2	Pipe (livestock water)	P (l/stock)
3	Water treatment (for domestic use)	WT (dom.)	7	Water (domestic), Wastewater (domestic)	W, WW	2		
4	Irrigation	Irrig.	8	Water (irrigation)	W	3	Pipe (irrigation water)	P (irrig.)
5	Pump	Pump	9	Water (pumped)	W	4	Pipe (domestic water)	P (dom.)
6	Agriculture	Agric.	17	Vegetables, Manure, Green manure, Fish feed, Petrol, Biomass (medium moisture content), Biomass (wet), CO ₂	Veg., Man., G. man., F. Feed, Pet., BM (med), BM (wet), CO ₂	8	Vehicle (manure), Vehicle (green manure), Vehicle (petrol), Vehicle (vegetables)	V (man.), V (g/man.), V (pet.), V (veg.)
7	Livestock	L/stock	18	Meat	Meat	9	Vehicle (meat)	V (meat)
8	Stove	Stove	20	Heat (stove), Firewood	H, F/wood	10	Vehicle (firewood)	V (f/wood)
9	Biomass drying (medium moisture content)	BMD (med.)	20			10		
10	Biomass drying (high moisture content)	BMD (wet)	20			10		
11	aquaculture	Aqua	21	Fish	Fish	12	Vehicle (fish), Vehicle (fish feed)	V (fish), V (f/feed)
12	Cooking	Cook.	24	Meat (cooked), Fish (cooked), Vegetables (cooked)	Meat (c), Fish (c), Veg. (c)	12		
13	Agricultural machinery	Agric. Mach.	24			12		
14	Domestic appliances	App.	25	Appliance use	App. use 12			
15	Heating	Heat.	26	Heat (domestic)	H	12		
16	Water heating	WH	27	Hot water	HW	12		

5.5.1 Results: comparison of formulations

Figure 5.15 shows how the number of equations and variables, run-time, and objective function value change with the number of processes in Tat's network. These plots show that as the number of conversion processes added to the network increases, then so do the number of equations and variables. When comparing the formulations, the number of variables and equations have the same order of magnitude. More interesting however, is the comparison of objective function values and run times, which exhibit two phenomena. First, unlike for the numbers of equations and variables, the objective function and the solution time do not monotonically increase with the number of processes (note in particular the spike in objective value for eight conversion processes, which does not find a solution within the 1,000 second limit imposed on the run-time). This unpredictability is because the speed at which nonlinear optimisation algorithms arrive at an optimal solution is sensitive to the way the model is formulated, even being affected by the order in which equations, variables, and components are defined. Second, a difference in the order of magnitude of solution time opens up from the point at which the network contains six or more conversion processes. Note that these solution times are to achieve objective function values that are very similar to those produced by the linear formulations (this can be more clearly seen in the plots where outliers have been removed). These behaviours give insight into how the formulations behave with respect to fidelity, generality, tractability, and usability, which are discussed in the following sections.

5.5.2 Discussion: which formulation should be used?

There are two important questions, the interaction of which will determine which formulation should be carried forward:

1. How well do the Null, PRaQ and Nonlinear formulations perform according to the characteristics of fidelity, generality, tractability, and usability (Section 5.1)?
2. What are the relative importances of these characteristics for this thesis' aims?

These questions are discussed in the following two sub-sections.

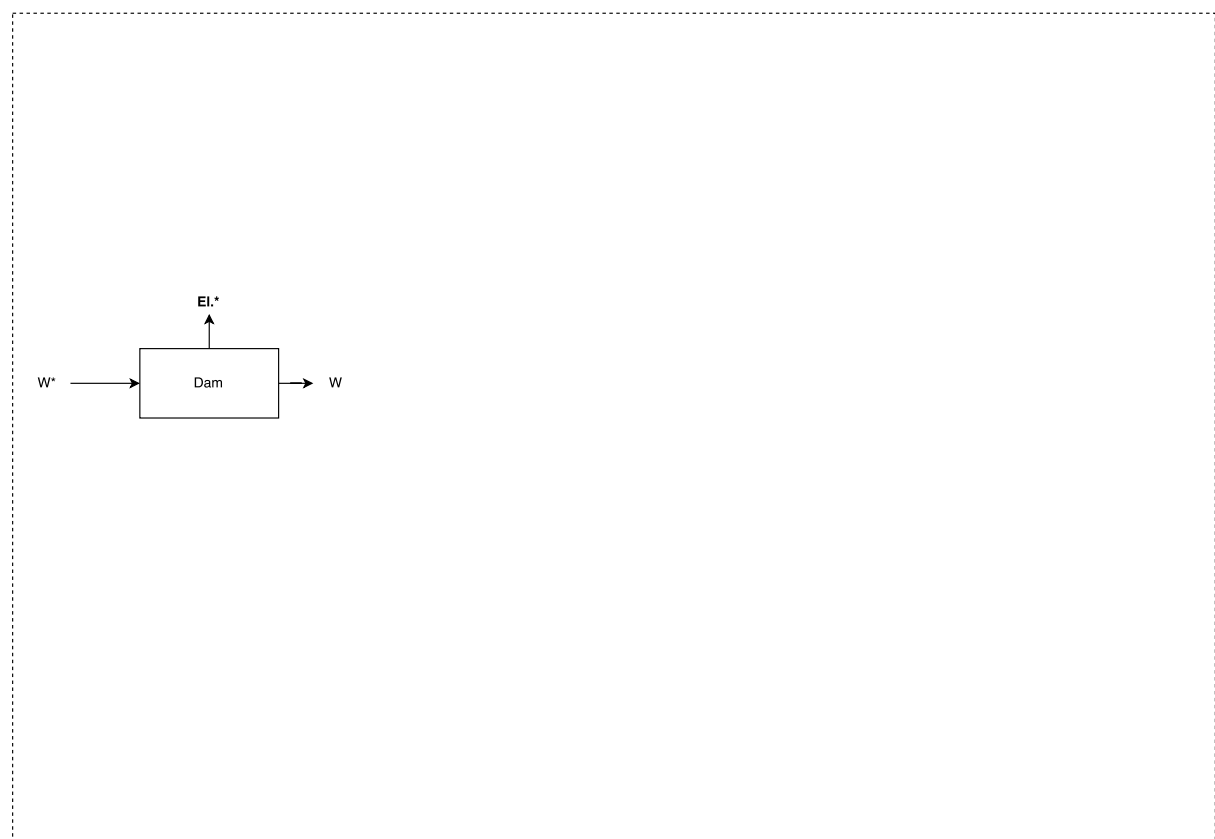


Figure 5.14: The first network to which the three formulations are applied. In this network, water and electricity can be imported in order to meet electricity demand.

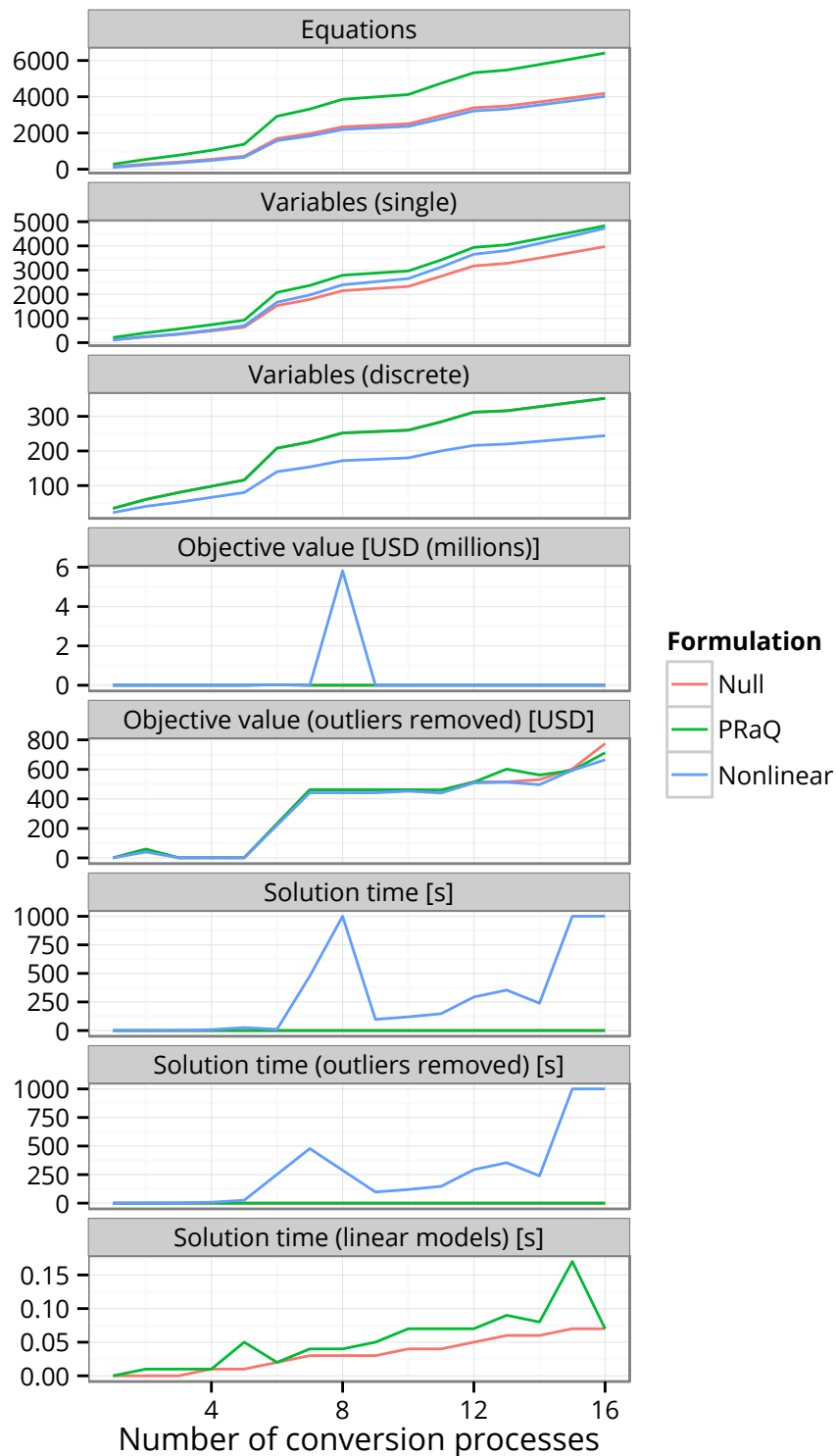


Figure 5.15: Comparison of model formulations. The plots headed with “outliers removed” show the same information as their counterparts, however with the data for 6 and 8 conversion processes removed. (The explanation for these outliers is given in Section 5.5.1.)

The trade-offs between the Null, PRaQ and Nonlinear formulations

One way to assess a model's fidelity would be to verify its results against real data. One could measure resource demands of Tat and the resource flows within the system, and then run the models using the measured demands to see if the model chooses a similar system and schedule of resource management. However, this would be impractical given the sheer number of variables involved (the sixteen-process networks have at least 4,000 variables in their models). Each of these variables represents a decision (for example, on where processes should be located, how they should be linked, and at what rate they should operate, as well as the resource quantities which should flow between them). Furthermore, the Tat Hamlet benchmarking problem is just a small-scale example of a resource management system, and does not even contain a temporal component. Due to this, it is impossible to validate models of this type by comparing its results to those of the real world (and as pointed out in Section 2.2.1, practical limitations are one reason that models can be useful). Moreover, even if such validation were practical, this method would assume that the inhabitants of Tat are trying to optimise the same objective as the computer model – given that a premise of this thesis is that urban resource management is generally sub-optimal, this approach would beg the question of why this thesis is even necessary. Furthermore, for the purposes of developing the model, Tat Hamlet has been re-imagined with simplifications, adjustments and assumptions, and hence there are some ways in which the modelled system and the real-world system are not comparable.

The inability to validate the model with real data is not unique to this thesis; many other models which optimise the systems at the urban scale cannot be validated in this manner, including the earlier-cited model of Keirstead and Shah (2013). This means that assessing the fidelity of the models must be achieved theoretically, with reference to the formulations themselves. As discussed in Section 5.1.2, on this view of fidelity, the nonlinear formulation is the most faithful to reality. The nonlinear formulation can model phenomena that linear models cannot. In second place is the PRaQ model, because it can attribute multiple properties to a resource, which is the case in the real world. The lowest fidelity version is the null formulation because it limits the representation of process behaviour to linear mathematics, and the representation of resources to single attributes (see Section 5.3).

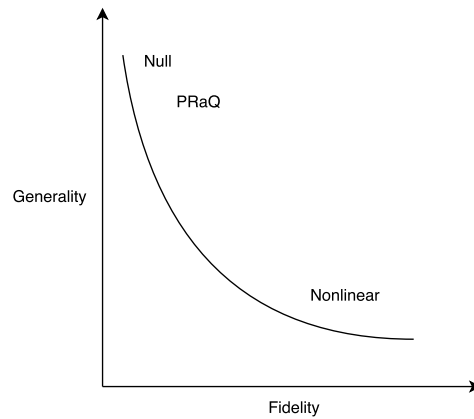
However, while the nonlinear formulation might have the greatest fidelity, it ranks lowest for generality, because nonlinear processes need Equation 5.38 to be defined specially for any nonlinear pro-

cess, so a single form of equation cannot be generally applied to all processes. In contrast, the linear models can apply the same equations for any process type (Equations 5.9 and 5.22–5.23 for the null and PRaQ models, respectively). The differences in resource definitions in the linear formulations arguably means PRaQ is slightly less general than Null – the need to attribute qualities to PRaQ’s resources could be seen to decrease generality because not every resource has the same number or combinations of qualities attributed to it (some may have just energy, some have mass, some may have both). However, the difference in generality between PRaQ and Null is small.

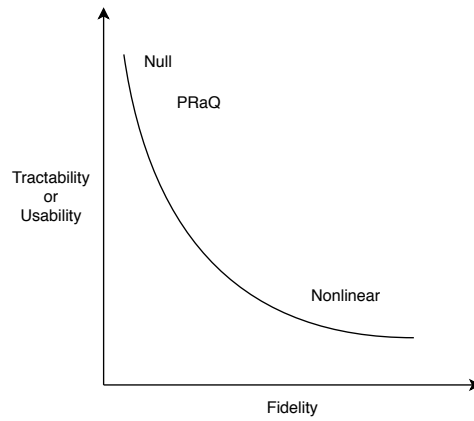
The most straightforward measure of tractability is computation time. The nonlinear model is the clear loser here, hitting the run-time limit (1,000 seconds) when running the full network, while the linear formulations run in fractions of a second. Figure 5.15 shows that these runtimes are driven by non-linearity. This is because the relationship between the number of conversion processes and the number of equations or variables is linear for all three formulations, and furthermore, the nonlinear model never has the highest number of equations or variables, yet as the model adds conversion processes, the nonlinear solution time increases exponentially, but linearly for the linear models. Note that these times are for models with only 16 processes, yet the library assembled in Chapter 4 contains 202 processes; moreover, these solution times are for models with neither temporal disaggregation nor nonlinear models of transport processes, both of which would further widen the runtime between linear and nonlinear formulations. In summary, nonlinear models are much harder to solve than equivalently sized linear models.

Usability is a more qualitative metric than tractability, and so harder to quantify precisely, but it can be measured by the ease of model construction. The simplest model to build is the null model, because the equations which model the processes and the resource balances can be defined generically, with only the production coefficients (k_{pr}^P and k_{prq}^P) needing to be specified. The PRaQ model is in theory harder to construct because of the quality set q and the additional variables¹¹. However, the model architecture described in Section 5.4 means little extra effort is required to gain the benefits of attributing multiple qualities to a resource – both Null and PRaQ are built from the same library of process behaviour and resource properties – the R-script does the hard work of converting these YAML files into the GAMS code. On the other hand, the NL model is harder to construct, because the conversion-process equations require much more customisation (note how this relates usability and

¹¹These are X_{rq} , $G_{prqz}^{(qual)}$, $V_{rrqz}^{(qual)}$, δ_{rq}^R , δ_{prq}^P , δ_{rrq}^T , k_{prq}^P , k_{rrq}^α , k_{rrq}^β , $k_{rrq}^{\alpha'}$, and $k_{rrq}^{\beta'}$.



(a) The trade-off between fidelity and generality.



(b) The trade-off between fidelity, tractability, and usability.

Figure 5.16: The trade-off between model formulations.

generality). The generic way in which the system resources are balanced in null and PRaQ gives way to a need to define each resource balance individually in the NL model – this is because the way a resource balance is defined needs to be customised according to which processes exist in the network.

In summary, the nonlinear formulation has the highest fidelity, but as a consequence has lowest generality, usability and tractability. The null and PRaQ models have lower fidelity, but are more general, tractable and usable. The PRaQ model has a very slightly lower generality, usability and tractability than the null model, but it has a higher fidelity. These performance features are represented in Figures 5.16(a) and 5.16(b).

The relative importance to this thesis of each performance characteristic

The discussion so far demonstrates a claim which opened this chapter, namely that the four modelling features “trade off against one another” (Section 5.1.1, page 124). Therefore, to decide which formulation to carry forward requires determining which features are most important for the purposes of this thesis.

