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Exploring analyses, methodologies, and theoretical dilemmas

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LINKING ENERGY SYSTEM MODELS

EXPLORING ANALYSES, METHODOLOGIES,
AND THEORETICAL DILEMMAS

BY
MIGUEL CHANG

DISSERTATION SUBMITTED 2023



AALBORG UNIVERSITY
DENMARK

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**EXPLORING ANALYSES, METHODOLOGIES, AND
THEORETICAL DILEMMAS**

by

Miguel Chang



AALBORG UNIVERSITY
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CV - Miguel Antonio Chang Ojeda

I am originally from Lima, Peru. I hold a B.Sc. in Applied Mathematics and a B.Sc. in Petroleum Engineering from the University of Tulsa, USA, and earned my M.Sc. in Sustainable Energy Planning and Management at Aalborg University, Denmark.

Previously, I worked as a Production Engineer at Schlumberger (2011-2015) in different project assignments in South America. From 2017 to 2022, I worked at the Sustainable Energy Planning Research Group at Aalborg University, initially as a Research Assistant and then as a PhD Fellow in Energy Planning. Parallel to my research work, I participated as a board member and representative at the university's PhD Association and at the PhD Association of Networks Denmark (PAND). Currently, I work at the Institute for Energy Technology (IFE), in Norway.

My research focuses on energy system modelling and developing scenarios for implementing sustainable energy technologies in the transition toward smart energy systems. The publications listed below show literature produced during my PhD, both as a main author and other contributions.

Primary publications

Paper [1]: Chang, M., Thellufsen, J. Z., Zakeri, B., Pickering, B., Pfenninger, S., Lund, H. & Østergaard, P. A., Trends in tools and approaches for modelling the energy transition, (2021), *Applied Energy*, 290, 18 p., 116731.

Paper [2]: Chang, M., Lund, H., Thellufsen, J. Z. & Østergaard, P. A., Perspectives on coupling energy system models, (2023), *Energy*, 265, 126335. doi: 10.1016/j.energy.2022.126335

Paper [3]: Paardekooper, S., Lund, H., Chang, M., Nielsen, S., Moreno, D. & Thellufsen, J. Z., Heat Roadmap Chile: A national district heating plan for air pollution decontamination and decarbonization, (2020), *Journal of Cleaner Production*, 272, 122744.

Paper [4]: Chang, M., Thellufsen, J. Z., & Lund, H., Aggregated versus disaggregated energy system modelling approaches: The case of Chile's energy system (2020). 2nd Latin America SDEWES Conference Buenos Aires.

Paper [5]: Chang, M., Paardekooper, S., Prina, M. G., Thellufsen, Lund, H. & Lapuente, P., Smart energy approaches for carbon abatement: Scenario designs for Chile's energy transition, (2023), Submitted to *Smart Energy*.

Additional publications during the PhD:

[6] Korberg, A.D., Thellufsen, J.Z., Skov, I.R., Chang, M., Paardekooper, S., Lund, H., Mathiesen, B.V., On the feasibility of direct hydrogen utilization in a fossil-free Europe, (2022), International Journal of Hydrogen Energy, In Press. doi: 10.1016/j.ijhydene.2022.10.170

[7] Lund, H., Thellufsen, J.Z., Sorknæs, P., Mathiesen, B.V., Chang, M., Madsen, P.T., Kany, M.S., Skov, I.R., Smart Energy Denmark – A consistent and detailed strategy for a fully decarbonized society, (2022), Renewable and Sustainable Energy Reviews, 168, 112777. doi: 10.1016/j.rser.2022.112777

[8] Lund, H., Skov, I.R., Thellufsen, J.Z., Sorknæs, P., Korberg, A.D., Chang, M., Mathiesen, B.V., Kany, M.S., The role of sustainable bioenergy in a fully decarbonized society, (2022), Renewable Energy, 196,195-203. doi: 10.1016/j.renene.2022.06.026

[9] Thellufsen, J. Z., Lund, H., Sorknæs, P., Østergaard, P. A., Chang, M., Drysdale, D., Nielsen, S., Djørup, S. R. & Sperling, K., Smart energy cities in a 100% renewable energy context, (2020), Renewable and Sustainable Energy Reviews, 129, 109922.

[10] Aliana, A., Chang, M., Østergaard, P. A., Victoria, M. & Andersen, A. N., Performance assessment of using various solar radiation data in modelling large-scale solar thermal systems integrated in district heating networks, (2022), Renewable Energy. 190, p. 699-712 14 p.

[11] Kany, M. S., Mathiesen, B. V., Skov, I. R., Korberg, A. D., Thellufsen, J. Z., Lund, H., Sorknæs, P. & Chang, M., Energy efficient decarbonization strategy for the Danish transport sector by 2045, (2022), Smart Energy, 5, 11 p., 100063.

ENGLISH SUMMARY

Under the current context of climate change, the transition to sustainable energy systems is essential. Energy system modelling tools can facilitate the energy transition by providing insights about the impacts of redesigning the energy system. This is especially relevant to illustrate the effects of large shares of sustainable energy supply sources and assess the impacts of different developments across energy demand sectors, technologies, and society.

In recent years, the analyses conducted with such tools have grown in scope and complexity, leading to more integration of tools across a range of modelling paradigms. This development leverages a wide range of scientific disciplines to overcome the limitations of using a single-model approach for generating insight. While the benefits of linking energy system models with each other and across disciplines are widely assumed, significant knowledge gaps remain in terms of fully understanding its benefits under archetypical situations and the trade-offs of adding additional layers of modelling complexity through model coupling. On a more fundamental level, this presents a dilemma between the principle of using models as simplified versions of reality and increased modelling complexity.

This thesis provides a view on this matter by exploring the practice of model coupling with applied cases of energy system modelling through a collection of articles. The findings of the studies and the thesis discuss some implications of model coupling from theoretical, methodological, and analytical perspectives.

On a theoretical level, aligning domains and models can be beneficial to get a broad range of answers from different perspectives about the energy transition, yet this must be managed with urgency, given the context of climate change. Therefore, model coupling developments must happen at a pace that can provide meaningful and timely insight and where insightful approaches can emerge from simple purpose-driven model coupling configurations with ESMs. From a methodological perspective, the ESM cases showed different levels of complexity and extra modeling efforts, that compounded with the increased resolution provided by model coupling approaches.

Finally, the analyses show the case of Chile's energy system under different potential future scenarios and modelling perspectives. The results of these analyses show that a redesign of the energy system is possible and can go beyond Chile's nationally designed scenarios and climate targets.

DANSK RESUME

I den aktuelle kontekst af klimaforandringerne, er omstillingen til bæredygtige energisystemer af højeste prioritet. Værktøjer for energisystemmodellering (ESM) kan give indsigt i hvordan energisystemer kan redesignes mhp. at lette energiomstillingen. Desuden er disse værktøjer især relevante for at illustrere effekten af store andele af bæredygtige og vedvarende energikilder i energisystemet, og hvad kan ske under forskellige udviklinger i teknologi, energiforbrug, og i samfundet.

I de senere år er energisystemanalyser udført med ESM værktøjer vokset i omfang og kompleksitet. Dette har resulteret i bedre integration mellem modeller med kontrasterende modelleringsparadigmer og med modeller fra forskellige videnskabelige discipliner via modelkobling. Denne udvikling forsøger at overkomme begrænsningerne ved at bruge en enkelt-model tilgang til at generere indsigt. Mens fordelene ved at koble energisystemmodeller indbyrdes og tværfagligt er bredt accepteret, er der stadig usikkerheder om, i hvilke arketyperiske situationer, der er fordele ved dette, og afvejningerne med at tilføje yderligere lag af modelleringskompleksitet gennem modelkobling er stadige usikre. Dette præsenterer også et dilemma mellem princippet om, at bruge modeller som forenklede udgaver af virkeligheden, og stigende modelleringskompleksitet.

Denne ph.d. præsenterer et overblik over disse spørgsmål og dilemma, ved at udforske praksis med modelkobling, og anvendte ESM-casestudie gennem en samling af artikler. Resultaterne af analyserne i artiklerne og afhandlingens implikationer af modelkobling diskuteres på et teoretisk, metodisk og analytisk synspunkt. Fra et teoretisk perspektiv bør modelkobling fokusere på at være problembaseret i stedet for at være universelt omfattende, så det kan give rettidig og meningsfuld indsigt i den presserende energiomstilling. Fra et metodisk perspektiv viser de anvendte ESM cases forskellige niveauer af kompleksitet og ekstra modelleringsindsats. Endelig viser analysen, at modelkobling og energisystemmodellering kan illustrere forskellige alternativer til at opnå dekarboniseringen af Chiles nationalt energisystem.

PREFACE & ACKNOWLEDGEMENTS

This thesis sums up my PhD project, undertaken from August 2019 to January 2023 in the Sustainable Energy Planning Research Group at Aalborg University (AAU). However, my academic adventure in Sustainable Energy Planning at AAU started much earlier when I decided to join their Master's program back in 2015.

Since then, I have always had a penchant for some of the modelling aspects of energy planning. Indeed, this came rather organically with my background in engineering and math but was also rooted in a sense of curiosity and experimentation. I found in energy system models a lab where it is possible to explore what the future could hold. The PhD project reflects some of those aspects and synthesizes the findings from Papers [1–5], diving into energy system modelling and exploring the niche of coupling modelling tools. Hopefully, energy system modelling practitioners can find some use and benefit from this undertaking. Elsewise, I'm equally glad if this opens up new interesting questions rather than answers.

This PhD project and the thesis work have received funding from the SENTINEL project of the European Union's Horizon 2020 research and innovation programme under grant agreement No 837089, and the RE-Invest project, which is supported by the Innovation Fund Denmark under grant agreement No. 6154-00022B. I want to extend my gratitude to all the project partners involved.

Special thanks are due to my supervisors: Henrik Lund, for his mentorship and for introducing me to a range of interesting projects during my time at the Sustainable Energy Planning Group, and Jakob Zinck Thellufsen, who has been a constant source of advice, sparring and interesting discussions – academic and otherwise. I would also like to thank Susana Paardekooper for proofreading the final draft of this thesis, and the rest of my former colleagues at AAU, from whom I've learned a lot in these last few years and shared great moments, be it during project work, lunch, Friday breakfasts, or other extracurriculars. In the same manner, I would like to extend my gratitude to my colleagues at the Department of Energy Systems Analysis at the Institutt for Energiteknikk (IFE) in Norway, for welcoming me with open arms and for their encouragement during the last few months of wrapping up the PhD.

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Without further ado, I wish you a pleasant reading!

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ACRONYMS AND ABBREVIATIONS

<i>ESM</i>	Energy system model
<i>GIS</i>	Geographical information systems
<i>MAC</i>	Marginal abatement cost
<i>PELP</i>	[Chile's] Long-term energy planning process
<i>RE-Invest</i>	Renewable Energy Investment Strategies project
<i>SENTINEL</i>	Sustainable Energy Transitions Laboratory
<i>VRES</i>	Variable renewable energy sources

*“Scientists supposedly study nature, but in reality much of what they do is constrict
and study models of nature.”*

– *Melanie Mitchell,*

Complexity [12]

CHAPTER 1. INTRODUCTION

What are models? One definition, from Lave & March [13], describes models as a *“simplified picture of part of the real world. It has some of the characteristics of the real world but not all [...] A model is simpler than the phenomena it is supposed to represent or explain”* [13]. We use models to inform decisions ranging from providing someone with a simple mental image for planning some desired outcome to intricate computational representations of complex systems [14].

In the current global context, models are used extensively to understand a vast range of important issues, including climate change mitigation actions. Among these actions, the transition toward low-carbon energy systems with sustainable supply sources will be critical in the coming years to lower the effects of climate change [15]. Therefore, energy system models (ESMs) are often used to illustrate how we understand current and future energy systems. With those representations, it is then possible to show and quantify the impacts of planning pathways and to represent potential energy system redesigns, such as increased levels of variable renewable energy sources (VRES), reduced fossil fuel consumption, and new developments in technology and energy carriers [16,17].

The challenge of the sustainable energy transition is characterized by rising complexity of energy systems, as more technologies and more interaction between technologies and infrastructures is foreseen [18]. In turn, energy system models are developing to capture this growing complexity to inform decision making [1,19].

Indeed, a wide range of energy system modelling tools are broadly available and used by decision-makers and modelling practitioners [1]. At their core, these tools all provide mathematical constructs and formulations of the energy system, but consider different modelling paradigms, scopes, technical capabilities, and methodologies [20–25]. In practice, this means that throughout the landscape of energy system modelling tools, specific tools will be suitable for certain intended uses and have capabilities to address specific questions, that can support policy development. However, when managing the increasing complexity of energy systems and their real-world interactions, the limitations of a single model can become a challenge [26].

Complementary approaches with models of diverse technical scopes can provide ways to bridge some of the initial limitations of using a single model. The synergies between technical scopes and modelling capabilities of different modelling tools can provide added insight into complex questions and complementary perspectives. Multiple studies have applied methodologies with linked models, outlining the benefits of multi-model suites for the particular cases they address. Nevertheless, practical hurdles also arise from complexity of a given modelling exercise. Additionally, it is uncertain how and to what extent these benefits can be generalized across modelling

exercises that link tools together [2]. Especially, when model complexity can be an issue for model users and those using the results [19,27,28].

This then raises the question, what is the role of coupling or linking energy system models in planning and analyzing the energy transition? Ultimately, what are the implications of model coupling? This thesis tries to address part of these underlying questions.

1.1. BACKGROUND

Over the past decade, several efforts have been conducted to portray the continuous developments in energy system modelling tools, which are constantly evolving in response to new technology innovations, planning practices, and emerging challenges around the energy transition.

In a 2010 study conducted by Connolly et al. [22], multiple energy system modelling tools were surveyed to assess their potential for analyzing the integration of variable renewables in energy systems along several dimensions. At that time, several modelling tools were found to lack adequate resolution to fully capture all the intricacies of representing the technical elements of 100% renewable energy systems. Even the handful of models that had represented energy systems with high integration of renewable energy sources fell short in their technical representation of one or more modelling dimensions.

For example, the temporal resolution to model short-term supply variability was found to be a major open challenge, as were the limited representations of the different energy sectors and end-uses corresponding to the modelling tools' focus. While on the other end, some of the tools ticking these boxes lacked resolution in other aspects like their technical, geographical, or long-term horizon representations of energy system scenarios [22].

Similarly, in a 2015 review by Pfenninger et al. [26], modelling with high temporal resolutions –both short-term fluctuations and long-term scenarios – was still an unresolved challenge for energy system models. Moreover, other key challenges were identified regarding the models' capabilities to represent high spatial resolutions, increase energy system complexity, integrate human and societal factors, and balance uncertainty and transparency.

More recently, many studies have looked into specific trends and features found in the landscape of energy system modelling tools. Some of these studies highlight advances in increased modelling resolutions [24,25,29], complexity [30], and open-source and transparency developments [31,32]. At the same time, other analyses have looked more laterally into broader modelling efforts, illustrating how energy system analyses can capture other dynamics of the energy transition by integrating the human

and social dimensions [33,34], representations of energy demands [35], supply chain and life-cycle assessments [36], analysis of material flows [37], or geospatial planning methods [38].

The first publication of this PhD project, Paper [1], outlines key trends in energy system modelling tools and approaches via a review of previous literature and a survey gathering inputs from ESM developers. Similar to past studies, Paper [1] shows that energy system modelling tools today offer – in general – more detailed depictions of the energy system compared to a decade ago. Challenges do remain in the simultaneous representation of multiple energy sectors and end-uses, as well as the use of high-resolution demand data as input assumptions (often modelled externally) and the models' real-world application for decision support.

Furthermore, Paper [1] shows that energy system modelling tools are often linked to other tools. While this occurs across the whole modelling landscape, it becomes an even more recurring practice across tools linked to decision support as opposed to other tool developments. At the same time, it is associated with great modelling detail in other technical aspects of the energy system representation.

Paper [2] explores this further, describing past cases where model coupling with ESMs occurs. From this study, it is possible to identify a few common occurrences and archetypical cases. First, a large portion of studies present instances in which ESMs were linked to other ESMs, which have contrasting modelling resolutions. Alternatively, the ESMs were linked recursively with themselves, with the purpose of adapting the original operational purpose of the model and the underlying modelling paradigm. Another common occurrence happened in cases where ESMs were linked to other disciplines and model classes, often only considering a limited set of disciplines being linked. Lastly, other developments try to provide more comprehensive linkages encompassing multi-model ensembles.

However, as discussed in Paper [2], there is a limited generalized understanding of the overall practice of model coupling and how complex model coupling approaches align with the energy transition landscape—which requires accurate and timely insight. This is highlighted by the fact that in the reviewed modelling exercises, not only models are linked but also their embedded disciplines, with their respective paradigms, vocabularies, their data flows, and their own model developments and complexities. Moreover, ensuring mutual clarity and comprehensibility across these areas also poses an extra challenge [39]. This is even more critical given the already existing challenge of transparently communicating single model results and balancing complexity with the needs of decision-makers and model users [19,27,28]. In the face of this, striving for both a comprehensible and comprehensively universal model might prove infeasible.

Consequently, there is a need to understand the extent, conditions and context in which model coupling makes sense and how coupling modelling exercises can be adequately designed. On paper, benefits can be seen when one tool can cover the gaps of another. In practice, considering more compartmentalized purpose-driven approaches can prove to be just as valuable.

Therefore, there is a need to develop critical cases that present model coupling approaches, analyzing the broad implications of this practice. Ultimately, this can provide new insight into how and when the benefits of model linkages outweigh their added complexity and when more straightforward non-coupled energy system modelling approaches can provide comparable outcomes.

1.2. PROBLEM STATEMENT

As explored thus far, a number of issues are present around the current energy systems modelling landscape. These can be summarized as follows:

- Models are meant to be simplified representations of reality.
- Accurate and timely insight is needed to inform the energy transition.
- The energy system is becoming more complex, and so are ESMs.
- It is not always possible to calculate or answer all questions about the energy system and the transition with a single model.
- Model coupling brings about further complexity both in terms of modelling and comprehensibility.
- It remains uncertain when and how simpler or more compartmentalized approaches can provide comparable outcomes to complex model coupling.

The issues mentioned above present some fundamental dilemmas. Intrinsically, models are meant to be simplified representations of reality. Models can help us capture the specific parts of reality that we want to represent to address specific purpose-driven questions. As the energy transition furthers, our energy system and understanding of this reality are becoming more complex, and in turn, models must continue being useful representations while potentially losing their core simplicity.

Indeed, a balance is needed between providing adequate answers with simple-enough models, and adequate levels of complexity and coupling new perspectives. While it is not always possible to answer all questions about the energy transition with a single model, it is also likely that we do not wish to answer everything all at once, for the sake of comprehensibility and methodological practicality.

Therefore, it is important to understand when model coupling makes us wiser in capturing the specific aspects of the real-world energy system that we want answers for, how we get those answers, and when it just provides additional detail with marginal or no gain to the analyses. In this context, three main questions can be

outlined that this thesis explores and aims to address related to energy system modelling and the practice of model coupling:

- 1) How does the dilemma of increasing model complexity through model coupling and models being simplified versions of reality align – from a theoretical perspective – with providing insight to manage the energy transition?*
- 2) What are the gains and shortcomings of additional modelling complexity when applying model coupling methodologies to energy system analyses versus applying a single-model approach with an ESM?*
- 3) What are the impacts on analysis results when applying single-model and model coupling approaches with an ESM?*

1.2.1. PROJECT SCOPE

To address the problem statement presented above, this thesis delves into some theoretical perspectives in order to understand the implications of model coupling on a meaningful conceptual level. After that, the scope of the study prioritizes specific critical cases of model coupling aligned with the archetypes discussed and presented in Paper [2]. For this, established energy system scenario design methodologies are considered alongside coupling approaches and a widely validated energy system modelling tool like EnergyPLAN. Lastly, the cases are applied to an energy system on a national level (in this case, Chile) since this represents a typical case and policy interface where energy system models would be applied for decision support.

1.3. REPORT STRUCTURE

The main body of this thesis is divided into five chapters. These can be summarized as follows:

Chapter 1 – Introduction: presents the current landscape of energy system modelling, focusing on the current trends in modelling tool developments. The background discussed corresponds to a state-of-the-art review conducted in Paper [1] and [2]. Following this, the problem statement and the scope delimiting the thesis are presented.

Chapter 2 – Conceptual Framework: outlines some of the key concepts considered through the thesis as well as some concrete theoretical perspectives that guide the research design. This serves as a common framework for understanding the thesis's perspective and outcomes. The discussion provided here aligns with the concepts presented in Paper [2]

Chapter 3 – Methodology: discusses the different choices of methods and tools applied across the research studies, their procedural approach, and their limitations.

Chapter 4 – Publication Summary and Research Contributions: presents a brief overview of the five publications, highlighting the findings in connection to the theme of model coupling presented in this thesis.

Chapter 5 – Discussion & Conclusions: presents the conclusions of the thesis and addresses the research question presented in Section 1.2. Thematic reflections of the theoretical, methodological, and analytical findings are also discussed.

Finally, the papers written as part of the PhD project are included as *Appendices*, which supplement the discussions carried throughout the text, especially the summaries and conclusions presented in Chapters 4 and 5.

CHAPTER 2. CONCEPTUAL FRAMEWORK

This chapter sets a common ground of understanding for the themes, methodologies, and analyses presented throughout the thesis and research papers. This is first done by defining the terminology and key concepts applied. Then, this chapter presents and discusses the main theoretical perspectives embedded in the analyses of this work and the research papers.

2.1. KEY CONCEPTS

Throughout this thesis, a number of foundational concepts are used. These sections elaborate on their definitions in the context of this work to avoid potential misunderstandings and present conceptual delimitations.

2.1.1. ENERGY SYSTEMS

The concept of energy systems is central to this thesis, since models largely aim to represent this concept.

Here, an energy system is understood as a set of interrelated components structured around energy supply, energy conversion processes, energy transport, and energy end-use demands across different activity sectors. This set of interdependent components encompasses both physical and societal elements and constructs, their interactions and the emerging properties from these interactions and interdependencies.

From a physical or technical point of view, an energy system is understood to be constituted of components such as fossil fuels and other energy carriers; power generation plants, renewable generation technologies, and energy storages; transmission lines, gas infrastructures, and district heating grids; and demands for energy services from buildings, transport vehicles, and industry [40]. From a broader perspective, energy systems can also be said to include societal, economic, institutional, and political elements. These, in turn, can consist of individuals' behaviors, organizations, energy markets, and existing policies and regulations [33].

Naturally, the scale of these systems can vary from the very local implementation of a photovoltaic panel on the rooftop of a house to large and complex systems spanning inter-continental transmission systems. In this thesis, the concept alludes to large-scale energy systems that cover multiple economic activities and sectors with a critical mass of aggregated end-use demands and supply technologies and that also fall under an aggregated organizational unit. This underlying consideration relates to the notion of applying energy planning to inform decisions and for policy support, which often

happens at some non-trivial geographical aggregation level. It also relates to the idea that the different sectors are not self-contained but rather have synergies and interactions.

2.1.2. SMART ENERGY SYSTEMS

The concept of sector coupling is frequently used to refer to the broad idea of integrating (coupling) sectors in the energy system. However, it can conceptually span a varying number of sectors and different extents of integration. For example, the concept can refer to an electricity-only focus, where energy demands are electrified across a wide range of applications. Or it can also have broader connotations, like integrating the surplus heat from power production and industrial processes or the production of electricity-based fuels [41].

A more integrative notion of sector coupling can be found under the Smart Energy Systems concept formulated by Lund [42,43], as depicted in Figure 1.

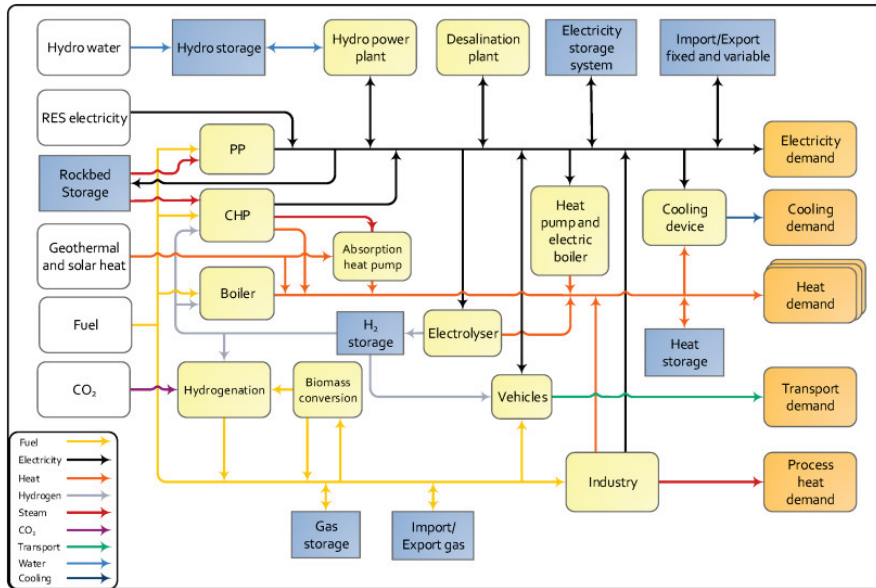


Figure 1. Conceptual representation of a Smart Energy System and the interrelation between supply, conversion technologies, energy carriers, and end-use demands [43].

This concept refers to energy systems where large shares of renewable energy sources can be integrated into the system while balancing the supply and different energy demands across the various sectors by integrating the latter's infrastructures, storages, and carriers to provide flexibility and energy efficiency. This holistic conceptualization can enable the design of 100% renewable energy systems with high levels of efficiency and cost-effectiveness [44–48].

This concept is widely used in this thesis to guide the design of energy system scenarios since it provides a comprehensive approach that can enable the efficient use of energy resources, enabling technologies and exploiting the existing and new potential synergies across sectors.

2.1.3. ENERGY SYSTEM MODELS, MODELLING TOOLS & PARADIGMS

Energy system models (ESMs) provide mathematical representations of energy systems. At their core, the underlying mathematical formulations of ESMs often follow simplified constructs that attempt to replicate the operation of an energy system. These can provide insight into system operations, cost-optimal capacity investments, emission reductions, energy balances, and the effects of introducing policy measures, among other things already discussed in Chapter 1, and presented in more detail in the research studies.

However, it is important to point out that in this work, the term ESMs has – in most occurrences – a slightly different connotation to the term “energy system modelling tools”. Here, the latter is used in connection to software or modelling frameworks that have a set logic and mathematical formulation used to generate models, but they by themselves do not necessarily have any data inputs to actually represent a particular system. On the other hand, the term ESMs typically describes instances where these modelling tools have already been used and populated with inputs to construct a modelled representation. So, to use Paper [5] as an example, the energy system modelling tool employed to simulate the energy systems was EnergyPLAN. The ESMs described are not the tool, but the model representations of the different scenarios designed in the research and generated by populating inputs into the tool.

Many different classifications of ESMs exist in connection with the underlying mathematical formulations of the models, methodological approach, and modelling resolutions [20,29]. One categorization, provided by Lund et al. [49], distinguishes between ESMs based on two modelling paradigms, differentiating between simulation and optimization models. It is essential to highlight this distinction since it is an aspect further explored in Paper [2] from a theoretical perspective and in Papers [4,5], where simulation and optimization approaches are linked together to provide an applied practical perspective on the complementary aspects when coupling paradigms.

Under this framing, simulation models are understood as models with fixed rulesets in their algorithms that replicate how an energy system operates and where the user(s) can directly configure how to represent a system best based on their criteria of analysis. On the other hand, optimization models present mathematical formulations of ESMs as optimization problems that endogenously decide the configuration of the energy system based on its optimization criteria and constraints. In [26,49], these modelling paradigms are also linked to contrasting planning practices and approaches for scenario analysis.

2.1.4. MODEL COUPLING OR LINKING

The concept of model coupling, or linking models together, is explored throughout this thesis, and both of these terms are used somewhat interchangeably. The process of model coupling implies establishing connections between different models to answer research questions that a model on its own might not be entirely able to answer or alternatively, to provide complementary perspectives to said answers. As presented in Paper [2], multiple types of links can be seen in past studies.

Early categorizations of link types emerge from the nexus between energy-economy models [50], although these are also used for describing the links between ESMs and other model classes [1,51]. Helgesen & Tomasgard [52] provide a synthesized view of these different types of links based on their level of integration or data exchange, presented in increasing complexity as soft-linking, hard-linking, and full integration of models.

The most frequent of these is soft-linking [1], which in this thesis is understood as a process with “*coordinated purpose-led data exchange between models or modelling algorithms*” [2]. The analyses presented in Papers [3-5] refer to model coupling under that framing. This specific linking approach allows for the integration of models that were not explicitly designed to be used together and enables the use of different models for different purposes or at varying levels of detail. This is particularly relevant since it facilitates the use of already well-developed models and tools. It also allows exchanging data exogenous to one of the models and internalizing these as new input assumptions within the scope of the whole model coupling exercise without significant model redevelopment required.

Different strategies of varying complexity can be applied when soft-linking models. These strategies include having manual or automatic data exchange protocols, unidirectional links of data, or bidirectional links where models feed each other data in an iterative process until some convergence between these is reached [53]. On the one hand, unidirectional linkages offer a simple approach to exchanging data between ESMs and other models, for example, from different disciplines or with dissimilar coverage of modelling resolution.

In contrast, bidirectional linkages can make more extensive use of the modelling outputs creating a feedback loop that can improve the cohesiveness of results across models. Still, differences across models might also lead to convergence issues. Bidirectional links can also provide recursiveness to an ESM, linking the latter as a core calculation engine with algorithms that provide additional rules and logic to exchange data across model runs, thereby expanding the original resolution and coverage of the ESM. Both of these strategies are explored in the analyses presented in this thesis.

2.2. THEORETICAL PERSPECTIVES

This section elaborates on the main theoretical considerations of this thesis. More specifically, it expands on discussions presented in Paper [2], relating model coupling to Choice Awareness and the multi-level perspective framework applied to transitions.

2.2.1. CHOICE AWARENESS AND MODELLING PARADIGMS

The notion of choice awareness is explored in various scientific fields, often addressing the idea that an individual's awareness of alternatives available to them will manifest in their behavior and decision-making process [54–57]. In the context of energy planning, Choice Awareness theory, as argued by Lund [42], parallels this on a societal level suggesting that, in order to enact radical technological change in the energy system, society needs to be aware of the range of alternatives available. However, Choice Awareness theory also argues that society's awareness of radical technology alternatives is influenced by the discourse of entrenched institutions and organizations, which will hinder or seek to eliminate certain options, creating a perception of limited or no choice.

This can manifest as choice-eliminating mechanisms such as the exclusion of alternatives from the public arena, methodological biases leading to the exclusion of key technologies, or portraying them as unfeasible to society under a specific set of conditions. Conversely, raising awareness of radical technological change is possible, and it can be achieved by promoting the development of concrete and comparable technical options, methodologies that can incorporate addressing political targets, and regulation to foster the implementation of these new alternatives [42].

In this thesis, an underlying consideration linked to Choice Awareness is that not only institutions or organizations can hinder awareness of options, but this can also happen as an unintended consequence of embedded practices associated with analytical paradigms. For example, the modelling paradigms presented in Section 2.1.3. – simulation and optimization – have corresponding elements associated with contrasting scenario planning approaches [26,49].

Simulation models lend themselves to a descriptive scenario planning approach. Under this scenario typology, scenarios focus on both predictive and explorative aspects, like answering “*what if?*” and “*what can happen?*” questions [58,59]. Indeed, the flexibility to represent different future states and radical change alternatives lies in the modeller's hand and may lead to a wide range of analysis criteria and perspectives that explore the consequences of potential changes rather than finding an optimal solution [60].

In contrast, optimization models are normative in nature. Normative scenarios focus on having a prescriptive approach that can answer the question of “what should

happen?” [58,59]. Under this framing, they can provide a view of the desirable end state of the energy system and its transition based on specific optimality criteria and the bound of their modelling set-up [61]. This means that an “optimal” alternative will precede other options that might be desirable under different perspectives or criteria.

Explorative approaches have been developed with optimization ESMs to identify near-optimal alternatives [62–64], thereby expanding their scenario planning approach and raising awareness of choices. However, as argued in Paper [2], this does not fully address potential issues intrinsic to their modelling resolution. Furthermore, potential limitations in a model’s construct to represent key enabling technologies might still hinder its ability to produce choices, potentially leading to presenting solutions with technology lock-ins. So, additional perspectives might be needed by linking other ESMs together to explore alternative energy system designs and capture different viewpoints corresponding to the envisioned modelling spaces inherent to the models [2]. This notion is conceptualized in Figure 2.