It is argued here that generality is the most important characteristic – the whole purpose of this thesis is to develop a method which considers the production, consumption and transport of energy, water and waste management together, in a general way. It is therefore helpful that processes from different types of system can be defined in similar ways, because this generality brings about usability. Modellers can easily assemble models in order to derive insights on how the systems should work together. Moreover, Chapter 4 means that linear definitions of process behaviour already exist, avoiding the need for the modeller to go to the effort of writing bespoke equations of process behaviour. Tractability is also desirable because it allows the modeller to quickly explore different options for planning a network of resource management processes. Furthermore, models which are more tractable and usable can be used more widely, requiring less specialist knowledge and software (such as nonlinear solvers).

Relative to the above considerations, the greater theoretical fidelity of the nonlinear model is less important. Increasing fidelity reduces generality, usability and tractability, such that it is worth sacrificing fidelity. For now, nonlinear process behaviour may be too much of a luxury for a more generic model, where the equations should apply to multiple real world systems which are being investigated at a high-level. Given that there is very little difference between Null and PRaQ, it would make sense to carry forward with the PRaQ model; the cost of increased fidelity is barely noticeable in relation to generality, usability, and tractability. Furthermore, if the modeller so chooses, the PRaQ can be reduced to the null formulation by only attributing a single quality to each resource.

5.6 Conclusion

One of the aims of this thesis is to develop a model which can optimise how systems of different types can work together to manage resources in such a way as to improve an area’s metabolism. This chap-

ter has established three possible model formulations, and has discussed the relative merits of each method with respect to fidelity, generality, tractability and usability. The linear models were shown to be the most general, tractable and usable, whilst the nonlinear model is in theory the most faithful to the reality being modelled. The above discussion proposed that the importance given to these four characteristics should be determined by the model's purpose, which – like the precedent model of Samsatli et al. – seeks a generic approach to urban resource modelling.

Therefore, it is proposed that the PRaQ model is carried forward for future use. However it is noted that improvements can be made to the formulations, and thus the Tat Hamlet case study has been made publicly available as a benchmarking study for the UM field. It is important that the considerations of the above discussion inform how the model is used – this thesis has chosen to prioritise generality over fidelity, and so PRaQ should not be used for detailed design decisions. Rather, it provides high-level guidance on how systems might improve an area's urban metabolism. This shall be the focus of the next chapter, where the PRaQ model is used in a case study, to help optimise the intersectoral synergies of a Chinese urban development.

5.6.1 Developments to the optimisation model

The methods in this chapter can be made more sophisticated in a number of ways. Four such developments are inspired by the urban energy systems model on which PRaQ was originally based (Keirstead, 2013, Samsatli et al.):

- *Enable the model to distinguish between domestic and non-domestic conversion processes and resources.* For processes and resources belonging to the domestic set, constraints could ensure that (i) a household has a maximum of one type of domestic technology; (ii) households have a minimum of one technology that can provide each required domestic resource; (iii) domestic technologies do not provide more than a household requires; and (iv) domestic production must equal domestic demand. These four constraints are formulated in Equations 9 to 12 of Samsatli et al.
- *Introduce processes which store resources.* Such storage processes might hold biomass, water and other resources over a period of time. These would need to be able to quantify the resources required to keep a resource in storage (for example heat required to keep biomass dry), and losses over time (for example, in the case of stored heat). Such constraints are formulated in

Equations 9.3–9.10 of Keirstead (2013).

- *Take greater advantage of PRaQ's geographical representation..* Each zone, z , could have spatial area A_z^Z defined for it. Processes p could also be defined with a spatial area (i.e. its 'footprint'), A_p^P , and then a constraint could be defined which restricts a zone's process selection to those that fit inside it. This constraint is formulated in Equation 37 of Samsatli et al.
- *Model demand variation over hourly, daily, weekly, and seasonal periods, in a computationally efficient manner.* In practice, the computational cost of using small time steps may become prohibitive as it multiplies the number of variables. One way to address this is to use 'hierarchical non-uniform time discretization', as described in Keirstead (2013) (Section 9.2.1, p161). This method considers time at different levels (e.g. yearly, weekly, daily, hourly, etc.). By definition, each level is defined by the next level down (e.g. a week is seven days). This means a city's demand profile can be constructed by combining these units of time in appropriate proportions. For example a week can be made up of two day types (weekday and weekend), which repeat five times and two times, respectively. These two day types are each assembled from types of hour (e.g. morning peak, evening peak and rest-of-day average). In this way, a 90 day season could be modelled at hourly granularity (for example) with just $3 \text{ hour types} \times 2 \text{ day types} = 6 \text{ intervals}$, rather than by $90 \text{ days} \times 24 \text{ hours} = 8,760 \text{ intervals}$.

One thing that the developments above cannot do is deal with nonlinear process behaviour. This is not to say that over the longterm, there is no hope for a nonlinear formulation (especially given that computation times are reducing all the time). Two possibilities present themselves:

- One approach is to adopt 'piecewise linear modelling'. In this approach, nonlinear functions are linearised by approximating them as being made up of several linear components (Figure 5.17).
- An alternative approach is to write a fully nonlinear formulation, but to use heuristic methods to find a solution. Such methods do not necessarily find the mathematically optimal solution, but they do get close to it, often in less time. They carry the added advantage that they do not get trapped in the 'local minima' which can exist in certain nonlinear problems (Williams, 1990, Section 7.2, p140).

Note that these approaches only solve the issues of tractability, and the lack of generality remains, because of the need to define nonlinear process behaviour. Any nonlinear formulations – however

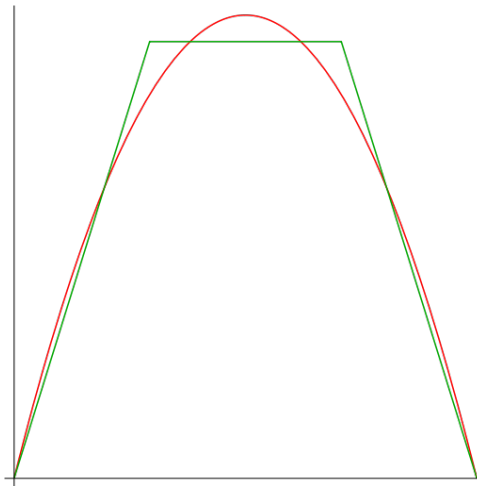


Figure 5.17: An example of a nonlinear function (red) which has been given a piecewise linear approximation (green)¹².

they are solved – would require Chapter 4’s database to be replaced by a set of equations which represent process behaviour. This will likely require sector-specific expertise; perhaps dividing up the 202 current processes among several specialists in the fields who can write necessary bespoke equations.

¹²Image available from Wikimedia Commons: https://commons.wikimedia.org/wiki/File:Piecewise_linear_approximation.svg.

Chapter 6

Case study: a Chinese urban development

“I don’t like novels that end happily. They depress me so much”

Cecily Cardew in *The importance of Being*

Earnest by Oscar Wilde

An early version of the work in this chapter was published as: Ravalde, T. and Keirstead, J. (2015b). Comparing performance metrics for multi-resource systems: The case of urban metabolism. *Journal of Cleaner Production*, 163:S241–S253.

This thesis has argued for the need for an optimisation model which can help plan urban energy, water and waste infrastructure, with a view to improving the urban metabolism of an area. To that end, the previous chapter introduced the PRaQ model – a MILP formulation that is generic enough to incorporate multiple resource types, user-friendly to construct, and can be solved without excessive computational effort. Such a model enables the evaluation of the hundreds of thousands of choices which could be considered when taking into account all the possible ways a system could be configured (which processes should be used, where they should be located, and the rates at which they operate, etc.). This chapter now applies the PRaQ model to a case study, using the library of resource management processes assembled in Chapter 4, and using some of the principles of Chapter 3 to assess the systems designed by the model.

This chapter first introduces the case study which is based on the site of a Chinese urban development

(Section 6.1), before outlining the site's spacial layout and resource demands, as well as the processes available to manage its resources (Section 6.2). Following this, Section 6.3 introduces several scenarios to which PRaQ is applied. These scenarios will all use the same patterns of resource demand, but vary in their objectives and/or the set of available resource-management processes. This will allow investigation of both currently proposed system designs, as well as other more speculative ideas. This section will then present and discuss the results for each scenario. In summary, this chapter's aim is to use a case study to show how the PRaQ model can improve an area's metabolism, to fulfill Aim 3 of the research question (Section 1.4.2).

6.1 The case study and its wider context

The case study is an ongoing Chinese urban development in the city of Xi'an, led by the Shann Gu Power Company (hereafter, 'SPC'). Historically, the SPC have provided turbo-machinery services (such as steam turbines, fans and energy recovery units) for industries requiring heavy machinery, including chemical production, power generation and construction (ShaanGu Power Company, 2014). The SPC are implementing plans to redevelop one of their industrial sites and its surrounding region. The site has an overall area of around 51 km²; the focus of this case study, however is a region of 7 km². This area has residential, commercial, industrial and recreational functions (roughly represented by Figure 6.1)¹ which each have their own energy, water and waste management needs.

In recent years, China has become the world's largest consumer of energy, resulting in nearly a seven-fold increase in energy-related carbon dioxide emissions between 1977 and 2013. This has led China to make efforts to reduce its reliance on non-renewable energy sources and decrease the concentration of pollutants in the air (Chen et al., 2016). With this broader context in mind, more attention is being paid to integrated systems management as planners and policy makers attempt to overcome the "technical, socio-economic and institutional barriers" to such approaches (Chen et al., 2016, p.357). Concerning the site more specifically, the SPC hope to address the inefficient provision of its heating (due to aging coal-fuelled boilers and electric heaters). However, a stated ambition of the SPC site re-development is to not only address issues of energy inefficiency, but to go further, by considering how integrated management of the energy, water and waste sectors can maximise energy efficiency, min-

¹There are six documents which provide background and data to the SPC redevelopment plans. However, the documentation is confidential and thus certain information (such as the precise site location) cannot be given here.

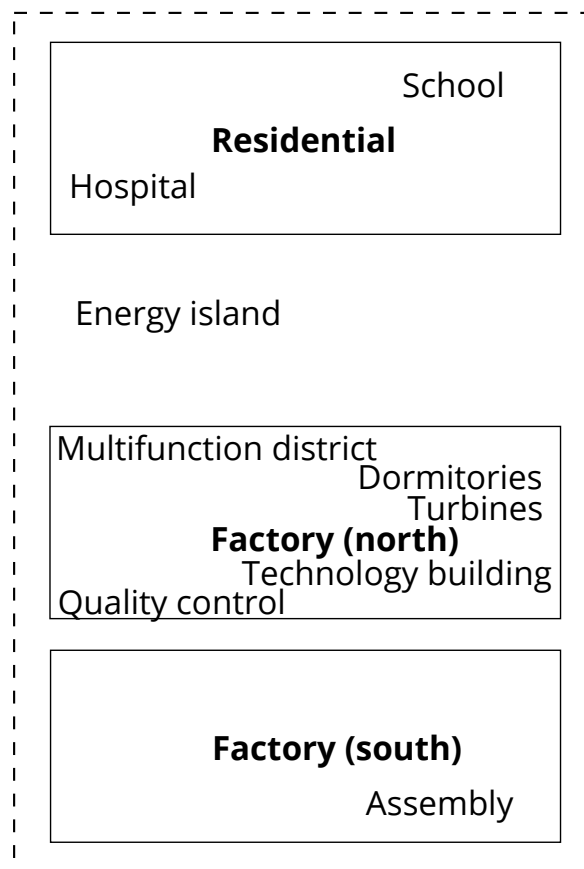


Figure 6.1: A schematic of the SPC redevelopment site showing its twelve zones, adapted from figures in the SPC documentation. The outer dashed rectangle encloses the full 7 km² site; the solid rectangles with **bold** labels represent broad regions within the site (e.g. the **residential** region); the unbolded text labels denote specific zones (e.g. a hospital within the residential region).

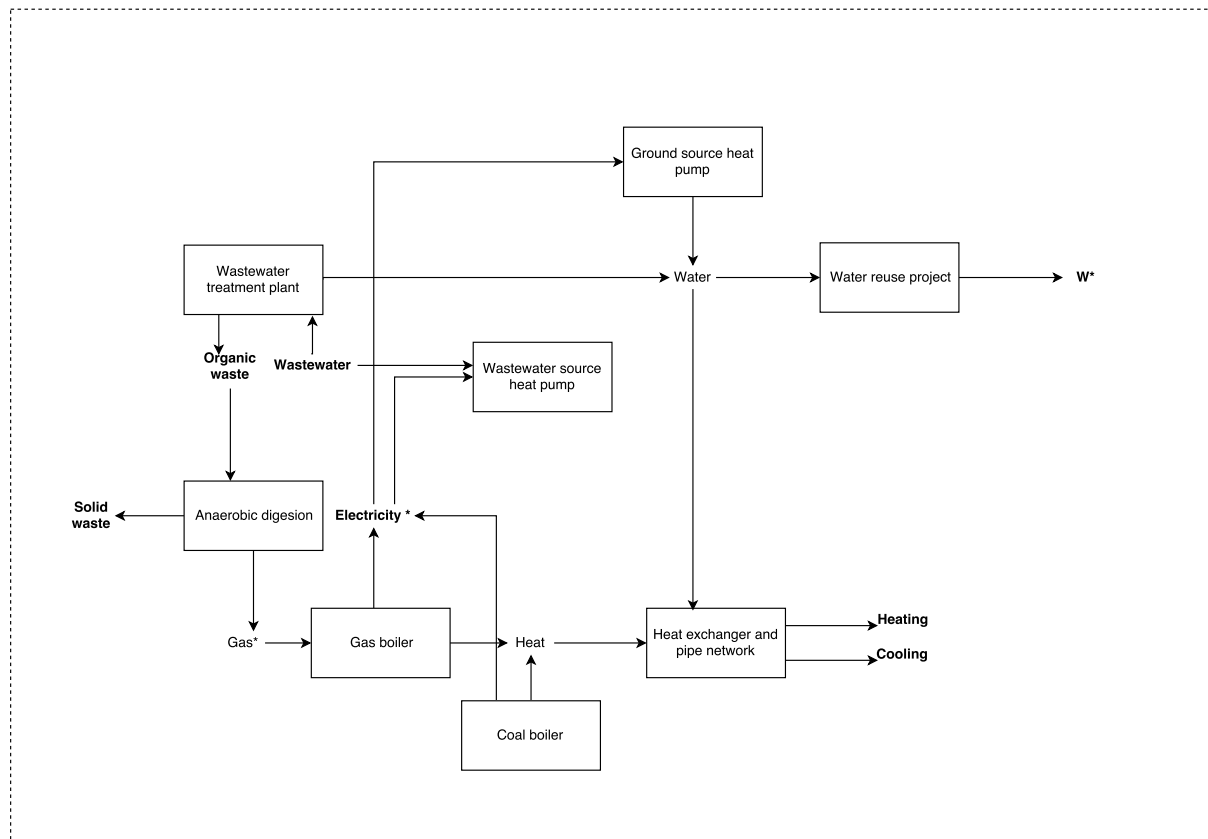


Figure 6.2: SPC's proposed interactions between energy, water and waste management. Resources with **bold** labels represent those resources either demanded or produced by the end-users in the zone of Figure 6.1; and * indicates a resource can be imported from outside the system boundary (represented by the dashed line). In the modelling that follows, these processes will be split between the zones of the site. The zones themselves can be connected by transport infrastructure.

imise the discharge of waste, and minimise economic costs. The SPC's proposals to that end include using heat stored within wastewater to feed a water source heat pump, and generating biogas from wastewater fermentation. The recreational area is also to include an artificial lake, which the planners hope to source via a water reuse project (Zhao and ShaanGu Power Company, 2013). These, and other intersectoral synergies are summarised in Figure 6.2, which shows part of the resource management infrastructure proposed by the SPC for the site's redevelopment.

In terms of the approaches used to realise such integrated planning of urban systems, Zheng et al. (2017) notes that optimisation methods are a poorly-established field in China, and hence the SPC site has presented an opportunity to demonstrate such methods of planning. Zheng et al's previous work looked at the energy management for the site's industrial and residential areas. This modelled the thermal properties of the buildings to derive the site's energy requirements as they fluctuate over a time horizon, and used a MINLP modelling framework to design the network of energy supply tech-

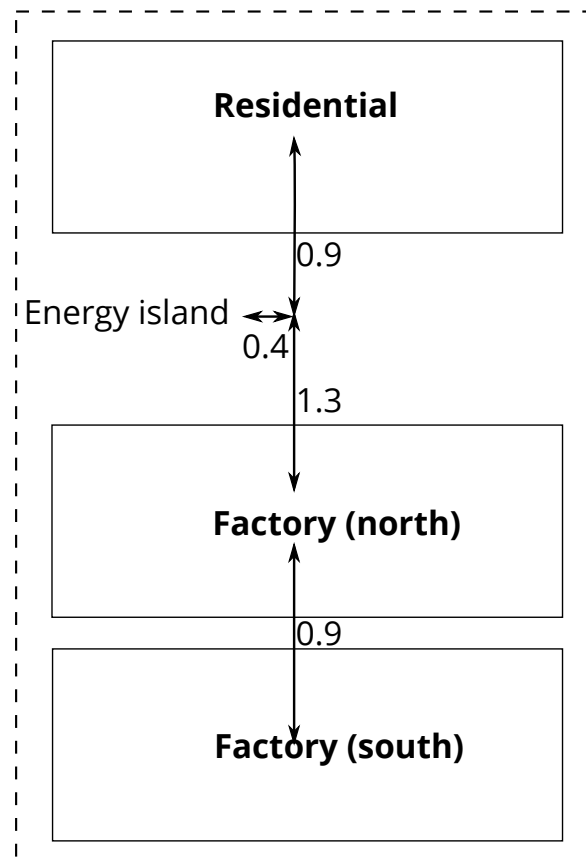


Figure 6.3: A re-representation of the SPC redevelopment site, with arrows indicating how zones can be connected (defined in set $nb(z, z')$). All distances are in kilometers. Each region centre connects to the other zones in the region (e.g. **Factory (south)** $\leftrightarrow$ Assembly) with a connection that is assumed to be 0.5 km in length.

nologies with minimum system cost under different scenarios of energy prices and limits on emissions. The work of this chapter is less detailed – it does not attempt to model the demands or apply detailed sensitivity analysis. However it takes a higher-level view by incorporating water and waste systems alongside the energy system, and considers not just the current proposals for a system design, but also those made possible when the full database of Chapter 4 is considered. In other words, this case study is concerned less with the detailed design of the SPC’s energy system, but more with optimising the site’s metabolism.

When considering how resource management networks affects a site’s metabolism, it is important to take into account seasonality. Xi’an weather exhibits fairly strong variation between seasons, with average summer high temperatures over 30°C and winter low temperatures dropping below 0°C (China Meteorological Administration, 2018). This means that demand for resources (particularly heating and cooling) will vary substantially between seasons, and may well require different management processes. This variation in processes which provide heating and cooling may also affect the optimal mix of processes from the other sectors with which they interact. For this reason, the site’s demands are defined at a seasonal level – this means a time component, t , needs to be introduced into the PRaQ model – the full formulation which includes t is presented in Appendix B.

6.2 Model data

When applying the model to a case study, the first step is to specify the zones and time periods used in the model, defined by sets $z \in Z$ and $t \in T$, respectively. With the zones determined, another set specifies whether any pair of zones (z, z') are neighbours, by defining them as belonging to the set, $nb(z, z')$. Following this, the sets of processes and resources available to the model can be listed ($p \in P$ and $r \in R$, respectively). At this point, there is enough information to define the two final sets: first, the qualities to be attributed to resources ($q \in Q$), and second, the transport technologies, $\tau \in \mathcal{T}$ which transfer the resources between zones.

With the sets in place, the parameters can be defined. First the distance between between two any two neighbouring zones defines the interzonal distances, $l_{zz'}$ (kilometers), while $\mathbb{S}_t$ defines the length of time of each time period, t (days). Resource management needs can then be assigned to each time and location with $D_{rzt}^{(qty)}$ and $D_{qzt}^{(qual)}$. Other parameters to define include the limits on imports and

exporting resources to particular zones, and the costs of resources and processes.

The following subsections outline how the sets and parameters above are defined from the SPC documentation (with further details provided in Appendix C). The explanations are deliberately comprehensive, reflecting on why certain choices and assumptions regarding data are made, to justify the modelling decisions taken here – recall that Section 2.2.1 noted that the value of modelling is found not merely in the results, but in making explicit assumptions and methods which would have otherwise been unstated in the decision-making processes. The following description walks the reader through how one might set up a model for a particular case study, and when it would be appropriate to take different decisions. The details are given in the recommended order of how a user might construct a particular case study model.

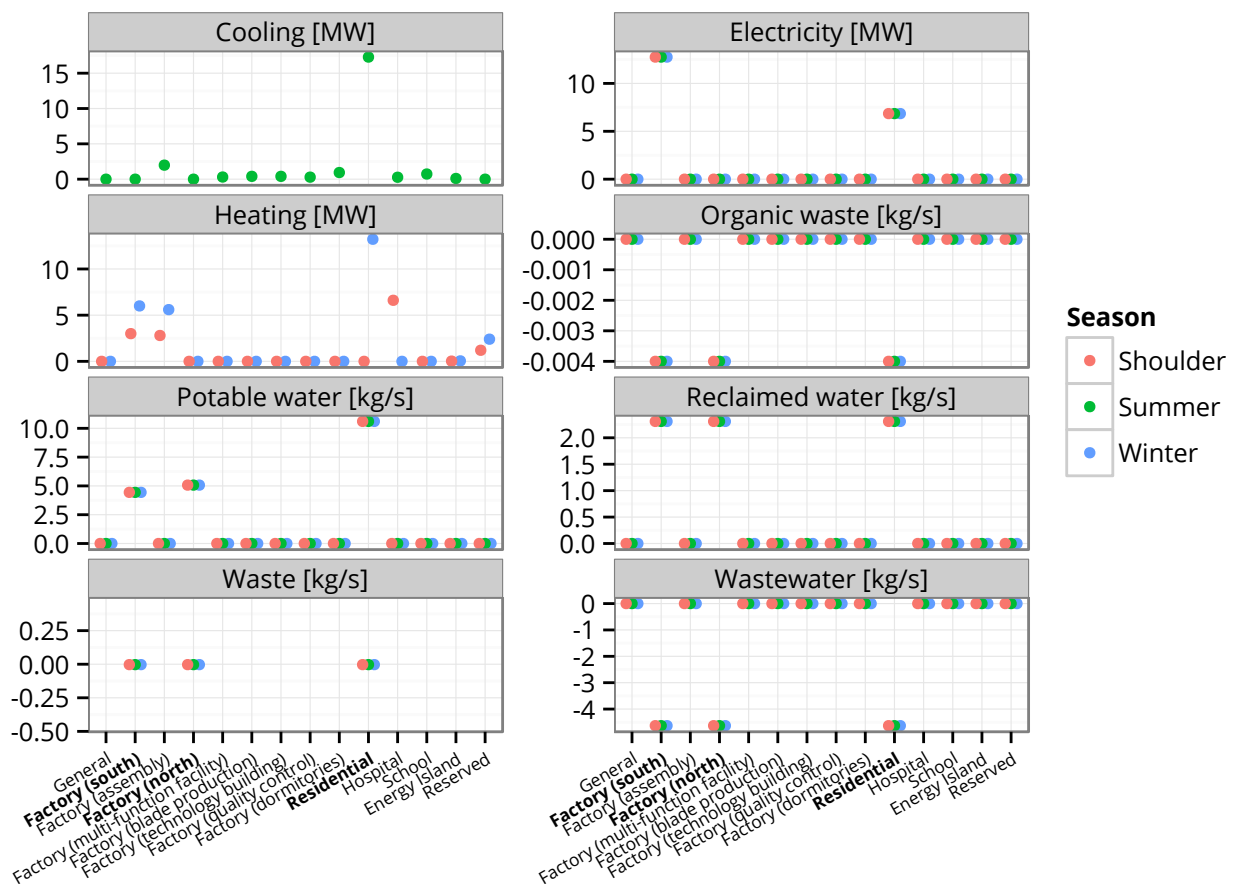


Figure 6.4: Resource management demands for the SPC site's zones (with the broader regions indicated by **bold** axis labels). Positive values indicate the resource is consumed by the end-users; negative values (i.e., for wastes and wastewater) indicate the resource is produced by the end-users.

Table 6.1: The zonal connections defined for set $nb(z, z')$ (with **bold** text denoting a broader region), and their corresponding lengths $l_{zz'}$ used in the SPC case study.

z	z'	Dimension on plan [cm]	Site dimension, $l_{zz'}$ [km]
Factory (south)	Factory (north)	3.4	0.9
Factory (south)	Assembly		0.5
Factory (south)	Multifunction district		0.5
Factory (south)	Dormitories		0.5
Factory (south)	Turbines		0.5
Factory (north)	Technology building		0.5
Factory (north)	Quality control		0.5
Factory (north)	Energy island	$4.8 + 1.3 = 6.1$	$1.3 + 0.4 = 1.7$
Factory (north)	Residential	$4.8 + 3.4 = 8.2$	2.2
Residential	School		0.5
Residential	Hospital		0.5
Residential	Reserved		Assume to be 1

6.2.1 Site layout

Each of the twelve zones shown in Figure 6.1 will be represented in the model, and thus each belongs to the set of zones $z \in Z$, where $|Z| = 12$. It is assumed that the three regions will be linked via a connection running north-south through the site, and also that the functions within a region are equidistant from the region's centre (with the exception of the energy island which does not belong to a region). This makes the size of set $nb_{z,z'}$ as $|nb| = 12$. The connection distances have been estimated from the site's dimensions. Assuming that the region-to-region connections join the regional centroids, distances can be estimated by scaling distances from the site plans in the SPC documentation. The region-to-function distances will be assumed as 0.5 km. In total, there are twelve two-way connections defined, which are given in Table 6.1. The transport processes used for these connections are detailed in Section 6.2.6, but briefly, roads are assumed to exist along any connection. Additionally, the model will have the option to run underground pipes and overhead cables along their length². Further details are given in Appendix C.1.

6.2.2 Times

The SPC documentation provides energy demands for winter, summer and the remainder of the year (Zhao and ShaanGu Power Company, 2014). This model therefore uses three timesteps, specified by

²As discussed in Section 6.2.6, this means that roads have no financial cost in the model, whereas pipes and cables will.

$t \in T$, where $|T| = 3$, representing the winter, summer, and shoulder seasons, having spans, $\mathbb{S}_t$, of 90 days, 90 days, and 180 days respectively. This means that the infrastructure selected by the model would be in place all year round, but could operate differently in each season. Consider the provision of domestic heating provided by district heating as an example. In the winter, the district heating could deliver heat to homes, and this would govern the operation of heat-generating processes upstream of the district heating network. However, these upstream operations would not be required in the summer, when the district heating does not run. As this phenomenon is applied in relation to all the resource demands, the network of processes emerging from the system interactions could operate differently in each season, in order to optimise the site's metabolism.

Of course, in reality operation might not just vary by season, but could vary for smaller time slices. For example each season could have alternative weekday and weekend resource demand (thus $|T| = 3 \text{ seasons} \times 2 \text{ day types} = 6$), which could be further divided into hourly demands (thus $|T| = 3 \text{ seasons} \times 2 \text{ day types} \times 24 \text{ hours} = 144$). The temporal resolution could become finer still, using demands at a minute-by-minute or second-by-second level. Thus the decision here to use seasonal timesteps is not as coarse as it could be (i.e. yearly), but neither is it as granular as it could be. Greater resolution would require additional assumptions by downscaling the data from the SPC documentation (which is given at a seasonal level), and furthermore, would come at greater computational expense³.

In summary, seasonal timesteps are appropriate to the exploratory early-stage planning purposes of this model. Further along the planning process when detailed designs are being examined, it would be justifiable to expend more effort, thus a finer temporal resolution may be warranted. Furthermore, at the more detailed design stages, some decisions will have been made (for example, the location of a particular conversion process), thus reducing the number of variables in the model, and thereby speeding up computation.

6.2.3 Resource demands

Having determined the seasons and the time steps in the model, it is now possible to define the resource demand parameter $D_{rzt}^{(qty)}$ for each resource, r . (As mentioned in Section 5.4, the code which assembles the model is designed such that $D_{rzt}^{(qual)}$ can be defined automatically once $D_{rzt}^{(qty)}$ is known.)

³Section 5.6.1 discussed possible modelling approaches which use more time steps without proportionately increasing the computational costs.)

The SPC documentation provides values which can be used in the modelling. However, these values do not necessarily cover all resources r , and may not be disaggregated to each zone, z and season, t . Thus, sometimes, assumptions and calculations need to be applied in order to translate a documented value into a set of values which can be used in the modelling. The details of these adjustments are provided in Appendix C.3.

The resource demands used here are summarised in Figure 6.4, which shows the seasonal demand for energy (electricity, heating, and cooling), water (potable, and reclaimed), and waste management (wastewater, non-organic solid waste, and organic solid waste). Resource demands are defined as rates, i.e. on a per-second basis (kg/s or MW). This is a common way to express energy quantities, which makes sense given that energy is most commonly demanded on such a basis, i.e. as a power⁴. This makes the demand parameter definitions consistent with PRAQ's definition of process behaviour, because process rates are also defined on a per-second basis.

6.2.4 Other resource parameters

The resource demands discussed above will define some of the r items in set R , but to complete this set requires the other resources which the available conversion processes can consume and produce. In total, there are 68 resources, including everything from algae to wood. Each resource has at least one associated quality q , which is attributed to the resource using the X_{rq} and δ_{rq}^R parameters. The qualities used in this case study are *mass* and *energy*. Most resources are only attributed with one of these (e.g. algae possesses mass, and heat possesses energy), though some resources are attributed with both (e.g. ground water has both a mass and an energy head). With the resources, zones and times determined, the remaining resource-related parameters can be defined, namely: limits on how many zones can import and export particular resources (N_r^I , N_r^E), the maximum allowable imports of a resource in a season (I_{rt}^{max} , E_{rt}^{max}), and the cost and emissions factors of resources (c_r^R and ϵ_r^R). Further details are given in Appendix C.4.

⁴This is in contrast to waste management services (to give one example) in which waste may be collected at regular intervals (e.g. weekly), and sent to a particular processing unit once a certain threshold (e.g. tons) has been met. Nevertheless, for the sake of model usability, there should be consistency between the definition of energy and other resource demand definitions.

6.2.5 Conversion processes

The contents of the process set P will vary for each scenario, and will draw from both technologies proposed by the SPC, and the database of urban metabolism processes outlined in Chapter 4. The information needed to define the processes are the coefficients which define the input and output resource quantities (k_{prq}^P), and maximum process rates ($F_p^{P,max}$). For the database processes this information already exists, but for the SPC proposals, this information needs to be derived from the SPC documentation.

In addition to these parameters, each process needs a cost, c_p^P , for use in the objective function. Estimating these is not without its difficulties. First, there is the sheer number of processes in the database (202 in total). Second, the process database includes processes which have not yet penetrated into the market or are still to be developed (i.e. those with a technology readiness level marked as ‘long-term’, p.112), thus there are no values which can be easily lifted from the literature. Third, currency exchange rates and purchasing power parities around the world make it difficult to attribute a cost to a process with any degree of certainty. For these reasons, costing is approximate.

The broad approach to estimating process costs is to assemble a number of ‘process categories’ (PC), to which processes from the database – ‘database processes’ (DP) – are assigned. As an example, ‘biogas-fuelled CHP’ is defined as a PC, which includes four types of biogas-fuelled CHP conversion processes in the database. Costs are assigned to the PCs, in relation to a process’s capacity (i.e. USD/MW or USD/kg/s)⁵. These costs are obtained from the literature – this may require some assumptions and adjustments to the numbers – details are given in Appendix C.5). A guiding principle of these estimations is that process costs exhibit economies of scale⁶. For this to be captured in the model, each PC is assigned both a lowerbound and an upperbound unit cost, Cost^{LB} and Cost^{UB} respectively. Thus, the total cost of any particular DP with a given capacity (unit = MW or kgs/s) can be calculated from:

$$\text{DP Total Cost [USD]} = \text{PC Unit Cost [USD/unit]}^* \times \text{DP capacity [unit]},$$

where * can indicate either LB or UB. The lowerbound costs are applied to larger instances of a process,

⁵Recall that these capacities have been defined in each processes’ YAML file.

⁶For example, if a system demand requires 10 MW, then it should be cheaper to meet that demand with two 5 MW power plants than ten 1 MW power plants.

and upperbound costs are applied to smaller instances, and thus DPs become cheaper as they get larger. For the conversion processes which do not yet exist in the market, costs are based on existing processes which have the same main resource⁷. This approach is justified due to its conservatism, because it assumes that new processes will not penetrate the market unless they deliver a particular service (i.e. to manage a main resource) at lower cost than a more traditional method of conversion⁸.

In summary, the conversion processes in this case study are drawn from both the SPC documentation (18 in total), and the database assembled in Chapter 4 (202 unique process types, which increases to 363 when including the same processes at various capacities). Each modelled scenario is given a subset of these processes it is allowed to choose from (as outlined in Section 6.3). Cost estimates have been provided for these processes, which enable PRAQ to take into account economies of scale, and the cost of processes which do not yet exist in the market. In summary, the SPC case study modelling can choose from up to 381 conversion processes from which to design an integrated resource management system, for which a rough overall system cost can be computed.

6.2.6 Transport processes

Many of the resources (with some exceptions such as heat⁹) can be transported between zones, via three types of transport infrastructure: roads, along which vehicles can transport everything from municipal solid waste, to gases and liquids carried by tankers; pipes, which transport water and gases; and cables, to carry electricity. As noted in Section 6.2.1, the roads are assumed to already exist to connect neighbouring zones of set $nb_{zz'}$, whilst underground pipes and overhead cables can be optionally added by PRAQ to follow the roads, if and where necessary.