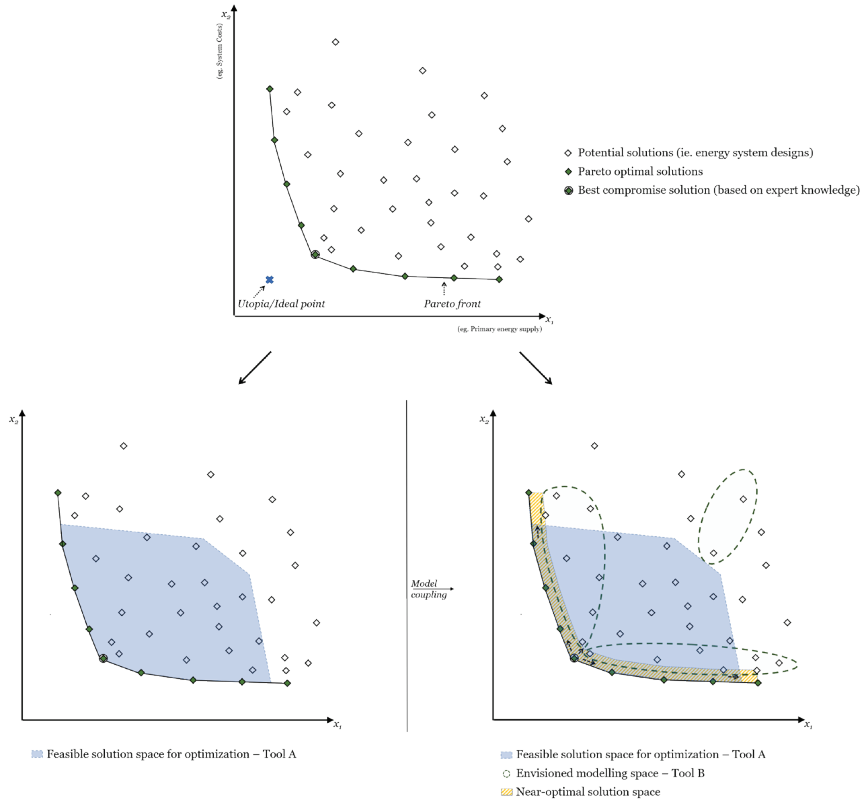


Figure 2. Conceptualization of the exploration of alternative and near-optimal energy system design options in the feasible and envisioned modelling space [2].

The exploration of different perspectives in the solution space and Choice Awareness theory naturally converges. In this thesis, these aspects are explored through the scenario design. Awareness of the methodological aspects is also raised as key to understanding how those scenarios were formulated and their implications. In addition, the scenarios considered later in the analyses portray technology choices by presenting scenario comparisons that incorporate political targets and contribute to the societal debate with new alternatives for the transition of the energy system.

2.2.2. TRANSITIONS, MODEL COUPLING, AND A MULTI-LEVEL PERSPECTIVE

A key question in energy planning is *how* the shift towards sustainable and low-carbon energy systems should take place. Indeed, in socio-technical systems like the energy system, such a process requires a redesign of its current physical elements, but it also encompasses other complex challenges that include – among other things – social, political, and institutional change, as well as changes in current practices and interactions across relevant actors.

In the context of transition theory, a transition is seen as a change in a socio-technical system [65]. For example, a redesign in the current energy system to a future decarbonized and sustainable energy system represents a process of drastic reconfiguration of technological elements, and – inherently –, it also embodies a shift towards a vastly different society, with different organizational features, value chains, policies, and shifts in behavioral patterns.

In addition, transitions – as characterized by Grin et al. [65] – have other intrinsic features such as:

- involving technical development and innovation through new knowledge and its applied use in societal domains
- integrating the interaction between groups in society
- radical reconfigurations of the socio-technical system
- being long-term processes
- observable at an aggregate level of institutional life or organizational network.

Another element in transitions, suggested by Geels [66,67], is that they are not easy to achieve due to stability (i.e., inertia, lock-in effects, path dependencies) in a current system. Geels describes the different elements in socio-technical systems as lying in a nested hierarchy and argues that transitions can be driven by the alignment of interactions and mutual influences between the different elements in this hierarchy. These elements are: (i) Niches – representing emerging and novel solutions developed by actors and societal domains; (ii) Regime – referring to the structures locked in place within the system, like current institutions, policies, and practices; and (iii) Landscape

– referring to broader and slow changing contextual aspects that shape the socio-technical system, like climate change, geopolitical developments, or global trends.

Indeed, this thesis portrays some of these features as underlying dimensions. For example, technical innovation and new knowledge from niches are often considered part of the scenario formulations in the ESMs used for analyzing the impacts of new and emerging technologies. This also relates to themes in Choice Awareness theory, where new choices emerge from societal domains. The scenarios in the analyses often showcase radical reconfigurations of the energy system, with both a long-term perspective and a meaningful spatial aggregation at a national and regional level. The cross-cutting integration of societal domains is considered to a limited extent and implicitly in the integrative approach embedded in the scenario analysis. Namely, when considering sector coupling of demands and infrastructures applying the Smart Energy System concept, and the implicit coordination happening across different elements in the system. On a methodological level, integration is expected between different societal domains (e.g., scientific communities, decision-makers) when coupling models from different disciplines and approaches to ESMs for new knowledge generation.

On a more fundamental level, the practices of systems modelling and model coupling can also be portrayed as elements in a nested hierarchy, with the developments in this practice being an embedded reflection of the transition on the broader socio-technical system. In other words, the broader transition of the energy landscape also reflects a potential transition within the embedded modelling practices. Paper [2] elaborates on this conceptualization, representing it from a multi-level perspective, as depicted in Figure 3.

In this conceptualization, different disciplines (e.g., energy planning, operations research, earth sciences, etc.) can be thought of as niches of societal domains where new novel knowledge and model developments can emerge. On the regime level, the patchwork of models emerging from these disciplines represents current practices that can inform planning decisions and policy. These models both influence and are influenced by the niche domains. For example, current modelling practices guiding decision-making and scenario developments co-produced in the science-policy interface often emerge from interdisciplinarity among knowledge domains and established institutions.

With increased structuration and development, these patchworks of models coupled together can increase their realism and representation of the energy transition. However, this also increases the complexity and the inherent challenges of coordination across the domains. Finally, at the top of this hierarchical perspective, the context of the energy transition forms the general landscape, which includes climate change mitigation actions, geopolitics, and other global trends exerting pressure on the lower levels.

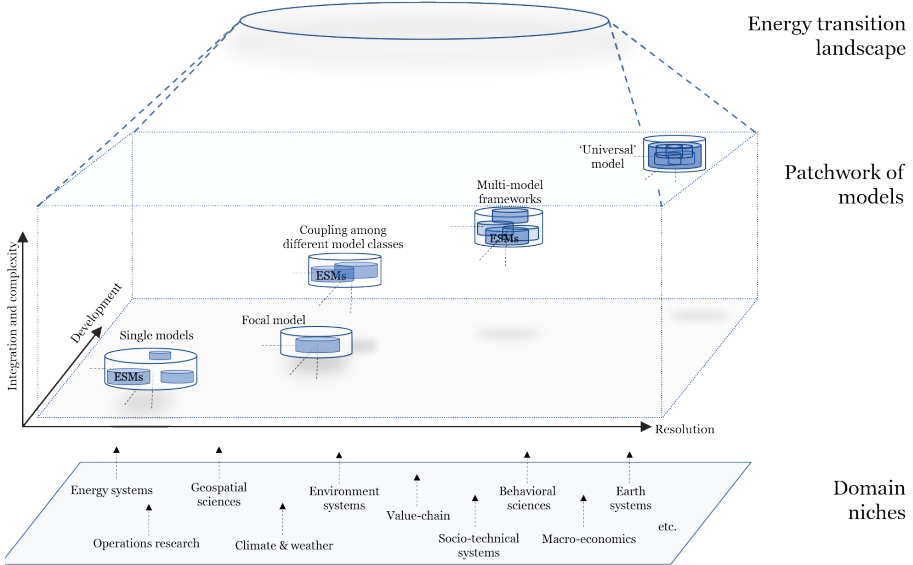


Figure 3. Model coupling structured from a multi-level perspective, adapted from [2].

The multi-level perspective framework presented above also illustrates certain shortcomings of model coupling practices from a theoretical viewpoint. Indeed, more realism could be achieved by increasing the integration across domains, leading to complex patchworks of models coupled together with a greater resolution to form comprehensive models. However, challenges could arise in the form of understanding and building standard vocabularies across disciplines, aligning practices, contrasting disciplinary paradigms, modelling scopes and resolution, data exchanges, and both computational time and development time for models. This increased structuration can become even more of a challenge when considering the interplay in the science-policy interface, which requires comprehensible insights from models in a timely manner. In some instances, this added model complexity might not necessarily be aligned with model user needs [19,68,69].

As highlighted in [65,70], managing transitions in the context of climate change should also be balanced with a sense of urgency for drastic action. Making adequate investment decisions early on for the energy transition can pay off, considering lock-in effects and the long-term nature of investments needed in the energy system [71]. In this context, striving for a universally comprehensive model or coupled approach might contravene the need for timely yet valuable insight to drive the energy transition forward if the former need time to be extensively developed, used, understood, and widely adopted.

As argued by Max-Neef [72], interdisciplinary approaches with a narrower focus could be more practical solutions in the face of these challenges. In this thesis, this consideration translates to limiting the model coupling approaches to a subset of

commonly used and already interdisciplinarily linked modelling tools for energy system analysis. Additionally, the analyses supported in this thesis by ESM coupling exercises are carried out to identify opportunities for national-level smart energy system development. This provides a scope where models are being coupled with the purpose of creating better realism and broader coverage without losing immediate focus.

CHAPTER 3. METHODOLOGY

This chapter provides an overview and critical discussion of the different choices of methods applied throughout the research papers appended to the thesis. For ease of navigation, Table 1 provides a summary of the research methods presented in each Paper. The methodological discussions are presented in sequential order in the following sections of this Chapter.

Table 1. Overview of research methods for each of the articles.

Study	Literature review	Survey questionnaire	ESM	Model coupling / linkages		
				Geospatial model	Powerflow model	Optimized MAC curve model
Paper 1	X	X				
Paper 2	X					
Paper 3	X		X	X	(X)	
Paper 4	X		X		X	
Paper 5	X		X			X

3.1. LITERATURE REVIEWS

Critical overviews of the existing research were necessary for each of the studies presented in this thesis. This was done to identify existing gaps and trends in the universe of related studies in the field. To that end, it was essential to conduct literature reviews.

For each paper presented here, the first step in their respective literature review was to narrow down the specific problem areas and research questions to address. This was followed by searching relevant keywords in scientific databases. These keywords included terms such as “energy system models”, “smart energy systems”, “energy system analysis”, “model coupling”, “soft-linking”, “energy models”, among other terms related to the key concepts outlined in Section 2.1. Additional search keywords were included in the Papers [3-5] about the specific case of energy system scenarios for Chile. The results of all these searches were then inspected and narrowed down based on their actual relevance to the different papers.

Compared to the other studies, the literature reviews presented in Papers [1] and [2] took a more prominent role as central elements of their respective analyses. This choice was made given the nature of these two papers since they were not tied to specific modelling exercises. As summarized later in Chapter 4, both of these publications utilized the reviews to provide comprehensive meta-analyses, and classifications of past cases and to infer direct conclusions and ways forward from the underlying findings of their respective classifications rather than solely synthesizing

past findings. In practical terms, it meant that the reviews had to follow a more systematic approach where the relevant scientific literature was organized by themes, conceptual categories, and the types of modelling tools they covered. This was especially valuable for Paper [2] since no unified review or perspective specific to the article's subject matter existed priorly.

However, a key challenge of this approach lies in the fact that it only provides a snapshot of the current situation. Thus, certain relevant publications might not have been included in the reviews. In the case of Paper [2], another potential shortcoming arises from the way in which other publications report their methods and research design. Here, omissions explaining parts of their methods (e.g., not explicitly reporting soft-linking models as part of their approach, even if this was the case) might cascade into omissions of potentially relevant papers in the literature review.

3.2. SURVEY QUESTIONNAIRE

In Paper [1], an online survey to model developers was used as means of data gathering. The choice of conducting a survey rather than relying solely on reviewing the literature or the modelling tools' documentation had the goal of establishing a direct line of dialogue with model developers. This engagement was needed for two main reasons: (i) to have a common vocabulary about the features of the modelling tools surveyed, and (ii), to uncover aspects about the use of the tools that are not captured in documentation or scientific articles.

The latter of these reasons came as a direct conclusion from the meta-analysis of past energy system modelling review articles conducted in the first part of Paper [1]. As mentioned in Section 4.1, the meta-review showed that past reviews had limited insight into specific areas of application of energy system modelling tools with regards to how these are subsequently used for policy-support or whether models tend to be linked with other modelling tools. Therefore, gathering input on these matters was necessary.

The questions in the online survey were designed to have broad coverage of the different aspects of the modelling tools. The survey was then sent to model developers for the various modelling tools identified in the meta-review presented in Paper [1]. The questions were segmented into 6 different parts, which included:

- General information about the tool (e.g., Name of the tool)
- Modelling specifications (e.g., Main purpose, user-interface, licensing, etc.)
- Application (e.g., Case studies, use for policy-support, coupling with other tools, etc.)
- Modelling resolution (e.g., modelling timestep, time horizon, geographical coverage, technical aggregation, etc.)
- Key inputs (e.g., technologies considered, demand representation, etc.)

- Additional information (e.g., documentation, short description)

The full list of questions is presented in Appendix A. (as an Appendix to Paper [1]), and a database with the full results of the survey questionnaire is available in [73].

The survey gathered responses for 54 modelling tools, including many well-known and widely-used ESMs in the field. This means that it only represents a fraction of all the available energy system modelling tools. Moreover, it also presents a static snapshot of a field that is in constant development. Nonetheless, the results are still capable of providing insight into current trends, and therefore have to be complemented with the additional level of validation provided by comparisons with similar past studies, as was done in Paper [1].

3.3. ENERGY SYSTEMS ANALYSIS

This section describes the tools and approaches used throughout the energy system analyses presented in Papers [3-5], which are applied to the case of Chile's energy transition. A brief discussion on the choice of energy system modelling tool is presented, followed by an additional discussion on the methods and tools coupled to the ESM.

3.3.1. CHOICE OF ESM TOOL: ENERGYPLAN

Papers [3-5] present applied cases where Chile's national energy system is modelled. To this end, a tool capable of representing the energy system was needed. As identified in Paper [1], many potential options would be able to capture the dynamics of the energy system. That being said, a few key considerations were taken into account for selecting the adequate choice of tool:

- Hourly timesteps for modelling the energy system
- Coverage of multiple sectors and the synergies between their infrastructures
- Aggregated technical detail
- Validated use for national and regional Smart Energy Systems
- Fast computational time
- Openly accessible
- Linkable with other modelling tools.

The EnergyPLAN tool was selected as it ticked all of the categories mentioned above. EnergyPLAN is a bottom-up simulation modelling framework for designing models of the energy system. The tool provides an hourly representation of the energy system for a target year, and it can model the hourly balances of the energy system representing the system as an aggregated geographical node (i.e., as a copperplate model) with aggregated technology groups [74].

To do this, it considers as inputs different user-specified energy supply sources, efficiencies and volumes for conversion technologies and storages, and demands across all energy end-use sectors. Moreover, if costs are provided, it can estimate both total system costs and marginal production costs, depending on the type of simulation strategy selected. The main outputs of the model are annual and hourly balances which include primary fuel consumption, energy demands, production, imports, exports, and theoretical curtailment (expressed as a critical excess electricity production parameter, CEEP). Moreover, the outputs can also provide estimates of emissions and a breakdown of system costs. These outputs are finalized within seconds of starting a model run. Figure 4 presents an overview of the tool's setup.

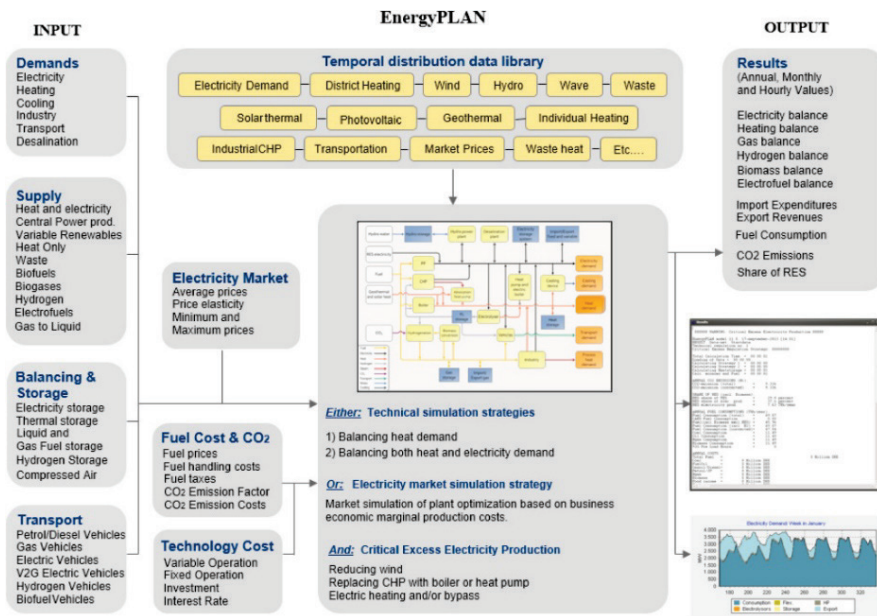


Figure 4. Overview of the EnergyPLAN tool's setup, including a list of user-defined inputs, simulation strategies, and outputs. Source: [74].

EnergyPLAN also benefits from being a widely used tool, validated across various scopes of studies, and with several applications where it has been linked to other tools for answering questions about the energy systems' transition [2,75]. Its application is also quite flexible, capable of analyzing multiple performance indicators of the energy system rather than fixed optimization criteria [60].

Nonetheless, the tool also has some limiting factors. For instance, the geographical representation in EnergyPLAN is quite coarse since it only represents the energy system as a single node. This means that geographically dispersed supply and demand volumes need to be aggregated, and bottlenecks in the transmission system cannot be represented endogenously. In addition, the tool is also limited in terms of only modelling a target year. This means that it cannot provide endogenous decisions about

capacity expansion options along the energy transition. Similarly, other optimization objectives need to be assessed analytically by the modelling practitioner rather than being endogenous decisions made by the model. These limitations, however, can be complemented by linking the EnergyPLAN tool with other modelling tools and approaches.

3.3.2. SCENARIO FORMULATION

In Papers [3-5], energy system scenarios are designed to help analyze the energy system's future redesign and test different relevant model coupling approaches. Here, the analysis is done comparatively, taking Chile's energy system as a case. As a first step in the different analyses, a reference scenario for benchmarking was generally identified, corresponding to conservative developments in the energy system and policy measures (i.e., following current trends). In Papers [3] and [4], the reference scenarios were derived from a past iteration of Chile's national long-term planning process (PELP). In Paper [5], new scenarios were used corresponding to the latest and most updated projections from Chile's new national long-term energy planning process.

The second step of the scenario analysis then included the evaluation of impacts when considering new developments and the introduction of measures that translate into changes in energy demands, the implementation of energy-efficient technologies, and exploiting the synergies across all sectors. This evaluation was conducted by representing the scenarios' data assumptions as inputs in EnergyPLAN-based models.

Throughout Papers [3-5], the specifications of their corresponding scenarios and their data assumptions are presented within the individual papers (available in the Appendix to this thesis). However, key uncertainties remained that required additional insight and the use of other tools and approaches linked to the ESMs to fill in the gaps in their respective analyses. These approaches and tools are described in the following sections.

3.3.3. SOFT-LINKING ENERGYPLAN WITH GEOSPATIAL ANALYSIS

As mentioned in Section 3.3.1, energy systems modelled in EnergyPLAN tend to have a coarse geographical representation. Furthermore, while the model can provide insights into the system's energy supply and demand balances, it cannot determine by itself the value of final or end-use energy demands or how these can be aggregated on a national or regional level. As explored in Paper [1], it is common for energy demands to be exogenous variables in energy system models. This often means that these types of inputs need to come from existing databases or other modelling results.

In the case of Chile, heat demand estimates were unavailable on a national level from statistics or prior projections. In Paper [3], and the study presented in [76], a joint

effort was made to align a geospatial heat demand model and an energy system model of Chile to bridge this gap. The geospatial model was built using a Geographical Information Systems (GIS) tool. In the GIS tool, geo-referenced data was compiled for buildings, population, and climate, as well as costs of pipework for the district heating infrastructure. A regression model was then used to estimate geo-referenced space heating demands at a high spatial resolution for the whole country. Along with this, estimates for district heating grid cost curves and grid losses were also calculated. For these results to be used in the energy system scenarios, the data outputs from the heat demand model had to be aggregated on a country level. The same was done for the cost estimates and grid losses, although these were also provided at varying penetration levels for district heating, to assess the impacts of introducing larger shares of this technology across the energy system scenarios. Figure 5 provides an overview of the data flows and the links between the models and the resulting scenarios.

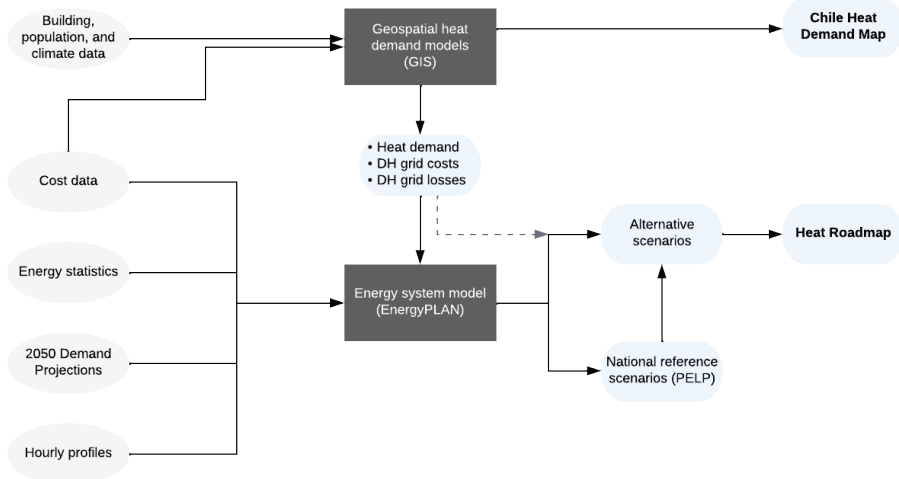


Figure 5. Data flows and linkages between the geospatial and energy system models. Adapted from [76].

Having established purpose-made aggregations and a streamlined flow of data between the geospatial and energy system models facilitated quick runs and iterations of the scenarios when new heat demand estimates were ready, without having to undertake substantial work.

Paper [4] applies a finer energy system aggregation considering four interconnected macro-regions, each as an individual EnergyPLAN model. In this study, the already established links allowed for quick aggregations of the heat demand data for these regions. Similarly, cost estimates and grid losses were easily exchanged for this modelling exercise, given the already established links across the models.

3.3.4. OPTIMAL POWER FLOW ACROSS DISAGGREGATED ESM

As mentioned in the previous sections, the energy system representation provided by EnergyPLAN tends to have an aggregated copperplate approach, modelling the energy system as a single node. This means that electricity transmission across transnational or regional borders and bottlenecks in transmission lines are not captured in the model. Hence, to account for this missing dimension and potential limitations of modelling energy systems as single nodes, EnergyPLAN has to be coupled with external tools.

An early example is the multi-node representation proposed by Thellufsen & Lund with the MultiNode tool [77]. This tool, however, groups together the transmission volumes and does not account for the specific details of which individual nodes are connected to each other in the network. However, another method has been developed under the EPlanFlow tool, where EnergyPLAN simulations are linked with an optimal power flow approximation algorithm [78].

The links provided by EplanFlow can identify optimal transmission flows across nodes based on the minimum costs of power generation while considering the specific connections between networks and line capacities [78]. Paper [4] applies this approach to capture the impacts of having disaggregated representations of the energy system scenarios for Chile and to test how this affects the overall results from a national perspective. The procedure applied with the EPlanFlow tool can be segmented into three major steps, as seen in Figure 6.

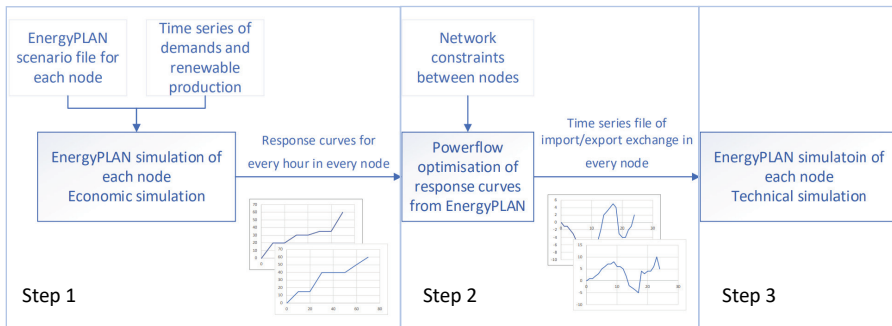


Figure 6. Overview of the links and approach with EPlanFlow. Adapted from [78].

These steps, based on the methodology presented in [78], can be explained as followed:

1. Individual EnergyPLAN simulations initialized for each node.

This first step consists of executing the energy system models for each node independently to generate hourly response curves. For illustration, in Paper [4],

the countrywide model for Chile was disaggregated into four smaller models. Each of these represented a macro-region of the country, and each of the corresponding regional models was also conceptualized as a node in the EPlanFlow tool. These disaggregated models also required their own set of hourly time series inputs for demands, renewable production, and inputs for fuel prices and variable costs.

Then, separate EnergyPLAN model runs were conducted for each regional model. These runs applied a specific simulation strategy in EnergyPLAN (“market economic”), generating a response curve for every hour. These response curves include the electricity import and export potential for different marginal production costs.

2. Power flow optimization of the response curves generated in EnergyPLAN.

The response curves from EnergyPLAN are fed into the power flow algorithm. Details about the network must be included in the algorithm, consisting of the list of connected pairs of nodes and the line capacity between these connections.

Once inputs are set, the algorithm utilizes a DC power flow approximation to optimize the electricity flow at each hour across the network, minimizing the electricity production costs and subject to the constraints in transmission line capacities. The results of this procedure yield hourly profiles of the electricity import and export at each node as text file inputs for EnergyPLAN.

3. New EnergyPLAN simulations with optimized import and export profiles

The power flow optimization algorithm outputs are fed back into EnergyPLAN as import and export time series and as aggregated annual import volumes for each node. Then, new EnergyPLAN model runs are executed to capture the operation of the systems and the resulting energy balances with the new import and export flow specifications.

While this procedure can improve the technical and spatial granularity of the energy system model, certain shortcomings arise from its implementation. On one end, additional details could also enhance the realism of this approach. For example, the power flow approximation applied to the case of Paper [4] neglects effects such as the thermal capacities or reactive power in AC lines. Nonetheless, approximations like the one presented in [78] are common in the power market industry to reduce data and computational complexity [79–81].

On the other hand, applying this approach instead of an aggregated model still means that data requirements and computational time will compound depending on the number of nodes modelled, and scenarios considered thereafter. This applies both due

to additional individual EnergyPLAN simulation runs for each node, and also a more complex formulation of the network and the optimization problem in the power flow algorithm. Moreover, the optimization remains sensitive to the additional data assumptions and uncertainties in variable costs and fuel prices – which would affect the generation of the marginal production costs for the response curves.

Finally, while the algorithm provides a perspective on optimal import and export flows, it does not look into the potential optimality of other key components and criteria for the energy system at large, such as optimal capacity expansion options or carbon abatement measures in all sectors along the transition.

3.3.5. OPTIMIZED MARGINAL ABATEMENT COST CURVE GENERATION

A theme explored in the analyses is how scenarios can be optimized while still providing a view of multiple planning perspectives, aligning energy system modelling paradigms, as suggested in [2]. The analyses in Paper [5] explore this aspect by applying an energy system optimization method to generate sequential scenarios with capacity expansion and carbon abatement alternatives. The method implemented in Paper [5] employs a modified version of the algorithm from the EPLANoptMAC tool, initially developed by Prina et al. [82].

The EPLANoptMAC tool operates by coupling an EnergyPLAN model to an optimization algorithm to generate marginal abatement cost (MAC) curves. A MAC curve is a valuable visualization tool that shows the incremental costs of reducing a given type of emission relative to the reduction (abatement) achieved by introducing new reduction measures at increasing abatement levels. MAC curves have a widespread use for decision-making since they can help to identify cost-effective abatement alternatives and priorities in an energy system's redesign (e.g., introducing new onshore wind capacities, energy efficiency measures, fuel replacements in transport). Moreover, they can provide a view of which measures would benefit from policy support or incentives to become cost competitive. However, MAC curves often fail to capture system dynamics which can lead to double accounting of abatement potentials [83,84]. Therefore, MAC curves need model-based approaches to consider the system perspective, like in the EPLANoptMAC tool.

The tool generates step-wise MAC curves by applying a hill-climbing optimization algorithm. This type of algorithm works by finding a solution for a single-objective problem at a given step, then iteratively evaluating new solutions in each subsequent step until reaching a peak value or a pre-determined number of evaluation steps. In the specific case of the EPLANoptMAC tool applied in Paper [5], this logic is embedded in the optimization procedure, as outlined by [85].

The steps of this procedure can be described as follows and are similarly illustrated in Figure 7:

1. Initializing a reference EnergyPLAN scenario and optimization parameters:

The algorithm is fed the value of total number of iteration steps, a list – or vector – of decision variables (dv) representing the separate abatement measures, the target end-values for these variables, and the incremental values (I) to be added at each step. A reference EnergyPLAN model is also linked to the algorithm, providing the initial set of starting values for the list of decision variables that will be modified in the subsequent step.

2. Evaluation and generation of new scenario alternatives:

The reference model is modified, changing separately and one-by-one the values of each decision variable by adding their respective incremental values. The newly generated modified scenarios are then executed in EnergyPLAN, saving the output results.

3. Assessment of the costs of carbon abatement (CCA):

The output results of the different runs are evaluated. For each new modified scenario, the total system costs from the reference scenario are subtracted from the new resulting costs, which shows the incremental costs of implementing a measure. Then, the CO₂ emissions for each new scenario are deducted from the reference emissions, showing the potential carbon reductions. A cost-effective indicator for the cost of carbon abatement (CCA) is then calculated for each of these scenarios by taking the ratio between incremental cost differences and emission reductions. The option yielding the minimum CCA value is then selected as the optimal solution, and the newly estimated CCA values are saved with the output results.

4. New reference scenario selection for the next step, re-initialization and repeat:

The optimal solution is set as the new reference scenario system. Then, the algorithm moves to the next step and checks if the values for the decision variables have reached their target end-values. If that is the case, these are no longer considered for the following iterations. Finally, the procedure is repeated with the new modified reference until the algorithm reaches the specified number of total steps or all options fail to provide carbon reductions.

In Paper [5], an additional condition is added so that in the third step, the assessment also considers a maximum biomass value from the output results. If this value is exceeded, then the option is no longer evaluated until the next step.

After this procedure is executed, the results are plotted together, depicting the optimal CCA values and cumulative CO₂ reductions for each of the selected measures.

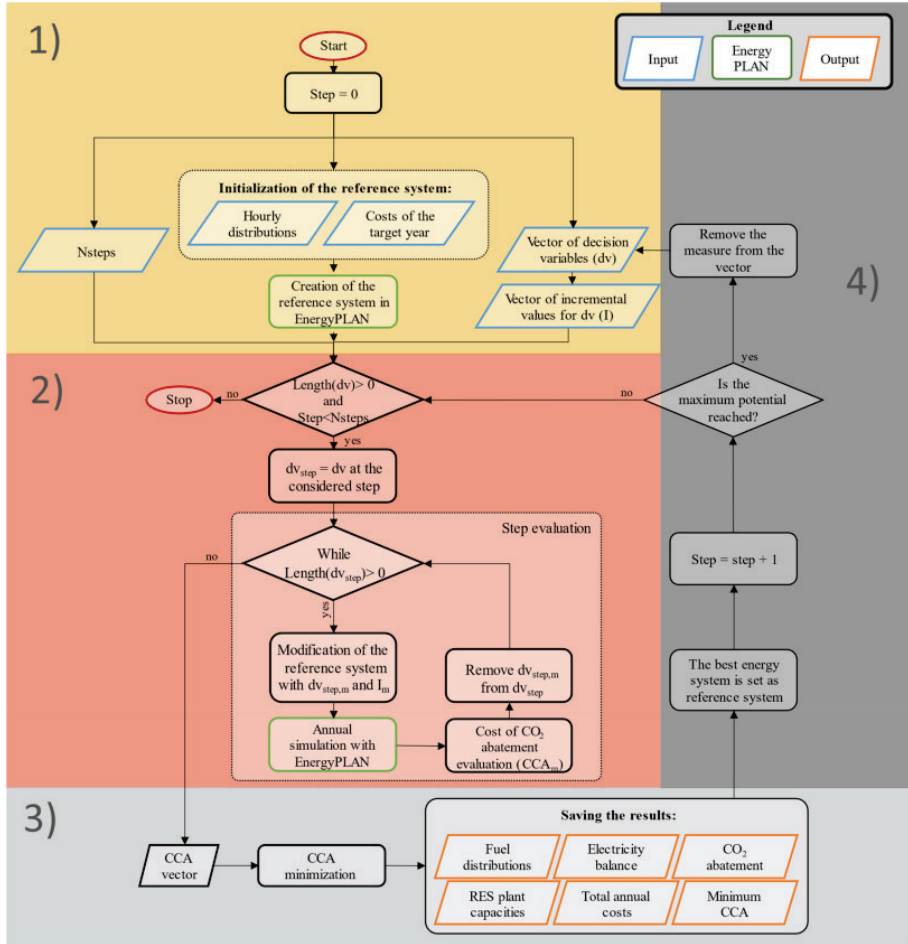


Figure 7. Flow chart explaining the optimization procedure considered by the algorithm in the EPLANoptMAC tool [82].