Transport processes are defined by the origin-to-destination resource input and output coefficients, k_{trq}^* (where $*$ stands for α , β , α' , and β'), and define quantities for the resource carried (e.g. water through a pipe); the energy resources required to carry that resource along the length of a connection (e.g. electrical energy to pump water along a pipe); and any by-products, wastes, and emissions from

⁷Recall from Chapter 4.2.2 the idea of a 'main' resource being the (e.g. electricity output for a power plant, or wastewater input to a treatment facility), and always has a value of $k_{pr} = \pm 1$.

⁸Though one may argue against this principle on the basis that a novel process may be more expensive than existing methods due to other benefits (e.g. environmental benefits). However, this thesis can only hope to be approximate with the cost of conversion processes, and indeed, such estimations warrant their own separate research focus (Morrow et al., 1979, Roy et al. (2005)).

⁹Though whilst heat itself cannot be transported, it can be carried by water, e.g. in a district heating pipe network.

Table 6.2: Coefficients for the three categories of transport processes used in the SPC case study.

τ	r	q	Source		Destination	
			$k_{\tau r q}^{\alpha}$	$k_{\tau r q}^{\beta}$	$k_{\tau r q}^{\alpha'}$	$k_{\tau r q}^{\beta'}$
Cable	Electricity	Energy	-1		1	
Water pipe	Water	Mass	-1		1	
	Electricity	Energy		-0.0054		
Gas pipe	Gas	Mass	-1		1	
Vehicle	Transported goods	Mass	-1		1	
	Gasoline	Mass		-0.18		
	CO ₂	Mass		0.3		0.3

the process. The main resource typically leaves the origin zone and arrives in the destination (perhaps minus some losses, such as power along a cable), the energy resources and by-products should be appropriately shared between the origin and destination. The specifics of transport process coefficients are outlined below, for the three main types of transport technologies, with example values of $k_{\tau r q}^*$ given in Table 6.2.

Cables This is the simplest type of transport process, because they can be defined with respect to just a single resource ($r = \text{electricity}$). Electricity transported via cables incur losses at rates of between 3–7 per cent over 1,000 km distances (IEA, 2016), however, given the whole site is only 7 km², these losses are considered negligible here. Thus cables can be defined simply with $k_{\tau r q}^{\alpha} = 1$, $k_{\tau r q}^{\alpha'} = -1$, and $k_{\tau r q}^{\beta} = k_{\tau r q}^{\beta'} = 0$ when $\tau = \text{cable}$, $r = \text{electricity}$, and $q = \text{energy}$.

Pipes These can transport $r = \text{water}$ or $r = \text{gas}$, and require electricity to provide pumping energy. Hydraulic calculations given in Appendix C.6.2 derive the amount of energy required to overcome friction between the water and the pipe in a pipe of zero slope¹⁰. The modelling assumes that all this electricity is provided in the zone of the water's origin. For gases it is assumed that friction is low enough so as to make the energy requirements negligible for the distances in the SPC site.

Vehicles Other resources are carried by vehicles. As well as the carried resource (e.g. $r = \text{biomass}$), vehicles require gasoline. It is assumed this is provided entirely by the source zone. As well as this, CO₂ emissions are emitted, with these being shared equally between the origin and destination zones. The $k_{\tau r q}^*$ values are derived in Appendix C.6.3.

¹⁰This assumes the nonlinearities in the relationship between transport mass and volume can be ignored.

As with the conversion processes, transport processes each need to have an associated cost, c_T^T . As the roads already exist, these are not costed in the model, as their total cost would be the same, whatever the system designed by the model. The cost of cables and pipes are defined per kilometer, and the values and sources for these calculations are linked to in Appendix C.6.

6.3 Application to model scenarios

Having detailed the data sources, assumptions, and calculations used to determine the model's parameters, PRaQ is now applied to seven scenarios (1–3c, below) to give insights on how to satisfy SPC demand using different sets of available processes and objective functions:

1. *Base case.* This assumes that the required quantities of electricity, fuels and water are imported directly from the grid (with wastewater treated on site). Thus, in this case, there is no attempt to take advantage of synergies. As such, this scenario provides baseline results to which other results can be compared.
2. *Design case.* The site developers intend to take advantage of intersectoral synergies to minimise resource consumption. This scenario considers the processes suggested in the SPC documentation, including combined heat and power (CHP), a wastewater source heat pump, and a district heating network. This scenario has three sub-scenarios to test how the process mix changes, with different objectives:
 - a. Design case – minimum cost
 - b. Design case – minimum emissions
 - c. Design case – minimum waste
3. *Wildcard case.* This scenario finds the minimum-cost process mix, when the processes of the database from Chapter 4 are made available, using three time horizons of process-availability:
 - a. Wildcard – current (using currently available processes)
 - b. Wildcard – medium-term (using technologies available in the current- to medium-term)
 - c. Wildcard – long-term (using technologies available in the current- to long-term, such as the solar electrolysis of water to produce hydrogen)

Scenario 3c forms the largest programme, and thus indicates the computational effort required to solve the problems, having 1,220,809 single variables, 7,670 discrete variables, and 1,248,035 equations. These values indicate the difficulty of the problem by highlighting how many decisions need to be made, and in doing so, demonstrate a reason to use optimisation models – they can tackle problems which would be impossible to solve by other means. Note, this number of variables also shows the impossibility of validating such a model – it would be impossible to compare the results of any such model with those of a real-world system.

These scenarios enable testing of a network’s sensitivity to fairly broad design considerations (such as technology availability and objective functions). More detailed design problems should be more narrowly focussed, by applying sensitivity analysis to understand how a system’s design responds to varying demand, resource and technology prices, and other factors (see Saltelli et al. (2008), Keirstead et al. (2012b) and Zheng et al. (2017) for examples). These detailed considerations are beyond the scope of this study due to the nature of the model itself, and – more importantly – the aims of this thesis, namely to understand the possible benefits of intersectoral synergies in improving urban metabolism (5.5.2).

When GAMS runs a scenario¹¹, it outputs the results into a set of CSV files, which are passed into an R script for processing so the output data can easily be used to describe the system designs (namely the resource flows and network of processes), and compute quantities such as cost, emissions, water footprint, exergy efficiency, as well as perform ENA. The following subsections visualise and describe the results, and discusses their implications for optimising an area’s metabolism. Appendix C provides links to all results in CSV format.

6.3.1 System designs and metabolic flows

A key premise of this thesis is that the aggregate metabolic flows into and out of a city are governed by the middle of the system, i.e. a network of resource management processes. This is observed in Figure 6.5, which shows how aggregate metabolic flows differ for each scenario, and Figure 6.6 which shows that making more processes available to PRaQ tends to design networks made up of a larger number

¹¹As with the benchmark study (Chapter 5), the project architecture separates the data and formulation, to facilitate running, reproducibility, modification, and development of the scenario models. Also to that end, the data and formulation are available at <https://github.com/tomravalde/shann-gu-case-study>, along with the results of the modelling.

of processes and resource types.

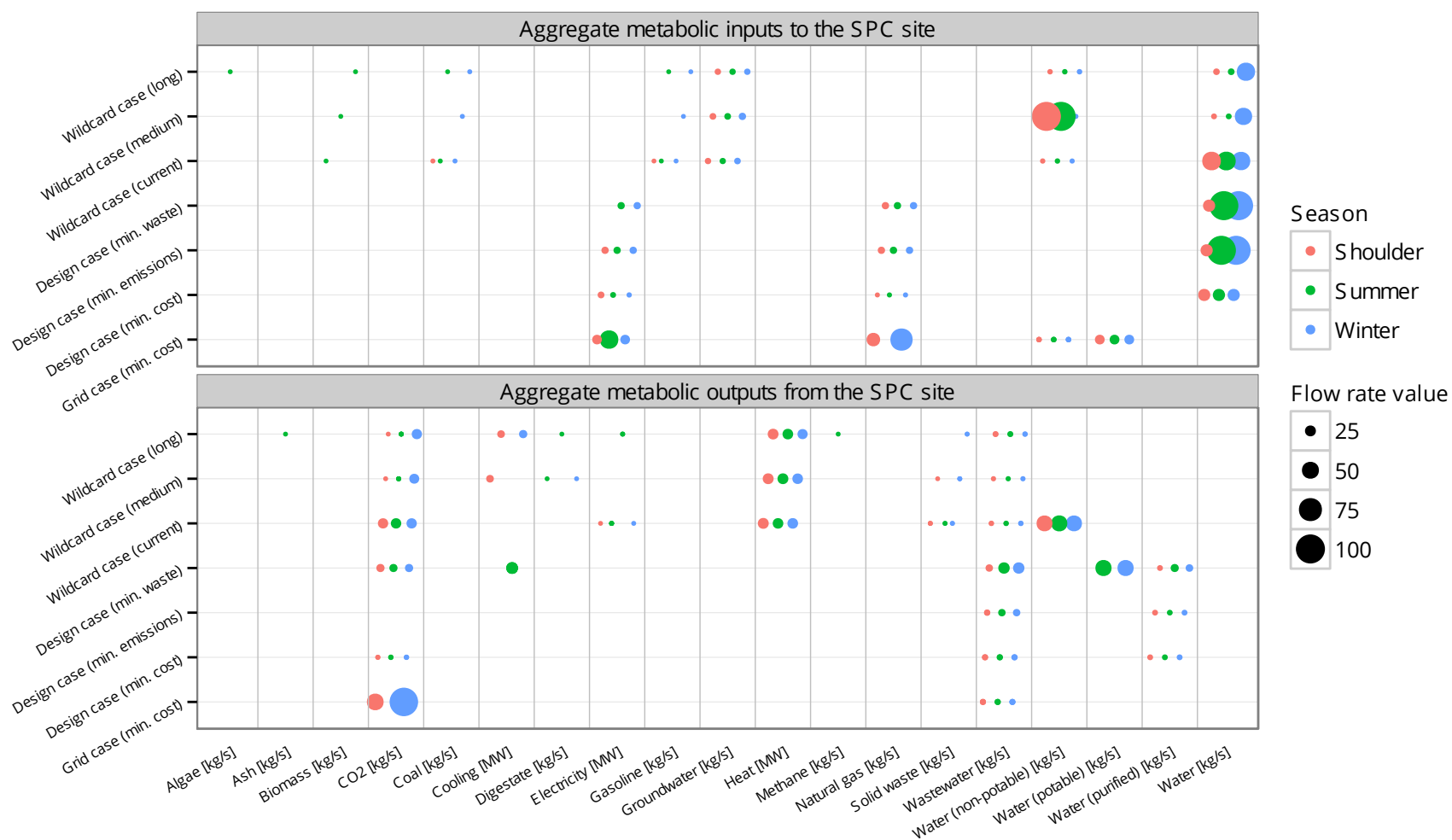


Figure 6.5: Metabolic flows into and out of the SPC site.

The process networks for each scenario are visualised in Figures 6.7 to 6.12 as undirected node-link graphs (these are in the same style of the graph introduced earlier in Figure 4.4). Processes that transfer resources from one to another are connected by lines; the proximity of any pair of linked processes is proportional to the quantities of resources transferred. From this, it follows that the more central a process is to the plot, the more integral it is to the network because it is linked to more processes. Conversely, the closer a process is to the plot's fringe, the less that other processes depend on it. The processes have been coloured according to the management sector to which they belong¹² to help visualise the intersectoral interactions and synergies. Inputs, outputs and demands are also represented to show which processes import and export resources. In each scenario, the system middle differs according to the design objective and/or available processes. All scenarios are dominated by processes whose main function is to produce energy, but the networks nevertheless exhibit intersectoral interactions (such as the energy demands of water and wastewater treatment), and synergies (such as heat generated by the water-source heat pump) in the design Case scenarios (Figures 6.7–6.9).

Design Case scenarios

The design case scenarios have up to twelve unique processes available to use, with each using a common set of seven processes: (1) water treatment plants, (2) wastewater treatment plants, (3) an anaerobic digestion facility (which generates gas from the organic fraction of waste), (4) ground-source heat pumps, (5) water-source heatpumps, (6) absorption chillers, (7) heat exchangers (to deliver hot and cold water through a district heating network), and (8) electrically-powered HVAC systems (to provide cooling). In addition to these processes in common, the different objectives cause the selection of processes unique to each scenario. These differences are summarised in Table 6.3, and further explained below.

The minimum cost scenario keeps costs down by importing less electricity, natural gas and water than the other scenarios. Importing no electricity forces the site to generate its own with the CHP plant. Importing less gas means that PRAQ avoids choosing gas-fuelled boilers – this means that heating is provided by electrically-powered HVAC systems (to supplement the heat from the CHP plant), rather than district heating networks. The knock-on effect of this is that water imports are reduced, because water is not required to run the district heating network. Note that other models (such as the urban

¹²This is determined by the 'main' output of each process.

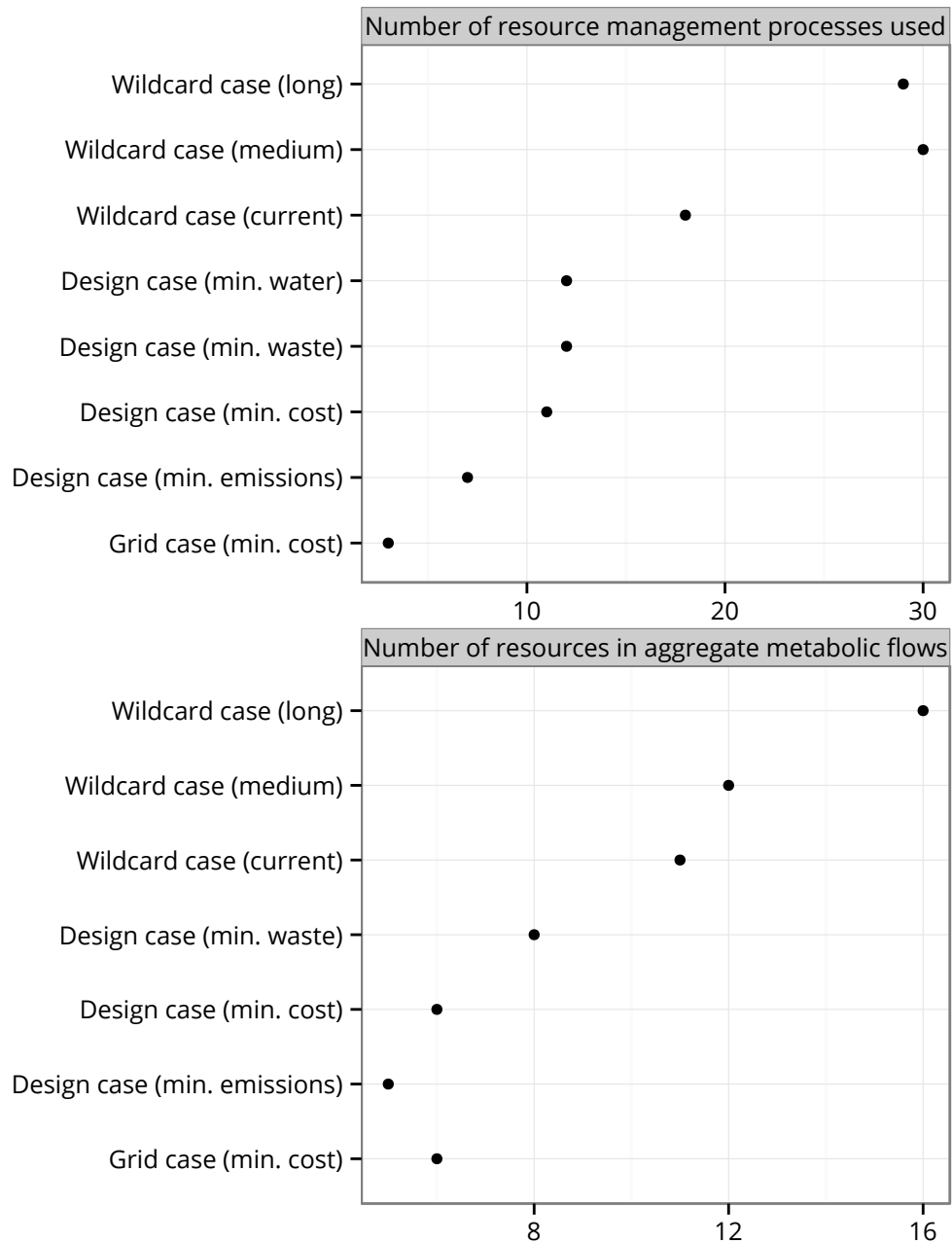


Figure 6.6: Making more processes available results in the model choosing more management processes and a more diverse mix of aggregate metabolic flows into and out of the SPC site.

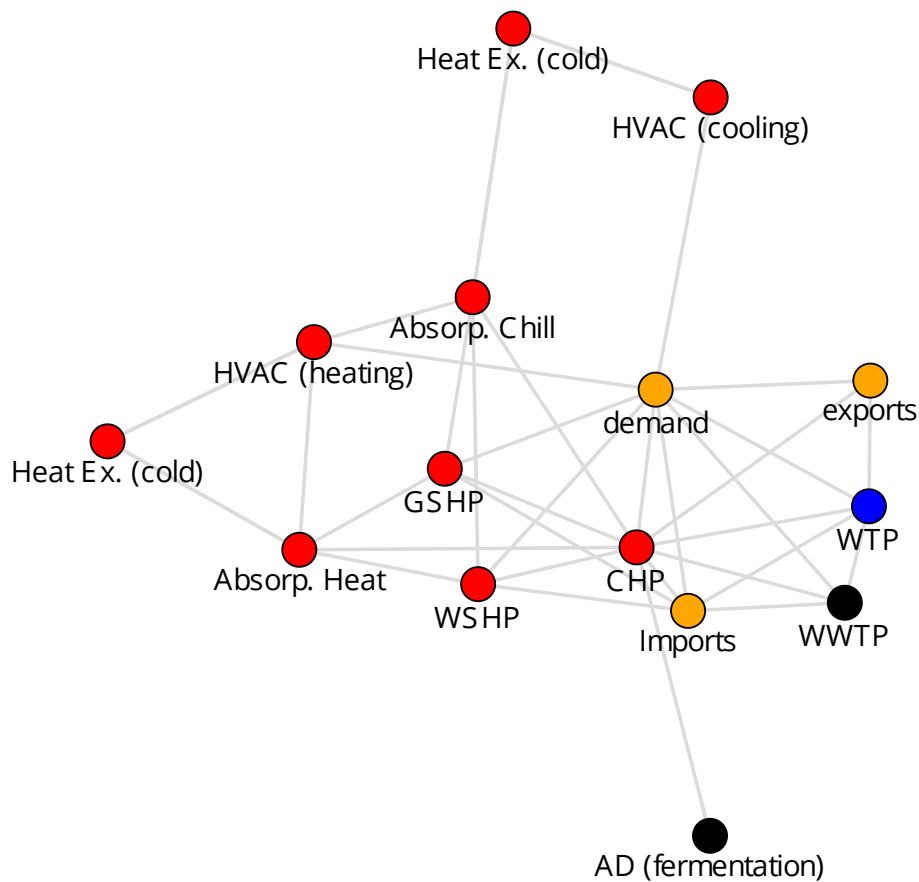


Figure 6.7: Process network for the design case (minimum cost) scenario. Colours indicate the management sector to which the processes belong (red = energy, blue = water, black = waste, and orange = imports or exports).

energy system of Keirstead and Shah (2013) would not be able to provide these integrated insights).

For the minimum emissions scenario, PRaQ avoids using CHP to meet electricity demand, or gas-fuelled boilers to meet demand for heating (both of these technologies burn fossil fuels). Instead, the system meets electricity demand by importing it directly from the grid, and meets heating demand by using electrically-powered heat pumps.

The minimum waste scenario minimises the site's waste output by sending organic waste to feed anaerobic fermentation. This generates natural gas which supplies the both CHP and boiler (which does not happen in the previous two scenarios). In addition, all the wastewater generated by the site is treated (which actually means the site produces more potable water than it needs). The site's heating and cooling needs are met via a district heating network and HVAC systems, which are fed by heat and electricity respectively. CHP produces both heat and electricity, though in summer and winter, the CHP's electricity output needs to be supplemented by imports – note that this leads the minimum

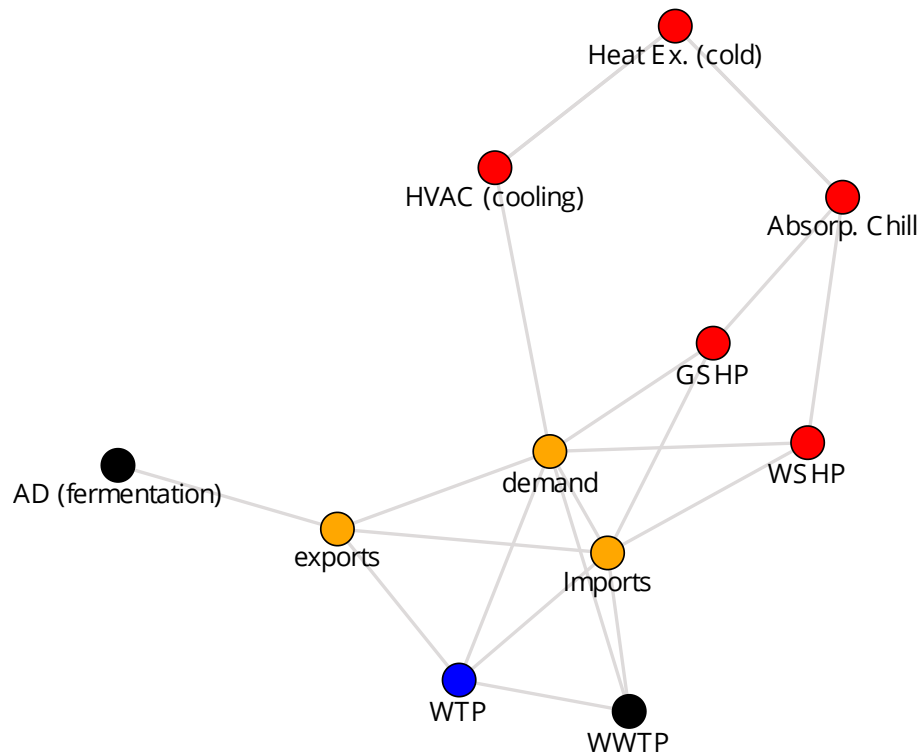


Figure 6.8: Process network for the design case (minimum emissions) scenario. Colours as for Figure 6.7.

waste scenario's aggregate metabolic flows to exhibit seasonal variation (i.e. there are no electricity imports in shoulder season).

In summary, the results of the design case scenarios demonstrate that PRaQ meets design objectives by changing the network of processes in the middle of a system. These network engage in intersectoral interactions and synergies which in turn, affects the aggregate metabolic flows into and out of an area.

Wildcard scenarios

The wildcard scenarios each have the same objective of cost minimisation, and their optimised networks share eleven processes types in common¹³ as well as processes unique to each scenario. The resulting networks exhibit intersectoral interactions and synergies, for example: waste gasification (a synergy between the waste and energy sectors), wastewater reuse (a synergy between the waste and water sectors), and groundwater pumping (an interaction between the energy and water sectors).

¹³This value of eleven partly depends on how processes are categorised into types. The types in common are: central heating, CHP (gas-, biomass- and hydrogen-fuelled), air conditioning, evaporative cooling, absorption cooling, hydrogen generation, waste gasification, groundwater pumping, heat exchanger networks, water treatment, and wastewater reuse treatment.

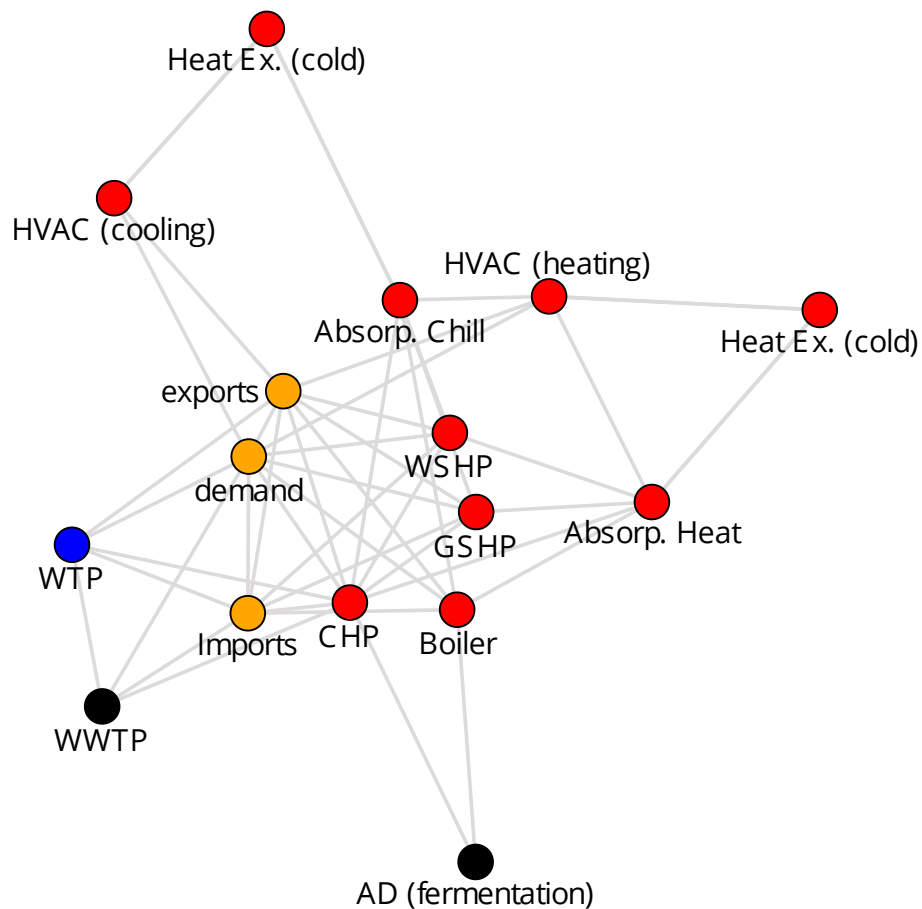


Figure 6.9: Process network for the design case (minimum waste) scenario. Colours as for Figure 6.7.

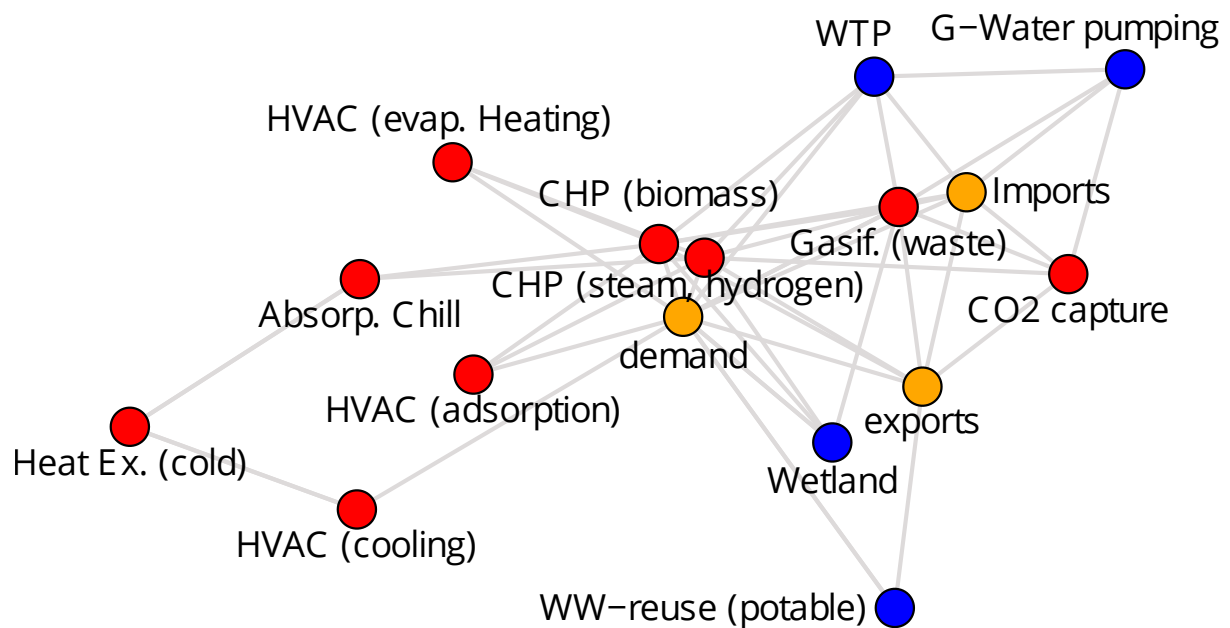


Figure 6.10: Process network for the wildcard case (current) scenario.

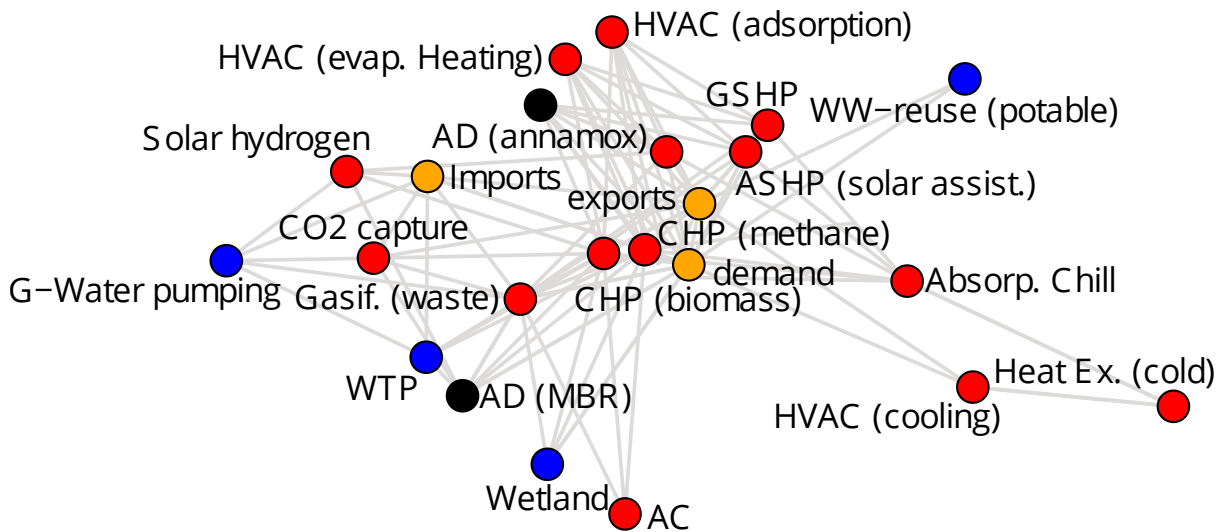


Figure 6.11: Process network for the wildcard case (medium) scenario.

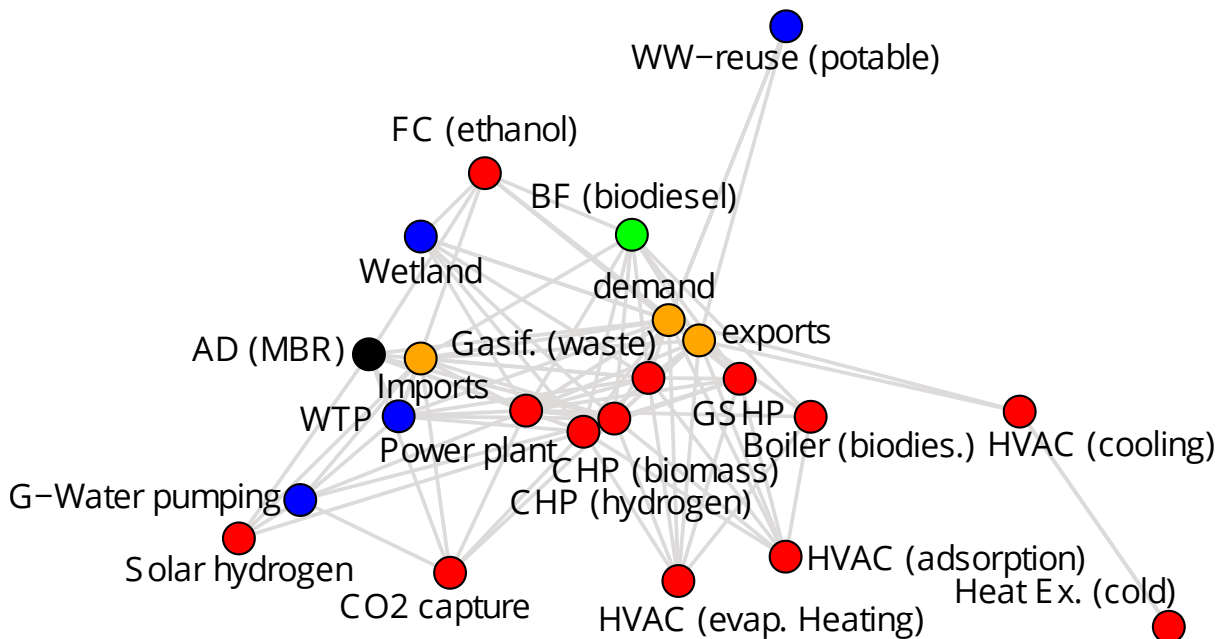


Figure 6.12: Process network for the wildcard case (long) scenario.

As with the design-case scenarios, different process mixes drive variations in the overall metabolic flows. In particular, these wildcard scenarios are less reliant on imports of electricity and natural gas than the design-case scenarios. The systems are more complicated than the design cases, so not all the differences can be explained here; the following examples, however, show how the middle of the system affects site's aggregate metabolic flows.

Aggregate inflows of coal and gasoline are a notable variation between the wildcard scenarios: the current scenario imports them in all three seasons, whereas the medium-term scenario imports them

Table 6.3: The conversion processes unique to each design case scenario. A checkmark indicates that the technology was picked for a scenario.

Scenario	CHP	Boiler	HVAC (cooling)	Absorption heating	Comment
Minimum cost	✓		✓	✓	Removes need for electricity imports, lowers gas imports, and lowers water imports
Minimum emissions					Greater electricity imports than the minimum cost scenario
Minimum waste	✓	✓	✓	✓	No output of organic waste or wastewater

in the winter only, and the longterm scenario imports them in winter and summer. This is due to the presence of additional energy-generating processes in the medium- and long-term scenarios, (such as include heat pumps, fuel cells, anaerobic digestion and biodiesel generation), which make these scenarios less reliant on fossil fuels.