It is worth noting that although the algorithm can provide the optimal sequence of carbon abatement steps, this sequence will be limited by the choice of decision variables and the representation of the energy system within the modelling tool. Also, the algorithm will be sensitive to input assumptions, such as costs or the magnitude

of the incremental values used for each decision variable. Furthermore, the algorithm applies a metaheuristic approach, and as such, it only provides a good-enough approximation of the best possible optimal solution [86].

In addition to the above, other planning perspectives or optimality criteria might be desirable. This means that, for example, reductions of other emission types could be applied to the algorithm and yield contrasting results. Similarly, more cost-effective or energy-efficient system redesigns could be achieved that wouldn't necessarily follow this optimal sequence of carbon abatement steps. Therefore, this perspective needs to be complemented in order to effectively explore other desirable options in the solution space, as is done in Paper [5] by contrasting this approach with analytically-designed scenarios.

CHAPTER 4. PUBLICATION SUMMARY AND RESEARCH CONTRIBUTIONS

This chapter briefly synthesizes the main research contributions of each of the primary publications attributed to the PhD project. Each section in this chapter summarizes the main findings of the respective papers highlighting the aspects linked to problem statement presented in Section 1.2. The full texts and results for each of these studies are available in the Appendices.

4.1. PAPER I – TRENDS IN TOOLS AND APPROACHES FOR MODELLING THE ENERGY TRANSITION

Paper [1] presents a status of energy system modelling tool developments. In doing so, the study covers two main broad aspects. The first of these aspects branches out into a meta-analysis of previous literature review studies looking into modelling trends. At the time, 42 different articles presenting reviews of energy system models were identified. The second aspect presented in Paper [1] dives into the results of a survey questionnaire sent out to modelling tool developers, gathering responses for 54 tools.

The meta-review, presented in the first part of Paper [1], categorizes seven focus areas addressed by previous review papers of energy system models, identifying two understudied areas across most of these. This showed that past studies had limited focus on the policy relevance of energy system modelling tools and even less emphasis on the application of model linking. This first part of the paper also touches on the way in which previous reviews have conducted their analyses, showing that – mostly – review papers on energy system models do not establish a direct dialogue with model developers to uncover the features of said tools or their subsequent use.

The issues raised in the meta-analysis were then considered in the second part of Paper [1]. Here, a survey was used to establish a dialogue with energy system modelling tool developers and to establish a common vocabulary about model features to avoid misrepresenting the technical details of the models. Moreover, the survey allowed gathering inputs about the use of these energy system modelling tools in connection to policy support and their application in model linking or coupling with other tools.

Some key and novel contributions of this paper are the findings pertaining to these latter aspects. First, based on the responses from tool developers, it shows that energy system modelling tools used for policy support tend to have more detailed representations of the energy system (i.e., higher temporal, spatial, technical, and cross-sectoral resolution). Likewise, it shows that these tools are often soft-linked to

other tools to gain more insight. Although the specific details of which type of models are being linked with each other is not covered in the paper, the results map for the first time this application, which was found as a gap in the meta-review.

In addition to these findings, other contributions of the paper include mapping the features of energy system modelling tools. For example, the results explore the type of user interfaces and licensing present across modelling tools, and how these relate to their access and usability. Furthermore, the survey shows that a wide range of tools have the ability to model the energy system with high temporal resolutions, which is an advancement relative to how the modelling landscape looked a decade ago [22]. However, model development is still lagging in other areas, including higher sectoral resolution beyond the electricity sector and the representation of end-use of demands. These limitations further highlight the need for expanding modelling perspective.

4.2. PAPER II – PERSPECTIVES ON PURPOSE-DRIVEN COUPLING ENERGY SYSTEM MODELS

Paper [2] deals with a key gap uncovered in Paper [1]. Namely, it provides a deeper and cohesive view into cases where energy system models have been linked and presents a status and perspectives on the practice of model coupling. In the study, two high-level typologies are conceptualized around how model coupling with energy system models takes place.

On the one hand, Paper [2] illustrates that model coupling occurs when linking energy system models together with other ESMs of varying resolution or with algorithms that expand the coverage of a single model. Under this typology, model coupling can add value by bridging the limitations of one ESM with the capabilities provided by the other. This provides additional modelling resolution and can help explore new scenarios and feasible near-optimal design options for a given energy system compared to a single-model approach. The study finds that this exploration is occurring under specific modelling paradigms like linking simulation and optimization models or with single energy system optimization models, but models linked with simulation-based optimization approaches could benefit from including this in the future. The discussion presented in this part of the study expands the theoretical positions presented by Lund et al. in “*Simulation versus Optimization: Theoretical Position in Energy Systems Modelling*” [49], elaborating further on the role of coupling energy system modelling paradigms.

The second typology illustrated in this study deals with coupling energy system models to other disciplines and their respective model classes. Links to certain knowledge domains are found to be relatively well-established. For example, there are ample cases linking energy system models with end-use demand models, macro-economic models, life-cycle assessment tools, and geospatial analysis tools, among others. However, there are other dimensions that are not as often explored through

model linkages. Examples of these include links to material flow models, and models that capture the human and social dimensions. This aligns with past studies looking into the individual dimensions mentioned above [37,87–90].

The study also presents a theoretical viewpoint on the practice of model coupling, linking it to transition theory and a multi-level perspective framework. Under this theoretical framework, Paper [2] contributes to the discussion of model development by highlighting that increasing the complexity of model linking – while necessary to an extent for providing robust representations of real-world systems – can also contravene the urgency of having actionable insight that can influence the landscape of the energy transition promptly due to the need for coordination, data alignment, bridging paradigmatic and ontological gaps across models and disciplines, and challenging incumbent modelling approaches already informing the energy transition landscape. Therefore, a key contribution of the study is contextualizing and highlighting the need to design purpose-driven coupling approaches based on specific research questions rather than striving for a universal, comprehensive model.

4.3. PAPER III – HEAT ROADMAP CHILE: A NATIONAL DISTRICT HEATING PLAN FOR AIR POLLUTION DECONTAMINATION AND DECARBONISATION

Paper [3] is a collaboration with another PhD student and co-authors, where my contributions focused on developing an energy system model for Chile, and the corresponding data gathering, curation, and scenario analysis for the model. The study tries to answer questions around what are the potentials and impacts of including clean and efficient heating technologies in Chile’s energy system, at a national level. Furthermore, it is the first analysis of its kind applied to Chile and applies a modified version of methodologies from the Heat Roadmap Europe series of studies but in a global south context [91–94].

To capture viable choices of heating technologies and infrastructure in the scenarios, the study had to consider the expansion of district heating as a key enabling technology. For this, a geospatial analysis tool – used to model heat demands and generate estimates for infrastructure costs and thermal grid losses – was linked to the energy system model of Chile, developed with the EnergyPLAN tool. Here, the results from the geospatial analysis were aggregated on a national level so the data transfer could be coordinated as direct inputs to the ESM scenarios.

Although clearly linking models, the methodology presented in this paper also illustrates that coupling is not always explicitly mentioned in the methodological approach. Nonetheless, the approach still follows a very clear intended purpose: providing a missing perspective on heat demands and infrastructure estimates that is not attainable by only designing scenarios with a single model or within a specific discipline.

The study's main findings contribute to the discussion of Chile's energy transition by providing alternative national scenarios to those designed under Chile's long-term energy planning process. The results of the analyses show that a redesign of the energy system where district heating is included can provide reductions in the amount of air pollutants from heating while still using nationally available biomass resources and could facilitate further penetration of fluctuating renewables. Moreover, it shows that up to 40% of the space heating demand can be covered with district heating without additional total system costs compared to the reference scenario for 2050.

4.4. PAPER IV – AGGREGATED VERSUS DISAGGREGATED ENERGY SYSTEM MODELLING APPROACHES: THE CASE OF CHILE'S ENERGY SYSTEM

Paper [4] expands on the analysis from the previous study addressing the implications of modelling a national energy system – like Chile's – as a countrywide aggregated copperplate model, versus having a finer disaggregated geospatial representation (e.g., representing regions or other subnational aggregations as separate interconnected nodes). This is of particular relevance to understanding the extent of the impacts of the scenarios presented in Paper [1], given the geographical distribution of the country, its energy demands, and the available energy supply options.

For the disaggregated approach, EnergyPLAN was coupled with an optimal power flow algorithm and applied with the EPlanFlow tool. This disaggregated approach represents the energy system in 4 nodes, each for a macro-region in Chile modelled in EnergyPLAN. Then, linking EnergyPLAN with EPlanFlow resulted in scenarios with optimized volumes of electricity transmission.

Comparing the aggregated and disaggregated approaches shows the trade-offs of applying each. Coupling models to gain additional detail of the energy system transmission does provide an improvement in capturing more realism in the model. Although the disaggregated approach provides a marginal gain in detail, showing slightly higher energy consumption and total system cost than the aggregated approach, it comes at the price of additional analytical effort and data requirements. Meanwhile, the comparison showed that despite the added detail, both methods still had congruent results on a country level. Here, the benefits of the added complexity are somewhat eclipsed when answering questions about the expansion of thermal grids and new VRES capacity across related scenarios when high levels of flexibility are already present in the energy system.

A key contribution of the study, thus, is that it provides validation for the potential use of aggregated approaches when dealing with the assessment of scenarios on a national scale. Nonetheless, the disaggregated approach remains valid when

answering questions related to a finer geographical resolution, or in connection to addressing questions about bottlenecks in the transmission system.

4.5. PAPER V – SMART ENERGY APPROACHES AND CARBON ABATEMENT: SCENARIO DESIGNS FOR CHILE’S ENERGY TRANSITION

Paper [5] presents two scenario design methodologies applying the Smart Energy Systems approach to the case of Chile. The resulting country-level scenarios explore the potential for carbon abatement, reaching climate neutrality targets by 2050 and a transition towards a 100% renewable energy system across all sectors. These scenarios are the first to compare results with the most recent scenarios from Chile’s new long-term energy planning process and with their assessment of Nationally Determined Contributions (under the framework of the Paris Agreement), which show the carbon abatement measures and priorities in Chile’s nationally-designed carbon neutrality scenarios [95–97]. Moreover, the study showcases the first application of the Smart Energy Systems approach coupled with the generation of model-based optimized marginal abatement cost curves outside a European context.

The EnergyPLAN tool is applied first as a standalone model generator to design scenarios. Then, it is coupled with a hill-climbing algorithm under the EPLANOptMAC tool to generate step-wise scenarios minimizing the cost of carbon abatement at each step. A key contribution of this study is showing how coupling the two scenario design methodologies can complement one another.

The results of the analysis with a single-model approach show that a 100% renewable energy system is, in principle, possible in Chile and could present similar total system costs to the current national carbon neutrality scenarios. The coupled approach shows that following carbon abatement priorities only based on the optimal cost of carbon abatement measures can also lead to more cost-compelling alternative carbon neutrality scenarios than the current national scenarios. However, this approach on its own can hide other desirable energy system design alternatives that go beyond carbon neutrality, like a 100% renewable energy system. In contrast, the complementarity of the two approaches can illustrate the full potential of a system redesign and a view of which discrete carbon abatement measures could be prioritized at different stages of the transition, as well as showing which abatement measures and technologies require additional support to be implemented cost-effectively.

CHAPTER 5. DISCUSSION & CONCLUSIONS

This PhD thesis provides perspectives on the practice of linking energy system models to other models. The conclusions of this work can be divided into three main themes, related to the problem statement presented in Section 1.2.: Theoretical conclusions, discussing the dilemma between the principle of model reductionism and increased complexity in model development and in model coupling of ESMs; Methodological conclusions, presenting the gains and shortcomings of applying model coupling methodologies; and Analytical conclusions, which discuss comparatively the results of the analyses in the applied cases presented in Papers [3-5]. These conclusions are expanded in the following corresponding sections.

5.1. THEORETICAL

How does the dilemma of increasing model complexity through model coupling and models being simplified versions of reality align – from a theoretical perspective – with providing insight to manage the energy transition?

Aligning domains and models can be beneficial to get a broad range of answers about the energy transition. Managing this transition in the context of climate change also elicits a sense of urgency for drastic action. Meanwhile, the fundamental essence of a model is to provide a simplified representation of reality, or in this case, simplified view of real-world energy systems. Therefore, model coupling developments must happen at a pace that can provide meaningful and timely insight, and where insightful approaches can emerge from simple purpose-driven model coupling configurations with ESMs.

These can then be used to answer specific questions rather than striving for universally comprehensive model coupling designs, with longer development and alignment across domains and incumbent practices. In turn, this can help balance the challenge of complexity with providing comprehensibility of results and adequate scope.

In this context, links between ESMs and other modelling tools must be purposefully designed to provide appropriate alternative perspectives to foster the generation of new options and awareness of new solutions and radical technology change needed in energy systems. This can be achieved by illustrating the impacts of going beyond the idea of optimal solutions, highlighting both near-optimal yet radically different scenarios based on different planning objectives and applying different modelling paradigms.

5.2. METHODOLOGICAL

What are the gains and shortcomings of additional modelling complexity when applying model coupling methodologies to energy system analyses versus applying a single-model approach with an ESM?

As discussed in Chapter 3, different model coupling methodologies applying ESMs were explored in the scenario development for the analyses presented in Papers [3-5]. Three overarching methodological cases were explored: coupling to other disciplines and dimensions, coupling to expand the resolution of an ESM's original modelling scope, and coupling modelling paradigms.

From a methodological perspective, stepping out of the ESM silo was necessary to acquire inputs regarding aggregated demand data at a meaningful custom-fitted aggregation level. While this meant additional coordination to communicate assumptions and establish data exchange where essential, it also meant compartmentalizing the complexity of both approaches within their respective self-contained analysis and expertise. This provided a valuable purpose-driven coupling of models without a significant increase in model complexity for either type of analysis.

When expanding the resolution of the ESM via coupling, a major shortcoming was encountered in having increased complexity in the required input data, and in the post-processing steps while interpreting a larger set of results. Moreover, additional computational time was also compounded with the increased level of disaggregation (e.g., for each geographical node modelled) and the number of scenario analyses required. While the outcome of this approach provided more detail, the results of the national-level analysis did not present major differences compared to the more aggregated approach.

Finally, the issue of using methodologies that link modelling paradigms provided a similar outlook in terms of additional complexity in data requirements and computational time, as well as showing issues in terms of discontinuous scenarios due to the complex interactions in the energy system representation. The end results show that expert-based simulation can yield fairly similar results to an optimization approach independent of each other, and together can provide complementary perspectives at the cost of added complexity

5.3. ANALYTICAL

What are the impacts on analysis results when applying single-model and model coupling approaches with an ESM?

The specific outcomes of the analyses show the practical implications regarding the development of the energy transition in Chile, under different scenarios.

The analysis shows that by introducing VRES and key enabling infrastructure for sector coupling, multiple political targets set by Chile's government could be reached. For this, it is critical to link the perspective regarding energy demands to fully understand the potential of new technologies like district heating. Moreover, the analysis also shows that in a system with said enabling infrastructure, more flexibility will be achieved in the energy system, so capturing transmission effects will provide more detail but not necessarily drastically different insight in terms of long-term scenarios at the national level.

Finally, the analyses also present updated scenarios that align with a different planning goal: carbon neutrality in the national energy system. Here, the results show that a transition is possible and can take different paths, which different modelling paradigms can illustrate. The result of the analysis also shows that a 100% renewable energy system is possible in Chile, but cannot always be fully captured by all modelling approaches.

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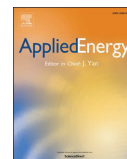
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APPENDICES

APPENDIX A. PAPER 1

Trends in tools and approaches for modelling the energy transition [1]



Trends in tools and approaches for modelling the energy transition

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HIGHLIGHTS

- Survey of current trends and challenges in energy system modelling tools (N = 54).
- Tool features, linkages, user accessibility and policy application were reviewed.
- Growing coverage of cross-sectoral synergies, open access, and improved temporal detail.
- Challenges in representing high resolution energy demand in all sectors.
- Key issues remain in understanding tool coupling, accessibility & perceived policy-relevance.

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ABSTRACT

Energy system models are crucial to plan energy transition pathways and understand their impacts. A vast range of energy system modelling tools is available, providing modelling practitioners, planners, and decision-makers with multiple alternatives to represent the energy system according to different technical and methodological considerations. To better understand this landscape, here we identify current trends in the field of energy system modelling. First, we survey previous review studies, identifying their distinct focus areas and review methodologies. Second, we gather information about 54 energy system modelling tools directly from model developers and users. Unlike previous questionnaire-based studies solely focusing on technical descriptions, we include application aspects of the modelling tools, such as perceived policy-relevance, user accessibility, and model linkages. We find that, to assess the possible applications and to build a common understanding of the capabilities of these modelling tools, it is necessary to engage in dialogue with developers and users. We identify three main trends of increasing modelling of cross-sectoral synergies, growing focus on open access, and improved temporal detail to deal with planning future scenarios with high levels of variable renewable energy sources. However, key challenges remain in terms of representing high resolution energy demand in all sectors, understanding how tools are coupled together, openness and accessibility, and the level of engagement between tool developers and policy/decision-makers.

1. Introduction

The transition towards a decarbonized and sustainable energy system is expected to play a crucial role in halting the effects of global warming while furthering human wellbeing, security, and sustainable development [1]. Energy system models - mathematical representations of energy systems - are often needed to quantify the impacts of this

transition, and plan potential pathways [2,3] due to increasing complexity. Numerous energy system modelling tools¹ are available, providing energy modelling practitioners and planners with a wide range of alternatives to represent energy systems according to different technical and methodological considerations, which can help inform policy- and decision-makers in their planning processes and policy recommendations [4,5]. These tools are in continuous development in

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¹ We refer to modelling tools as computational software, or modelling frameworks, that generate energy system models.

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response to the emerging challenges in the energy transition and new technological breakthroughs [3,5]. For this reason, multiple efforts have been made in the energy modelling community to review the ever-changing pool of tools available to energy modellers, to classify their features, outline their applications, and point at the issues that these aim to tackle [4,6–8].

In this paper, we survey how these reviews have been conducted and what issues they address. Moreover, we show current trends found in energy system modelling tools by gathering some of their key features and applications, including their apparent role in decision-making support. To do this effectively, we have gathered inputs from tool developers to better assess some of the key considerations and to gather information that is not necessarily readily available from written academic sources or tool documentation.

The work presented here is divided into four parts. Section 2 gives an overview of different reviews and surveys of energy system models and tools, outlining how these reviews were conducted, their respective focus areas, and existing gaps in the literature. The purpose of this review is to not only identify emerging trends, but to also identify how some of the lessons learned in past reviews are captured. In Section 3, we detail the analytical approach followed in our survey of energy system modelling tools. In Section 4 we present the results from this survey and identify the key features and trends in tool developments. In Section 5, we put into perspective some of the emerging challenges and discuss potential ways forward.

2. Literature review

This section presents an overview of different reviews and surveys of energy system models and tools found in the literature. These are then categorized according to their respective focus areas and their review approach, to show existing gaps in the literature.

2.1. Background

Energy system modelling tools are used for assisting energy policy making and assessing different energy pathways [9]. The range of available energy modelling tools is significant and continuously expanding. Several studies have investigated the developments of the above with a focus on different aspects of these models and reported different challenges faced in the field of energy systems analysis. For instance, Connolly et al. [4] present an overview of computational modelling tools capable of analyzing the integration of renewable energy sources (RES) in energy systems at large, looking into survey responses from 37 model developers.

In Foley et al. [10], a literature review of system models with a focus only on the electricity sector is presented. Similarly, Després et al. [11] conduct a review of modelling tools focusing on the integration of variable renewable energy (VRE) mainly in the power sector. Mahmud and Town [12] reviewed modelling tools with a focus on the integration of electric vehicles in the energy system. More recently, in a study by Ringkjøb et al. [6], a thorough review of 75 energy and electricity system modelling tools is presented, assessing modelling scopes, characteristics and limitations, and validating most inputs with tool developers.

In addition to these broader overviews of energy system modelling tools, a relevant body of work exists about the underlying implications that models have on a broader energy planning level. In this regard, a key aspect to consider is the classification of the energy system model, and the choice of specific types of modelling frameworks according to the purpose of a given planning exercise.

Different classifications of energy system modelling tools have been discussed by a number of studies, which reflect upon the characteristics and challenges of bottom-up applications [8], the suitability of tools for decision support in local planning [13], as well as their applicability worldwide [14], their general effectiveness for energy planning

purposes [15], their level of technical complexity [16], and the classification of modelling approaches with direct feedback from modelling tool developers [17].

Another critical consideration examined in the literature is the applicability of models in specific context-areas. This has been the case, for instance, in reviewing and narrowing down the applicability of various energy system modelling tools and their limitations for analyzing the energy transition in a European context [18], in a regional Nordic perspective [19], on a country-specific level [20,21], in developing world countries [22,23], in energy systems of urban scale [24–29], and standalone and grid-connected hybrid energy systems [30,31].

Over the past years, a number of studies have shifted the spotlight from a pure overview of modelling tools towards the study of emerging issues for energy system modellers and planners, as developers and users of such tools, under the context of climate change and the transition towards sustainable energy systems. For example, Pfenninger et al. [5] outline different modelling paradigms and emerging methodological challenges faced in the energy system modelling arena, highlighting the way current modelling methods could be revised by benefiting from cross-discipline and cross-sectoral synergies.

Similarly, Lund et al. [32] put into perspective the theoretical positioning with regards to selecting a modelling approach and how these should be considered when addressing and debating different future energy system scenarios based on sector integration.

Correspondingly, the complementarity of these modelling paradigms and approaches, and the potential to integrate models with different features for answering emerging research questions has also been a matter of recent study [33–35], as the focus towards more cross-sectoral integration [12,36–38] and socio-technical considerations becomes more apparent [39–43].

Meanwhile, Savvidis et al. [7] review and discuss the gaps between energy policy questions and modelling capabilities found in a selected sample of modelling tools. In addition to these, the openness of energy data and models have been discussed in a number of studies [44–48] and by expert groups. These include the *Open Energy Modelling Initiative* [45,49], which collects information on a growing number of open-source energy system models and frameworks in addition to open energy data; and combined efforts in the modelling community like the Energy Modelling Platform for Europe and other energy system modelling related projects [50–55].

However, some key gaps remain present. As pointed out by Hall and Buckley [20], the lack of clarity found in the literature about models' characteristics can hinder side-to-side comparisons. Moreover, the target audience and the main area of application of these modelling tools are not always explicit in the literature, often leaving these aspects open to interpretation [25]. Furthermore, potential misinterpretations or misrepresentations while reviewing modelling tools can arise if no form of dialogue with developers take place. Taking as an example the EnergyPLAN tool as portrayed in recent literature review studies, the tool is described as having an optimization methodology [56], geographical coverage [8] and being developed in a programming language [21] which do not necessarily correspond to the tool as described by its developers [57]. Thus, having open lines of dialogue, such as surveys and personal communication, can be a valuable approach when reviewing and validating the technical characteristics of modelling tools, as has been shown in past studies [4,6,16,17].

Nonetheless, this more direct review approach has had limited use when probing aspects such as the policy relevance of the tools, the ability to couple multiple modelling tools to answer complex research questions, or the level of accessibility of the tools with a perspective on not only the licensing but also on the user interaction. This becomes especially crucial as the value of modelling tools and scenarios for decision support is not always fully appreciated by energy planning practitioners and decision-makers [58], despite the intent of models and tools to be relevant for decision-support [59].

2.2. Classification of energy system modelling reviews

As described in the previous section, the current landscape of reviews assessing energy system modelling tools is quite vast. To better understand how these studies have been conducted and their focus areas, we have put forth a classification scheme of these reviews. This classification scheme also has the purpose of outlining new potential focus areas to survey modelling tools, and potential areas of actionable research. At the same time, it provides a useful view into past research that has listed some existing modelling tools, including their attributes and applications.

For this, we have used a modified and expanded categorization scheme compared to that initially proposed by Savvidis et al. [7], where the reviews were catalogued into four groups based on their underlying purpose.

In the present study, we reformulate the four original categories with additional details and propose three new additional categories based on recurring themes found in previous literature but not explicitly mentioned in the previous categorization effort. Namely, these new categories cover reviews that examine real-life policy application of the tools, model linking, and the transparency, accessibility and usability of the tools. In addition to this, we contextualize these studies in terms of their review approach, as well as their area of application and delimiting scope. This allows identifying existing trends and new potential study areas while putting in perspective how modelling lessons are gathered, and how future review exercises can potentially be conducted.

In this paper, the categories considered are divided as follows, considering their corresponding purpose(s):

- Category 1 [Descriptive overview]: Provide descriptive overviews of the technical features of modelling tools, such as their methodological approach, mathematical formulation, and resolution (spatial, temporal, techno-economic, sectoral).
- Category 2 [Classification]: Provide a new classification scheme, and/or focus on grouping modelling tools to provide an overview of existing modelling typologies (based on their technical attributes or modelling approaches).
- Category 3 [Practical application]: Identify the use of energy system modelling tools based on previous applied studies, and to identify areas of suitability for addressing current and future issues based on the tools' modelling capabilities.
- Category 4 [Inter-comparison & suitability]: Compare modelling features side-by-side in order to identify the suitability for a particular application.
- Category 5 [Transparency, accessibility & usability]: Identify transparency and licensing/accessibility of the modelling tool, outlining issues such as result reproducibility, validation and testing, and open source code, and the user interaction with the tool.
- Category 6 [Policy relevance]: Identify policy-relevance of modelling tools based on real-world applications and policy-making case studies².
- Category 7 [Model linking]: Identify combined capabilities of modelling approaches through the linking of modelling frameworks.

It is apparent that these categories are not mutually exclusive. In fact, most reviews fell into more than one single category. It is also important to note that there is a degree of overlap between the categories, where some elements of one category could be sub-categorized within another

due to some of the studies having more general purposes. However, a degree of differentiation is needed to zero in on the key issues and insights contributed by the reviewed literature. For instance, when considering reviews of the modelling tools' practical application (category 3), an overlap with potentially reviewing their suitability to access policy applications. However, the latter warrants deeper analysis to determine actionable research and real-life application of the reviewed tools, as conveyed by Category 6.

In addition to these categories, we have categorized the reviews by their focus area and delimiting scope, by outlining whether the reviews focused on – for example – urban scale modelling tools, power sector models, bottom-up tools, socio-technical energy transition (STET) models, etc. Similarly, the review approach was also outlined. Here, we noted three distinct approaches: literature reviews, reviews with developer/user inputs (from survey questionnaires, presentations, or review validation with tool developers), and web searches. Concretely for the last approach, the review paper by Markovic et al. [24], presented results without further procedural description and solely referencing websites.

A summary of the categorization, focus and approach of the reviews is seen in Table 1.

As observed in Table 1, several purposes can be identified in previous review studies of energy system models and tools. This survey shows that a clear majority of the studies provide some type of descriptive overview (Category 1) of the features found in models and tools, while also providing classification schemes (Category 2) or prescriptive narrowed-down lists of tools suitable to address a specific issue or scope of analyses. In general, these reviews are useful at mapping the technical aspects and considerations for modellers to select a tool and to pinpoint issues within specific modelling approaches. This is especially the case when these tools are assessed in tandem with applied case studies, where their application provides further insight into how the tools are able to tackle questions about the energy system and different energy policy scenarios.

Although dialogue with tools developers is often suggested by a number of reviews to improve clarity on modelling purpose and scope, assumptions and categorizations; the reviews are not always conducted in such ways. Instead, as seen in Table 1, most of these studies rely on reviewing the existing literature to formulate their interpretation of modelling features or to assess the applicability of models or their policy-relevance.

In more recent years, the issues of transparency and model accessibility have come into focus, being key issues covered by a growing number of studies. This often refers to having open access to a model or to a modelling framework's underlying mathematical formulation - i.e. making the underlying software code in some tools being open source. However, the broader accessibility of the tools in terms of the readiness with which end-users can use tools to construct an energy system model and generate energy system scenarios is not commonly evaluated in previous studies.

Moreover, from this survey we have seen that the policy relevance of the modelling tools is often evaluated in terms of the tool's capabilities to assess the impacts of current policy and potential future developments in academic studies. Given the technical features found in the current landscape of modelling tools, evaluating techno-economic aspects of policy implementations could be routinely performed. However, the focus has been more limited in terms of reviewing the tools used for official policy-making – including both whether the tools have been used directly or as a reference to support official policy choices and their subsequent impact on official planning and decision-making processes. Finding out about these types of applications requires going beyond the tools' technical documentation, and sometimes even beyond written academic outlets. While, this information might be available in official documents, it becomes increasingly complicated to compile when considering the multitude of national, regional and local official plans (often only published in their local language) documenting the use of

² While the technical features of some energy modelling tools enable the analysis of policy relevant questions, the actual use of these to support official policy is more limited. Here, we refer to reviews that follow up on whether the modelling tools have been used to support official (government) policy, rather than their ability to technically evaluate policy and generate insights solely on an academic level.

Table 1

Overview of the 42 review articles surveyed with their corresponding classification and review method, sorted by year of publication.

Source	Category							Focus topic	Spatial/Technical/Access delimitation	Review method	Year published
	1	2	3	4	5	6	7				
Van Beeck [13]	X	X		X				Classification of tools for local energy planning	Local	Literature review	1999
Jebbaraj and Iniyar [14]	X		X					Review of energy models' applications	Global	Literature review	2006
Connolly et al. [4]	X			X				Suitability of tools for modelling integration of renewables	Local/National/Regional	Survey questionnaire	2010
Bhattacharyya and Timilsina [22]	X			X				Comparison of suitable tools for developing countries	Developing countries	Literature review	2010
Mundaca et al. [60]	X		X		X			Review of tools for evaluating energy efficiency policies	Bottom/up energy economic models	Literature review	2010
Foley et al. [10]	X		X					Overview of tools for electricity system modelling	Electricity sector models	Literature review	2010
Unger et al. [19]	X	X	X				X	Coordinated use of modelling tools	National/Regional	User inputs, Literature review	2010
Mendes et al. [61]	X		X	X				Review of integrated community energy system tools	Local (district/ community)	Literature review	2011
Markovic et al. [24]	X			X				Tools suitable for modelling urban energy systems	Local (urban/district)	Web searches	2011
Manfren et al. [62]	X	X		X				Tools for distributed generation projects	Local (urban/district)	Literature review	2011
Keirstead et al. [25]		X	X					Review of urban energy system models approaches	Local (urban/district)	Literature review	2012
DeCarolis et al. [63]	X		X		X			Modelling results transparency and reproducibility	Energy economic optimization	Literature review	2012
Mirakyan and De Guio [64]	X		X	X				Tools & methods for integrated energy planning in cities	Local (urban/district)	Literature review	2013
Pfenninger et al. [5]	X	X	X				X	Modelling categories and outline emerging challenges	National	Literature review	2014
Allegrini et al. [26]	X		X	X				Modelling approaches and tools for district-scale systems	Local (urban/district)	Literature review	2015
Huang et al. [65]	X	X	X	X				Modelling approaches and tools for community systems	Local (urban/district)	Literature review	2015
Van Beurkom et al. [27]	X		X	X				Suitable optimization tools for urban development	Local (urban/district)	Literature review	2015
Li et al. [39]	X		X					Review of socio-technical energy transition models	STET models	Literature review	2015
Despres et al. [11]	X	X	X					Energy modelling tool typologies for renewable integration	Power sector	Literature review	2015
Hall and Buckley [20]	X	X	X					Systematic review of energy models and classification	National (UK)	Literature review	2016
Olsthoorn et al. [36]	X	X						District heating systems and integrated storage	Local (urban/district)	Literature review	2016
Mahmud and Town [12]	X		X					EV modelling	EV modelling included	Literature review	2016
Lund et al. [66]		X	X			X		Modelling approaches and planning support	Simulation/optimization	Literature review	2017
Ringkjøb et al. [6]	X	X	X	X	X			Renewable energy integration	Active models (2012<)	Lit. review, developer inputs	2018
Lopion et al. [21]			X					Historical trends in energy system models' development	National	Literature review	2018
Müller et al. [17]		X				X		Discussion of approaches and categories of energy	EU developed models	Developers' presentations	2018
Crespo del Granado et al. [33]		X	X					Review of nexus between energy and economic models	Economic/bottom up models	Literature review	2018
Lyden et al. [67]	X		X	X				Community-scale energy systems with storage & DMS	Local (district/ community)	Literature review	2018
Morrison [46]						X		Modelling transparency, reproducibility and openness	Open modelling projects	Literature review	2019
Oberle and Elsland [47]	X	X	X		X			Suitability and application of open access models	Open access models	Literature review	2019
Ferrari et al. [28]	X		X	X				Suitability of tools for urban energy planning	Local (urban/district)	Literature review	2019
Scheller and Bruckner [29]	X	X		X				Optimization models & approaches for municipal systems	Local (urban/district), ESOMs	Literature review	2019
Savvidis et al. [7]				X		X		Suitability of models to answer policy questions	Active, policy relevant models	Literature & expert review	2019
Groissböck [48]	X		X	X	X			Review of tools for power system modelling	Open access tools	Literature review	2019
Abbasabadi and Ashsayeri [68]	X	X	X					Outlook of modelling approaches in urban energy systems	Local (urban/district)	Literature review	2020
Hirt et al. [34]	X		X				X	Applied cases of linking energy system and STET models	STET models	Literature review	2020
Prina et al. [8]	X	X		X				Classification of bottom-up energy models	Bottom-up models	Literature review	2020
Ridha et al. [16]		X		X				Profiles and categorization based on modelling complexity	Available data in MODEX database	Survey questionnaire	2020

(continued on next page)

Table 1 (continued)

Source	Category							Focus topic	Spatial/Technical/Access delimitation	Review method	Year published
	1	2	3	4	5	6	7				
Weinand et al. [31]			X	X				Suitability of modelling autonomous systems	Local (district/community)	Literature review	2020
Musonye et al. [23]	X		X	X				Suitability of modelling in Sub-Saharan African context	National/Regional (Sub-Saharan Africa)	Literature review	2020
Fattahi et al. [35]	X	X	X				X	Linking of modelling approaches	National	Literature review	2020
Klemm and Vennemann [56]	X		X	X				Suitability of tools for modelling district energy system	Local (urban/district)	Literature review	2021

energy system modelling tools.