Other differences include the long-term scenario's inflow of algae (to feed a biodiesel generation process), the long-term scenario's outflow of ash (due to the presence of a coal-fuelled power plant) and methane (which is a by-product from the biodiesel generation mentioned above). Finally, solid waste outputs are lower in the medium-term scenario, and lower still in the long-term scenerio, due to the presence of digestion processes which are fed by the organic fraction of solid waste.

In summary, the results of the wildcard-case scenarios support the findings of the design-case scenarios, by showing that PRAQ selects a network of processes which interact in such a way as to affect an area's aggregate metabolic flows.

6.3.2 System designs and grey-box metrics

The aggregate metabolic flows and costs considered above are black-box metrics (Section 3.1). The results show how these metrics or metabolic flows are affected by the mix of management processes (as hypothesised throughout this thesis). However, Chapter 3 showed that the so-called grey-box metrics of exergy analysis and ENA can further understanding of an area's use of resources, by delving into the details of process mixes and their governance.

Exergy analysis

Chapter 3 showed exergy analysis to be useful because it did not disqualify any type of resource from its study, and therefore made it possible to quantify the efficiency of any type of processes, and hence a system as a whole (Section 3.3.1). Here, exergy analysis is carried out for each scenario, using a simplified version of the method described in Section 3.2.2 in which system exergy efficiency is calculated as $\eta_{ex} = \alpha_{ex}^{prod} / \alpha_{ex}^{in}$ (Equation 3.4), where α_{ex}^{prod} are the system demands, and α_{ex}^{in} are the site's aggregate metabolic inflows. The results of exergy analysis for each minimum-cost scenario are given in Table 6.4 – this has been limited to the minimum-cost scenarios because these all have the same objective functions, which means they can be fairly compared according to the same metric. Further details are provided in Appendix C.8.

Table 6.4: Results of exergy analysis for each of the minimum cost scenarios; $\alpha_{ex}^{prod} = 47$ MW for each scenario.

Scenario	α_{ex}^{in} [MW]	η_{ex} [per cent]
Baseline case	377	12
Design case (min. cost)	85	55
Wildcard case (current)	79	59
Wildcard case (long)	78	60
Wildcard case (medium)	78	60

The results show that exergy efficiency is sensitive to the designed network. The baseline case, has the lowest efficiency, which is mainly driven by the high electricity imports required to meet demand for electricity (both for end-use, and to power HVAC systems). The grid case does not allow these demands to be met by the by-products of other processes resulting in lots of wasted exergy leaving the system, hence the low exergy efficiency. The design case and wildcard cases benefit from synergies (such as CHP, which allows both electricity and heating to be derived from coal imports, and gasification, which generates energy from waste). This enables these cases to achieve higher exergy efficiencies.

Ecological network analysis

Section 3.3.1 showed how ecological network analysis (ENA) reveals how city's resource-management sectors work together. The results of ENA will quantify the extent to which a system exhibits inter-sectoral synergies and interactions by computing the degree of network mutualism. The results of this analysis is given in Table 6.5 for the minimum cost scenarios (with the exception of the baseline

scenario, which, by design, has no network mutualism). This shows that network mutualism exists in all cases, but is higher for the wildcard cases – networks with more processes tend to have more intersectoral interactions. This result is in line with this thesis’ hypothesis – namely that intersectoral synergies bring metabolic efficiency. However, it also shows the need for the agents who manage each sector to work together, and highlights the risk of system vulnerability – if one sub-system (e.g. the energy sector) fails, then the rest of the system may go down with it.

Table 6.5: Network mutualism for SPC scenarios calculated from the Indirect utility matrix.

Scenario	Network mutualism
Design case (min. cost)	0.57
Design case (min. emissions)	0.67
Wildcard case (medium)	0.80
Wildcard case (long)	1.00

6.4 Summary and conclusions

This chapter has demonstrated how to apply the PRaQ model to the SPC site using its seasonally and spatially disaggregated demands to design highly integrated urban resource management systems – such optimised design would be impossible without a model such as PRaQ due to the number of choices which need to be evaluated. The analysis of the results uses the principles of Chapter 3 to quantify the ways in which a mix of resource-management processes affects the site’s metabolism. Alongside the PRaQ modelling itself, this chapter has also described and applied a rule-of-thumb method to estimate the costs of processes, taking into account economies of scale, even for conversion process which are still only in a research-and-development stage.

For the SPC site specifically, the PRaQ modelling justifies the planners’ decision to integrate resource management systems. The modelling of the design-case scenarios show the SPC’s proposals to use integrated energy management and a water-reuse project (Figure 6.2) are an improvement over direct imports of resources and exports of wastes of the baseline case. The PRaQ modelling has also shown how the optimal mix of resource management processes and resource imports needs to vary by season (especially so in light of the strong seasonal variation in heating and cooling demand). The wildcard scenarios challenge the planners to consider a more complicated network of processes which is less reliant on imports of electricity and natural gas, and has a greater exergy efficiency and net-

work mutualism. Within the broader Chinese context, this work has complemented that of Zheng et al. (2017), by showing how optimisation approaches to integrated urban resource management can be introduced in China, especially given environmental concerns (for example, those pointed out by Chen et al. (2016) at the start of this chapter).

More generally, this chapter contributes to fulfilling Aim 3 of this thesis' research question (Section 1.4.2), by showing that an area's metabolic flows (at the top of a system) are indeed affected by the mix of processes (in the middle of the system), whether this process mix varies due to design objectives (as in the design cases), or process availability (as in the wildcard cases). The case study shows that the synergies which drive high exergy efficiency and network mutualism can be achieved through larger and more varied networks of processes (as in the wildcard cases). This demonstrates the power of PRaQ, which can propose networks too complicated to design without such a model, and enables consideration of ever-increasing variety of resource-management technologies.

6.5 Further work for the SPC case study

Section 5.6.1 suggested developments to the PRaQ formulation, all of which could have implications for the SPC study (for example, the inclusion of storage processes). However, even without making changes to the formulation, there are several areas of further work, which could provided further useful insights for the SPC site:

- *Parameters.* Currently, the system costs are very rough – these could be refined, for example, taking into account local prices, exchanges rates, and purchasing power parities.
- *Processes.* It may be possible to rule out some processes as not available or feasible for the SPC. On the other hand, the SPC decision makers may know of processes not currently in Chapter 4's database which could be included.
- *Temporal resolution.* It is possible the networks designed in this chapter are incorrectly sizing processes. For the sake of exploratory early-stage planning, this case study has disaggregated seasonal demands to a single per-second value, however, in reality demands will vary throughout the day, which means the process operation rates will also vary. It would therefore be useful to run PRaQ at finer temporal resolutions (as briefly discussed in Section 6.2.2). The simplest way to consider operation is to split demand into two periods, average and peak (though finer reso-

lutions could also be chosen). By taking into account demand variation within a day, it will be possible to more appropriately size the system's conversion processes, and thereby investigate networks which are plausible at an operational level (and not just for exploratory planning). This would require more detailed resource demand management data. Increasing temporal resolution would have a computational cost (Section 5.5.1), so this might happen after a technology mix has been chosen, so the technology choice variables (N_{pz}^P) can be fixed.

- *Objectives.* Another area of further work is to alter the objective function. Examples include incorporating revenue from the selling of exports (this would increase exergy efficiency as waste exergies are re-defined as useful products, Ex_p^{prod}). Other alterations to the objective could be to include environmental taxes on carbon dioxide emissions.
- *Sensitivity analysis.* This case study has shown how a system's middle and its metabolic flows responds to different objectives and the available set of conversion processes. However, further sensitivity analysis could show how a system responds to changing demands (for example, to investigate the effect of population growth, changing consumer behaviour, etc.), the cost of resources, and the cost of processes. It would be particularly interesting to study a system's resilience; i.e. how much change it can bear before it becomes over-reliant on importing resources, no longer achieving the metabolic efficiency objectives intended.

Chapter 7

Discussion and conclusions

“...when you close your eyes and imagine an epidemic spreading, or any other social dynamic, you are running some model or other. It is just an implicit model that you haven’t written down ...At least I can write mine down so that it can, in principle, be calibrated to data ...The choice, then, is not whether to build models; it’s whether to build explicit ones. In explicit models, assumptions are laid out in detail, so we can study exactly what they entail. On these assumptions, this sort of thing happens. When you alter the assumptions that is what happens. By writing explicit models, you let others replicate your results.”

Van Der Leeuw (2004)

This thesis began in Chapter 1 by highlighting both the socioeconomic importance of cities, and the challenge they face in managing their resources in an environmentally- and economically-sustainable way. One way for cities to address their challenges is to take advantage of their co-located infrastructure, by using the wastes and by-products of one process as the inputs to another, and thus responding to the call for urban planning to adopt the ‘urban harvest’ approach. In this way, cities could use

principles of industrial ecology (as often practiced in eco-industrial parks) in order to meet their inhabitants' demands for energy, water and waste management, in ways which reduced environmental and economic risks. However, the complexity of a city presents a technical challenge for planners and decision makers leading to the suggestion that the complex network of processes and resources should be considered as a system. This system can be represented mathematically and subjected to mathematical programming in order find a mix of resource-management processes which serves urban resource demand while meeting some minimum objective. This methodology makes it possible to evaluate the hundreds of thousands of choices which can be involved in optimising a city's resource management infrastructure (for example, the choice of technologies, their location and their schedule of operation). This work to improve the sustainability of urban resource use is situated within the field of urban metabolism – an area of study which provides the ideas to consider the relationship between a city and its resources. Using the language of this concept, the challenge of this thesis is to offer insights on how cities could move from linear to circular metabolisms, by answering the following research question:

By how much can an area's metabolism be quantifiably improved by an optimisation model which integrates the planning of energy, water and waste systems?

This question was broken down into three aims, the first of which was to “*Investigate the opportunity and methodology*”. Chapter 2 addressed this by conducting systematic literature reviews to explore how the UM field currently understands issues of urban resource management, and the ways in which optimisation modelling has been applied to urban resource management. This review identified two research gaps to be filled:

- First, there was a need to consider an area's metabolism as emerging from an *engineered-system*. This novel conceptualisation seeks to understand a city's aggregate metabolic flows (at the 'top' of a system) as a function of the network of processes that manage energy, water and waste within a city (in the 'middle' of the system).
- Second, there was a need to go beyond current approaches to urban resource optimisation, in which resources were generally siloed according to their type (i.e. energy, water, or waste). Instead, models are needed which would consider the optimisation of urban resources in a *highly integrated* manner. These models would simultaneously optimise the design of energy, water and

waste systems.

This conceptualisation of a city's metabolism as an engineered system, together with the need for the highly integrated modelling of resources would subsequently facilitate and motivate the formulation of a mathematical model which could optimise the mix of urban resource management processes in order that energy, water and waste systems could be considered in a highly integrated manner.

With a new conceptual model proposed, Chapter 3 showed how metabolism could be quantified by different metrics, and proposed that exergy analysis and ecological network analysis were particularly suited to offer insights on how closely different resource-management processes work together. Chapter 4 assembled a publicly-available dataset of energy, water and waste management processes. The content of these two chapters would subsequently be useful in the modelling: the former gives methods which could quantify the extent to which the model could improve an area's metabolism; the latter provides data for the model to use.

With the groundwork laid in Chapters 1–4, the thesis' second aim was to *“Develop a model which computes the optimal mix of resources to meet demand for goods and services”*. To that end, Chapter 5 extended an existing formulation for an urban energy systems model, to incorporate energy, water and waste resources and processes. A particular requirement of the model was generality, so that the model could handle multiple resource types in a user-friendly and tractable way. Of three test formulations, the PRaQ method most suited these priorities, though the formulation has been made public with a benchmarking study to facilitate future improvements of the formulation.

The thesis' third aim was to *“Assess how well the models improve urban metabolism”*. This was addressed in Chapter 6, by applying the PRaQ model to the ShaanGu Power Company case study. This demonstrated that an area's metabolic flows, and the degree to which resource-management sectors worked together, could be quantifiably affected by the mix of processes in the middle of the system, where this process mix itself can be determined by design objectives and process availability.

7.1 Research contributions

In general, this work responded to calls for cities to become more sustainable in their resource management through moving from linear metabolisms to circular metabolism, by using the wastes of one

sector as the inputs to another. In the cause of this broad aim, this thesis made the following novel contributions, which are summarised in Table 7.1 and are explained in more detail below:

1. *A new conceptual model of urban metabolism.* Since a city's metabolism was first conceptualised by Wolman (1965) as a black-box, others have been extending the idea to increase its explanatory power. For example, Girardet (1990) added the idea that UM models could conceptualise the re-use of a city's outputs as inputs, in order to describe how a city's overall resource throughput could be reduced. Zhang et al. (2009c) took the UM concept further, by opening up the black box, to show that inside it was a network of economic sectors between which resources could be exchanged. The main theoretical contribution of this thesis was to extend Zhang's network concept to include the engineered systems which convert and transport resources.

The power of conceptual models is that they provide the ideas and language to relate components of real-world systems to one another in ways that allow people to think through the effects on a system when one or more of those components change. This thesis contributes a new way to conceptualise how energy, water and waste management processes in the middle of a system affects the aggregate metabolic flows at the top of a system.

2. *Guidance on how best to measure the efficiency of an area's metabolism.* To measure the performance of a system which handles a single resource type (e.g. an urban energy system) is fairly straightforward. But this thesis was proposing that energy, water and waste systems should be considered together, which raised the challenge of how to quantify how efficiently a city used resources across multiple resource types. Chapter 3 classified a city as a multi-resource system which exhibited the multi-resource trade-off problem. Such systems could be measured by black-box methods (such as water footprint and energy efficiency) or grey-box methods (such as exergy analysis and ecological network analysis). This thesis showed that grey-box analysis could quantify how well different sectors worked together, and advocated for their use in urban metabolism studies.
3. *The database of resource conversion processes.* This database lists 202 processes which can manage energy, water and waste (both now and in the future), and for each process, records their relative quantities of resource inputs and outputs. This contribution adds to the growing collection of open-source tools within the field of industrial ecology, for use in PRaQ and other models.

4. *The PRaQ model.* This was the thesis' main methodological contribution. PRaQ mathematically formalises the conceptual model described above, in order to perform highly integrated systems optimisation which simultaneously optimises the design of energy, water and waste systems. Previously, optimisation models for urban areas only considered one or two sectors, and therefore could do little to optimise metabolism as a whole. With the PRaQ model, the field of urban metabolism now has its own optimisation model. This makes it possible to consider the hundreds of thousands of decisions involved in integrated networks of energy, water and waste management systems in a computationally tractable manner. As such, this work adds another voice to the discussion on urban sustainability, by providing a tool which helps planners and policy makers take calls for systems integration from idea to reality.

In summary, this thesis has provided methods and tools to help researchers and decision makers consider the interactions and synergies between energy, water and waste systems. Moreover, further research into this 'process-oriented' approach to urban metabolism is encouraged by the fact that two of the above contributions above are open-source. The database can be used by others, who can also edit and extend it; the PRaQ formulation can also be developed, and these developments tested against one another by using the benchmarking problem. Adding these tools to the growing open-source ecosystem within urban metabolism and industrial ecology (Davis et al., 2010), facilitates the study of urban metabolism from a process-oriented perspective.

In addition to the contributions above, this thesis has also made two smaller contributions, which can be considered as 'by-products' of this research.

1. *Urban metabolism literature review.* Chapter 2 provided a review of the urban metabolism research landscape, which encompassed: the origins and purposes of UM studies, the way UM is conceptualised, the methods UM studies employ, and the models used to understand how components of UM systems relate to one another.
2. *Method of systematic literature review.* The data for Chapter 4's database was gathered using a systematic literature review. This method used the bash and R programming languages to: filter research according to quality, identify relevant articles, and categorise articles according to resource type. These search and organisation methods might find useful application in urban metabolism and other fields.

Table 7.1: Summary of how this thesis answers the call for systems integration.

Chapter	Thesis aim	Contribution to field	Further work
2	1	Conceptual model	
3	1	Assessed the ability of various ways to evaluate the efficiency of multi-resource systems (such as cities), to provide metrics which can be used to quantify the efficiency of an area's metabolism.	From Section 3.4: Confirm conclusions regarding metrics with other UM datasets; perform grey-box analysis at a higher resolution, to quantify the trade-off between insights obtained and data required to obtain them; explore additional metrics; and apply this analysis to other types of multi-resource system.
4	1	Open-source database providing quantitative information on behaviour of processes which manage energy, water and waste.	From Section 4.4: Continuous improvement of the database (new processes, more information such as process costs, extend to other processes important to metabolism such as steel manufacture); nonlinear models of process behaviour; developing the eco-system in which the database lives, so it can link to other open-source UM data.
5	2	The PRaQ model formulation and benchmarking study which can be used to help further develop the formulation	From Section 5.6: Continuous improvement of formulation and solutions, including piecewise linear and nonlinear formulations (requiring nonlinear models of the database processes), and heuristic-based solution methods such as genetic algorithms.
6	3	Demonstration that model can quantifiably improve UM	From Section 6.5: Test PRaQ with more finely-resolved demand data; apply model at an operational level; investigate other objectives; further sensitivity analysis.

7.2 Shortcomings and further work

Some specific proposals for further work have been given in the concluding sections of Chapters 3, 4, 5 and 6, and summarised in Table 7.1. The further work of Chapters 4 and 5 (namely, the extension of the database and the development of PRaQ), are helped by the fact that these contributions are open-source. Building on this thesis through numerous incremental developments made by the industrial ecology and urban metabolism communities could lead to a model and database that includes many more features, while remaining tractable and user friendly. Other proposals for further work are broader, and are considered in the following subsections.

7.2.1 The application of PRaQ

In addition to the applications of PRaQ suggested in Chapter 6, PRaQ could be applied in the following ways:

1. *Inform investment decisions for existing cities.* This thesis applied PRaQ to a new urban development, however, it would be possible to use PRaQ to offer guidance as to how an existing city should change its processes to meet particular design objectives (e.g. minimising emissions). In these applications, the city's resource-demand profile would be fed to the model as before, but unlike before, so would the city's processes. Some of the variables (e.g. N_{pz}^P and F_{pz}^P) would be pre-defined. PRaQ could then choose to operate the processes to a different schedule, or to add-to and/or replace processes, in order to meet an objective. This application would require datasets which provided the data to define the demands, processes and geography of existing cities.
2. *Application at different time scales.* In going to a greater temporal resolution, planners can go beyond investigating how system design affects metabolism, to investigate the effect of process operation on metabolism. Using larger time intervals (for example, varying demands over several years, perhaps corresponding to changing populations and demographics), can inform the long-term investment decisions which achieve design-objectives.
3. *Application at different spacial scales.* Increasing PRaQ's spatial resolution would enable the model to consider the resource flows into and out of and within buildings. This would require a database of building-level conversion and transport processes (such as sinks, water pipes, lavatories, elec-

tric heaters, compost bins, etc.). Such modelling could be used to show how building managers could invest to reduce their overall consumption and waste. On the other hand, PRaQ could be scaled up to regional and national levels to optimise the chains of resource conversions which occur over larger parts of an economy. Again, this application would require a database of larger processes (e.g. agriculture, livestock farming, forestry, etc.)

4. *Extension beyond energy, water and waste sectors..* Processes not belonging to the energy, water and waste sectors have not been considered in this thesis. Examples include the manufacture of iron and steel (which Chapter 3 showed was important in a city such as Sao Paulo). This would require extending the database of processes.

7.2.2 The place of PRaQ within broader socioeconomic considerations

This thesis has been limited to considering how the process mix in the middle of a system affects aggregate metabolic flows at the top. However, cities do not exist in a vacuum, free from other concerns – cities are not merely resource-managers. It is one thing to address the technical problem of how a city might best manage its resources; it is quite another to bring about such a technical solution in reality. As Chapter 1 noted, cities emerge and grow due to their socioeconomic desirability. This means that what drives development of a city is, in large part, the forces which give rise to socioeconomic improvements. These may be in tension with the typical ways cities are governed.

One such force that has arguably driven the prosperity of cities is the effect of liberalised-markets (Section 1.1). However, such markets are also one of the road-blocks to the integration of urban resource management. Energy, water and waste systems are typically managed separately, with each system's operators seeking to maximise their own profit. This does not necessarily sit well with an integrated system whose design needs to be imposed from the top-down. This criticism echoes those levelled at 'smart cities' – namely that they impose a technocratic vision of a city (Greenfield, 2013). It is not the place of this thesis to offer a view on which philosophies are preferable when it comes to governing cities. However, there is always ongoing debate as to the relative merits of planned versus free-market economies. Those in favour of the former (perhaps, in part at least, out of concern for the environment), may want to use PRaQ to show the benefits of integrated resource management.

7.2.3 Linking PRaQ to other models

PRaQ could be used in conjunction with other models¹. For example, there already exist models which optimise process use at a household level (e.g. Chen et al. (2013)). These could be used to define household demands at the bottom of the system, which could then be fed into PRaQ, to optimise resource flows at the urban scale. Similarly, demands at the bottom of the system could come from agent-based models (e.g. Keirstead et al. (2012a)); these derive consumer demands from the activities a population participate in (e.g. shopping, education, travelling, etc.).

At the top of the system, the aggregate metabolic flows arising from a process mix could be used to feed regional or national input-output economic models (e.g. Leontief (1986)), in order to investigate the larger economic impacts of an urban system's resource flows. In a similar vein, aggregate flows could be fed into environmental models, such as those which quantify local emissions or hydrological conditions – in this way, modellers can investigate some specific environmental impacts of an area's metabolism.

7.2.4 The development of the UM open-source ecosystem

It has been noted earlier in this chapter that the open-source contributions of this work facilitate its extension – particularly with regards to the database and the PRaQ formulation. However, as discussed in Section 4.4, open-source content often lives in an 'ecosystem', alongside other tools and data sources. This means that PRaQ's potential is realised not just by the developments to the model itself, but also by the presence of *other* open-source content.

Consider, for example, the application of PRaQ to existing cities (Section 7.2.1). This would be made much easier if there existed an open-source dataset of demand profiles for existing cities, and a database of the processes they use (in which records were defined in a form similar to the records of Chapter 4's database. This is a substantial project, and perhaps only the open-source community is up to such a task. Should it be achieved however, it would be a huge step forward towards realising PRaQ's potential.

¹Multiple models can either be soft-linked or hard-linked. In soft-linking, the models are run independently, with the results of one being manually fed to become the parameters of another. In hard-linked models, this transfer of one model's outputs to the others inputs is automated using code.

Finally, the contributions of this thesis are not yet fully open-source, because the compiler for the GAMS language (in which the PRaQ model is encoded) is proprietary. There do however exist examples of successful optimisation models written in open-source programming languages, for example, the Calliope energy systems model, which is written using the Python programming language (Pfenninger, 2017). The online repository of code and documentation of Calliope sets a standard to which PRaQ could aspire to achieve².

7.3 Modelling, PRaQ, and the future of highly integrated urban energy, water and waste systems

This work began with the premise that cities are vital, providing invaluable socioeconomic benefits to humanity, but at the same time, presenting significant environmental and economic challenges related to resource management. This work has advanced the field of urban metabolism by bringing together ideas and methods from urban metabolism, industrial ecology, optimisation modelling, and the open-source community, to understand how the urban energy, water and waste sectors can work together to enable more environmentally and economically sustainable resource management. Key to this is the development of a *model*. Models advance understanding of a system by explicitly representing it in a way that can be communicated and challenged – an insight powerfully expressed by Professor Joshua Epstein in the epigraph which opens this chapter. The PRaQ model seeks to do that for integrated urban resource management. There is of course still some way to go, and to that end the developments suggested above (as well as developments others will offer) will further the role of models in suggesting how energy, water and waste sectors might work better together.

In an increasingly resource-constrained world which faces the challenges of population growth, global warming, water scarcity, shrinking landfill capacity, economic stagnation, and other challenges, cities are being hailed as the most efficient means to provide goods and services to an ever-increasing global population. Reasoned-out model-based approaches can help cities become more economically and environmentally sustainable. This thesis is one step along the way, helping researchers and decision makers to think about urban metabolism as a whole, rather than individual sectors as a part, in an objective and user-friendly way.

²<http://calliope.readthedocs.io/en/stable/>

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Appendix A

Tat Hamlet – details of the benchmarking study

Section 5.2 noted that for the purposes of the benchmarking study, some simplifications, assumptions and additions were made. These are listed below.

Simplifications help ensure the benchmark study is user-friendly:

- The commercial sector (i.e. the shops, which sells 'final goods') will be ignored. These goods are directly imported, and are thus not managed by processes, so add nothing to the benchmark study
- Amalgamate all livestock (chickens, dogs, buffalo, and cows) into a single 'livestock' category which produces all livestock products in the village (meat, dairy, and manure).
- Amalgamate all agricultural activities into a single 'agriculture' category which produces all agricultural produced in the village (firewood, swidden, green manure, vegetables)

Assumptions account for the fact that the literature does not resolve Tat's energy flows down to their final use:

- Tat's total electricity use are split equally between domestic, agriculture, and water pumping purposes.
- Tat's total heat output = 5375.6 GJ/year (Heezen, 2003). Assume this is split between do-

mestic heating, cooking, and domestic hot water

Additions give the benchmarking study greater ability to test different types of formulation:

- For the purpose of this study, a dam is added to the village. This generates electricity from the river water. As shown below, this will enable two types of linear formulation, and one type of nonlinear to be compared for their performance.
- Each household will include cooking, space heating, and hot water heating processes.
- The literature does not provide any spatial information regarding the point of demand and the location of processes. In order that the benchmarking can consider spatial disaggregation, Tat will be divided into four zones (each of which have equal demands for resources).

Appendix B

PRaQ formulation for the SPC case study

The formulation of PRaQ given in Chapter 5 does not contain the temporal element (indexed by t , for example, resource demands which vary with time, D_{rzt}), whereas the case study in Chapter 6 does. For the sake of completeness, this appendix presents the formulation used in the SPC case study.

Resource quantity and quality balances:

$$I_{rzt} + \sum_{\tau}^{\mathcal{T}} J_{\tau rzt}^{(qty)} + \sum_p^P G_{przt}^{(qty)} = D_{rzt} + E_{rzt} \quad (\text{B.1})$$

$$X_{rq} I_{rzt} + \sum_{\tau}^{\mathcal{T}} J_{\tau rrqzt}^{(qual)} + \sum_p^P G_{prqzt}^{(qual)} = D_{rqzt}^{(qual)} + X_{rq} E_{rzt} \quad (\text{B.2})$$

Limits on imports and exports:

$$I_{rzt} \geq \delta_{rz}^I I_{rt}^{min} \quad (B.3)$$

$$I_{rzt} \leq \delta_{rz}^I I_{rt}^{max} \quad (B.4)$$

$$E_{rzt} \geq \delta_{rz}^E E_{rt}^{min} \quad (B.5)$$

$$E_{rzt} \leq \delta_{rz}^E E_{rt}^{max} \quad (B.6)$$

Conversion processes:

$$G_{prqzt}^{(qual)} = k_{prq}^P F_{pzt}^R \quad (B.7)$$

$$X_{rq} G_{przt}^{(qty)} = k_{prq}^P F_{pzt}^P \delta_{rq}^R, \quad \forall \delta_{prq}^P = 1 \quad (B.8)$$

$$F_{pzt}^P \leq N_{pz}^P F_{pt}^{P,max} \quad (B.9)$$

Transport processes:

$$J_{rrqzt}^{(qual)} = \sum_{z'} (k_{rrq}^{\alpha} + k_{rrq}^{\beta} l_{z'z}) F_{\tau z z' t}^T \quad (B.10)$$

$$+ \sum_{z'} (k_{\tau rrq}^{\alpha'} + k_{\tau rrq}^{\beta'} l_{z'z}) F_{\tau z' z t}^T \quad (B.11)$$

$$X_{rq}V_{\tau rz}^{(qty)} = \left[\sum_{z'} (k_{\tau rq}^{\alpha} + k_{\tau rq}^{\beta} l_{zz'}) F_{\tau zz't}^{\mathcal{T}} \right. \quad (\text{B.12})$$

$$\left. + \sum_{z'} (k_{\tau rq}^{\alpha'} + k_{\tau rq}^{\beta'} l_{z'z}) F_{\tau z'zt}^{\mathcal{T}} \right] \delta_{rq}^R \quad \forall \delta_{\tau rq}^{\mathcal{T}} = 1 \quad (\text{B.13})$$

$$F_{\tau zz't}^{\mathcal{T}} \geq \delta_{\tau zz'}^{\mathcal{T}} F_{\tau t}^{\mathcal{T},min} \quad (\text{B.14})$$

$$F_{\tau zz't}^{\mathcal{T}} \leq \delta_{\tau zz'}^{\mathcal{T}} F_{\tau t}^{\mathcal{T},max} \quad (\text{B.15})$$

$$\delta_{\tau zz't}^{\mathcal{T}} = 0, \quad \forall (z, z') \notin nb \quad (\text{B.16})$$

$$\delta_{\tau zz'}^{\mathcal{T}} = \delta_{\tau z'z}^{\mathcal{T}} \quad (\text{B.17})$$

Costs of system components:

$$C^R = \sum_{rzt} c_r I_{rzt} \quad (\text{B.18})$$

$$C^P = \sum_{pz} c_p N_{pz} \quad (\text{B.19})$$

$$C^{\mathcal{T}} = \sum_{\tau zz'} c_{\tau} \delta_{\tau zz'}^{\mathcal{T}} l_{zz'} \quad (\text{B.20})$$

Objective function for minimum cost:

$$\min \left\{ \gamma^R C^R + \gamma^P C^P + \gamma^{\mathcal{T}} C^{\mathcal{T}} \right\} \quad (\text{B.21})$$

where $\gamma^P = \gamma^{\mathcal{T}} = 0.1$ to represent an annualised cost over an assumed ten-year life-span of the model, and $\gamma^R = 1$.

Objective function for minimum emissions:

$$\min \left\{ \sum_{rz} \epsilon_r I_{rz} \right\} \quad (\text{B.22})$$

Objective function for minimum waste:

$$\min \left\{ \sum_{rtz} I_{rtz} \quad \forall r \in R^{\text{waste}} \right\} \quad (\text{B.23})$$

where R^{waste} is the subset of resources R which are considered waste resources (i.e. MSW, organic waste, waste water, ash).

Appendix C

Shann Gu Power Company case study: data, assumptions, and calculations

This appendix provides further detail on the data used in the case study outlined in the Shann Gu Power Company (SPC) case study in Chapter 6, including, summaries of the data, links to the full data sets (recorded in CSV and YAML formats), and notes regarding data sources, along with assumptions and calculations (e.g. those used to convert the data into appropriate units of measurement). The following sections outline the data in the order in which it was presented it in Section 6.2. Note that the documentation regarding the SPC redevelopment plans is confidential and thus certain information (such as the precise site location) cannot be given here.

The data discussed in this appendix can all be found online at the GitHub repository for the case study¹. Moreover, because this thesis has been written using the R-markdown format, the R code used to summarise and manipulate the data is embedded in the source of this page², which maybe useful for those who want to study the data for themselves.

¹<https://github.com/tomravalde/shann-gu-case-study>

²https://github.com/tomravalde/thesis/blob/master/C_spc-data.Rmd

C.1 Site layout

The zones z and their interzonal-distances $l_{zz'}$ (km) given in Section 2.6.1 (Table 6.1) are defined in the zone-matrix³. Any origin-destination pairs which are not neighbours are denoted by NA (e.g. factory-northDistrict). This matrix is lower-triangular, so there is no need to define a distance in both directions (because they are assumed to be equal).

C.2 Times

The case study's time steps $\mathcal{S}_t$ (seconds) given in Section 2.6.2 are defined in the times table file⁴. They are calculated assuming a 360 day year, with the winter, summer and shoulder seasons taking lengths of 90 days, 90 days, and 180 days, respectively. So for example, the length of the shoulder season is calculated as $180 \text{ days} \times 24 \text{ hours} \times 3,600 \text{ seconds} = 1.5552 \times 10^7 \text{ seconds}$.