Finally, another recurring area suggested in the surveyed review articles is the application of interdisciplinary approaches, and model coordination and integration. However, few reviews try to map how tools have been coupled together beyond a specific set of modelling traditions [34]. This opens questions as to how model coupling is done, with which tools, and to what extent coupling approaches are used to answer specific energy planning questions.

2.3. Observed trends and findings in past energy system modelling reviews

Looking beyond the scope and methodologies of past reviews listed in Table 1, several trends and findings emerge from the literature over the past 10 years. In Connolly et al. [4], the typical application of different modelling tools is provided. While this study has a comparative nature, it outlines that – at the time – only seven energy system modelling tools were identified capable of modelling 100% renewable energy systems, four considering hourly time-steps and different sector coverage, and three with coarser (annual) temporal resolutions but with multi-year perspectives.

From there, several suitability studies have looked further into the technical descriptions of different energy modelling tools, having as main outcome shortlists of applicable tools that could address specific research cases. This has been predominantly the case of reviews looking into the suitability of energy system modelling tools to represent local scale energy systems (ie. Urban, district, community scale), though similar cases apply for other geographical scales. As early examples, Mendes et al. [61] identify a handful of tools highlighting the importance of hourly modelling and spatial scale flexibility to conduct their assessment; while Allegrini et al. [26] call for adequate representation of district heating, renewable energy and adequate integration of the urban microclimate and resulting effects on building demands when conducting energy system analyses. By contrast, studies conducted over the past 5 years incorporate into their model-finding exercises far more comprehensive criteria about high modelling details such as multiple sector representation, high spatial and temporal resolutions, uncertainty analysis, storage and demand side management representation [29,36,67]; but also user-friendliness [28] and openness of these tools [56]. Meanwhile, other studies point at a lack of representation of additional dimensions, like increased social aspects in energy system modelling tools [31].

Similar to Connolly et al. a decade ago, Foley et al. [10] also raised the issue of modelling renewable energy, finding that electricity system models were ill suited to properly consider energy storages, flexibility services and variable renewable energy sources. More recently, Ringkjøb et al. [6] found that several studies address the effects of integrating variable renewable energy sources to varying degrees, with models capable of representing grid expansion, storages and demand-side management technologies. However, representing the variability of these sources in long-term energy models was found as a challenge due to the coarser time-step of these modelling tools. Likewise, the integration of energy sectors was also found as an outstanding challenge to be addressed in model development. Prina et al. [8] also makes this point, after identifying the current status of bottom-up models in their spatial,

temporal, techno-economic and sectoral resolutions. In their study, bottom-up modelling tools are found incapable of addressing these four dimensions fully.

Similarly, in Lopian et al. [21], key trends are also examined around the development of energy system models over the last decades. In this review, they found new developments around increasing spatial and temporal flexibility of energy system models and state the need to have modelling efforts align to answering energy policy questions. This is also touched upon by Savvidis et al. [7], when reviewing gaps between modelling capabilities and technology-specific policies. From this study, the representation of the distribution grids, endogenous demands, the systems technical flexibility and policy constraints were found as areas of improvement for energy system models.

Other key areas found among recent reviews, include the prospect of expanding modelling dimensions to increase realism in addressing energy and climate challenges, and increasing modelling transparency. In the case of the former, linking energy system modelling tools with socio-technical energy transition approaches [34] or macro-economic models [33] has been found as a potential avenue for inter-disciplinarity and better representation of the energy system. Fattahi et al. [35], also highlights this potential, after noting the shortcoming of energy system modelling tools in generating insight about micro- and macro-economic aspects of the energy transition.

On the issue of transparency, much has been said in recent years. For instance, Morrison [46] and Pfenninger et al. [45] find that energy system models are lagging behind in adopting best practices for transparency, such as those found in the open modelling community, pointing out the need to enhance transparency of modelling analysis and reproducibility. Following from this, Oberle and Elstrand [47] look into the current landscape of open access tools to outline their features, finding them technically suitable to address research questions regarding a variety of energy scenarios.

3. Methods

In this paper, we opted to review the features and applicability of energy system modelling tools by gathering inputs directly from tool development teams and key users. As seen in the literature review, some aspects of the tools and their applications can be overlooked, are rather difficult to come by from only analyzing publications or are altogether misinterpreted due to a lack of a common language found in the existing literature describing modelling tools. This becomes increasingly relevant when considering the application of some modelling tools outside the realms of academia, where modelling outputs can translate into local or national policy discussion in white or green papers (sometimes in their original language), while being less accessible to external inspection or by reviewing traditional sources and model documentation.

By establishing some line of dialogue, in this case through a survey questionnaire, we try to bridge this methodological gap and establish a common language to describe the tools and their applications from the developers and users own perspectives.

In this process, 137 different modelling tools were identified from the existing literature and survey studies referenced in the previous section. The conceptualization of the questionnaire took the work

presented in Connolly et al. [4] as a starting point of inspiration, with several reconsiderations and new aspects added to the questionnaire presented in that study corresponding to new developments and considerations in the practice of energy system modelling and tool development.

A web-based questionnaire was designed on the SurveyXact platform, which then was sent to the developers of each tool identified.

From this survey, 54 complete responses were gathered, plus an additional six partially completed entries. Although, additional tools and model descriptions can be found in the literature, these are not considered in the following result interpretation in order to preserve the consistency of the analysis. It must be noted that the overall survey results, while not necessarily providing a comprehensive sample of all existing tools, are still indicative of general trends found in the energy system modelling field. The tools covered in the analysis ranged from commercially available software, to in-house proprietary developments, and open access, widely used modelling tools. In addition, a deliberate choice was made to only include one modelling tool in cases where multiple branch-out versions exist; for example, in the case of MARKAL-TIMES [69], and its family of models [70–74], or similarly in the case of OSeMOSYS [75] and GENESYS-MOD [76]. The list of tools surveyed is presented in Table 2.

The survey questionnaire covered questions regarding the tools' access and licensing, user interface, methodological approach, mathematical formulation, spatio-temporal resolutions, sectoral representation, technical attributes and technology detail, and area of past application, including use for official policy-support. In addition to this, data regarding typical application of tools and descriptions from the respondents was also gathered.

An overview of the questionnaire is provided in Appendix A, while a summary of the inputs for the 54 modelling tools is provided in Appendix B as a supplementary data repository.

4. Features and trends in energy modelling tools

In this section, the results from the tool survey are presented with a focus on approach, scope, coverage, access, policy relevance and model coupling.

4.1. Approaches and formulation of the objective

As identified in the literature, several schemes exist to classify modelling tools according to their methodological approach and mathematical formulation [13,17,20,129]. In this study we examined the modelling tools under three broad categories according to their analytical approach: Simulation, Optimization and Equilibrium models. In the case of the latter, further subcategorizations were defined by model developers about their modelling tools, namely to clarify if these are computable general equilibrium (CGE) or partial equilibrium. In addition to the above, some simulation tools made further specifications to describe the novelty of their underlying methodology; for instance, by elaborating on their operation and iterative simulation approach [107].

In terms of the mathematical formulation, several objectives were identified across the sampled energy system modelling tools. More recurring across optimization modelling tools was the characterization of one or more purpose-fit objective functions, including the minimization or maximization of indicators such as total system costs, investment costs, dispatch costs, fuel consumption, system emissions, renewable energy penetration, and social welfare. In the case of simulation tools, the main approaches identified behind their mathematical formulation included scenario development, what-if analysis, multi-criteria analysis and agent-based analysis.

Irrespective of modelling approach and formulation, the definition of multiple objectives or purposes for a given single tool was readily apparent from the gathered data, as is the fact that a significant portion of the models can serve multiple purposes with their underlying

Table 2

List of the 54 modelling tools surveyed where full responses were gathered.

Modelling tools surveyed (completed questionnaire responses)
Balmorel [77]
Calliope [78]
COMPOSE [79]
DER-CAM [80]
DIETER [81]
Dispa-SET [82]
E2M2 - European Electricity Market Model [83]
EMLab-Generation [84]
EMMA [85]
EMPIRE[86]
Enerallt [87]
Energy Transition Model [88]
EnergyPLAN [57]
energyPRO [89]
energyRt [90]
EnergyScope [91]
Enertile [92]
ENTIGRIS [93]
ESO-XEL [94]
EUCAD [95]
EUPowerDispatch [96]
Global Energy System Model (GENESYS-MOD) [76]
GridCal [97]
Homer Grid [98]
iHOGA [99]
IMAGE [100]
IMAKUS [101]
Integrated Whole-Energy System (IWES) model [102]
INVERT/EE-Lab [103]
LIBEMOD [104]
LIMES-EU [105]
LOADMATCH [106,107]
LUSYM [108]
Maon [109]
MESSAGEix [110]
National Energy Modeling system (NEMS) [111]
OpenDSS [112]
OptEnGrid [113]
POLES-JRC [114]
POTEnCIA [115]
PRIMES [116]
PSR – SDDP [117]
Pymedeas [118]
PyPSA[119]
RamsesR [120]
Regional Energy Deployment System (ReEDS) [121]
REMIND [122]
Sifre [123]
System Advisor Model [124]
TIMES [69]
TransiEnt Library [125]
UniSyDs.0 [126]
WEGDYN [127]
WITCH [128]

formulation. Overall, we observed that most modelling tools can use multiple assessment criteria in their studies depending on the specific case and the underlying context, resulting in a wide range of choices as highlighted in [31,130].

4.2. Modelling scope: temporal, spatial, and technical resolution

4.2.1. Temporal resolution

The integration of high levels of variable renewable energy sources (VRES) poses a challenge for energy planning, which calls for models capable of representing the corresponding variability. Similarly, the level of detail used for modelling the energy system can also result in more accurate system representations capable of capturing synergies and resource availability that are spatially dispersed by nature.

The choice of temporal resolution used in energy system studies can

have a significant impact on capturing the actual dynamics of a modelled system and adequately balancing supply and demand. This is illustrated, for example, by Poncelet et al. [131] when assessing the impact of temporal resolution in systems with high uptake of renewables, concluding that low temporal resolution can potentially underestimate operational costs and overestimate generation capacity.

Similarly, Deane et al. [132] determined that higher temporal resolutions are better able to capture system loads, the inflexibility of large thermal power units, and renewable energy generation; thereby assessing more accurately the corresponding system costs. Nonetheless, increasing the time resolution can be computationally expensive. Thus, temporal resolution should be selected with caution, especially when considering resolutions coarser than 1-hour to represent renewable generation fluctuations [133].

In the modelling tools sampled for this study, the 1-hour modelling time-step was the most frequently observed, as seen in Fig. 1. Other time-steps observed, although to a lesser extent, were the yearly and multi-year resolutions, as well as seasonal time-slices. In the “Other” category, the modelling tools were reported capable of adjusting their modelling time-step to even higher levels like minutes, seconds, or having user-defined steps, as well as having lower resolutions e.g. daily, using representative hours and hour-blocks and weekly resolutions. In addition, some tools had higher (hourly) resolutions in certain aspects of their system representation while using coarser (annual) resolutions for others.

Interestingly, modelling tool developers also highlighted that the capabilities of their models not always correspond to their typical application. For example, some tools although technically capable of operating with an hourly resolution, are typically used with other modelling time-steps, such as using a time-slice representation [69] or with a reduced yearly time-series produced from aggregation algorithms [76]. For some tools, this can be explained by the fact that high modelling resolutions and temporal detail can translate to higher computational effort and calculation times [5]. However, the choice of lower time resolutions can also driven by a lack of empirical high resolution data for future time horizons, or from the use coarser temporal detail of the energy demands represented in energy system modelling tools [134].

An additional temporal aspect considered is the time horizon of the modelled outputs, as seen in Fig. 1. This shows that a large majority of the modelling tools can provide more than just a single snapshot of the energy system, but rather have the capability to outline multiple stages of the energy transition by providing multi-year outlooks, with some being capable of having more than one fixed time horizon. This modelling capability is reflective of the intent to outline the pathways of policy scenarios and sequential decision-making [135], as seen – for example – for capacity expansion at a country level [136], to formulate energy policy at the EU level [137–139], or to assess regional and global decarbonization pathways [140].

On the other hand, a smaller yet significant share of the modelling tools surveyed can also use a 1-year modelling time horizon or even shorter-term horizons. This comes with the potential advantage of lower computational effort and less uncertainty due to the number of assumptions and data inputs going into the modelling. While less detailed in outlining potential energy transition pathways, the application of a 1-year time horizon can still outline end- and mid-point snapshots of technical developments or policy scenarios at selected years. This can provide high levels of detail of an energy system redesign to strive for, as illustrated in studies about urban energy transitions [141,142], national energy system redesigns [143–146], and regional studies [147–149]; in turn, acting as potential points for policy backcasting [150–153].

Putting these results into perspective, we can see that over the past decade advances have been made in how time is represented in modelling tools. Taking the study by Connolly et al. (2010) as an example, we can see that now a larger share of energy system modelling tools are capable of using hourly time-steps, compared to roughly half

capable of such identified at the time for the 37 tools surveyed in that study [4]. In terms of the modelling time horizon, the results found in this survey are to an extent similar to those presented by Connolly et al. [4], which shows that most models surveyed then were already capable of handling multi-year time horizons, as well as yearly, and to a lesser extent coarser resolutions.

Similarly, Pfenninger et al. [5] raises the issue of higher temporal detail as a pending challenge in energy system modelling development. As seen today, increased development has been given to capture high temporal detail in the modelling tools surveyed.

4.2.2. Spatial and technical resolution

Across the surveyed modelling tools, a levelled distribution was observed between tools working with aggregate technical specifications and those capable of representing individual plants or energy system components. Out of the 54 tools surveyed, 31 reported using individual plant details, while 23 reported using aggregate technical details. This reflects – in part – the nature of the tools sampled since some of them are capable of modelling large spatial aggregations on the global and regional scale (and in some cases even at the urban level), where aggregate operational detail provides adequate representation of the energy system [154,155], having an overall less significant impact than the temporal resolution [131].

On the other hand, some of the tools working with finer operational detail are tuned based on the purpose and scope; for instance, to flexibly represent project-specific components [156,157] or set up to represent specific dispatchable units or plants [158,159].

Interestingly, the survey pointed that even if some of these tools are capable of representing individual plants and conversion units, the standard modelling representation for larger spatial scopes – like on a national scale – would still rely on aggregated values. This raises an interesting point when considering the features and intended flexibility of use, with the standard practical use of the tools.

4.3. Cross-sector coverage

As the global focus shifts towards higher penetration of renewable energy sources to decarbonize the energy system and to halt global warming, more effort has been put towards coupling the main energy sectors to benefit from their potential synergies. A vast range of reviews identify the challenges of integrating more renewable energy, mainly considering electricity sector [5,10,11]. However, as identified by Lund et al. [37], cross-sector integration can also be a pivotal aspect to incorporate larger shares of renewables, by facilitating additional flexibility in the energy system. This has been the subject of a number of studies (e.g. [149,159–162]), which have analyzed the potential of integrating the electricity, heat, transport and industrial sectors, and thereby allowing 100% renewable energy shares in future energy system scenarios.

The potential for sector coupling was investigated in the survey of modelling tools by looking into their sectoral coverage. This is shown in Fig. 2 and Table 3, and outlined in further detail in Appendix B.

As seen in Fig. 2 and Table 3, the inclusion of the electricity sector is shared across almost all the tools examined. For roughly half of these tools, it is furthermore possible to explicitly model both the transport sector and heating (including individual and district heating). However, it must be noted that when considering tools representing only the electricity vector, non-explicit approaches to represent scenarios where heating and transport are electrified can arise and, thus be partially covered. Additional sector coverage is seen to a varying degree when looking at industry or cooling applications, and it is much less prominent considering biofuel production, being modelled by only one-third of the tools examined.

The common theme of the electricity sector is key to sectoral integration, since thermal, transport, and industry sectors are considered in the context of electrification in a smart energy system [163]. Indeed, it is



Fig. 1. Modelling time-step by time horizon of the 54 surveyed tools. Note that the sum exceeds 54 as some tools can operate with different user-defined time resolutions.

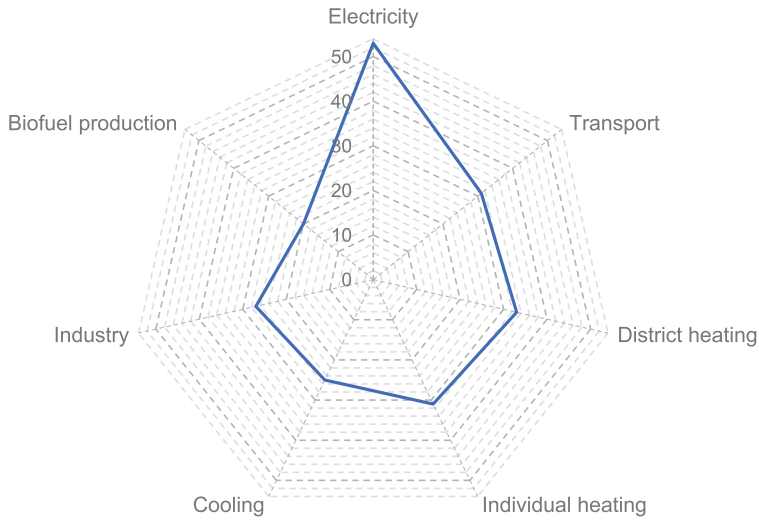


Fig. 2. Sector & end-use coverage in the 54 surveyed modelling tools.

expected that when incorporating these demands, the total electricity demand will markedly increase [160]. More importantly, however, these sectors can act as sources of demand response, having promising prospects to provide flexibility and improve the efficiency of the energy system [164]. This has been shown in prior studies when analyzing the potentials to shift industrial [165], thermal [166], and electric transport loads [167]. This flexibility can also be reaped within the electricity sector, by considering flexible demands responsive to the costs of generation dispatch, which could cover second priority loads. This can be done by covering these lower-priority demands in off-peak hours, or in

the presence of excess electricity from fluctuating renewable sources when generation costs are lower [164,168,169]. In our survey, about 23 of the 54 models were capable of representing elastic demands responsive to supply costs (Fig. 3).

4.4. Demand representation

Common across all energy system models is the need to balance energy supply and demand. As seen in Fig. 3, energy demand is rarely a modelling outcome, but rather an exogenous input assumption, either as

Table 3
Sector coverage overlap by number of tools in the 54 surveyed modelling tools.

No. of sectors/ end-uses covered	Number of modelling tools	Sectors/end-uses excluded by number of tools
7	15	n/a (ie. all sectors covered)
6	5	biofuel production (3 tools), industry (1), cooling (1)
5	4	biofuel production (4), cooling (1), industry (1), district heating (1), transport (1)
4	7	cooling (5), biofuel production (4), individual heating (4), industry (4), transport (3), district heating (1)
3	3	biofuel production (3), cooling (3), industry (2), district heating (2), individual heating (1), transport (1)
2	8	biofuel production (8), cooling (7), industry (7), individual heating (6), transport (6), district heating (5), electricity (1) ^a
1	12	All but electricity generation (12)

^a Partially covers electricity as contributions for heating purposes.

a static demand or with some elasticity. This requires that modellers represent energy demand for the variety of aforementioned sectors at the relevant temporal and spatial resolution of their modelling tool.

Focusing in on specific studies undertaken by some of the surveyed modelling tools, we see that the same data sources are often used, or that the hurdles to data acquisition are dealt with in similar ways.

In the European context, hourly electricity demands are readily available from the European Network of Transmission System Operators for Electricity (ENTSO-E) [170]. ENTSO-E data is used in several national scope studies [81,147,171–174], although others source data directly from relevant national bodies [133,166,175–177] or as a synthesis of ENTSO-E and national statistics, via the Open Power System database [178]. When data is unavailable for countries, or subnational regions are being modelled, scaling factors are applied based on aggregated demand statistics [147,179], relative population magnitudes [133,142,177], or additional economic parameters and weighting ratios [180]; in all such cases, it is not possible to verify validity.

The inclusion of additional sectors beyond electricity poses additional difficulties, since high resolution measured data is not readily available outside the electricity sector. Instead, national statistics are usually mapped to representative profiles of demand [161,175]. In the case of thermal demand, heating degree days or hours are used in this process, whereby the deviation of outdoor temperature from a reference

temperature indicates a requirement for heating or cooling. Several projects have endeavored to simulate thermal demand using both bottom-up and top-down approaches [169–171], but their incorporation by energy modelling tools is currently limited.

Although sources exist to understand historical demand at some resolution, future demand is understandably unknown. Frequently, historical demand is used directly when modelling a scenario of a future energy system, without altering its magnitude or shape [172,175,181]. The same approach has been used when projecting further back in time than available data allows, whereby a single year is used to represent all historical years of interest [133]. Yet, it is clear that demand changes over time. Roadmaps for energy systems, such as the EIA international energy outlook [182], include estimations of the increase in demand and have been used to scale the magnitude of model input profiles accordingly [166,183]. However, the magnitude of demand is not the only element that will change, the profile shape is also variable. Indeed, at the high (one hour) temporal resolution we see to be increasingly important to modellers, the dynamics of demand are as important as variable renewables; the two may even be coupled [184,185]. As with thermal demand, reliance on demand modelling tools is key to understanding future profile shapes, but is underutilized. An example of how they could be used is shown in [171], where the DeSTINEE [186] simulation tool is used to estimate electricity demand in Italy for the year 2050, considering full electrification of heat and transport sectors.

4.5. Cross-platform modelling integration: Model coupling

With the expanding number of energy modelling tools available, and with these having different focus points, it is interesting to see to what extent different tools are linked with each other. By linking tools, more issues can potentially be scrutinized by investigating multiple aspects or to complement their methodological approach and coverage. This has been the case in studies looking into combining the capabilities of energy system modelling tools and demand modelling [187], energy system modelling tools with different technological and temporal resolution [188], and linking bottom-up and top-down modelling approaches [189].

Based on the survey of energy tools, the most common linking approach is the so-called “soft-linking” of tools: 33 of the 54 tools have been run with other tools, by applying an external workflow or a linking tool. Soft-linking is in the scope of this review, defined as a clear definition of an approach towards how inputs and outputs from different tools can be utilized in combination. Thus, soft-linking does not interlink source-code specifically between two tools to operate automatically

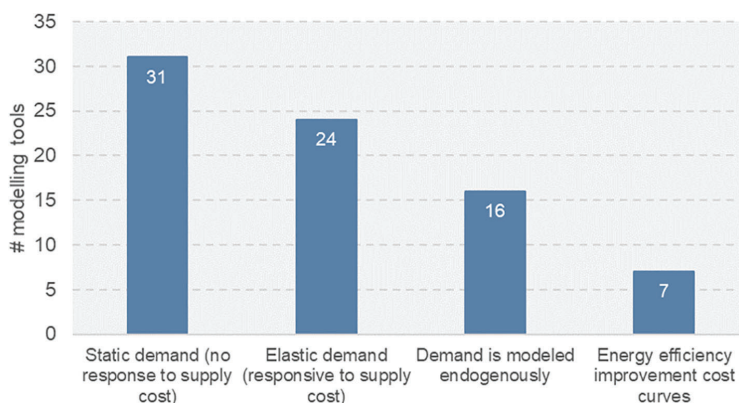


Fig. 3. Overview of how energy demands are handled across the 54 surveyed modelling tools. Note that the sum exceeds 54 as some tools can represent different energy demands in multiple ways.

together. An example of soft-linking could be the energy scenario of one tool modelled in another energy system tool that can capture a finer temporal resolution and sectoral or technological details.

If two or more tools are linked through their source code, we specify that as hard-linked tools. An example of this would be if the code of two or more energy system optimization tools are linked together in such a manner that they can be solved as a single, yet complex, optimization problem. Three of the tools in the survey have been hard linked to other tools. Five of the tools have been integrated into other tools, making new merged tools. The difference between an integrated tool and a hard-linked tool is as follows. In principle, with hard-linking, two separate tools still exist but linked to each other to exchange input/output data automatically. However, when two tools are fully integrated, the linked tools evolved into a new tool with a common set of input and output data. So, in total nine tools have been integrated with specific coding between tools. Out of all tools examined, 11 have not been linked to other tools, and for one the linking status was unknown for the tool developer. Further information regarding the type of tools connected between each other was not collected in the survey.

These results hint at a growing trend where complementary methodological approaches are used in tandem to leverage their capabilities and potential for additional insight. Fattahi et al. [35] present an example of this by reviewing the features and gaps of current energy system models and proposing a conceptual framework of how model coupling can take place between energy system modelling tools and regional models presenting infrastructure and resource constraints, electricity market, and macroeconomic modelling tools. Otherwise, more focused coupling efforts can also be found in the literature, including cases coupling top-down and bottom-up energy system modelling tools to gain insight about appropriateness of technology choices in the energy system and wider macroeconomic and welfare effects [189–191], linkages between technology-rich modelling tools and long-term planning ones to get more nuanced representations of the systems' sector coupling and flexibility options [159,192–194], coupling tools forecasting fuel and transport demands with energy system simulation tools [195], or even combined efforts linking spatial analysis [146,196], and behavioral aspects of end-user transport demands [197,198] with energy system modelling tools. Likewise, linking socio-technical transition aspects with energy system tools can prove beneficial to capture more realism in modelling [34].

In all, the coordinated use of modelling tools and different approaches opens a world of possibilities to capture greater detail of the real-world and its dynamics with the energy system. Moreover, this could help in tackling modelling uncertainty, as a better representation could be captured by linking approaches. However, increasing modelling realism should not trump the functionality of modelling tools. While it is certainly impossible and impractical to create an all-encompassing model [19], the added complexity of model coupling could also be detrimental for uptake by relevant users, or for an eventual use of modelling outcomes which are perceived as being too-complex [58]. At its core, the interpretability of modelling outcomes will be rooted in a clear understanding of the underlying modelling assumptions and formulations rather than the increase realism of integrated modelling tools [3]. Thus, a balance between modelling complexity and interpretability and usability is necessary when considering tool coupling exercises.

4.6. Tool usage: accessibility and transparency

There is a current trend and focus on openness of energy system modelling tools [44,46,47,199,200], which, as gathered by Oberle & Elstrand [47], are well suited technically to model current challenges in the energy transition. As mentioned in Section 2, this open development is also one of the drivers behind the *Open Energy Modelling Initiative* [45,49], which gathers a growing number of open-source energy system models and frameworks. While this openness generates a natural exchange of knowledge between researchers and modellers and allows for

a transparent modelling framework for modellers and users, it is essential to focus on user accessibility and third-party replicability [63].

As explored in other fields of study, prospective users of open access tools still require adequate levels of guidance to learn how to use these, and enable subsequent model implementations [201]. In some cases, this can be facilitated by dedicated graphical interfaces as opposed to direct manipulation of the source code, especially when considering occasional users³ of a tool [202]. However, the selection of interface should accommodate the specific user-needs [203]. This is especially relevant as the uptake of energy system models as tools for decision-support can be hindered by the functionalities and complicatedness of use perceived by target users [28,58].

Therefore, we compare the tool openness with the tool's user interface. In Fig. 4, the same tool might appear more than once, but in total, 36 of the 54 models and tools surveyed can be free for other users. Of those, 22 are open source, and eight of these require additional commercial software or solvers to run. Only two freeware applications were reported which were not also open source, while 11 tools commercial (paid) software were identified. In addition, 11 tools were observed to be in-house tools that are not sold or provided to outside users. Moreover, 11 tools report being free under special conditions, or being available under request for academic purposes, and overlapping with some of the previous categories otherwise.

The open-source category, as well as most of the other categories, are to a large extent dominated by tools with direct coding options. For many of the tools, this is the only option to use the tool, although human-readable text interfaces are also available to more easily handle the code of some tools' code. In addition, under the "other" category for user-interface we identify that some tools can be used in diverse ways via other external applications such as Excel, Jupyter Notebooks, via bash controls, etc.

Within the non-open source tools, whether they are free or commercial, the share of tools with a dedicated graphical user interface is more significant, while there is a lower number of tools with web-based interfaces.

Many energy tools are dependent on mathematical solvers to operate and find solutions. Talking about the accessibility of free tools, it is important if a tool can operate on open-source/free solvers. Of the 37 tools that indicated they use a solver, 23 are dependent on commercial software while only 8 of these are reported as being open source. This potentially also limits the accessibility of such open and/or free tools, especially looking outside of academic settings with special educational licensing agreements to access some of these solvers.

4.7. Perceived policy-relevance

A key aspect of energy system modelling is the ability to quantify the impacts of changes in the energy system and in this manner contribute to the public debate, while also supporting decisions to guide the energy transition [5,32,204]. Although it is commonly understood that energy policies are political decisions, the use of energy system modelling studies is important to inform and substantiate the policy-making process [7].

In the survey, we attempt to quantify the number of tools that have made some policy contributions. We differentiate between those that have been used directly by an official governmental or public institution for guidance in official policy and indirectly by contributing to the discussion or used as a reference to contrast and/or validate official policies. An outline of this can be seen in Table 4.

Many of the surveyed tools have been used for policy support, both directly (e.g. PRIMES [205]) and indirectly, with some overlapping

³ Casual or occasional users refers to those who are using a tool intermittently rather than having constant interactions, regardless of their level of expertise in the field of study for which the tool is applied.

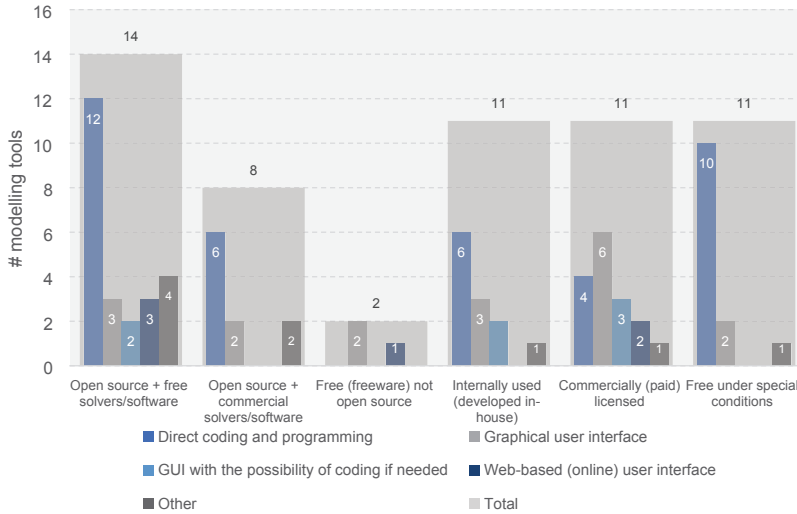


Fig. 4. Comparison of tool types with user-interface among the 54 surveyed tools. Note that the sum of each bar and the total exceed 54 as some tools can fall under multiple licensing/availability and user interface categories.

Table 4

Modelling tools and policy support status among the 54 surveyed tools. Note that the sum exceeds 54 as some tools have had more than a single policy-support application.

Use for policy-making and/or support	# of tools
No	8
Not known	16
Yes, directly	16
Yes, indirectly referred in a relevant official document	17

usage between these two categories (e.g. [EnergyPLAN \[206,207\]](#)). On the other hand, over a third of the models did not have any identifiable policy contribution. This could correspond to the fact that some of these tools are rather new in-house developments used within academic research, or they have been used for a limited scope of projects.

While this certainly shows a gap between modelling and policy, it does not reflect on the modelling potential of such tools to answer policy-related questions. It does however raise a question regarding awareness of modelling tool application beyond initial development, and the involvement of policy-makers in discussions about modelling features and results. Such an involvement could enrich the end-use of energy system models, particularly to produce scenarios answering policy-related questions [7,17]. Ultimately, having this interaction with policy-makers and putting the models to use in decision-support also serve as form of legitimacy and could be viewed as a real-world validation of the energy system model in question [59].

For this reason, it is important to understand the characteristics of the tools used for policy support applications. The attributes of these tools vary in terms of technical modelling characteristics, but also in their accessibility, target user-base and interfacing. In [Fig. 5](#), an overview is presented of the different attributes found in those tools. From the results shown in [Fig. 5](#), a few clear trends can be observed.

First, the tools used for policy-support tend to have high temporal resolution, relying mostly on hourly modelling. This has been specially the case for those tools reported to have direct policy applications, which responds to the need to model the energy system's dynamics when considering fluctuating demands and supply sources, as well as energy balancing. For the tools with indirect application, the hourly

time resolution is apparently used as much as yearly resolutions. To a lesser extent, some tools also consider seasonal time-slices or multi-year resolutions to conduct their modelling.

In terms of modelling time-horizon, a multi-year outlook is seen to be most predominant among the surveyed tools with policy applications, while yearly horizons are less used. The ability to represent multiple years facilitates outlining long-term policy pathways, making it a valuable attribute when modelling transition scenarios for the energy system. On the other hand, 1-year horizons, while not explicitly modelling transition pathways, can still aptly model different end- and mid- point scenarios for the energy system, making them equally valid tools for policy analysis and support.

As seen in [Fig. 5](#), the ability to represent multiple energy sectors and end-uses is widely considered in the tools with policy applications. Here, the electricity sector seems to be slightly more well represented, however other key sectors and end-uses are also considered to an almost equal extent. Interestingly, those tools used indirectly for policy support report having higher representation of some of these sectors, with a slight edge on modelling transport, industry and cooling. By contrast, the overall number of tools surveyed, shown prior in [Fig. 2](#), show a gap between modelling the electricity and other sectors and end-uses.

The energy demand representation in the tools used for policy support falls mostly under static demand representations, with elastic demands also being represented. On the other hand, endogenous demand modelling does not seem to be a common feature present in these models. This aligns with the discussion in [Section 4.4](#). However, endogenous demand representations is slightly more predominant in the tools used for indirect policy support. On the other hand, we see that most of the energy system modelling tools with policy applications rely on connections with other tools, likely to supplement their modelling capabilities.

Finally, regarding the access and use of the tool, it is possible to see some clear cut distinctions between the tools used directly and indirectly for policy support. For instance, while open source access seems to be a preferred attribute in the observed tools, the use of commercial and non-open source freeware seems more prevalent in direct policy applications. Similarly, tools used for direct policy-support seem more likely to provide graphical user interfaces, in contrast with direct coding, mostly found in those modelling tools used indirectly for policy support

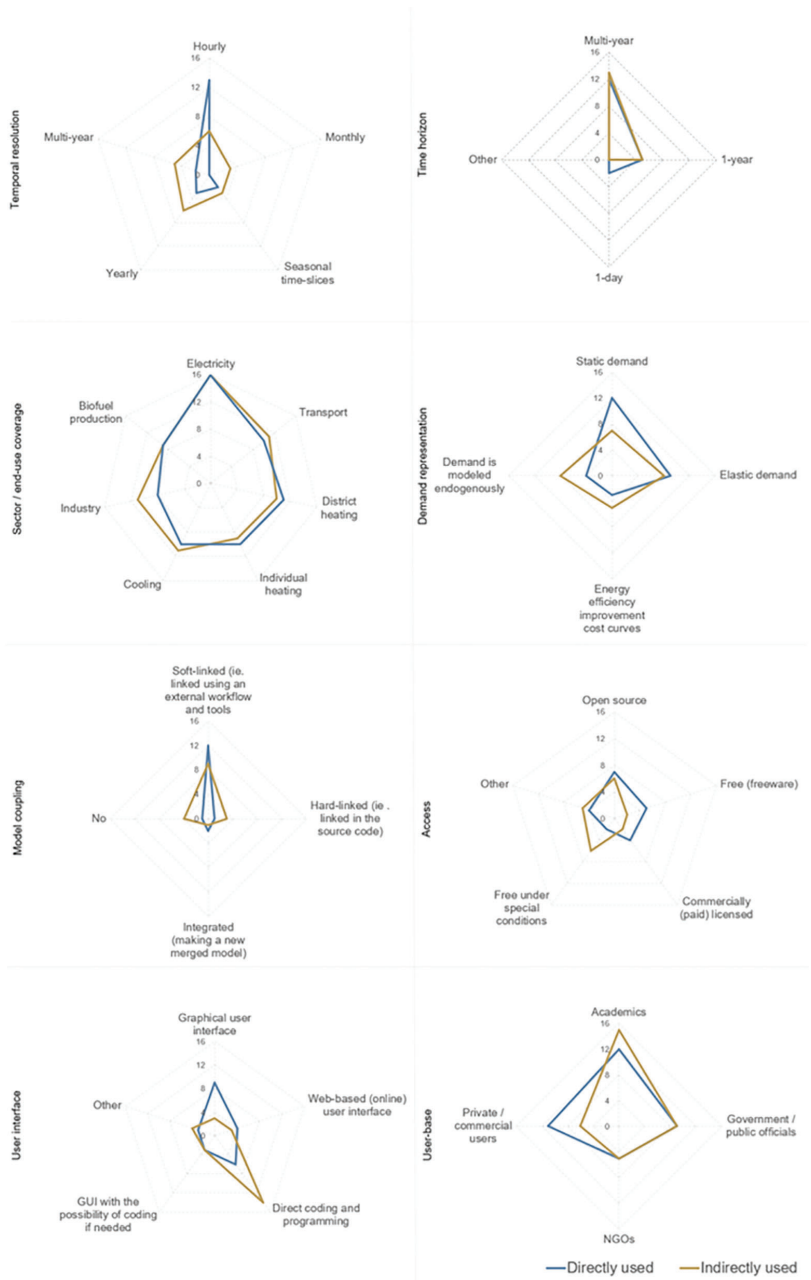


Fig. 5. Characteristics of the tools reported to be used directly (in blue) and indirectly (yellow) for policy support represented as radar plots of temporal resolutions, time horizons, sectoral coverage, demand representations, model coupling applications, access/licensing, type of user interface and user-base of the tools. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

applications. Ultimately, this could potentially be associated to the target user-base of the modelling tools as seen in Fig. 5, where we see that for direct policy support the main user-base consists of private/commercial users, as well as academics and government/public officials;

while, academic users make up the main user-base of those tools used for indirect policy-support.

5. Summary and discussion

This study reviews recent trends in energy system modelling tools by surveying the existing literature and gathering inputs directly from tool developers about the features and applications of their modelling tools. Unlike previous review studies found in the literature, this contribution establishes a direct communication with modellers and developers of the tools through a questionnaire, to reflect the way these developers understand their tool under a common terminology, while also addressing issues that previous survey-based studies have not put much focus on, such as the factual policy-relevance of studies conducted by an energy system modelling tool, the accessibility, openness and usability of the tool, and possible model coupling applications. This reduces the risk of misinterpretation or biased assessment of different tools by relying on their published information, although with a limited sample of tools surveyed. Moreover, the survey offers an avenue to gather information about the real-world application of the tools directly from their developers.

This, of course, does not come free of downsides, like the potential exclusion in the current survey of some well-documented modelling tools, in cases where no responses were gathered for the questionnaire, or by considering representative 'members' from a family of models which might have different technical attributes to their source. Moreover, potential biases in the survey can arise as the majority of the past reviews, and the models surveyed stem from European research, which could hint at a focus on modelling specific aspect of European energy transition paradigms. Nonetheless, we recommend this line of dialogue with tool developers when conducting future review exercises in order to gather insight about the modelling applications of a particular tool or for validation purposes, and more generally to identify trends in the field of energy system modelling. From this, the following points appeared to be evident after the process of conducting the survey, including both literature reviews and modelling tools.

First, it is challenging to agree on a specific vocabulary that all tool developers reach consensus in the same way. For instance, multiple studies have focused on proposing new classification schemes and to categorize different modelling approaches or methodologies. While some of these categories are unambiguous, other descriptive labels assigned to tools might fall within an overlapping spectrum which is harder to define. This is not surprising as an overlap between modelling methodologies does exist; it highlights, however, the importance of communication between modellers when discussing different modelling methods and would be relevant when interpreting the tools application or when working on linking different tools. Similarly, expanding this dialogue can also provide a better understanding of a tool's intended design versus its inferred potential applications obtained from only reviewing modelling features, as seen in Section 4.2. regarding the typical modelling time-step used by some tools and the clarifications from tool developers, or in Section 4.6 regarding their policy-related applications. However, it is important to point out that surveying can only be fully effective if there is a common understanding of terminology and a clear framing of survey questions. As a case in point, a survey question like "How is energy demand modelled in the tool?" can be understood in many ways, such as in terms of energy carriers (e.g. a country's demand for oil) or in terms of end-uses (e.g. demand for energy from households). In turn, this could lead to potential misunderstandings on whether the demand is modelled endogenously or exogenously depending on how the respondent interprets demand in the first place.

Second, modelling tools rely on exogenous demand datasets. Yet, there is still a lack of accessible data for modellers to understand projected and uncertain changes in demand, and to model high spatial and temporal resolution systems. Where available, standard input datasets are relied upon in energy system models, irrespective of their research focus, representing the frontier of data availability. The modelling of cross-sectoral decarbonization will open new challenges, including the

integration of sectors for which ever more data is required and the need to specify demand that is matched to the weather conditions influencing the increasing prevalence of variable renewable generation. For this, coupling with demand modelling tools is necessary, but nascent. In addition to issues of data availability, greater energy system complexity and reliance on non-dispatchable technologies exposes the inadequacy of exogenous demand. Instead, modelling tools must embrace elastic and endogenous demand to develop highly interconnected energy systems.

Third, when investigating many tools that can do different things in terms of modelling energy transitions, it becomes clear that it is impossible to build a tool that can do it all. Most of the tools have been developed to fulfil a specific task within a defined scope or according to specific user-needs. It might have received updates and an increased number of capabilities, but the underlying general architecture, technology, and terminology remains the same. We would argue that efforts should be targeted towards linking these different tools to each other, utilizing the many capabilities that are already present. Individual tool development is obviously still required and necessary, but there is a trade-off between the details and granularity of a model and computational resources. In line with this, future review efforts could also study in more detail model coupling exercises and identify more specifically which tools are coupled together, which specific typologies exist and the trade-offs of coupling approaches. For instance, this could be done by examining the coupling of energy system modelling tools with demand models, socio-technical energy transition models, etc.

Finally, the transparency and policy-relevant applications of energy system modelling tools should be put into a real-world perspective. For example, the complexity of linking modelling tools should not jeopardize the interpretability of the underlying modelling assumptions and outcomes, as this would detract modellers and output consumers (e.g. decision/policy-makers). In line with this, model development should be conducted in such a way that it leads to actionable research, and in which policy and decision support takes center stage. In this regard, further research could be conducted to identify how user-needs and policy-making processes mark the development of modelling tools actually used for decision-support, and which features these have and need.

In line with this, modelling interpretability goes beyond the access to open code and the perceived transparency that this provides. While open development and open source development is laudable and a recommended practice, the "out-of-the-box" usability of a tool also needs to be accounted for as an additional dimension of accessibility. Doing so could enhance the application of energy modelling tools and allow for a more active engagement with a wider multiplicity of actors that can actively contribute and enrich the energy policy debate by using modelling outcomes, while also validating the appropriateness of energy system modelling tools in the real-world arena.

CRedit authorship contribution statement

Miguel Chang: Conceptualization, Methodology, Formal analysis, Investigation, Writing - original draft, Writing - review & editing. **Jakob Zink Thellufsen:** Conceptualization, Methodology, Writing - original draft, Supervision, Project administration. **Behnam Zakeri:** Conceptualization, Methodology, Investigation, Writing - review & editing. **Bryn Pickering:** Conceptualization, Formal analysis, Investigation, Writing - original draft, Writing - review & editing. **Stefan Pfenninger:** Conceptualization, Writing - review & editing. **Henrik Lund:** Conceptualization, Methodology, Supervision, Writing - review & editing. **Poul Alberg Østergaard:** Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence

the work reported in this paper.

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Appendix A. Survey questionnaire structure

1. General information

Name of the modelling tool

2. Modelling specifications

2.1. Modelling method

Simulation//Optimization//Equilibrium (specify)//Other (specify)

2.2. Purpose of the model's mathematical formulation

Investment cost minimization//Dispatch cost minimization//Electricity import/export minimization//Social welfare maximization//Fuel minimization//Multi-criteria analysis//Agent-based analysis//Other (specify)

2.3. User interface:

Graphical user interface//Web-based (online) user interface//Direct coding and programming//GUI with the possibility of coding if needed//Other (specify)

2.4. Accessibility of modelling tool:

Open source//Free (freeware)//Commercially (paid) licensed//Free under special conditions//Other (specify)

2.5. Additional modules or solvers needed to run the model

Yes/No

2.5.1. Based on the above, are the additional module/solver: (check all that apply)

Open source//Free (freeware)//Commercially (paid) licensed//Free under special conditions//Other (specify)

2.7. Possibility to add equations/sectors/technologies/add-ons or other details to the structure of the model

Yes//No//Specify parts (specify)

2.8. Derivative/branch-out versions based on the original modelling tool

Yes//No//Not known

3. Application

3.1. Previous case studies

(Specify)

3.2. Previous linkages with other modelling tools

Yes, soft-linked (ie. linked using an external workflow and tools)//Yes, hard-linked (ie. linked in the source code)//Yes, integrated (making a new merged model)//No//Not known

3.3. Main user-base

Academics//Government/public officials//NGOs//Private/commercial users//Not known//Others (specify)

3.4. Previous use for policy-making

Yes, directly (reference below)//Yes, indirectly referred in a relevant official document (reference below)//No//Not known

3.4.1. Policy-relevant reference

(Specify)

4. Modelling resolution

4.1. Geographical resolutions represented in the modelling tool (multiple choice)

Global//Regional//National//Local//Project-specific resolution//Other (specify)

4.2. Minimum level of granularity to represent a technology (multiple choice)

Aggregated values//Individual plant/component(s) inputs//Other (specify)

4.3. Typical scale of technology representation in national level modeling (Specify)

4.4. Sectors represented in the model (multiple choice)

Electricity generation//Individual heating//District heating//Cooling//Transport//Industry//Biofuel production//Other (please specify)

4.5. Temporal resolution (multiple choice)

Hourly//Monthly//Seasonal time-slices//Yearly//Multi-year//Other (specify)

4.6. Time horizon of modeled outputs (multiple choice)

1-day//1-year//Multi-year (specify) //Other (specify)

5. Key inputs

5.1. Representation of demand

Static demand (no response to supply cost)//Elastic demand (responsive to supply cost)//Energy efficiency improvement cost curves//Demand is modeled endogenously//Others (specify)

5.2. Demand-side flexibility to integrate variable renewable energy

Yes, electricity and heat//Yes, only electricity//No//Other (specify)

5.3. Electricity generation technologies considered (multiple choice)

Power plants (Thermo electric)//CHP plants//Nuclear//Hydro power (dam)//Run-of-river hydro//Wind//Photovoltaic//Solar Thermal//Geothermal//Wave and/or Tidal//Other (specify) //Any (user-defined)

5.4. Heat supply technologies considered (multiple choice)

Heat pumps//Fuel-based boilers//Electric boilers//Solar thermal//CHP plants//Geothermal//Industrial excess heat//Other (specify) //Any (user defined)

5.4. Storage technologies considered (multiple choice)

Pumped hydroelectric energy storage //Battery electric storage//Compressed-air energy storage//Rockbed storage//Hydrogen production i. e. electrolysis//Power to gas//Power to liquid//Power to heat (electric heat pump and heat storage)//Liquid & Gas fuel storage//Smart charging of electric vehicles//Other (specify) //Any (user-defined)

5.5. Transport technologies and sub-sectors considered (multiple choice)

Internal combustion vehicles//Battery electric vehicles//Intelligent battery electric vehicles//Hybrid vehicles//Rail//Aviation//Other (specify) //Any (user-defined)

5.6. Representation of electricity transmission and bottlenecks in the grid

Yes, as a transshipment network//Yes, as a DC or AC load flow network//Yes, a point-to-pool network (no explicit bilateral trade)//No//Other (please specify)

6. Additional information

6.1. Overview of the modelling tool (developers' description)

(Specify)

6.2. Specific modelling focus on a technology or group of technologies listed in the previous sections (ie. if the modelling tool has more level of detail on a specific technology)

Yes (specify)//No

6.3. Public availability of tool's documentation

Yes (please provide source)//No

6.4. Format of modelling tool documentation

Documentation file available online//Documentation file published//Online documentation//Online documentation linked to the mathematical model//Other (specify)

Appendix B. Supplementary data – Survey inputs

The following is the supplementary data to this article: [208].

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APPENDIX B. PAPER 2

Perspectives on purpose-driven coupling of energy system models [2]



Perspectives on purpose-driven coupling of energy system models

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ABSTRACT

Energy system models (ESMs) are essential for planning the energy transition and understanding its impacts. However, this transition is inherently complex and cannot always be understood by using just one model. Consequently, efforts linking different model classes are common practice to get insights into the energy system and the different dimensions around it. While existing literature has focused on proposing how such multi-model analyses could be structured, presenting applied cases, or looking into how specific aspects of other knowledge domains are included in energy modelling, a high-level overview of the practice of model coupling with ESMs is lacking. This article puts this practice into perspective by providing an outlook on two aspects: coupling ESM paradigms and model coupling with other knowledge dimensions. Coupling ESMs paradigms have often been used to expand modelling resolution, yet further emphasis should be placed on illustrating contrasting near-optimal system designs and expanding the solution space beyond optimality criteria. Model coupling across knowledge domains is desirable when providing meaningful insights about specific themes, yet, increased complexity of data, multi-model frameworks, and coordination across practices would make an all-encompassing model impractical and calls for purpose-driven model coupling to answer specific questions about the energy transition.

1. Introduction

To mitigate global warming and meet global climate action commitments, a transition towards a decarbonized, clean, and sustainable energy system needs to take place [1]. Abstract representations of the energy system, or energy system models (ESMs), are instrumental for exploring and assessing the impacts of different energy system scenarios that could outline this transition [2]. Moreover, the insights provided by ESMs can support decision-making by providing the means to answer research questions validating existing energy policy, assessing new policy options, setting targets, and driving decisions contributing to the energy transition [3].

A wide range of ESMs exists, possessing distinct technical attributes, methodological considerations, and varying degrees of complexity [4–8]. While ESMs with more complex representations of the energy system are widely used for policy support, modelling efforts often still rely on coupling more than one tool together to complement their capabilities [7]. Model coupling – or linking – can take place by, for example, unilaterally feeding the outputs of one model to another via systematic protocols; iteratively exchanging data between models;

creating links in the code to resolve a mathematical problem jointly; or integrating models altogether running as one [9,10].

Different linking categories have been described in the literature [11–13], with Helgesen and Tomasgard [9] synthesizing these categorizations: defining soft-linking as a user-controlled information exchange between models, hard-linking as a formal computer-led transfer of data with shared code from the models, and integrated models as the combination of models running and handling data as one. In the present study, soft-linking is understood as a coordinated purpose-led data exchange between models or modelling algorithms. Among the above, soft-linking is most common across ESM tool developments, while hard-linked and fully integrated models are less frequently observed [7], typically presenting a simplified focus of one of the models over the other [14]. Other than additional model development, hard-linking or fully integrating models present challenges in both the computational effort to solve more complex mathematical constructs and data reconciliation and consistency. This is the case, especially when accounting that data assumptions, model formulations, and outputs can be quite heterogeneous across models [15–20], and across established modelling frameworks to consider (e.g., TIMES [21–42], OSeMOSYS [43–48],

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LEAP [44–46,49–53], EnergyPLAN [30,31,34,49–51,54–102], MES-SAGE [11,103], Calliope [104,105], etc.).

Interlinkages also facilitate an integrated modelling approach where complementary features can be used to obtain a cross-cutting representation of the energy system. This also allows parameters exogenous to a single model to be internalized within a model coupling exercise. In turn, this can arguably provide more holistic multidisciplinary insights and realism than what can otherwise be achieved with a single-model approach. Past studies have relied on model linking to expand their scenario analysis by coupling ESMs with life cycle assessment (LCA) [21], behavioral [22], energy demand [43], and economic models [23–27,54], as well as power market models and with other ESMs [28–35,106,107].

Other cross-cutting representations of the energy systems also exist in the form of integrated assessment models (IAMs), which are widely used within the context of climate policy and planning the energy transition. These tools model the complex interactions between the energy, economy, environment, and other Earth systems, thereby providing encompassing representations of transition scenarios and their climate impacts often on a global and macro-regional scale [108]. However, these models present tradeoffs between their wide analytical range and lack of detailed bottom-up resolution of supply technologies and local energy demands [109]. Therefore, IAMs may need to be combined with other support tools like high-resolution bottom-up ESMs to provide a more nuanced view of the energy system [110]. Past studies have focused on linking IAMs to bottom-up models to assess, for example, the impacts of developing gas infrastructure [111] or to have better assessments of variable renewable integration including high spatial, technical and temporal modelling resolutions [36,112].

The trend of model coupling is further highlighted in recent studies that conceptualize multi-model frameworks and their key considerations and apply linked modelling approaches to energy system analyses [10,41,113,114]. In general, these frameworks present different model classes linked together to address questions about the energy transition, representing multiple dimensions of the energy system and its socio-technical context.

For example, Crespo del Granado et al. [113] propose a modelling framework coupling bottom-up ESMs with top-down macro-economic models to broaden the analysis of energy-economic systems and highlight the strengths and limitations of both types of modelling classes. McCullum et al. [114] put forth a framework to link different bottom-up tools, including ESMs, energy demand models, and statistical tools, to represent the impact of end-user behavior on energy demands and the overall system. Similarly, Fattahi et al. [10] propose modelling frameworks consisting of ESMs linked to spatial and economic models to address the existing shortcomings of energy modelling methodologies. Gardumi et al. [42] propose a modelling framework consisting of multiple tools of varying scales and outline the challenges and benefits of such an integrated modelling approach. In the same context, the implications of developing applied multi-model frameworks are put into perspective by Nikas et al. [115], providing an outlook of the challenges and recommended practices and highlighting the need for future actionable research under the context of the European energy transition. Meanwhile, a growing body of work is emerging at the European level, with projects aiming to establish cross-cutting links between ESMs and other model classes to provide answers about different aspects of the energy transition [116–119].

At the same time, recent studies have looked into the broader integration of ESMs and other approaches or with specific aspects of other knowledge domains, although not specifically focusing on the practice of model coupling. For instance, studies have reviewed energy demand modelling and their integration with ESMs [120], the role of geospatial analysis in energy modelling [121–123], the integration of behavioral aspects [124], socio-technical transition theories [125], social and environmental factors in energy modelling [126,127], LCAs [128], and climate and weather models with ESMs [129,130].

However, a high-level overview of the general practice of coupling ESMs, putting into perspective modelling paradigms and coupling dimensions is lacking in the existing literature. Thus, this paper provides a perspective on current research within the growing field of model coupling, looking beyond previous studies which have mostly focused on proposing blueprints for multi-model frameworks or providing specific practical outlooks and cases. Here, a conceptual framework is presented to better understand why coupling across ESM paradigms is needed, then we contextualize coupling of ESMs to models in other knowledge domains and how this aligns within the landscape of the energy transition.

2. Exploring new solution spaces via coupling of ESMs

A recurring theme in energy system analysis is the coupling of ESMs of different scopes among each other. This is often done to reap the benefits of complementary features found across ESMs with different attributes and mathematical formulations. Such features represent different methodological approaches and socio-technical dimensions, and ultimately the modelling outcome of these can lead to representations of vastly different energy system designs and societal configurations.

Two predominant paradigms can be found in energy system modelling: simulation and optimization. Accordingly, these reflect the type of algorithm applied to the underlying mathematical model formulation of a given ESM. Henceforth, a “simulation model” can be broadly understood as a model resolved via a fixed set of rules that seek to replicate the operation of an energy system, where the modeler can heuristically refine parameters and potential systems for analyses. On the other hand, “optimization models” formulate a given energy system as an optimization problem solved by reaching target criteria such as endogenously minimizing or maximizing values for specified parameters or reaching an optimal equilibrium point, under a set of constraints. Lund et al. [131] present these approaches and contrast their theoretical aspects and practical applications; explicitly, they outline how these approaches are used in energy planning to devise scenarios.

The scenarios formulated with simulation models can usually be associated with predictive scenario planning and thus show what can happen in the future under different assumptions without necessarily portraying an optimal solution, and are rather used for openly exploring the impacts of different alternatives and metrics [132]. In contrast, optimization models are more often associated with normative scenario planning, where scenario outputs are prescriptive, showing what should optimally happen under a given set of assumptions, constraints, and optimality criteria [2,131].

Coupling these two approaches can broaden the range of scenarios and analyses that would otherwise be achieved with only a single ESM by enabling complementary features or enhancing an existing framework's capabilities and providing a consistent and transparent framework to generate different scenario alternatives. For example, complementarity can be seen when linking a long-term spatially explicit cost-optimization capacity expansion ESM with technology-rich bottom-up system modelling [30,31], in spatially explicit power flow optimization models that feed cross-border transmission balances to a simulation model [55,56], or also across energy system optimization models with different formulations and resolution [32].

The linking of simulation and optimization approaches is not limited to coupling pre-established ESMs together. Hybrid models can also emerge from linking these approaches together, taking one model as a black-box calculation engine [133]. This is well illustrated in simulation-based optimization analyses, which often originate from a pre-existing energy system modelling framework being linked to a custom-fitted metaheuristic optimization algorithm. These types of algorithms can be simply described as optimization methods based on a high-level strategy or specific solution-search rationale to find optimality.

Metaheuristic optimizations can be particularly useful due to their ease of applicability with ESMs, ability to solve multi-objective problems with conflicting objectives (e.g., minimizing costs, emissions and/or primary energy supply, maximizing renewable energy shares), and reasonable computation time [134]. Moreover, they allow practitioners to expand the search space that would otherwise be considered for scenario development and potential system designs. Examples of this can be found in simulation-based optimization analyses that coupled ESMs with different algorithms, such as exhaustive search algorithms [57,58], multicriteria decision analysis [59], evolutionary algorithms [60–76] and swarm intelligence algorithms [77–79] for system design and capacity expansion, multi-objective algorithms for transition pathways analysis [80,81], hill-climbing optimization of marginal CO₂ abatement [82,83], and power flow optimization for analyzing cross-border electricity transmission [55,56].

Whether coupling ESMs of different approaches or expanding their modelling approach dimension, it can be said that feature complementarity can be found. As broadly illustrated in Fig. 1, the feasible solution

space for one model can be expanded for exploring new system alternatives (which represent both potentially feasible energy system designs and societal configurations), and includes both near-optimal or even contrasting sub-optimal options for a fixed set of optimality criteria and assumptions. This application aligns with recent studies where single energy system optimization models are used to generate a wide range of results representing diverse and vastly different nearly-optimal energy system configurations rather than a single optimal solution [135–141], which can cater for the potentially different perspectives and choices of result-users and decision-makers. In Fig. 1, an analogous exploration of near-optimal alternatives happens in the proximity of a Pareto front, which presents a set of optimal system representations (here, assuming a 2-dimensional view of competing optimization objectives, such as system costs and primary energy supply).

Meanwhile, simulation-based optimization studies typically explore the set of optimal solutions along the Pareto front, focusing on the best compromise solutions as defined by the modeler's criteria, or generating new optimal sets of results by changes in assumptions [64,68,71,75].

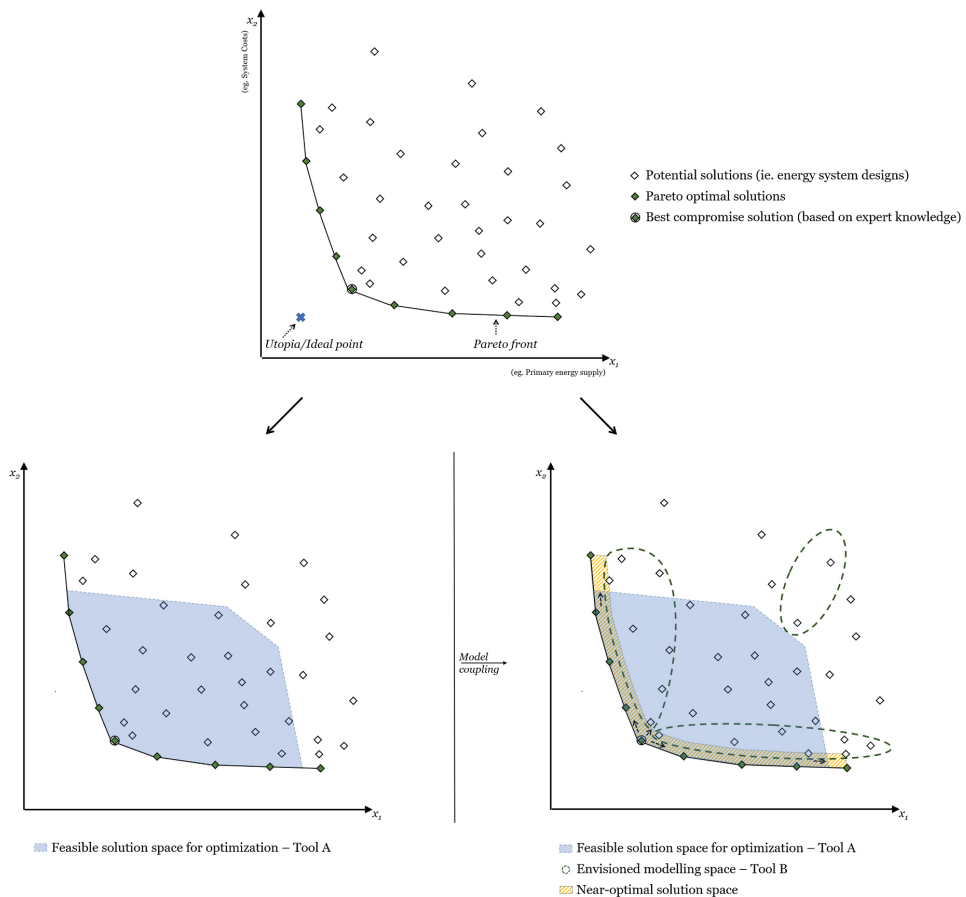


Fig. 1. Conceptual illustrations of the feasible space for energy system designs under a fixed set of assumptions and overlays of the feasible modelling spaces for distinct ESM tools. The axes on the charts represent a simplified 2-d view of competing optimization objectives. The squares represent potentially feasible energy system configurations bounded by the set of Pareto optimal solutions. In the upper chart, the compromise solution (based on modelers' criteria) is depicted as the closest one to the utopia or ideal point, where objectives are at practically unrealizable minima. In the lower-left chart, the shaded area represents the feasible solution space of a given ESM (i.e., Tool A). In the lower right chart, the dashed ovals represent envisioned modelling spaces for a different tool (i.e., Tool B), which overlaps and goes beyond the solution space of Tool A. The top-most right oval encapsulates sub-optimal feasible solutions for the given objectives, while the other ovals cover near-optimal solutions. The cross-shaded area represents the near-optimal solution space, which can be further explored when coupling models.

The diversity of near-optimal options close to the Pareto front, or the compromise solutions, is often not explored to contrast maximally different alternatives. However, studies have contrasted optimal solutions with manually-resolved scenarios from single-model simulations [60,77], showing how these can be found in the near-optimal space. Similarly, coupling ESMs of different scopes could provide a different avenue for exploring said space, or for exploring solutions beyond the feasible scope of one tool by means of the other (in Fig. 1, illustrated by the rightmost oval furthest away from the Pareto front). This is especially relevant when considering computational overhead and solution times of large optimization models [142], which can be complemented with fast resolve times of simulation ESMs [143]. Henceforth, simulation-based optimization studies and coupling of ESMs could further illustrate the diversity of near-optimal and contrasting system designs within the solution space.

3. Coupling knowledge domains and modelling dimensions

Other knowledge domains and their respective modelling classes can provide different perspectives and supplement the capabilities of ESMs to represent parts of real-world systems. This section presents a brief status of linking ESMs across these domains. Then this practice is conceptualized under a multi-level framework.

3.1. Archetypical coupling dimensions

3.1.1. Energy demand

While ESMs are often able to capture both the demand and supply side of the energy system, these models often rely upon demand data as exogenous inputs [7]. Energy demand models are therefore needed to better address questions regarding future demand developments, changes in demand profiles, effects of energy efficiency policy on demands, the location of demands relative to supply sources, and projected changes in the sectoral demands with increased levels of electrification and sector coupling [120].