C.3 Resource demands

The SPC site's demands for resource management $D_{rzt}^{(qty)}$ introduced in Section 6.2.3 are derived from the SPC documentation, which gives demands for the following regions and time-periods:

##	resource	zone.region	season	value.doc	units.doc
## 1	heat	south	wint	6000	kW
## 2	heat	south	wint	5600	kW
## 3	heat	residential	wint	13220	kW
## 4	heat	energyIsland	wint	50	kW
## 5	heat	Unspecified	wint	2400	kW
## 6	cool	south	sum	1985	kW
## 7	cool	production	sum	304	kW
## 8	cool	production	sum	400	kW

³<https://github.com/tomravalde/shann-gu-case-study/blob/master/modelling/model/data/model-definition/zone-matrix.csv>

⁴<https://github.com/tomravalde/shann-gu-case-study/blob/master/modelling/model/data/model-definition/times.csv>

## 9	cool	production	sum	400	kW
## 10	cool	production	sum	288	kW
## 11	cool	production	sum	940	kW
## 12	cool	residential	sum	17280	kW
## 13	cool	residential	sum	272	kW
## 14	cool	residential	sum	730	kW
## 15	cool	energyIsland	sum	100	kW
## 16	elec	south	wint	1117	1e5 kWh
## 17	elec	residential	wint	600	1e5 kWh
## 18	elec	south	sum	1117	1e5 kWh
## 19	elec	residential	sum	600	1e5 kWh
## 20	elec	south	shoulder	1117	1e5 kWh
## 21	elec	residential	shoulder	600	1e5 kWh
## 22	waterPotable	south	wint	140000	tons/year
## 23	waterPotable	production	wint	160000	tons/year
## 24	waterPotable	residential	wint	335000	tons/year
## 25	waterPotable	south	sum	140000	tons/year
## 26	waterPotable	production	sum	160000	tons/year
## 27	waterPotable	residential	sum	335000	tons/year
## 28	waterPotable	south	shoulder	140000	tons/year
## 29	waterPotable	production	shoulder	160000	tons/year
## 30	waterPotable	residential	shoulder	335000	tons/year
## 31	wastewater	Unspecified	wint	-1200	tons/day
## 32	wastewater	Unspecified	sum	-1200	tons/day
## 33	wastewater	Unspecified	shoulder	-1200	tons/day
## 34	waste	Unspecified	wint	-275100	kg/year
## 35	waste	Unspecified	sum	-275100	kg/year
## 36	waste	Unspecified	shoulder	-275100	kg/year
## 37	waste_organic	Unspecified	wint	-360	tons/year
## 38	waste_organic	Unspecified	sum	-360	tons/year

```
## 39 waste_organic Unspecified shoulder -360 tons/year
## 40 water_reclaimed Unspecified wint 600 tons/day
## 41 water_reclaimed Unspecified sum 600 tons/day
## 42 water_reclaimed Unspecified shoulder 600 tons/day
```

These demands need to be distributed to appropriate zones z , and converted to a consistent set of units (MW for energy, kg/s otherwise). The resource-demands table⁵ shows how the demands are allocated to zones, and the assumptions and calculations used to determine this. The table's columns (denoted by monospace text carry the following information:

- `zone.region` and `zone` are those regions and zones referred to in Section 6.2.1
- The SPC documentation for a resource demand in any given season is cited using the `resource`, `season`, and `value.doc` columns, with the units and reference given in `units.doc` and `reference`.
- When the Shann Gu documentation gives little detail about the spatial disaggregation of the demand (i.e. demand is only attributed to a region, rather than a zone), the demands need to be divided this demand up between zones. Similarly, when the documentation has not provided a value for a particular season, assumptions need to be made (e.g. that the shoulder heat demand is half the winter heat demand). These assumptions are recorded in `assump.redist`, with the new values listed in `value.redist` (and units given in `units.redist`)
- Finally, `notes.conv` notes any necessary changes in units, such that `value.conv` and `units.conv` contain resource demands in a consistent set of units.

In summary, the reasoning for every demand value which appears in the case study can be justified by the chain of sources, assumptions, and calculations embedded in the table.

C.3.1 A note on waste and wastewater generation

Waste and wastewater generation rates are defined as negative demands.

The waste generation figures from the SPC documentation are not provided in the same units (total solid waste is given as 8 m³/day, organic waste is given as 360,000 kg/year), so the following calculations separate the documented values into quantities of `waste` and `waste_organic`, on the assump-

⁵<https://github.com/tomravalde/shann-gu-case-study/blob/master/modelling/model/data/model-definition/resource-demands.csv>

```
resource: coal
quality:
  mass: 1
cost: 0
notes:
```

Figure C.1: An example YAML record for a coal.

tion that solid waste has a density of 217.5 kg/m³.⁶

$$\begin{aligned}\text{Total solid waste} &= 8\text{m}^3/\text{day} \\ &= 1,740 \text{ kg/day} \\ &= 635,100 \text{ kg/year}\end{aligned}$$

Subtracting the organic waste fraction:

$$\begin{aligned}\text{Non-organic waste} &= 635,100 - 360,000 \text{ kg/year} \\ &= 275,100 \text{ kg/year}\end{aligned}$$

C.4 Resource parameters

As well as the resource management demands specified above, the case study considers other resources which can play a part in the conversion chain of processes which meet demand (e.g. coal can be used in a power plant which also requires cooling water, and emits carbon dioxide). Each resource has its own YAML file which defines its properties⁷, specifying a resource's name and its quality attributes X_{rq} , for example:

The YAML files define resource properties in and of themselves. But each resource must also be associated with several parameters which are specific to the case study. These are recorded in the resource

⁶From Chandrappa and Das (2012), Table 2.2 gives a density range of 87–348 kg/m³. This thesis uses the median value.

⁷<https://github.com/tomravalde/shann-gu-case-study/tree/develop/modelling/model/data/libraries/resources-yaml>

parameters table⁸, which records the following information:

- Limits on resource import and export quantities (I_{rt}^{min} , I_{rt}^{max} , E_{rt}^{min} , E_{rt}^{max})
- Limits on the number of zones which can import and export a resource (N_r^I and N_r^E)
- Resource costs (c_r^R). There are several columns in the table which show the sources, assumptions and calculation steps used to estimate resource costs:
 - `currency` records the cost for a particular quantity of resource in the currency it was found in the literatures
 - `notes` provides sources and for a resource's cost
 - `conversion notes` contains notes on the calculation required to convert costs into appropriate units
 - `cost.converted` is the cost of the resource in USD used in the model
 - `unit.flow` is the units which the `cost.converted` values are given in (per MJ for energy resources; per kg otherwise)

C.5 Conversion process parameters

Each process needs to be associated with resource conversion parameters (k_{prq}^P) and maximum process rates ($F_p^{P,max}$). These are defined in YAML files⁹ – an example of a coal-fuelled power plant was given in Figure 4.2. A few of the processes have been defined using information from the Shann Gu literature, but most of them are adapted from the publicly available database introduced in Chapter 4¹⁰.

Each process's costs are defined in `process-costs.csv`, using the procedure described in Section 6.2.5, which can be summarised by the following steps:

1. Define 'process categories' (PC) (e.g. 'biogas-fuelled CHP')
2. Assign the processes from the database – 'database processes' (DP) – to each PC. The 'biogas-fuelled CHP' PC includes four types of biogas-fuelled CHP conversion processes in the database.
3. For each PC, obtain unit costs (USD/MW or USD/kg/s) from the literature (this may require

⁸<https://github.com/tomravalde/shann-gu-case-study/blob/master/modelling/model/data/model-definition/resource-params.csv>

⁹<https://github.com/tomravalde/shann-gu-case-study/tree/develop/modelling/model/data/libraries/processes-yaml>

¹⁰<https://github.com/tomravalde/urban-metabolism-process-database>

some assumptions and adjustments to numbers from the literature, of which details are given.

A guiding principle of cost estimations is that process costs exhibit economies of scale¹¹:

- a. For each PC, obtain upperbound and lowerbound costs, Cost^{LB} and Cost^{UB} .
- b. Calculate the total cost of any particular DP with a given capacity (MW or kgs/s) using

$$\text{DP Total Cost} = \text{PC Unit Cost}^* \times \text{DP capacity}$$

where $*$ can indicate either a *LB* or *UB*. The lowerbound costs are applied to larger instances of a process, and upperbound costs are applied to smaller instances, and thus DPs become cheaper as they get larger.

4. For the conversion processes which do not yet exist in the market, costs are estimated by basing them on existing processes which have the same main resource. This method is conservative in its approach, on the assumption that new processes will not penetrate the market unless they deliver a particular service at lower cost than a more traditional means of conversion.

Steps 1–4 above will involve making various assumptions and adjustments to the numbers – the details of these for each process are given in the process-cost calculation table¹², where `monospaced font` refers to the columns of the table:

- The PCs are listed in the `process-type` column. Each GP has lowerbound and upperbound versions, appending `_l` and `_u` to the process names, respectively (e.g. `CHP-biogas_l` and `CHP-biogas_u`).
- The costs for each PC are recorded in the `ref.cost` column, with the currency indicted in the `ref.currency` column.
- The `reference` cites the source of the number
- If necessary, the cost is converted to USD in the `ref.USD` column.
- The referenced cost will correspond to a particular resource and its production (or consumption) rate. For example, a CHP cost may be given per kW of electricity it produces. The resource, its quantity, and its units, are recorded in `ref.flow`, `ref.flow.value` and `ref.flow.units`, respectively.
- The `ref.flow.mult.factor` can be calculated, which is the number by which the `ref.flow.value`

¹¹For example, if a system demand requires 10 MW, then it should be cheaper to meet that demand with two 5 MW power plants than ten 1 MW power plants.

¹²<https://github.com/tomravalde/shann-gu-case-study/blob/master/modelling/model/data/model-definition/process-cost-calcs-kgysr.ods>

```

process: road_coal
inputs:
  coal: -1
  gasoline: 0
  CO2: 0
outputs:
  coal: 1
  gasoline: 0
  CO2: 0
dist_source:
  coal: 0
  gasoline: -0.18
  CO2: 0.3
dist_dest:
  coal: 0
  gasoline: 0
  CO2: 0.3
rate: 100
notes:

```

Figure C.2: An example YAML record for a vehicle which transports coal.

should be multiplied, in order to convert the flow into a consistent set of units (MW for energy resources, kg/s otherwise). Any notes relevant to the calculation (e.g. the density of a material) are recorded in `mult.factor.notes`.

- Finally the unit cost of each PC, `ref.unit.cost` (USD/MW or USD/kg/s) is calculated from `ref.USD/(ref.flow.value × ref.flow.mult.factor)`.

C.6 Transport processes parameters

Each transport needs to be associated with resource conversion parameters ($k_{\tau\tau q}^{\alpha}$, $k_{\tau\tau q}^{\beta}$, $k_{\tau\tau q}^{\alpha'}$, and $k_{\tau\tau q}^{\beta'}$) and maximum process rates ($F_{\tau}^{\mathcal{T},max}$). These are defined in transport process YAML files¹³. An example of coal carried by road is given below, where:

- `inputs` corresponds to $k_{\tau\tau q}^{\alpha}$
- `outputs` corresponds to $k_{\tau\tau q}^{\beta'}$
- `dist_source` corresponds to $k_{\tau\tau q}^{\beta}$
- `dist_dest` corresponds to $k_{\tau\tau q}^{\alpha'}$
- `rate` corresponds to $F_{\tau}^{\mathcal{T},max}$

¹³<https://github.com/tomravalde/shann-gu-case-study/tree/develop/modelling/model/data/libraries/transport-yaml>

Note, as per the assumptions stated in Section 6.2.6:

- All the coal which leaves the source zone arrives in the destination zone
- The quantity of gasoline depends on the distance travelled, as it is provided entirely by the source zone
- The quantity of CO₂ emitted depends on the distance travelled, as it is split equally between the source and destination zones

The transport costs (and their sources) are defined on a per-kilometer basis in the transport costs table¹⁴.

Section 6.2.6 noted there were three types of transport processes used in the case study: cables, pipes, and vehicles. The assumptions and calculations from which the parameters values were derived are given below.

C.6.1 Cables

Electrical energy is lost as electricity travels along a cable, typically at a rate of about 3–7 per cent over 1,000 km¹⁵. In the SPC case study, cable lengths are around 10 km, and thus losses will be assumed to be negligible, meaning that there is only a need to define parameters of -1 and 1 for k_{trq}^{α} and $k_{trq}^{\alpha'}$, respectively, and $k_{trq}^{\beta} = k_{trq}^{\beta'} = 0$.

C.6.2 Pipes

For pipes carrying gas, it is assumed that the distances involved make the pumping energy required negligible.

For pipes carrying water, it is assumed that pipes are horizontal, which means the only energy required is that pipe flow to overcome the head loss due to friction, h_f , quantified according to the so-called hydraulic slope S of a pipe of length L :

¹⁴<https://github.com/tomravalde/shann-gu-case-study/blob/master/modelling/model/data/model-definition/transport.csv>

¹⁵According to The Energy Technology Systems Analysis Program (see <http://iea-etsap.org/>).

$$h_f = SL$$

For turbulent flow, S is given by the Darcy-Weisbach equation:

$$S = f_D \frac{1}{2g} \frac{V^2}{D}$$

where f_D is the Darcy Friction factor, V is the flow velocity, and D is the pipe diameter.

The linear black-box representation of a pipe requires expressing h_f as a function $h_f = f(Q, L)$, where Q is the mass flow rate (m^3/s), calculated from the product of the cross-sectional pipe area (A) and flow velocity:

$$Q = AV$$

Rearranging yields:

$$\begin{aligned} V^2 &= Q^2/A^2 \\ &= \frac{16Q^2}{\pi^2 D^4} \end{aligned}$$

Thus:

$$\begin{aligned} h_f &= \frac{8f_D}{g\pi^4 D^5} Q^2 L \\ &= \frac{16Q^2}{\pi^2 D^4} \end{aligned}$$

For the black-box representation, by definition, the volume flow rate is $1 \text{ m}^3/\text{s}$, such that $Q^2 = Q$. It is also assumed that $D = 0.5 \text{ m}^3$, and $f_D = 0.04$, thus the energy required for pumping is given as:

$$\begin{aligned} k_{rrq}^\beta &= h_f \\ &= 0.0054\text{L} \end{aligned}$$

C.6.3 Vehicle transport

For vehicles, it is assumed that the resources being transported (e.g. biomass, coal, etc.) leave the source zone and arrive at their destination with no losses, i.e. $k_{rrq}^\alpha = -1$ and $k_{rrq}^{\alpha'} = 1$, and $k_{rrq}^\beta = k_{rrq}^{\beta'} = 0$. However, vehicles require gasoline, and emit carbon dioxide. The assumptions and calculations for the parameters which define these quantities are given below.

In calculating the mass of gasoline required to transport goods a given distance, it is assumed that:

- a heavy goods vehicle has a fuel efficiency of 11.3 miles/gallon¹⁶, which is equivalent to 0.25 l/km
- gasoline's density is 0.737 kg/l¹⁷
- all gasoline is provided by the source zone.

Thus:

$$\begin{aligned} k_{rrq}^\beta &= 0.737 \times 0.25 \\ &= 0.18 \text{ kg/km} \end{aligned}$$

In calculating emissions quantities, it is assumed that the specific CO_2 emissions for petrol (gasoline) is 3.3 kg of CO_2 per kg of fuel consumed¹⁸. Therefore, per kilometer travelled by a vehicle, the emissions are given as:

¹⁶ Adopting a conservative value from UK Government statistics: <https://www.gov.uk/government/statistical-data-sets/env01-fuel-consumption>

¹⁷ As given by http://www.simetric.co.uk/si_liquids.htm

¹⁸ From <http://www.engineeringtoolbox.com>

$$0.18 \times 3.3 = 0.6 \text{ kg/km}$$

These emissions are assumed to be split equally between the sources and destination zone, such that

$$k_{\tau\tau q}^{\beta} = k_{\tau\tau q}^{\beta'} = 0.6/2 = 0.3 \text{ kg/km}$$

C.7 Model scenarios

The data described above is used in the three scenarios described in Section 6.3. The GitHub repository possesses directories for each scenario which contain their own versions of the resource- and process-parameter files. These function to list the subset of resources and processes used in a scenario, and define some of the parameters (i.e. the costs, import limits, etc.)¹⁹. A YAML file then lists the files and parameters used for a scenario (Figure C.3) – this provides an R-script with the information it needs to be able to assemble the GAMS code for a scenario, by pulling the costs and other parameters from the aforementioned files, and using the listed resource and processes to pull in the remaining parameters from the YAML files (i.e. resource definitions and process behaviours). With the GAMS code for a scenario defined, the model can be run on a machine with the GAMS software²⁰.

C.8 Exergy analysis

The exergy analysis of Section 6.3.2 follows a simplified version of the method in Section 3.3.1, because the PraQ model enables exergy to be calculated without using Equations (3.5a) and (3.5b). In the original method, material- and energy-flow accounts for a city where matched with a city's processes so that every resource flow could be traced from its input to the city, through conversion processes and out the other side as a demand or a waste, i.e. exergy flows had to be derived from the bottom up, process-by-process. In the simplified method used here, there is no need to distribute the flows

¹⁹ An example for the Design Case scenario is available at <https://github.com/tomravalde/shann-gu-case-study/tree/develop/modelling/model/data/model-definition/designCase>.

²⁰ The results are exported to <https://github.com/tomravalde/shann-gu-case-study/tree/develop/modelling/model/results/cluster-results>. These can then be interrogated (see for example the R-code embedded in Chapter 6).

```

scenario: designCase_minCost
resources: data/model-definition/designCase/resource-params.csv
demands: data/model-definition/designCase/demands-nonzero.csv
conversion: data/model-definition/designCase/process-costs.csv
transport: data/model-definition/designCase/transport.csv
objective: "0.1*cost_prod+0.1*cost_transp+cost_res"
pareto:
  condition: "sum(Z, exports('gasNatural', Z, 'wint'))"
  limit: "1e8"
options: # These define options for GAMS
  filename: "options-short.gms"
  limrow: 0
  limcol: 0
  solprint: "off"
  decimals: 8
  optcr: 0.3
  reslim: 1000
notes:

```

Figure C.3: An example YAML record for a coal.

between the processes within the city, because PRAQ accounts any process products unused by other processes to become system outputs (Ex^{waste}). This means system exergy efficiency can be calculated at the whole-system level.

The simplification of Equations (3.5a) and (3.5b) can be formalised as:

$$\begin{aligned}
 \alpha_{ex}^{in} &= \sum_{p \in P} \sum_{i \in R^i} Ex_{p,i}^{in} \\
 &= \sum_{i \in R^i} Ex_i
 \end{aligned}$$

$$\alpha_{ex}^{prod} = \sum_{j \in D^j} Ex_j$$

where D^j is the set of a site's resource demands, and Ex_* represent the exergy value of a resource (for example the chemical exergy of a fossil fuel, or the exergy of heating).