A classic example of coupling between demand models and ESMs can be found in cases using bottom-up accounting tools (e.g., LEAP [144]) which feed long-term demand projections as inputs to ESMs like OSe-MOSYS [43–46,145] or EnergyPLAN [49–53]. Similarly, heating and cooling profiles from buildings can be captured by linking dynamic simulation models with ESMs [84–87]. Specific demand developments can be captured by coupling ESMs with sector-specific models, as has been the case in analyses looking into linking the data from transport sector scenarios [22,88–90]. Although capturing the fine details of the industry sector remains a challenge for ESMs [146], model linkages have been established to bridge this gap in studies analyzing electrification and fuel consumption scenarios in industry [90–92]. Additional linkages in the demand side can also occur when linking to models of consumer behaviors (e.g., consumer patterns, charging profiles of electric vehicles), or with geospatially explicit energy demand analyses.

3.1.2. Geospatial dimension

The spatial dynamics and geographical distribution of the energy system are accounted for to varying degrees in ESMs by considering different modelling resolutions and data aggregations [147]. Matching the level of detail and spatial aggregation of data inputs can be achieved via data processing with geospatial analyses and approaches. Geographic information system (GIS) tools are often used for this purpose to compile and process geo-referenced data which can then be aligned to ESM inputs [148]. Aside from GIS tools, other geostatistical methods can also be applied when aggregating climate and weather data for estimating wind and solar capacity factors at an adequate spatial resolution for these to be linked as inputs to ESMs [122,149].

For example, geospatial analyses have been conducted to estimate the distribution of energy demands, technical potentials of supply, and infrastructure expansion potentials and costs, subsequently linking these

into ESMs for national (e.g., Denmark [93,94], Chile [95], the United Kingdom [150], Germany [121]) and European studies [92,96,97]. Moreover, links between GIS and ESMs have been established to iteratively evaluated optimal shares of on- and off-grid electricity generation in rural areas based on estimated levelized costs from the ESMs [47], and for result visualization [37].

3.1.3. Macro-economics

Planning the redesign of future sustainable energy systems has, naturally, broad implications on public finances, economic competitiveness, employment and the economy at large. Therefore, a long tradition exists where top-down macroeconomic models are used to understand the broader socio-economic implications of the energy transition.

Examples of this can be found linking ESMs to econometric models to evaluate economy-wide effects of energy system scenarios [54], or with computable general equilibrium models to capture technological detail and investment flow, and how these affect economic parameters like gross domestic product, commodity prices, sectoral activities and consumption, which in turn result in changes in the energy service demands used by ESMs [14,23–27,103].

3.1.4. Social and behavioral sciences

ESMs typically consider social aspects as exogenous narratives, input assumptions and ex-post discussion of their scenarios, while gathering insights from social sciences on factors such as human behavior, actor heterogeneity, public acceptance, participation and ownership, and societal transformation [126,151]. Nonetheless, these factors can also be integrated into computer modelling and coupled with ESMs. For example, agent-based models (ABMs), which are capable of simulating actor decision-making and interactions, have been used in conjunction with ESMs to integrate EV charging patterns as demand profiles [98], the effects of market uptake of new vehicles [22], and building demand predictions [152,153]. Other standalone applications which could be linked to ESMs include agent-based modelling of capacity investment decisions [154].

System dynamic models – which can represent causal relations of activities and processes – can also be applied in the context of understanding broader societal and behavioral aspects. These have been used as standalone applications to, for example, capture the sociopolitical feasibility of energy transition pathways based on governmental decision-making dynamics, human behavior, and societal change [155–157]. Nonetheless, these aspects which can commonly be associated with the formulation of socio-technical pathways could also stem from other quantification approaches of social drivers and constraints of the diffusion of energy technologies applied to creating energy-related socio-technical narratives, such as those presented by Süsser et al. [158].

3.1.5. Environmental and earth sciences

The environmental effects of the energy transition and the reduction of greenhouse gas (GHG) emissions are core decision drivers in the modelling and policy interface. Indeed, this is reflected in ESMs which often include CO₂ and other GHG emissions in their core modelling capabilities. However, the scope of these calculations is usually limited to only include direct sector-specific emissions from combustion processes.

Therefore, a large body of work has utilized alternative tools to assess the energy-related emissions embedded in upstream processes of the system; namely, applying LCA tools [128]. These often focus on a specific sector or activity, gathering energy and technology mixes ex-post to derive life-cycle emissions and impacts. Examples of this include linking ESMs to LCAs assessing technologies in the electricity supply [38,39,99,100], buildings' renovation rates [159], the use and integration of electric vehicles [101,102], and system impacts when applying power-to-methane [21], as well as other system-wide impact assessment [160–162].

A key challenge of these remains in the accounting of future energy mixes and prospective new life-cycle inventories [163]. At the same time, a broader understanding of material flow models coupled to ESMs needs to be considered further, to assess the needs for rare earth minerals and resources required in the long-term energy scenarios' value chains, and to quantify how circular economy measures (e.g., recycling rates) influence material availability in energy systems [164]. Some of these aspects can partially be addressed by coupling ESMs with IAMs [108], which can include natural resource availability, however, the global scale and broad coverage of IAMs sit in contrast to simpler more targeted models [110]. Nonetheless, when linking ESMs to IAMs an additional interface to climate modelling is enabled, putting aspects of bottom-up energy modelling into perspective with regard to climate change mitigation.

3.2. Representing model coupling from a multi-level perspective

The dynamics of the energy transition include the interplay of a plurality of actors, disciplines, institutions, technologies and radical change. Neither energy systems modelling nor other science domains alone can capture all the aspects of said socio-technical transition [165]. Coordination across models is therefore needed and requires further development and structuration. However, these will be influenced by both model developments stemming from within specific expertise niches and the broad landscape discussions on climate change, energy, policy, geopolitics, grassroots movements and activism.

A multi-level perspective, which provides an analytical framework for socio-technical transitions [166–168], can illustrate how the practice of model coupling and the dynamics across knowledge domains shape the modelling interface in this context. The different levels can be conceptualized under a nested hierarchy, starting at the bottom with novelty and niche areas, in the middle with established configurations or regimes, and at the top with exogenous landscape developments [169, 170]. This is conceptually illustrated in Fig. 2.

In the bottom hierarchy, different domain niches appear,

representing the different disciplines and fields of expertise where modelling developments originate. This implies that at this level, modelers work on their own models, with limited external coordination. On the other end, the landscape level includes external mainstay factors such as climate change, sustainable development, global climate action commitments like the Paris Agreement, global trends, national and regional policy, geopolitics, and grassroots activism, all of which exert pressure on the lower levels driving their development and in the long term are also influenced by these. These two levels are connected by an intermediate level, which encapsulates the different pockets of connected niches, and which in turn is pressured by developments in the landscape level.

At the middle level, modelling exercises are conceptualized as different model patchworks and established practices, encapsulating elements stemming from the niches illustrated in Fig. 2, that can generate insight into potential energy transition pathways. Naturally, the structures presented at this level influence each other, drive model developments in the lower individual domains, and can seep through to broader and actionable developments at the landscape level, for instance, guiding long-term energy policy and target setting to reach global climate commitments. This can be exemplified in the current European energy system modelling scene, with projects driving both individual model developments and innovation with multi-model ensembles [42,115–117]. Moreover, some of these patchworks represent deep-rooted modelling practices and interdisciplinarity approaches, with developments of their own vocabulary and standards [171–173]. With increased structuration and model complexity, the idea of striving for an all-encompassing model or building highly coupled multi-model frameworks comes into question. These would require immense degrees of coordination in terms of aligning modelling paradigms, resolution, ontologies, data harmonization, computing power and transparency while keeping up with developments within the niche domains and the timeline and happenings of the energy transition, which also exert further pressure to model developments and the coupling of models to address specific issues. More so, when also

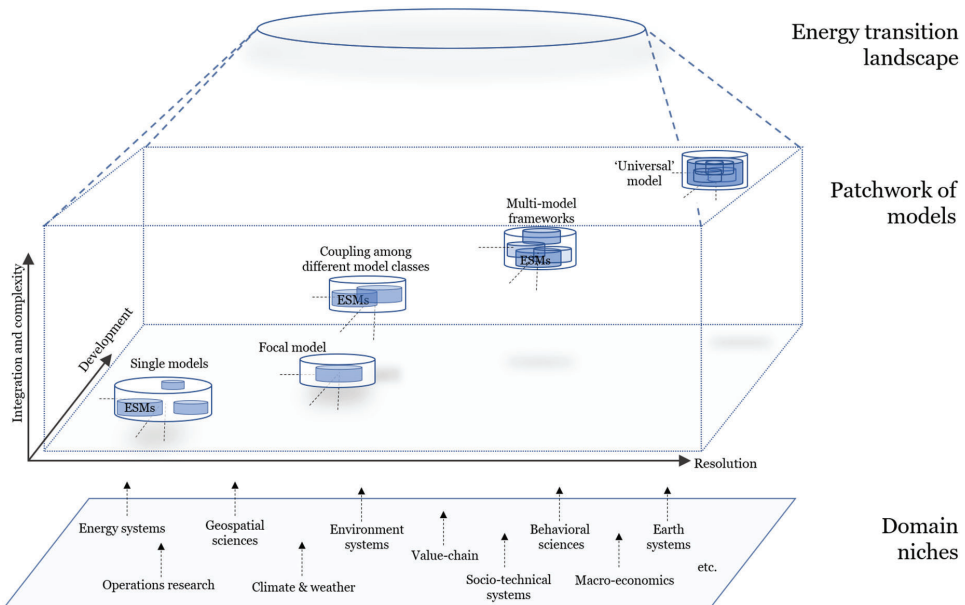


Fig. 2. Conceptual nested hierarchy of modelling dimensions and model coupling showing a multi-level perspective on the emerging practice of model couplings under the context of the energy transition. Inspired by Ref. [170].

aligning additional modelling complexity to the needs and capabilities of both modelers and result-users [174–176], as well as the needs of decision-makers to have timely yet robust insights. Therefore, model coupling should be purpose-driven: designed to address specific research questions, enabling manageable degrees of complexity, resolution, and coordination across knowledge domains, so that it can provide actionable and timely insight for the energy transition.

4. Summary and conclusions

In this perspective, we present the current landscape in the practice of coupling energy system models. Reviewing the current status of coupling ESMs shows that said modelling with multi-model frameworks is becoming ever more prevalent. Model coupling provides multidimensional views capable of addressing questions about the potential pathways of the energy transition in a more encompassing manner than what could be achieved with a single model.

Simulation and optimization approaches used by ESMs are commonplace and can provide mutually complementary aspects for analyzing different aspects of the future energy system. This can also be achieved by coupling one model class to optimization algorithms, as is the case in simulation-based optimization modelling. Nonetheless, these have mostly focused on providing a view of the Pareto optimal solutions under different assumptions without exploring near-optimal options with potentially drastically different system designs. This contrast with the growing field of analysis performed with optimization ESMs generating alternatives to explore near-optimal yet maximally different scenarios. Nonetheless, coupling approaches can enable a wider exploration of the solution space than would otherwise be obtained with a single-model approach. This can provide energy planners with more robust scenarios, and consistent scenario design frameworks, that can address not just near-optimality but also the incremental aspects of public planning that might be outside of the scope of certain optimality criteria.

Coupling ESMs with other model classes rooted in other expertise niches allows for a nuanced view of other dimensions to consider beyond only the setup of the energy system itself. In turn, model coupling or even devising multi-model frameworks can be a valid development to improve modelling realism once the tradeoffs in data and modelling uncertainty and additional complexity are weighted. That being said, certain types of archetypical connections present gaps in research. Overall, linkages between ESMs with demand-side models, geospatial models, macroeconomic models, and LCA models seem to have a long-standing presence. However, gaps remain in establishing model links addressing the human and social dimensions, and links to models capable of evaluating upstream value chains of the material flow of resources needed in the future energy transition, as well as the communication of methodological approach, including how and to what extent coupling is performed.

Finally, model coupling should not necessarily strive to be universally comprehensive but rather purpose-driven. That is, addressing specific and meaningful questions that can influence the energy transition landscape while adequately managing complexity, modelling resolution and interdisciplinary coordination.

Credit author statement

Miguel Chang: Conceptualization, Methodology, Formal analysis, Investigation, Writing – original draft, Writing – review & editing. **Jakob Zink Thellufsen:** Conceptualization, Writing – review & editing, Supervision, Project administration. **Henrik Lund:** Conceptualization, Supervision, Writing – review & editing. **Poul Alberg Østergaard:** Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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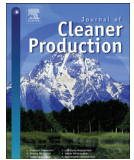
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APPENDIX C. PAPER 3

Heat Roadmap Chile: A national district heating plan for air pollution decontamination and decarbonisation [3]



Heat Roadmap Chile: A national district heating plan for air pollution decontamination and decarbonisation

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ABSTRACT

In many countries around the world district heating can play an important role in decarbonisation since it provides an efficient way of displacing fossil fuels and integrating renewable energy. Simultaneously, in some countries heating is based on the burning of biomass in individual stoves, which can be considered renewable but results in both inefficient heating and high contamination. In such countries, air pollution or decontamination is a more urgent problem. This paper presents the application of a methodology to analyse how district heating could be used as an important technology for coordinated decontamination and decarbonisation purposes looking towards 2050, based on an energy system analysis using hourly simulations, and using data based on spatial analysis to be able to explicitly include a Chile-specific cost for district heating. The results show that district heating also has the potential to be an important infrastructure to reduce air pollution from biomass combustion for heating, in addition to its better understood role of enabling decarbonisation and energy efficiency.

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1. Introduction

District heating (DH) has been proposed in various different contexts as a contributing solution for future energy systems—most notably for decarbonisation. However, that challenge does not apply to the heating sectors of many countries, since heating is based on the burning of biomass in inefficient individual stoves. In such countries, air pollution and decontamination can be a more urgent problem than decarbonising the heating sector; while the biomass can be considered renewable, it often results in both inefficient combustion of biomass for heating, low indoor thermal quality, and high level of air pollution and resulting contamination (Rodríguez-Monroy et al., 2018).

To address the problems of air pollution from heating, it is not possible to disregard the overall need to also decarbonise the energy system. This is especially important when considering the role that biomass has to play, since deeply decarbonised future energy systems are expected to largely reserve (scarce) bioenergy resources for transport, material, and certain industrial purposes.

This means that cleaner and more efficient solutions for the heating sector have to be sought that do not rely on fossil fuels and can fulfil secondary strategic energy planning objectives such as affordability and security of supply.

Chile is a signatory to the Paris Agreement (and has proposed legislation that would target greenhouse gas neutrality by 2050) and thus energy system planning includes a strategic objective of decarbonisation. Simultaneously, the country also has one of the highest level of (urban) air pollution in Latin America, so decontamination of the energy system is also a primary objective of the country (Ministerio del Medio Ambiente (Ministry of the Environment), 2014). Chilean cities represent 7 of the 10 most polluted cities in Latin America, with the impacts of outdoor air pollution causing an estimated 3500 deaths annually for the country (Ministerio del Medio Ambiente (Ministry of the Environment), 2018), since in some cities the air pollution can be double the level experienced in Beijing (IQAir Air Visual, 2018). At the same time, energy access in terms of being able to achieve sufficient comfort levels year round, and socio-economic factors that contribute to energy poverty – particularly during high pollution events, are important objectives (Reyes et al., 2019).

To address these issues for the heating sector, government and

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Nomenclature

Country/Region Codes

CL	Chile
EU	European Union

Abbreviations

CCS	Carbon Capture Storage
CHP	Combined heat and power
CO ₂	Carbon dioxide
DH	District heating
GIS	Geographic Information Systems
HP	Heat pump
HRCL	Heat Roadmap Chile
LEAP	Long-range Energy Alternatives Planning System
LSHP	Large scale heat pump
MUSD	Million United States Dollars
PELP	"Proceso de Planificación Energética de Largo Plazo", Long-term energy planning carried out by ()
PES	Primary energy supply: all energy that is used, before conversion, as input to supply the energy system
PM	Particulate matter
RES	Renewable energy sources

municipal policy approaches are based on both short and long-term measures. One option has been hard regulation, in the form of a prohibition of open biomass combustion during certain high-pollution days and events. Longer term approaches have been the promulgation of local atmospheric decontamination plans (PDSSs), which often include measures to promote higher levels of thermal insulation, better treatment of biomass to reduce humidity, more efficient biomass combustors, and switching to lower pollutant fuels such as electrification or natural gas.

These approaches are very strongly reflected in the governmental long-term planning energy planning strategies, for example in the form of the *Proceso de Planificación Energética de Largo Plazo* (Process of Long-term Energy Planning) (PELP), where heating demands are foreseen to be supplied through electrification, and by highly efficient biomass boilers using dryer wood, but governed by both an increasing access to heating and higher thermal efficiency standards for buildings (Ministerio de Energía, 2017a). In addition, the reduction of biomass consumption is also an important issue since the long term limited biomass becomes a high-value resource (Lund, 2014) and the use of sustainable biomass does not allow for burning the biomass for heating purposes (Connolly and Mathiesen, 2014). In the future, biomass should be used primarily for transport, material and certain industrial purposes.

This paper investigates the contribution that DH could make to the strategic energy planning aims of both decarbonising the energy system, but also the reduction in air pollution emissions using Chile as a case. DH has regularly been identified as a valuable infrastructure in term of creating potential to decarbonise energy systems conceptually at system (Lund et al., 2017b) and technology level (Rezaie and Rosen, 2012). Geographically, DH has been explored in the case of the EU (Colmenar-Santos et al., 2016) and for specific countries (e.g. (Thellufsen et al., 2019)). This is due to several mechanisms, including the ability to integrate otherwise wasted heat from power plants, waste incineration and industrial processes and thus create primary energy savings (e.g. (Persson and

Münster, 2016)); and the increased ability to directly integrate renewables such as geothermal and large-scale solar thermal (e.g. (Hansen and Mathiesen, 2018)). Furthermore, the increased ability to integrate (intermittent) renewable electricity (e.g. (Connolly et al., 2015a,b)), and the potential for increased efficiency of larger energy conversion units (e.g. (David et al., 2017)) are also valuable contributions of district heating.). These mechanisms all allow for the reduced reliance on (fossil) fuels, and overall decarbonisation of the energy system.

However, given the role that combustion processes, particularly of solid fuels, have in the emitting air-borne particulate matter (PM), DH is proposed as a potential solution to both decarbonise and decontaminate the energy system. So far, DH in the context of air quality has mostly been studied with the perspective of reducing the impact of coal combustion, with a geographic focus on (parts of) China (e.g. (Li et al., 2019 on a regional level; Zhang et al., 2018 at city level)). In Europe, there are various local studies that focus on DH and PM and NOx emissions, typically focussing specifically on the type of combustion processes in the heat supply technologies in existing DH systems in (e.g. (Fahlén and Ahlgren, 2012 in Sweden; Wojdyga et al., 2014 in Poland); (Ravina et al., 2017) concerning cogeneration in Italy. To the authors' best knowledge, this is the first national assessment of DH for PM reduction potential specifically in combination with decarbonisation based on energy system analysis methods.

2. Methodology

The methodology used in this study builds on the approach developed in the Heat Roadmap Europe studies, with the purpose of combining both the local analysis required to understand the costs and potentials of heating with national-level energy system analysis. This overall methodological approach was conceptualised for Denmark (Lund et al., 2010), iteratively further developed for Europe in 4 sequential studies: the first of which aimed to assess a cost-effective role for DH in Europe (Connolly et al., 2012), the second sought to combine DH with deep renovations (Connolly et al., 2014), the third which developed comprehensive heating and cooling scenarios (Connolly et al., 2015a,b), and the fourth which developed integrated low-carbon heating scenarios in line with the 2016 Paris Agreement (Paardekooper et al., 2018b). In this study, the methodology is being further advanced to include the strategic objectives and quantification of PM emissions, and is also now for the first time being applied directly outside of Europe.

The approach is closely linked to the Smart Energy Systems concept (initially explored in (Lund, 2010), defined in (Connolly et al., 2016), and described with regard to heat and storage in (Paardekooper et al., 2018a)) in that there is a shared approach to designing energy systems, as both are based on the coupling of energy sectors to exploit synergies and induce resource- and cost efficiency. They also have shared design objectives in terms of developing systems that to the largest extent possible are affordable, renewable, sustainable, and reliant on known and proven technologies.

The Heat Roadmap methodology takes its point of departure in the need to both combine (hourly) energy system modelling to develop future scenarios and assess their respective impact on national and local energy systems with outputs of local geospatial mapping of the heating sector. Since the Heat Roadmap approach aims to be congruent with the Smart Energy Systems concept and allow for a pathway towards full decarbonisation, and energy-system wide strategic objectives, the assessment for heating must include an explicit analysis of the wider energy system, in this case using hourly energy system model simulation. This is especially the case since many of the comparative advantages that DH can

provide, in terms of energy efficiency and renewable integration, arise from the coupling of the heating and industry and electricity sectors.

As the study explicitly aims to design and quantify an energy system that includes DH, inputs developed in Geographic Information Systems (GIS) are used for the cost and relative losses of the DH transmission and distribution system, which consider local climate and building conditions. This allows for the integration of the potential of DH into national energy system modelling, while respecting the spatial nature and cost of district heating.

In this paper, the Heat Roadmap methodology is developed to also consider the PM emitted. Given the background of a reference system that is already based on biomass (and thus could be considered renewable; if not necessarily sustainable), there is a need to include system design and quantification that addresses the dual objectives of decontamination and decarbonisation of the heating system. To do so, several design principles are applied in order to develop the alternative scenarios that fulfil these two goals to establish the methodology used in this paper: Assessing local heat densities: Since thermal energy travels badly, heat density and the availability of local heat sources are a large driver of the cost and potentials for DH infrastructures (Frederiksen and Werner, 2013). A spatially explicit heat demand model is used to determine at what cost different levels of DH distribution infrastructure could be implemented, so that this can be aggregated to the national level.

Introducing DH infrastructure at different market shares: An incremental increase of the heat demand covered thermal distribution networks (including losses) is simulated in an energy systems model. This step serves to integrate the cost of distributing thermal energy – which is inherently locally driven and therefore derived from a geospatial understanding – into national-scale energy model simulation.

- **Design of a diversified DH supply:** Including previously unavailable renewable and sustainable sources, such as excess heat from industries; renewable geo- and solar thermal heat; and heat cogeneration plants (CHPs) and large-scale heat pumps (LSHPs) allows for the simulation of the benefits that DH can have in terms of using cleaner technologies and substituting individual heat.
- **Integrating intermittent RES and final adjustments:** The previous steps, through their re-design of the heating sector, must also be viewed within context of their interactions with the other infrastructures in the energy system. The implementation of DH results in added flexibility provided to the energy system by the use of CHP and electric heating. This increased flexibility is expected to allow for a higher degree of intermittent renewable production and capacity to be integrated, reducing the need for electricity generation through combustion. Finally, several final alterations are made to all scenarios to ensure security of supply buffers in the form of sufficient backup capacity.
- **Assessing alternative and reference scenarios:** Quantification includes using total PM emissions in addition to CO₂ emissions, PES, socio-economic costs and cost structure as criteria to assess to what extent the scenarios are achieving the defined strategic energy planning objectives, and then propose one final Heat Roadmap scenario.

Using simulation tools to create an array of scenarios agrees with the exploratory nature of the research conducted; the objective is to understand the ways in which DH could contribute to the decontamination and decarbonisation of the Chilean heating and energy system, rather than merely prescribe one optimal solution

(Lund et al., 2017a). While one scenario is proposed as the Heat Roadmap scenario, the analysis of the role that DH can play in the reduction of air pollution and decontamination is also based on the step-wise approach and development of different scenarios reflecting the methodological steps described to better understand the mechanisms and impacts of particular parts of the DH system.

3. Scenarios

3.1. Scenario simulation

The energy system modelling is performed in the freeware simulation tool EnergyPLAN (version 14.2; available from <https://www.energyplan.eu>). EnergyPLAN is an hourly tool that covers the entire national energy system, specifically designed to enable the identification and analysis of potential synergies between energy sectors – including the electricity, heating, cooling, industry, and transport sectors (see (Connolly et al., 2010 for a more thorough and Lund et al., 2017b for the most recent description). This is particularly relevant for the Heat Roadmap methodology, since it considers the heating sector a key and integrated part of enabling a transition in the wider energy system. Since EnergyPLAN is a simulation tool, the results are based on the predefined inputs of the user regarding demands, capacities, and operation strategies, and the outputs include both the (hourly) optimised operation of the system and key assessment parameters like fuels, PES, CO₂ emissions, and costs.

The explicit value of EnergyPLAN as a simulation tool is also its ability to allow for user-defined scenario designs, meaning that it facilitates the development and comparison between different alternative scenarios along different optimisation criteria (Østergaard, 2009). This is deeply rooted within the concept of a dialogue model for planning, where the role of energy systems modelling is to inform, present (quantified and qualified) options, and facilitate participatory processes (Lund et al., 2017a).

3.2. Scenario development

The scenarios designed and compared in this study (Fig. 1) consist of a set of reference scenarios and several sets of iterative scenarios developed in support of the Heat Roadmap. This supports both the research aim to explore the effect DH can have on air pollution and other strategic criteria, and also present one alternative scenario in the form of a Heat Roadmap 2050 scenario for Chile (HRCL).

Looking towards 2050, the frame of reference is based on the study developed for Chile's Ministry of Energy, "Proceso de Planificación Energética de Largo Plazo" (PELP) (Ministerio de Energía, 2017a). Table 1 shows the additional data used for the development of the hourly energy systems.

The 5 scenarios given in PELP represent different potential future pathways based on different combinations of assumption variations (including different rates of optimism regarding technology development, projected energy demands and more or less optimistic costs assumptions). Based on modelling done in LEAP (the Long-range Energy Alternatives Planning System), PELP reports both capacities and energy produced for the reference scenarios (Ministerio de Energía, 2017b). To replicate the scenarios using EnergyPLAN, the general approach was to balance for energy produced, and adjust capacities. The exception is two types of hydropower, where the capacity constraints are tighter due to geographical restrictions so the estimated capacity in PELP is considered to be the maximum available. Since part of the modelling in PELP only extends to 2046, the yearly projections and results were linearly extrapolated to 2050 where necessary to align

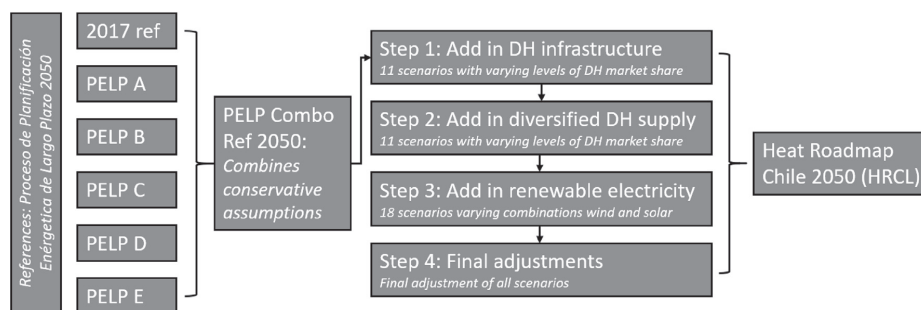


Fig. 1. Overview scheme of scenarios developed and simulated as references and in support of the final Heat Roadmap Chile scenario.

Table 1
Breakdown of the sources for the different technology, energy, and cost data used in the scenarios.

	Data type	Sources used
Time series	Electricity demand	Energía Abierta SEN (Coordinador Eléctrico Nacional (National Electricity Coordinator), 2019)
	Temperature data	Servicios Climáticos DGAC (Dirección General de Aeronáutica Civil (Directorate General of Civil Aviation), 2019)
	Hourly production profiles	Energía Abierta SEN (Coordinador Eléctrico Nacional (National Electricity Coordinator), 2019)
Aggregate data	Production capacities	Based on PELP (Ministerio de Energía, 2017a), (Ministerio de Energía, 2017b)
	Energy balance	Balance de Energía (Ministerio de Energía, 2019) & IEA (IEA, 2017)
	Energy demands & projections	PELP (Ministerio de Energía, 2017a)
	Fuel and CO ₂ prices	PELP (Ministerio de Energía, 2017a), (Ministerio de Energía, 2017b), Biomass reports (John O'Ryan Surveyors, 2016, 2012)
	Investment costs	PELP (Ministerio de Energía, 2017a), (Comisión Nacional de Energía (Chilean) National Energy Commission), 2018) Technology catalogues (Danish Energy Agency and Energinet, 2018; The Danish Energy Agency, 2019, 2018); DH distribution costs for Chile (Paardekooper et al., 2019)
	Emission factors	DEA technology catalogues (The Danish Energy Agency, 2019, 2018), for CCS (Rubin et al., 2015)
	Energy potentials	(IEA, 2017; Ministerio de Energía, 2017a; Poque et al., 2018)

with more common long-term climate and energy benchmarking.

3.3. Combined reference 2050

To have a common ground for the analysis, the 5 PELP scenarios were used to generate a combined reference 2050 scenario (Combo Ref, 2050). The Combo Ref 2050 scenario combines the most precautionary assumptions available to ensure a conservative approach, so the design of the final scenarios is robust even in the face of disadvantageous developments of e.g. technology developments. Specifically, the PELP assumptions are applied that include the exclusion of CCS; inclusion of higher electricity demands to account for shifts in transport; increased valuation of environmental externalities; and medium assumptions for battery technology development, renewable investments, and price developments. This Combo Ref 2050 scenario is both considered as the departure point for the development of the Heat Roadmap Scenarios and as the primary of the reference scenarios to function as a point of reference for comparison.

3.4. Heat Roadmap 2050 for Chile

The sets of scenarios simulated (Fig. 1) are a result of using an iterative approach of simulating multiple scenarios (with differing levels of DH and renewables) for each step, in order to establish the preferred level for the final recommended Heat Roadmap Chile scenario. The final Heat Roadmap Chile 2050 (HRCL) scenario combines the cheapest level of market share for DH and renewables while following the steps outlined in Section 2. The resulting energy demands, selected capacities, heating and electricity supply,

and fuel consumptions are displayed in Table 2 and Table 3.

To determine the cost of introducing DH infrastructure for Chile, results from a purpose-built nation-wide spatial DH model were used. A top-down model allocating heat demands based on a floor area and a regression model resulted in the possibility to estimate the investment costs of a DH distribution network, based on its relation to heat density. This allows for the market share to include the effect of decreasing returns to scale as DH expands into less dense areas. For a full description of the spatial analysis see (Paardekooper et al., 2019). The DH distribution network costs from the spatial model were further combined with costs for branch pipes and heat exchangers and the cost of the supply system.

To design the DH supply specifically for Chile, the availability of local sources of heat and potential for CHPs and LSHPs was simulated. For the availability of excess heat from industry, no appropriate dataset was available so a generalisation to determine the theoretical (Persson et al., 2017) and full recoverable potential was made based on previous studies, notably (Paardekooper et al., 2018b). Based on this, the level of recoverable excess heat in Chile is estimated to provide around 11% of the total DH production (Table 3).

For the case of both solar thermal DH plants and geothermal, no explicit data regarding their potential for the thermal sector existed, although inputs from the PELP identify a maximum potential for electricity generation. Overall, half of the respective total potential defined was assumed available for heat (Table 3), with the remainder available for electricity generation. This is likely to be an underestimation for geothermal, since the identified geothermal potential has far higher temperatures than required for DH (Ministerio de Energía, 2017a), and the more shallow and medium

Table 2

Electricity, heating, and transport demands and electricity and DH unit capacities in selected scenarios.

	Combo 2050 Reference	Heat Roadmap Chile 2050
Demands (TWh/year)		
Electricity (inc. transport)	204	204
Heating	106	106
Transport fuels	131	131
Installed capacities (MWe/MWth)		
Electricity (MWe)		
Condensing power plants	21 517	19 422
CHP plants (electric capacity)	0	10 100
Onshore wind	7576	20 000
Photovoltaic	17 508	17 508
River hydro	4556	4556
Dam hydro	3502	3502
Concentrated solar power	140	140
Geothermal plants	19	848
Electricity total installed capacity (MWe)	54 818	76 076
DH (MWth)		
Excess heat from industry		453
Solar thermal		113
Geothermal		848
Large scale heat pumps		4305
CHP (thermal capacity)		12 625
Boilers		16 320
DH total installed capacity (MWth)	0	34 664

Table 3

Electricity, individual and DH production in selected scenarios.

	Combo 2050 Reference	Heat Roadmap Chile 2050
Electricity (TWh/year)		
Condensing power plants	91.16	22.30
CHP plants (electric production)		22.39
Onshore wind	25.88	68.31
Photovoltaic	43.55	43.55
River hydro	23.09	23.09
Dam hydro	18.97	18.97
Geothermal plants	18.40	18.40
Electricity total supply (TWh/year)	221.05	217.01
Individual heating (TWh/year)		
Biomass boilers	53.00	31.80
Indiv. heat pumps	53.00	31.80
Individual heating total supply (TWh/year)	106.00	63.60
DH (TWh/year)		
Excess heat from industry		3.90
Solar thermal		0.28
Geothermal		1.00
Large scale heat pumps		9.64
CHP (thermal production)		27.99
Boilers		3.50
DH total supply (TWh/year)	0.00	46.31

temperature geothermal typically used in DH (<200°C) is not considered, resulting in a very low share of the heat supply coming from solar- and geothermal (van der Zwaan and Dalla Longa, 2019).

The potentials for CHP and LSHPs were not considered to be geographically limited, and were instead defined by their requirement for operation within the energy system (primarily in function of the electricity system). Both of these capacities (Table 2) are set in the different simulations so that they can both balance heat and electricity in terms of operational strategy and contribute maximally to the flexibility of the system. This means that they operate part load where necessary and can respond flexibly to electricity production from both wind and solar. In addition to determining the appropriate capacities and production levels for these main heat supply categories, the DH was supplemented with boiler capacity to cover the peak hour of demand and a 10% security of supply buffer; in addition, short term storage (equalling 48 h of average demand) was implemented.

As a final step the power capacities were adjusted to reflect the changes that result from the redesign on the heating sector. In particular, this meant decreasing the capacity for condensing power plants, and the maximal utilisation of geothermal energy –

even if only using half of the resources identified in the maximum potential for the generation of electricity. In addition, this included simulating increasing capacities for onshore wind and solar. The complementarity of using these sources must also be noted since the production by each of these types of variable renewable energies might be in direct competition with the other for given hours of the day, despite there being hours where one these resources might be available while the other is not.

Finally, several final alterations were made to all scenarios to ensure alignment and security of supply buffers. Coal was removed from power production in all the non-reference scenarios, to align with current government ambitions to phase out coal by 2040. Biomass consumption was capped at the highest level considered in the PELP scenarios. Similarly, to the security of supply buffer in the heating sector, an additional 10% buffer was added for the condensing power plant capacity.

4. Results and discussion

Using the EnergyPLAN results of the scenario simulations, it is possible to analyse the Combo Ref 2050 in comparison with the

HRCL scenario. The main metrics are the potential market share for district heating, PM to understand the role for decontamination, fuels and CO₂ for decarbonisation, and energy system costs to understand where investments would have to be targeted for such a system.

4.1. District heating market share

In the HRCL, 40% of the heat demand is shifted from the future heating solutions identified in the PELP scenario to DH. This results in the highest level of DH in a same-cost socio-economic energy system in 2050 (Fig. 2), although there is no radically significant increase in cost between a 10% and 50% market share. This represents the increasing costs as DH expands into less densely populated areas. Compared to the perceived potential today, this is partially explained by the high costs of the counterfactuals (individual HPs and (efficient) biomass boilers) and the effect of annualising infrastructure with a long life-span at a socio-economic discount rate (6%).

4.2. Decontamination: reducing PM

Fig. 3 shows that a 40% market share of DH can reduce the PM emissions from heating and electricity by almost 40% compared to the Combo reference scenario, and over 97% compared to 2017. Most of the PM reductions in the HRCL scenario result from decreasing use of individual biomass boilers. Even though future individual boilers are assumed to be far cleaner (10 mg/MJ PM emissions, compared to values today of between 20 mg/MJ (The Danish Energy Agency, 2018), 1600 mg/MJ (Ministerio del Medio Ambiente (Ministry of the Environment), 2018) or even higher (Vicente and Alves, 2018)), the combustion of biomass in a centralised DH boiler or CHPs is even cleaner, with centralised units emitting only 0.3 mg/MJ (The Danish Energy Agency, 2019). The scale of the centralised biomass combustion units in both DH boilers and CHP allows for better (and more cost-effective) flue gas and ash cleaning processes and dust filters to be available. This echoes the findings in e.g. (Giuntoli et al., 2015). This more efficient

combustion is the main driver behind the decrease in PM emissions in the HRCL scenario, and also allows for deeper decarbonisation overall.

Since the impact of outdoor pollution from heating stoves is worst in urban areas, the replacement of biomass boilers in urban areas is likely to be most important in terms of mitigating health impacts. It seems likely that the HRCL scenario would almost fully eliminate the emission of PM from heating in urban areas, because the development of DH is likely to target urban and suburban areas. However, to fully capture the spatial dimension of PM emissions (and through that a more detailed quantification of costs and health impacts and high air quality events avoided), it would be necessary to spatially redistribute the (local) need for CHP and biomass boilers. This is not possible given the current uncertainties regarding local heat sources and future building locations. While the methodology is effective in quantifying absolute emissions reductions, a feedback loop between the national potential for DH and local emissions would be necessary to quantify the impacts of reducing air pollution spatially. In addition, the quantification of the specific impact of reduced indoor air emissions is also not considered within this methodology, since its point of departure is the impact of outdoor air pollution.

4.3. Decarbonisation: fuel mix based on increased efficiency and renewability

The final fuel mix (Table 4) of the HRCL scenario uses 20% less primary energy (PES) for the entire energy system, and significantly reduces fossil fuel consumption compared to the Combo Ref 2050 scenario. In terms of CO₂ emissions from energy, it has the lowest level compared to all the 5 alternatives created in the PELP process and the Combo Ref 2050, which can contribute to the proposed target of greenhouse gas neutrality by 2050.

This efficiency and decarbonisation results from several of the changes made in the HRCL scenario, enabled by the widespread use of DH. Firstly, the availability of an infrastructure to transport heat allows direct use of renewables otherwise not available, such as geothermal and solar thermal energy. This principle is similar for

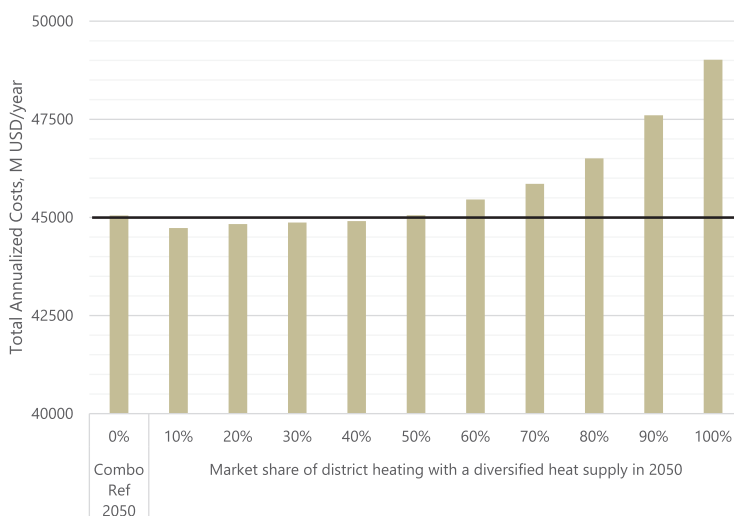


Fig. 2. Total annualised costs for different market shares of DH after integration of a diversified heat supply, compared to the combined reference scenario level (PELP Combo, 2050).

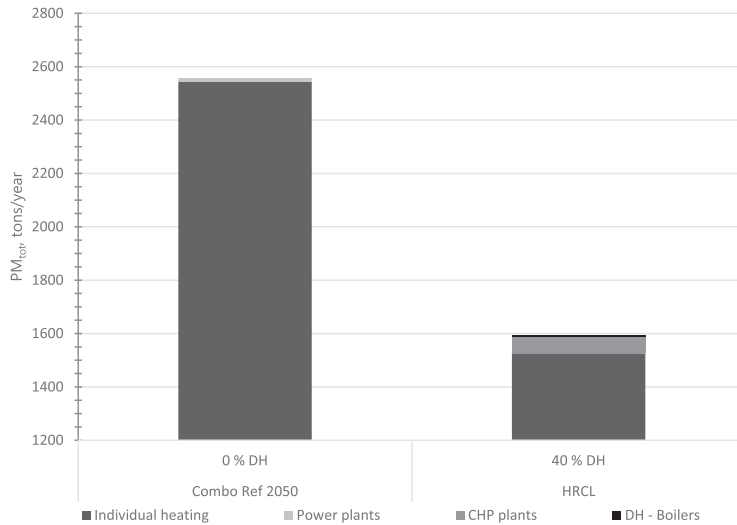


Fig. 3. Sources of particulate matter (PM_{2.5} + PM₁₀) in the Combo Ref 2050 scenario and Heat Roadmap Chile 2050 scenario. N.B. vertical axis starts at 1200 tons/year.

Table 4

Main types of fuel consumption and resulting CO₂ emissions for the energy system scenarios for transport, heating and electricity. CO₂ content of fuels based on (Howley et al., 2011) in (Aalborg University, 2015).

		Combo Ref 2050	Heat Roadmap Chile 2050
Fuels (including transport) (TWh/year)	Coal	118	36.46
	Natural gas	223	219
	Oil	114	58
	Biomass	133	153.43
Fuels Total (TWh/year)		588	467
CO ₂ emissions (including transport) (Mt/year)		123.75	82.26

the use of excess heat sources from e.g. industry and heat from power production, in the form of CHP. If the heating infrastructure is not available to use these sources, they would otherwise go wasted and heat would have to be provided in an alternative way, leading to more fuel use. This also enables substituting coal and oil in the electricity sector with biomass. Secondly, the better integration of renewable electricity sources (e.g. through LSHP and more flexible CHP plants) allows for the further substitution of the (inefficient) combustion of fuels for electricity generation and replacing it with wind and solar, also reducing the overall primary energy supply.

Reducing the reliance on fossil fuels by implementing DH and a higher level of intermittent renewables has further impacts for how the energy system performs in terms of the strategic objectives identified for the Chilean energy system that go beyond decontamination and decarbonisation. Firstly, the reduction in fossil fuels results in less need for imports, ensuring more stability and strengthening the Chilean position towards fuel price fluctuations and geopolitical considerations. Secondly, the increased use of local resources (including local biomass) and construction of renewables further encourages the potential for benefits to arise from the local development of energy and energy technology markets. Finally, the developments in the Heat Roadmap Chile scenario result in a system that is conceptually in line with a Smart Energy System, which in the long run supports and enables a full transition to 100% sustainable energy.

While the potential role for DH is clear, there are some

uncertainties associated with the estimations of the DH potential, especially on a national scale. This is especially the case for the identification of local heat sources, where more spatially explicit data could improve confidence levels. This is an important point for future development, since there are indications in other Heat Roadmap country applications that the level of excess heat may be one of the stronger drivers for the overall local and national potentials for DH (Moller et al., 2019 from a local supply perspective; Paardekooper et al., 2018b corroborating from an energy system perspective across countries). For example, there is a high degree of uncertainty as to what the actual amounts excess heat available are at a local level, since the analysis or datasets that would allow for determining spatially feasible amounts recoverable heat do not, to the authors knowledge, currently exist.

Similarly, further studies would be needed for a more accurate representation of the actual geo- and solar thermal heat potential could be integrated into both the mapping and the modelling. In the case of geothermal energy, the total potential identified is linked to high temperature sources more suitable for electricity generation (Ministerio de Energía, 2017a). Given the location of high temperature geothermal sources, it is likely that there could be a comparative advantage to using them for electricity generation and not for DH; however, shallower sources with lower temperatures that would suit DH better are not necessarily accounted for in the current estimation of potentials.

Likewise, the potentials for solar thermal energy consider a spatial availability linked to photovoltaic production. However, for

these sources, further studies that can give a district heating specific and better quantified potential and a better geo-referencing for these sources could be used to create more refined allocation models and develop the HRCL scenario further. However, given the relatively small impact of these two sources (Table 3), it would seem unlikely that they would change the overall prospective and mechanisms that exist in terms of the national potential for DH to contribute to the reduction of PM emissions.

Lastly, while the Heat Roadmap methodology is in line with and supports full decarbonisation, the application here does not represent a fully renewable energy scenario and does not make additional efforts to decarbonise the transport or industry sectors (where the majority of remaining fossil fuels is still used). If moving towards a fully renewable energy system, this would affect the scarcity and role of sustainable biomass as it could become reserved for the heavy transport/industry sector. This would obviously also affect the heating and electricity sector, and likely result in a higher need for excess and renewable heat utilisation (using DH infrastructure), combined with more intermittent renewable electricity.

4.4. Energy system costs

Fig. 4 indicates that overall, the HRCL scenarios show that DH can be implemented without a significant increase in total energy system costs. However, the structure of annual costs changes. This

shift is primarily because the changes in the HRCL scenario lead to a decrease in (fossil) fuel and exchange costs and a decrease in CO₂ emission costs. Conversely, the overall investment costs are higher in the HRCL scenario. This shift in energy system costs underwrites the attainment of energy planning objectives in terms of reducing fuel imports and sensitivity to price shocks, while also representing increased investments in local resources and local economic development.

Fig. 5 also shows the changes in investment needs at an annualised level for selected technologies. The largest need for investment is for individual HPs since the relative investment costs are high at smaller capacities, and they represent a substantial portion of the remaining 60% of the heating market. However, the required investments for individual HPs (and individual boilers) are reduced in the HRCL scenario, simply because a large portion of the heat demand is transitioned.

The largest single category of required investments for the DH system, on an annualised level, is the installations of heat exchangers at the individual building level. This is because the investment has to be made at every single building, and because the lifetimes are not as long as the other technologies associated with DH. Since the costs for DH transmission and distribution pipes are spread over the lifetime of the infrastructure, they do not represent the main cost of implementing DH when annualised.

Regarding supply technologies for DH, substantial investment is

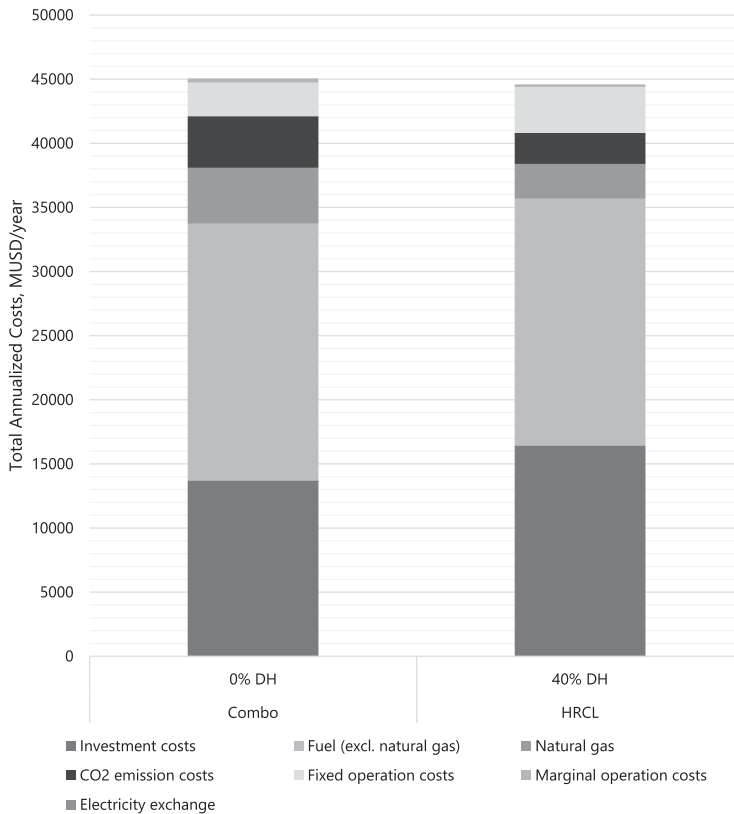


Fig. 4. Total annual energy system costs for the Combo Ref 2050 scenario and the Heat Roadmap Chile 2050 scenario.

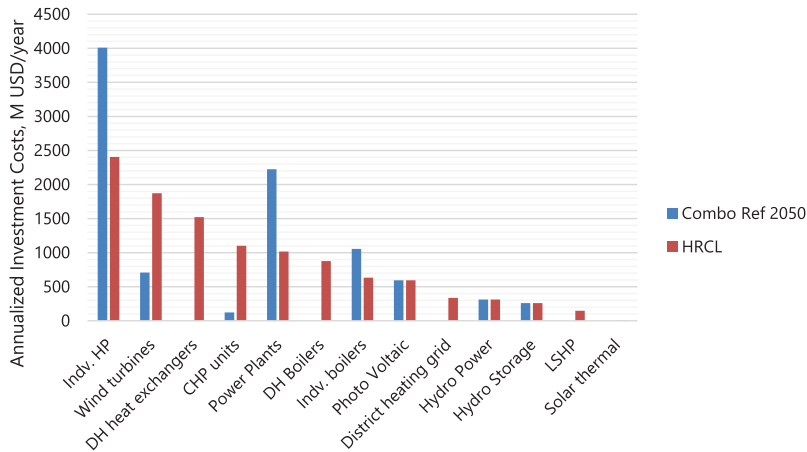


Fig. 5. Changes in annualised investment requirements for selected key technologies for heating and electricity between the Combo Ref 2050 and Heat Roadmap Chile 2050 scenario.

required for both the installation of LSHPs, CHPs (for DH), and DH boilers. The capacities were set to the maximum that was technically useful in terms of flexibility which results in some capacity having very low operating hours. In both the case for CHPs and LSHPs there was a slight economic argument to reduce the capacities slightly and in doing so reduce total annual cost – but the heat supply was then substituted with biomass boilers. Given the overarching objective to reduce air pollution from biomass combustion, and the overall comparability of cost efficiency compared to the reference scenarios, the normative decision was made to maximise CHP/LSHP capacity (and thus minimise boiler utilisation). However, this does imply that it would be possible to design a DH-based system that is cheaper, although it may not fulfil the other strategic objectives of air pollution reduction and decarbonisation as strongly.

The final important shift regards the investments needed to enable the transition in the electricity sector that is proposed in the Heat Roadmap scenario as a result of the higher level of flexibility through the sector interconnections. The required investments for large power plants are obviously reduced, while the investments needed for (onshore) wind turbines is more than doubled.

The transition to a HRCL based scenario would radically increase the amount of investment and market potential for some technologies (including DH related technologies and wind power), while simultaneously reducing the need for others (such as large power plants, and of course the different fuel transporting industries). Since it is very differently structured it is likely to be necessary to reallocate costs and benefits from different stakeholder in the value chain. To enable this, encourage investments where necessary, and avoid stranded assets in the long run, it is important to have scenarios that can make these quantitative impacts explicit, and support a long-term integrated energy planning approach that can support this process.

4.5. Implications

The purpose of this study has been to analyse the potential for DH to contribute to the reduction of air pollution on a national scale, by preventing the need for local biomass combustion in biomass boilers. This is done by analysing the impact and potential

of DH through the adaptation of a methodology that combines outputs of local mapping with (hourly) energy system scenario development to create and quantify alternative scenarios. The Heat Roadmap Chile scenario presented focusses on efficiency in heating, including the option of using infrastructures for heating so as to use local resources and exploits synergies with the electricity sector to analyse wider impacts.

Using the Heat Roadmap methodology, a scenario is developed for Chile in EnergyPLAN that shows that the DH market potential could be at least 40%, and reduce PM from heating, radically, compared to alternative solutions. A 97% reduction in PM emissions compared to today would hugely contribute to eliminating the yearly 3500 deaths nationally due to outdoor air pollution. However, it is important to note that there have been few national-level datasets developed regarding the heating sector specifically, so there is potential to increase the validity on the findings if assumptions for available excess heat and (geothermal) renewable energy potentials could be improved. While it is difficult to quantify the health and cost savings impact of reducing PM without more detailed spatial data, it is clear that by recovering excess heat from industry and CHP, utilising LSHP, and combusting local biomass resources in larger, centralised, cleaner facilities the overall emissions of PM from heating and electricity can be reduced by 40% compared to electrification and individual stove efficiency approaches, and more than 97% today. The application of the methodology in Chile also confirms the potential for DH to contribute to the decarbonisation of the energy system at similar cost. The success of this relies on a full redesign of not only heating, but also the electricity system to be able to take advantage of the synergies that are created as the thermal and electricity sectors become more interlinked.

The results show that, particularly in urban areas, DH can contribute to a deeper decontamination and decarbonisation of the heating sector, and should be considered complementary to the current approaches (which focus on increasing the thermal performance of buildings; introducing efficient electric heating and HPs and more efficient boilers, policies that can support and formalise biomass markets, etc.). This is especially important when viewing heating within a social context with regard to energy poverty and indoor air quality (Reyes et al., 2019). These findings

also highlight the need to develop tools and methodologies that can consider the local and national character of the heating sector in the context of the wider energy system, while being able to address different and multiple strategic energy planning objectives.

5. Conclusions

Using Chile as a case, this has been the first known application of the Heat Roadmap methodology outside of Europe, with a particular focus on achieving outdoor air pollution decontamination as part of the strategic energy planning objectives. Moreover, it shows the potential of a methodology applied in a broad international context, with mutability towards different planning objectives. This highlights the potential that the methodology has to further explore options for how to address carbon emissions, air pollution from energy, and biomass dependency in other countries as well.

This has also been the first national-level assessment of the potential for DH in Chile. In this way, this study builds on methodologies and results developed in a European context, investigating the potential of DH to contribute to the decarbonisation of the energy system, but also addresses the key objective of decontamination for the Chilean energy planning context.

The use of DH in the Heat Roadmap Chile has as a two-fold function to both decarbonise and decrease outdoor air pollution from the combustion of biomass solids. This is in many ways distinct from the role DH has been considered in from a European context, where the focus has been on energy efficiency and decarbonisation. This paper suggests that in countries where heating is mostly based on the (inefficient) combustion of local biomass resources, DH has a different role to play than in most places where its potential has been studied. This is partially because the heating sector is already largely decarbonised, so any benefits in terms of fossil fuel reductions result from the interconnection with the electricity sector. However, the role is mostly different since the strategic planning objective in these countries is often to reduce PM emissions to address (outdoor and indoor) air pollution, and the issue of decontamination is much more important than decarbonisation of the heating sector. Looking specifically towards the role of bioenergy in such energy systems, the discussion could be furthered by studying the role of heating within a 100% renewable energy system, since here bioenergy resources may need to be redirected towards transport, material, and certain industrial purposes.

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CRedit authorship contribution statement

Susana Paardekooper: Conceptualization, Methodology, Formal analysis, Project administration, Writing - original draft, Writing - review & editing. **Henrik Lund:** Supervision, Writing - review & editing. **Miguel Chang:** Conceptualization, Methodology, Formal analysis, Writing - review & editing. **Steffen Nielsen:** Conceptualization, Methodology, Formal analysis, Writing - review & editing. **Diana Moreno:** Conceptualization, Methodology, Formal analysis, Writing - review & editing. **Jakob Zinck Thellufsen:** Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to

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APPENDICES

APPENDIX D. PAPER 4

Aggregated versus disaggregated energy system modelling approaches: The case of Chile's energy system [4]

APPENDICES

Aggregated versus disaggregated energy system modelling approaches: The case of Chile's energy System

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ABSTRACT

The purpose of this paper is to compare energy system modelling approaches, taking the case of Chile's national energy system as a case. The Chilean government aims to decontaminate the heating sector and decarbonize the country's electricity generation by integrating more variable renewable energy sources into the energy mix. The availability of these sources is widely dispersed and not always located in proximity of high demand areas. This geographical spread affects the potential flexibility to be gained when considering scenarios with integration of energy-intensive sectors, like the electricity and heating sectors, and supplying them with fluctuating renewables. The integration of these sectors can be represented by either aggregated countrywide energy system models or with distinct interconnected models that capture local nuances of variable supply sources and demands, and the dynamics of electricity transmission between different areas. Under this context, this paper presents a comparison of a case where the country is represented as a single aggregated copperplate, using the EnergyPLAN modelling tool. For the interconnected approach, a combination of distinct EnergyPLAN models in conjunction with Power-Flow analysis are used applying the EPlanFlow tool. The results of this comparison show the trade-offs of each approach, namely a marginal gain in detail with additional analytical effort but overall congruent results on the country level.

KEYWORDS

Energy system analysis; Energy modelling; Model coupling; EnergyPLAN; Power flow; Decarbonization & decontamination; smart energy systems.

1. INTRODUCTION

The prospects of sustainable development and climate change are main driving forces for countries worldwide to shift towards clean and sustainable energy sources. In Chile this shift is of particular importance, given that residential heating is the main cause of air pollution [1], reaching hazardous levels for human health above those recommended by international guidelines and among the highest in the region [2]. Moreover, Chile's energy system is currently supplied with large shares of fossil fuels, making up around 67% of the primary energy supply (PES) in 2017 [3]. These issues have led Chile's government to develop actions and long-term plans to tackle both air pollution decontamination [4], and the decarbonization of the energy system [5,6], as well as to address these issues by considering different technology alternatives like district heating (DH), cogeneration through combined heat and power (CHP), and further integration of renewable energy [7–9].

In a broad context, these action plans are typically assessed using modelling approaches in order to quantify the impacts of different projected or desired changes in the energy system. In Chile,

the official long-term national plans have been based on modelling scenarios which combine different energy demand developments across different sectors, adopt energy efficiency measures and technologies, utilize the geographical disaggregated renewable energy potentials and projected system costs and fuel prices [6]. However, this study does not consider in detail, among other things, the potential of heat recovery from thermal power plants, nor DH, despite the latter being a proven solution in other locations for both air pollution decontamination [10,11] and decarbonization [12–14], as well as being an enabling element in sector coupling and integrating variable renewable energy sources (VRES) [15,16]. Other studies assess the potential of increasing the shares of VRES in the energy system and accomplishing emission reductions by using disaggregated optimization [17–19] or with integrated assessment models [20], although only focused on the electricity sector. Similarly, other efforts have focused on assessing specific renewable potentials and developments rather than taking a wider system approach [21–23]. In the working paper by [24], national scenarios are developed using a cross-sectoral modelling approach which considers the impacts of coupling the electricity and heating sectors, and utilizing both CHP and DH as potential solutions to the above-mentioned issues. However, the model developed in [24] only represents a national aggregated system, limiting the analysis of geographical locality and availability of resources, and the existing bottlenecks in the electricity transmission systems. Other cross-sectoral approaches integrating VRES have also followed a national aggregated approach to assess the future redesign of the energy system [25]. Following a 2-dimensional approach with both cross-sectoral integration and geographical interconnectivity, has been shown to provide a better overview of local nuances of the energy systems in a European context [26–28], however, to date no study of this kind has been identified for Chile.

In this paper, a 2-dimensional approach to model Chile’s energy system is presented which identifies the potential of cross-sectoral interconnection – namely in the electricity and heating sectors – while also considering geographical factors such as the interconnectivity between local systems, and the locality of resources and demands. This is then compared to a single, aggregated approach to identify if there are any trade-offs between each of the approaches, when analysing potential designs of a cleaner and geographically vast national energy system.

2. METHODS

In this section the methods and assumptions used in the analysis are described. These take as point of departure the national energy system scenarios presented in [6], and further developed in [24] to assess the potential of CHP, DH and increased in penetration of VRES in Chile.

2.1. Energy system modelling

In order to analyse Chile’s future energy system, a modelling approach was followed in which simulations of the energy system were conducted to generate different future scenarios representing redesigns of the energy system. This was done primarily using two freeware tools coupled together: EnergyPLAN [29] and EPlanFlow [30].

In EnergyPLAN, national and/or regional energy system models can be developed as single aggregated entities or nodes. EnergyPLAN simulates the operation of these systems and balances their energy supply and demands on an hourly basis while minimizing the amount of electricity imports/exports to the system. The main inputs used by this modelling tool are annual energy demands for electricity, heating, transport and industry; hourly time series of the electricity demand, heating demand, and variable renewable energy production; as well as the capacities and efficiencies for the different energy conversion technologies. In addition to the above, investment costs, operation costs, fuel prices, CO₂ prices, and emission factors are also considered [29].

Complementing the analysis done with EnergyPLAN, the EPlanFlow tool was used to conduct a geographically disaggregated analysis of the energy system with the additional dimension of considering the impacts of energy transmission. With this tool, multiple EnergyPLAN models can be connected as nodes, and the power flow between each node can be optimized to minimize marginal electricity costs, in line with the constraints of line capacity in the electricity transmission network. The resulting import/export flows are fed back to EnergyPLAN, which then simulates the operation of the system accordingly with these new inputs [30].

2.2. Design principles and scenario development

A key consideration for designing the scenarios in this study was to be able to identify trade-offs of modelling under a single national copperplate energy system versus multiple nodal systems with distinct demands, supply sources and electricity transmission constraints. Moreover, this had to be done under the context of also assessing the potential for cross-sectoral integration. For that reason, the scenarios considered in this study were built up from those developed in [24], which presents a national “Heat Roadmap” for the year 2050 and the only national energy scenario to-date with high integration between the electricity, heating, transport, and industry sectors along with high penetrations of VRES and district heating uptake, in congruence with current air decontamination and decarbonization goals held by the Chilean government.

The formulation of this parting scenario is based upon the Heat Roadmap Europe methodology and work towards the concept of Smart Energy Systems, as outlined in [16,31,32]. On those premises, the scenarios presented in [24] use as basic design principles the following considerations:

- 1) Using geospatially explicit heat demands to determine aggregated DH network costs and heat losses at different levels of market uptake.
- 2) Determining the effect on the energy system of introducing basic DH infrastructure (DH boilers and network pipes).
- 3) Including diversified DH supply sources in the mix to benefit from cross-sectoral synergies and from efficient heating technologies and renewable sources (e.g. surplus heat from industry, cogeneration plants, heat pumps, geo- & solar thermal heat, etc.).
- 4) Integrating VRES and adjusting capacities according to the gained system flexibility from having diversified heating sources and cross-sector integration, while allowing enough backup capacity for security of supply.

In line with the above, two main comparison approaches were considered for the scenarios.

Aggregated scenario approach. An aggregated scenario was constructed on the basis of the principles outlined above. The scenario models a completely aggregated national energy system, in which electric interconnectors are not considered within the country. In turn, the model does not distinguish the locality of supply sources and their actual potential to cover specific local energy demands, but rather favours a streamlined approach to assess the overall system as a copperplate model.

Disaggregated scenario approach. The disaggregation considers a split of the Chilean energy system into 4 parts, corresponding to the separated systems present in Chile up to the year 2017, which can be seen in Figure 1 (two of this – SING and SIC – which are interconnected as of that year by a 1500 MW interconnector to constitute the Sistema Eléctrico Nacional “SEN”). Each of these systems are then individually modelled, starting from the reference scenario established in [24] but split according to their projected energy demands. This split is done so that each system has an approximately representative share from the national total energy demand, as suggested in [33]. Each geographical aggregation is then redesigned according to

the principles outlined above for the copperplate national model. These systems are then taken as nodes in the EPlanFlow tool to optimize their import/export flow.

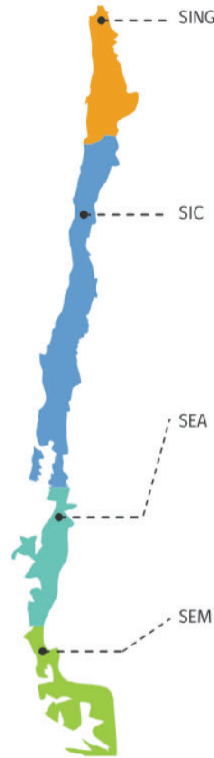


Figure 1. Geographical depiction of Chile's disaggregated systems (up to the year 2017) [34].

It must be noted that, as mentioned, only SING and SIC are interconnected. In contrast, the southernmost systems, SEA and SEM, currently operate with no interconnection either between each other or with the other two systems.

For this reason, the following scenarios were explored: 1) Aggregated country model; 2) A disaggregated approach with the 4 systems modelled without considering interconnection capacity; 3) A disaggregated approach in which the 4 systems are fully interconnected; and, 4) A disaggregated approach modelling the existing interconnection between only two systems (SING-SIC). In the case in which all the systems are interconnected, the assumption of having an interconnection equivalent to a minimum of 10% of the installed capacity will be followed, as suggested by other international power market guidelines for security of supply purposes [35].

2.3. Performance comparison

The performance of each scenario was analyzed by comparing some key outputs from the modelling. Namely, the total primary energy supply (PES), CO₂ emissions, and critical excess electricity production as a percentage of the electricity demand (i.e., the theoretical electricity production that would otherwise be curtailed).

2.4. Modelling inputs and assumptions

To adequately replicate and subsequently disaggregate the scenarios presented in [24], the national energy databases were used to identify the energy balances, geographical locality of power conversion units and their hourly production profiles [36], as well as fuel prices, and variable operational costs [37,38]. The projections for energy demands and investment costs of renewable energy technologies were supplied from [6], while the geographically disaggregated heat demands were extracted from [24,39]. The projections mentioned above were reported up to the year 2046. In the case of the scenarios developed in this study, the year of analysis considered is 2050, as this is the year up by which international targets must be met [40]. Thus, the projections were linearly interpolated up to the year 2050 when necessary.

The geographical and technical potentials were gathered from [6], which included the resource availability for solar, wind, hydropower, and deep geothermal for electricity generation for two of the systems (SING and SIC). The potentials for the other two systems (SEA and SEM) were only explicitly defined for wind energy, as per local reports presented in [41] and [42], respectively. At the time of this study, no potentials or sources for geothermal heating have been assessed in Chile. The latter are of importance since they can be used as a baseload supply source used for district heating, as has been found in cases elsewhere [32,43]. Given this limitation, an assumption of the available geothermal potential for heating is made whereby an equivalent potential to half of the geothermal for electricity generation is considered, based on the assumptions from [24].

Similarly, assessments of the potentials for using surplus heat from industry in district heating are lacking in Chile. To bridge this gap, the potential for recoverable heat suggested in [32,44] were considered, and used as recoverable fraction from the industrial energy demand as per [24]. In the case of the projected productions and capacities in 2050, aggregated estimates were used. For that reason, the disaggregation not only was conducted on a system level according to the respective share of energy demand in the 4 systems, but also in terms of the dividing the total installed capacities and productions to the different conversion technologies. In line with this, the share of the potentials for each technology were applied when available from [6] to allocate the aggregated installed capacities, otherwise the current shares of installed capacity were considered with their existing fuel distribution shares, namely for the case of the SEA and SEM systems [34].

An overview of the distinct input assumptions for the potentials of the different technologies and the demands in the modelled systems is provided in Table 1.

Table 1. Overview of assumed technical potentials and demand estimates considered.

Potentials/Demands	Unit	System nodes			
		SING	SIC	SEA	SEM
Wind		11.5	25.1	2.2	5.9
Solar PV		684.1	145.0		
Solar CSP		480.9	29.1		
River hydro	GW	0	6.1		
Geothermal (el.)		1.0	0.7		
Geothermal(heat)		1.0	0.7		
Solar thermal		461.8	97.8		
Surplus heat		3.9	0.7	3.1	0.1
Heat demand	TWh	12.4	84.1	1.3	0.7
Electricity demand		30.2	145.8	1.5	4.6

3. ANALYSIS & RESULTS

3.1. Scenario setup

Based on the approach and data assumptions described in the previous section, EnergyPLAN models were generated for the analysis. These EnergyPLAN models represented 5 systems: one aggregated copperplate model for the whole country, and 4 models representing the country as disaggregated systems. In order to perform the analysis, the power flow constraints representing the existing and assumed transmission capacity for the latter disaggregated systems had to be defined. These electricity transmission constraints are shown in Table 2.

Table 2. Matrix of existing and assumed interconnector capacity between nodes, based on [6], and in brackets the estimated assumptions of suggested interconnection capacity from [35].

Interconnection [MW]	SING	SIC	SEA	SEM
SING				
SIC	1500			
SEA	0	0 {6.1}		
SEM	0	0	0 {10.7}	

The Matrix presented in Table 2 shows the different possible interconnection scenarios that were used in the analysis. Other than these, the scenario setup for each of the different system nodes were based on the final scenario from [24]. That is, the scenarios represent a Chilean energy system with cross-sector integration where each of the macro regional nodes have varying levels of district heating, high renewable shares, and some use of excess heat in their district heating grids. In addition to these, reference scenarios with no sectoral interconnection are also considered as a benchmark of comparison based on [6,24]. These reference scenarios further illustrate the impacts of cross-sectoral integration on the interconnectivity across the different nodes, and are presented in Section 3.3.

3.2. Aggregated versus disaggregated energy system comparison

Using the constraints outlined as part of the scenario setup, it was possible to gather the results from EPlanFlow, and compare the results of running the country model as one or in its 4 main systems with and without full interconnection. This comparison of the scenarios is highlighted in Table 3.

Table 3. Comparison of primary energy, CO2 emissions and curtailment.

Indicator	Unit	Aggregated	Disaggregated			
			No interconnector	Existing transmission	Fully interconnected w/ constraints	Fully interconnected w/o constraints
Primary energy	TWh	629.4	650.5	650.5	650.4	649.8
CO2 emissions	Mton	74.7	76.1	72.74	72.74	72.77
Curtailment	%	4.40%	5.05%	4.48%	4.47%	4.43%

As illustrated in Table 3, and presented in more detail in Figure 2, it is possible to achieve lower levels of primary energy supply and CO₂ when a degree of interconnection is in place. This is due to the exchange of electricity that is tapped from renewable potentials across the systems, which displaces part of the fuel consumption. While these benefits can be readily observed from the results of the analysis as a gain in efficiency in primary energy supply, it is clear that the scale of these differences is relatively small.

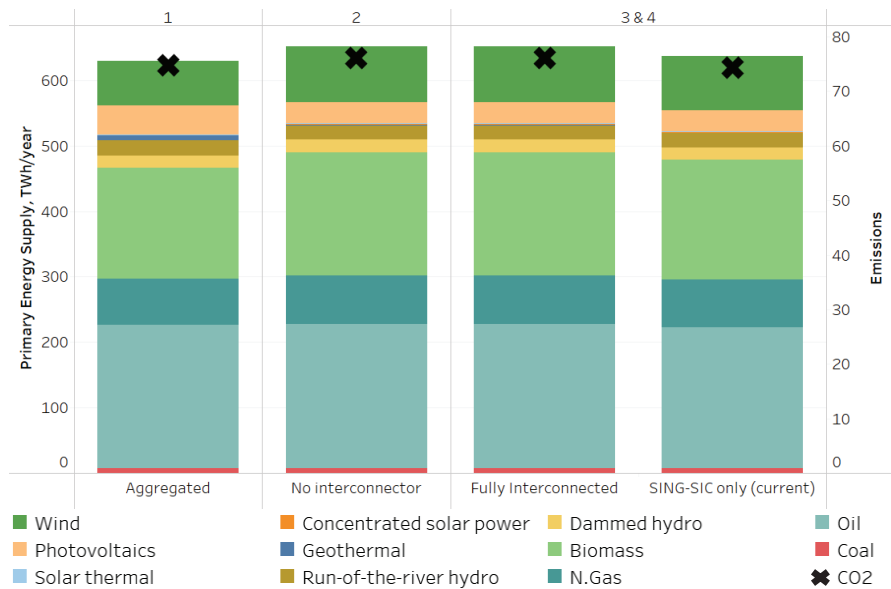


Figure 2. Comparison of PES and CO₂ emission for the 2050 aggregate and disaggregated scenarios.

This relatively small impact translates to other fronts. As illustrated in Figure 3, a relatively small difference can also be observed in the total annual costs of the systems when taking as a reference of comparison the aggregated country model.

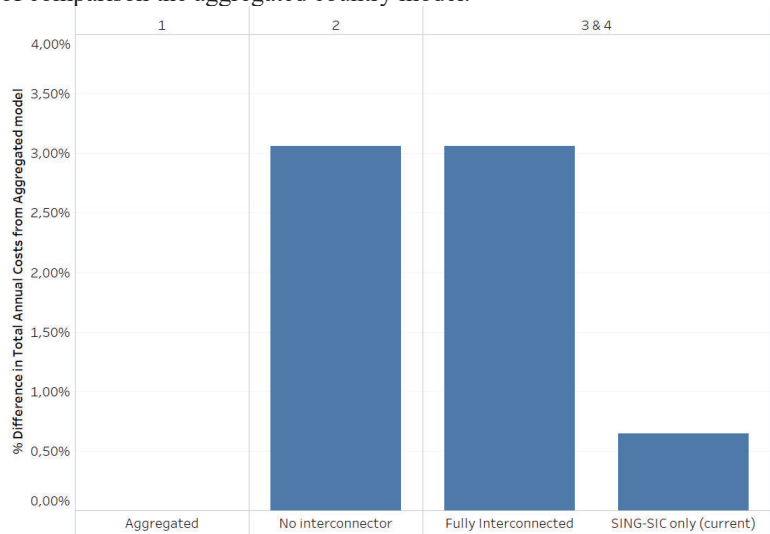


Figure 3. Percent differences in annual system costs relative to the aggregated system model.

3.3. Impacts of cross-sector integration

Although some of the observed difference seem rather small across the different interconnection scenarios, these can partially be attributed to the additional degree of flexibility from having district heating infrastructure and thermal storages embedded in these scenarios. Therefore, it is important to compare the operation of the system under different conditions. For example, when considering the reference scenarios outlined in [6,24], the system will be less able to integrate variable renewable energy sources into not only its electricity demand, but also into the demands for space heating. Figures 4 and 5 illustrate the comparison of both cases for the different interconnection scenarios, showing primary energy supply as a benchmark indicator.

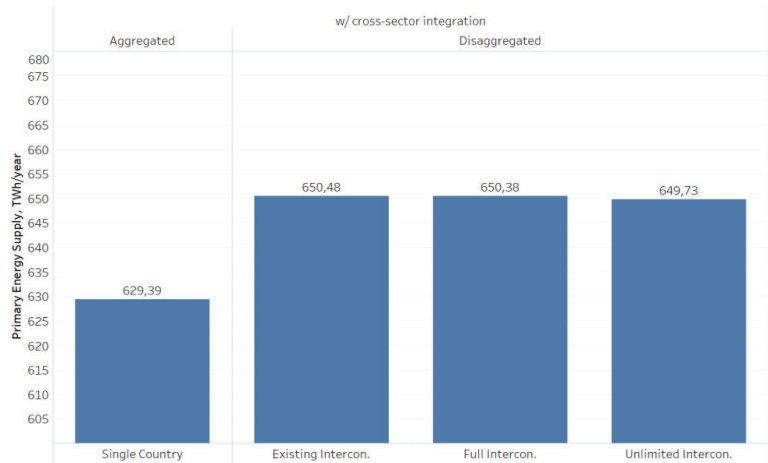


Figure 4. Comparison of PES for aggregate and disaggregated scenarios assuming cross-sector integration with district heating infrastructure



Figure 5. Comparison of PES for aggregate and disaggregated scenarios assuming no cross-sectoral integration with new infrastructure.

As shown in Figure 5, higher energy consumption is expected relative to the scenarios with district heating presented in Figure 4, since these do not yet consider efficient energy solutions in the systems. However, a slightly more pronounced difference can be seen across the different

interconnection scenarios. In Figure 5, since no cross-sectoral interconnection is yet considered, a lower potential is in place to utilize the excess electricity in the respective nodal systems. This leads to lower underestimation of the primary energy supply in the system when considering an aggregated copperplate model as compared to the interconnected scenarios that do capture some of the bottlenecks and additional need for primary fuel consumption. Figure 6 further illustrates this case, showing the differences in the theoretical excess electricity production, which would have to be curtailed across the different interconnection scenarios for both the cross-sector integrated cases and the disaggregated reference case from [6,24] with no cross-sectoral infrastructures.

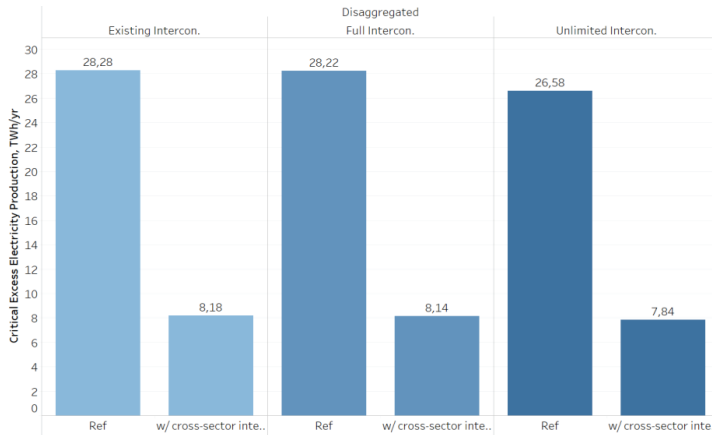


Figure 6. Comparison of PES for aggregate and disaggregated scenarios assuming cross-sector integration with district heating infrastructure

Across the different interconnection scenarios for each of the respective cases shown in Figure 6, small differences can be seen. However, when comparing across cases, the systems with district heating integration have a much theoretical excess electricity production. This means, that the energy system design allows for better utilization of variable renewable energy which causes in this potentially lower curtailment levels. The hourly profile presented in Figure 7 shows some of the nuances in the expected hourly curtailment for a 48-hour period. For example, it shows a more cyclical behaviour in the sector coupled cases due to the use of district heating infrastructure and storages. However, since more renewable capacity is in place, it also has curtailment in additional hours where the reference system is in balance.

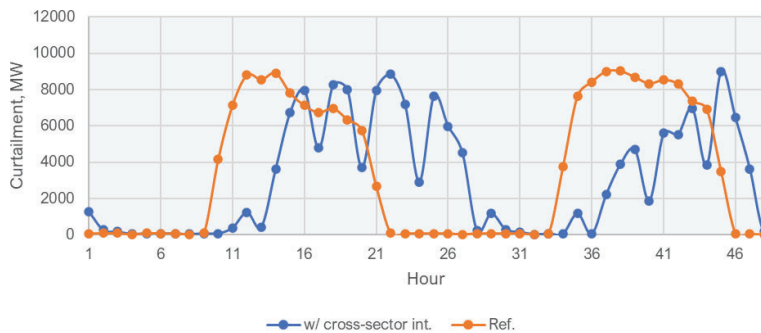


Figure 7. Comparison of PES for aggregate and disaggregated scenarios assuming cross-sector integration with district heating infrastructure

4. DISCUSSION

4.1. Trade-offs between modelling approaches

The results show that by following a 2-dimensional approach, where both cross-sectoral integration and geographical interconnection are considered, provides some insight into the gains of interconnectivity. For instance, the results show some differences between modelling isolated systems and an interconnection approach, that can be illustrate the potential role that implementing certain renewable energy technologies can play on lower geographical aggregations due to the local quality of supply. However, with mismatching renewable supply sources to the demands potential flexibility gains can be downplayed.

Nonetheless, the results show that these differences are not significant in the larger scheme of the national energy system, especially when considering systems with high levels of flexibility due to having in place enabling infrastructure and cross-sectoral synergies. So, although differences do occur, one could argue that for national planning an aggregated model does provide enough resolution to steer specific planning aspects of the energy system towards valuable insight at a lower analytical cost.

4.2. Robustness of assumptions

When conducting the disaggregation of the scenarios a number of assumptions had to be made about parameters with no finer resolution than the national level, as was the case for the potentials of solar thermal, transport demands, excess heat among other. The projected energy demands for each of the 4 systems had to be used as proxy for making a split. While this provides a reasonable estimate for the purpose of this modelling exercise, it widens the degree of uncertainty present in the results. Thus, further detail would be needed about the actual geographical potentials in order to make better assessments of the disaggregated analyses presented here.

In a similar manner, basing the scenario development on a previous study yielded somewhat divergent results when attempting to replicate the results with the disaggregate models. These differences can be traced to the additional detail used in modelling. This was the case for the distinct hourly distributions in each one of the systems, as well as district heating cost curves and technical potentials available for renewable energy sources, which were based on local data rather than country aggregates.

4.3. Further work

Some of limitations of this study have been discussed so far. These include the assumptions made and the steps followed when developing the scenarios. Further work would be needed to gather more geospatially detailed information for a more accurate split of the Chilean energy system, and for a better allocation of its potentials and demands. Furthermore, the scenarios developed could be supplemented by exploring an even higher degree of cross-sectoral integration, in the form of a Smart Energy System [16], along with the geographical electricity interconnectivity.

5. CONCLUSIONS

In this study, the Chilean energy system was represented both using an aggregated country model and a geographically disaggregated model with multiple interconnected nodes. The purpose of comparing these two approaches was to identify potential trade-offs between selecting each modelling approach when it comes to analysing the potential integration of renewable energies. Moreover, the analysis allows to assess some of the implications of having a finer geographical resolution when modelling an energy system and assessing its potential for cross-sectoral integration at a national level. In the case at hand, small differences were

observed between the two approaches, namely a small underestimation of the potential for renewable energy integration and primary energy efficiency gains in the aggregated country approach. These differences can be explained by the mismatch between available energy supply sources dispersed throughout the country and the demands modelled in the systems, which have different critical mass in the country's southern regions and bigger cities. Consequently, a major benefit of the 2-dimensional approach is the additional insight and level of detail gained from having a geographical representation closer to reality. That notwithstanding, the small difference in results could bring into question the additional analytical effort and data requirements of the 2-dimensional approach when having a broad assessment of a national energy system.

ACKNOWLEDGEMENTS

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APPENDIX E. PAPER 5

Smart energy approaches for carbon abatement: Scenario designs for Chile's energy transition [5]

Smart energy approaches for carbon abatement: Scenario designs for Chile's energy transition

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Abstract

This study develops scenarios aiming to transition the Chilean energy system in 2050 to 100% renewable energy; taking into account local resource potentials, demands, cross-sectoral integration of the electricity, heating, transport, and industrial sectors, and synergies in their related infrastructures. The energy system model EnergyPLAN is used to simulate the hourly operation of the energy system. The relationship between potential CO₂ emissions reductions and relative costs is estimated using marginal abatement cost curves with the EPLANoptMAC tool to assess the optimal sequence of capacity expansion and carbon abatement alternatives. The analysis demonstrates that it is possible to carry out this transition from a technical perspective more efficiently than what is proposed with current national scenarios while still aligning with climate neutrality targets; and that, in different phases of the Chilean energy transition, specific options could be prioritized based on an improved balance between carbon abatement and costs.

Keywords

Smart energy systems; Energy system analysis; EnergyPLAN; EPLANoptMAC; Model coupling; Marginal abatement cost curve;

1. Introduction

Countries worldwide are shifting towards clean and sustainable energy sources as part of a green energy transition. In Chile, this shift is of particular importance due to the country's issues with air pollution resulting from the inefficient combustion of fuels in the heating sector [1,2], and historical dependence on fossil fuel consumption and has had problems in the past securing natural gas. Chile's energy system is currently supplied with large shares of fossil fuels, making up around 67% of the primary energy supply (PES) in 2019 [3]. In response, Chile's government continues to develop long-term plans to tackle both air pollution decontamination [4] and the decarbonization of the energy system with secure energy supply sources [5,6], as well as specific climate actions which consider diversified technology alternatives like district heating (DH), cogeneration through combined heat and power (CHP), and further integration of renewable energy [7–9].

The country's legally established process of long-term energy planning (PELP) outlines potential scenarios corresponding to different expected energy demands and technology developments across end-use sectors. The current PELP scenarios include the adoption of different technologies, policy measures, technology costs, and fuel price developments to illustrate potential carbon neutrality pathways [10]. Yet, key enabling technologies and infrastructures are not fully represented in such national scenarios. Technologies such as district heating and Power-to-X (PtX) pathways for electrofuel production could prove essential in the transition towards a decarbonized energy system [11–13], as well as enabling

sector coupling and integrating variable renewable energy sources (VRES) as secure and locally available energy sources [14,15]. Thus, it is imperative to consider these options for the future of Chile's energy system.

In the context of Chile, past studies have assessed the potential of increasing the share of VRES in the energy system and accomplishing emission reductions through disaggregated optimization [16–18] or with integrated assessment models [19], but focused exclusively on the electricity sector. Similarly, [20–22] have focused on assessing specific renewable potentials and developments rather than taking a broader system perspective. More recent studies have actively considered system and cross-sectoral integration. Paardekooper et al. [23] developed national scenarios using a cross-sectoral modelling approach that considers the impacts of coupling the electricity and heating sectors, excess industrial heat, and utilizing CHP and DH as potential solutions to the issues mentioned above with a particular focus on the impacts of heating scenarios to reduce particulate matter emissions. Osorio-Aravena et al. [24,25] go beyond, analyzing 100% renewable energy scenarios for the power, heat, transport, and desalination sectors. However, the scenarios reviewed are not necessarily aligned with standard practices and tools used in Chile's nationally determined contributions (NDCs) plans [26] and most current energy planning process [10], including the use of marginal abatement cost (MAC) curves as means to show decarbonization priorities with explicit technological detail and system effects.

MAC curves in climate and energy policy are widespread, serving as tools to easily visualize the costs per unit of emission reductions for varying amounts of emission abatement and measures [27,28]. However, the application of MAC curves can have shortcomings in representing individual measures' costs and abatement potentials without a holistic system view, as is the case in Chile [26,29]. Likewise, when applied with energy system models, MAC curves will be limited and contextualized to the modeling tool's specific configuration and system resolution [30]. Studies have used MAC curve approaches to assess CO₂ abatement in the power and heating sectors [31–34], transport [35–37], industry [38], and all sectors representing the energy system as time-slices [39–41]. However, bottom-up representations of the energy system with an hourly resolution including all sectors can provide a more systematic and representative view of abatement potentials in the transition towards highly renewable energy systems [42]. While model-based MAC curves have been used in sector coupling scenarios [43], no prior application of these has been found to identify CO₂ reduction measures while incorporating a Smart Energy Systems approach or outside of a European context.

In this paper, we put forth alternative decarbonization scenarios for Chile's energy transition based on the Smart Energy Systems concept, which focuses on the integration of the whole energy system by including all sectors – with their synergies and related infrastructures – to find suitable energy efficient and cost-effective solutions to reach a low carbon energy system [15]. Here, this is formulated via a set of design principles and steps modelled as scenarios by simulating the energy system. Subsequently, this approach is complemented by designing optimized abatement scenarios yielding a marginal abatement cost curve, which – in turn – can graphically showcase the priority of the different measures relative to their cost-effectiveness and potential for CO₂ abatement, considering a system perspective.

In this way, the scenarios can be better assessed in line with Chile's current national determined contribution (NDC) targets and long-term energy planning process, presenting the different measures under a transparent and easy-to-visualize framework that can support policy-makers in designing energy transition strategies and supportive policies towards an alternative decarbonized future energy system. In addition, the application of the methodology presented in this paper illustrates how coupling modelling approaches can provide both different yet complementary perspectives to addressing a national energy transition more comprehensively than with a single-model approach.

2. Methods and research design

This section describes the methods and assumptions used in the analysis. First, the energy system analysis and models' descriptions are presented. Then, the principles behind the initial

scenario development are outlined. An overview of the data used across the modelled scenarios is also included, with additional details included as supplementary material in the Appendix.

2.1 Energy system modelling with EnergyPLAN

The scenarios presented in this study are formulated with the energy system modelling tool EnergyPLAN [44], which is a widely validated and used tool to simulate and analyze the operation of national energy systems, including the electricity, heating, transport, and industry sectors [45]. It simulates the operation of the entire energy system, hourly balancing the supply and demand, including the system's imports and exports of electricity. Scenario inputs include annual energy demands, aggregated capacities of conversion units and plants, and hourly time series for variable renewable energy production and electricity and heating demands. In addition, EnergyPLAN also includes investment and operation costs, fuel prices, CO₂ prices, and different emission factors [44,46]. Moreover, the tool can serve as a core calculation engine for simulation-based optimization models and has been coupled with several other optimization algorithms and energy system models [47].

In the present study, the Chilean energy system is modelled in EnergyPLAN, considering different scenarios for carbon abatement. These scenarios include the scenarios from Chile's long-term energy planning process and newly formulated scenarios applying a Smart Energy Systems approach to reach a 100% renewable energy system [15]. Furthermore, EnergyPLAN is used to develop the MAC curves in conjunction with an optimization algorithm, in order to identify alternative abatement priorities, as explained in the following section.

2.2. Model-based marginal abatement cost curves with EPLANoptMAC

The MAC curve optimization model presented by Prina et al. [48], EPLANoptMAC, is applied to the case of Chile. This model couples the energy system simulation tool EnergyPLAN – as the core calculation engine – with a single-objective hill-climbing optimization algorithm to sequentially simulate energy system scenarios with incremental values of different decision variables, and minimize abatement costs at each incremental step. These decision variables represent various abatement measures, such as the capacity expansion of renewable supply technologies, fuel replacements, and changes in energy demands.

The EPLANoptMAC model is configured with inputs for a reference energy system scenario, the set of measures as decision variables to be assessed with their respective incremental values, and the number of steps to evaluate these measures. The incremental changes to the decision variables are then fed as inputs to EnergyPLAN to generate scenarios. Subsequently, the outputs produced are evaluated across the competing scenarios, finding the scenario with the decision variable yielding the minimum cost of carbon abatement (CCA). This is defined in Equation (1) as the ratio between the difference in total system costs of the new resulting scenario and a reference case and the potential emission reductions.

$$CCA_i [MUSD / ton CO_2] = \frac{Cost_i - Cost_{ref}}{Emissions_{ref} - Emissions_i} \quad (1)$$

The measure with the lowest CCA is selected as the new reference in the next step of the iteration. After this, the procedure repeats, modifying the new reference scenario with incremental changes to the decision variables. Finally, the algorithm stops when CO₂ abatement is no longer possible for the given decision variables in case these have reached their maximum end-value or fail to converge or when the predefined number of steps is reached [48].

In addition to the steps outlined originally in [48], a new constraint has been included to the algorithm to limit at each step the amount of biomass to a maximum of 130TWh. This is done to ensure that each incremental scenario considers some technical and sustainability limitations of the system. The algorithm has been updated to consider additional effects of sector coupling in decision variables with dependent parameters such as the associated infrastructure costs and supply options when considering incremental shares of district heating to replace individual boilers, and fuel replacements when implementing biofuel and

electrofuel productions. Moreover, the original algorithm presented in [48] and developed in Python has been ported to run with the Julia programming language [49], and to perform the EnergyPLAN runs in batches (i.e., Spool mode) at each step rather than running each individual change in decision variable one-by-one with new instances of EnergyPLAN. These updates significantly increase the algorithm's performance, bringing down computational time.

2.3. Overview of modelling inputs and assumptions

The data inputs for modelling the energy system scenarios are obtained from Chile's national energy databases and previous studies, as outlined in Table 1. These inputs include the reference demand projections and installed capacities for power generation and renewable electricity generation potentials [10]. In addition, estimates related to district heating were obtained from the Heat Roadmap Chile project [23,50] including estimates for demand profiles, district heating potentials, losses and costs, and excess heat potentials. These estimates complement the heat demand estimated by carrier from the PELP's demand projections [10]. Furthermore, hourly profiles for electricity demand and VRES production were obtained from the national energy coordination agency [51], as were the estimated energy accounts for hydropower and storage [52]. Finally, cost assumptions and fuel prices were obtained from the national energy coordination agency when available [53] and supplemented with data from the Danish Energy Agency's (DEA) technology catalogues, which present comprehensive descriptions of investment costs and data for energy conversion technologies [54–58].

Table 1. Data sources for modelling scenarios.

Data	Source
Installed power capacity	PELP [10]
Renewable electricity potentials	PELP [10,59]
District heat potentials, excess heat supply & DH infrastructure costs and losses	PELP [10] & Paardekooper <i>et al.</i> [23,50]
Hourly distributions and productions from VRES, and energy demands	PELP [10], CNE [51,52], Paardekooper <i>et al.</i> [23,50]
Technology costs and fuel prices	CNE [53], DEA [54–58]

2.4. Scenario framework

2.4.1. Replication of Chile's long-term energy planning PELP scenarios

In the current PELP, three different scenarios are presented: (i) a scenario following “*current trends*” considering a conservative post-pandemic economic recovery and slow uptake of renewable energy capacities and energy efficient technologies; (ii) a “*carbon neutrality*” scenario with middle-of-the-road trends; and (iii) an “*accelerated transition*” scenario which also depicts a carbon neutral case but, happening earlier in time due to rapid economic growth and fast development of new technologies and ambitious implementation of energy efficiency measures [10].

These scenarios illustrate potential pathways for Chile's energy system towards 2050. While the scenarios above depict potential low-carbon futures of Chile's energy system, they do not fully showcase a fossil-free, 100% renewable energy system, but rather allow for some remaining shares of fossil fuels and their respective emissions. Moreover, the modelling behind these scenario results does not explicitly consider key enabling technologies for sector coupling, fuel replacements with different PtX other than hydrogen, nor an hourly resolution over a full year, which is beneficial to adequately capture the fluctuations across the different end-use demands across all sectors and the different energy supply sources [60].

Therefore, to initialize a comparison benchmark, these scenarios have been replicated and adjusted in EnergyPLAN. The input assumptions mentioned in Section 2.4 are applied, with adjustments made to power plant capacities in cases where the originally assumed capacities

from PELP become insufficient to cover the system's hourly energy demands. The comparison of these scenarios with the ones generated for this study are presented in Section 3.3.

2.4.2. Design principles to develop a Smart Energy System scenario for Chile

This study aims to explore alternative decarbonization scenarios to those present in Chile's national energy planning process. Namely, including a system redesign that allows for a 100% renewable energy and clean supply through energy efficiency, flexibility, and coupling of the different sectors and their infrastructures. This process is conceptualized via a series of steps and guiding principles following a Smart Energy Systems approach [15], similar to those outlined in past studies under different contexts [61–66] but adapted to fit the case of the Chile energy system, where at each step not only new technology and fuel replacements occur, but also more VRES capacity is introduced. The steps and principles considered can be formulated as follows:

- 1) **Identifying a “Reference” scenario:** This scenario is designed as a benchmark for comparison, which replicates capacities and projected energy demands for 2050 from Chile's PELP scenarios. Namely, it includes the estimated power generation capacities, space heating, and industrial demands from the PELP's “*current trends*” scenario while also including the developments from the “*carbon neutrality*” scenarios in both electricity demands and in the implementation of energy efficiency measures in transport [6], and hydrogen fuel replacements expected from Chile's hydrogen strategy [67]. The latter already includes measures such as the partial electrification of road transport and industry, heat savings, and fuel replacements with direct hydrogen use. Moreover, it includes the phase-out of coal in the electricity generation sector and a high carbon tax (70 USD pr. Mton) as defined in the PELP. Therefore, these measures will be embedded in the subsequent scenarios.
- 2) **Implementing diverse heating supply options including individual heating and district heating:** Building up from the previous steps, a redesign of the heating system is undertaken. This step entails expanding the share of the heating supply covered by district heating and upgrading to efficient individual heating solutions by electrifying the individual heat supply with heat pumps. The addition of district heating comes in hand with implementing a diversified supply, including combined heat and power (CHP) plants, large-scale heat pumps (LSHPs), heat recovery from industrial processes, and renewable heat sources such as solar thermal and geothermal. The excess heat supply also enables an additional level of cross-sectoral integration when considering the prospect of new fuel production technologies such as hydrogen and electrofuels. The Heat Roadmap Chile study results are considered to design adequate levels of district heating [23,50].
- 3) **Fossil fuel replacements in transport with biofuels and ammonia:** From the reference scenario, a significant share of the transport demands is not electrified or replaced with hydrogen. Therefore, this step examines some initial fuel replacements with biofuels and e-fuels from biomass hydrogenation across all transport demands and the use of ammonia for maritime fuel demands as abatement measures, as suggested in past studies [66,68]. In turn, this transformation requires the expansion of electrolyzer capacity, air separation units, hydrogenation plants, and electrofuel synthesis. Applying these technologies increases the expected electricity demand; thus, additional renewable capacity will be installed at this step. Moreover, these conversion processes and plants will yield reusable amounts of excess heat, contributing to the district heating supply and adding an extra degree of flexibility to the overall system.
- 4) **Fossil fuel replacements in industry with biogas:** This step in the transition consists in converting industry and mining demands from natural gas demands to biogas and synthetic gas. In turn, this transformation requires the increase of biomass gasification capacity, with its respective electricity demand. In addition, coal consumption in this sector is replaced with biomass.
- 5) **Replacement of remaining fossil fuels with CO₂-based electrofuels:** The final step considers replacing the last remaining fossil fuel consumption in the transport

fleet with electrofuels derived from CO₂. Converting the remaining liquid fuel demand requires new carbon capture and utilization (CCU) and expanding the technologies introduced in Step 3.

- 6) **Smart Energy Chile (SECL) scenario:** The last step considers the cumulative decarbonization developments in the energy system, and includes an additional biogas consumption as a final fuel replacement in the gas grid to the remaining fossil fuel demands corresponding to natural gas. This final adjustment in the modelled scenario starts yields a 100% renewable energy system. Although this scenario presents an overall increase in biomass consumption relative to the reference, it stays below the current consumption levels today, thereby ensuring a sustainable consumption level.

At each step, more VRES capacity can be incorporated into the system (while staying within their available technical potentials), namely additional capacities of solar photovoltaics (PV), onshore wind, and concentrated solar power (CSP). These steps, summarized in Figure 1, do not necessarily represent a sequential transition in terms of the priorities to implement change. However, for ease in the modelling, these are applied in bulk sequence, thereby facilitating the analysis of the different technologies' roles in the country's decarbonization goals and the comparison with current national scenario development.

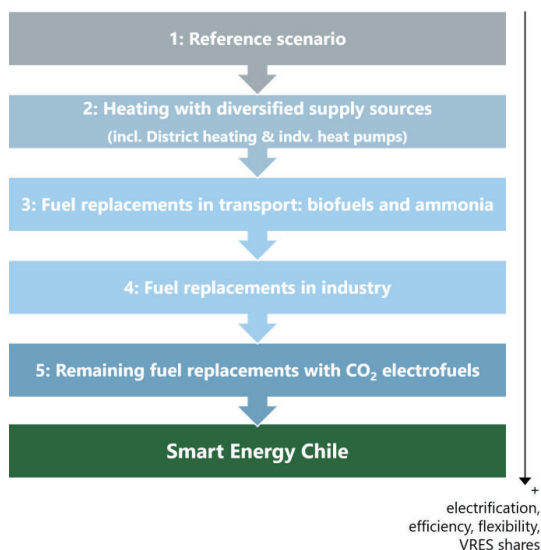


Figure 1. Depiction of steps leading toward a Smart Energy Chile scenario

2.4.3. Identification of abatement priorities and capacity expansion

To provide a complementary perspective of the different abatement priorities, the steps described in the previous section are contrasted with sequential scenarios generated via the marginal abatement cost curve optimization from EPLANoptMAC. In this way, the individual measures embedded in the bulk of each Smart Energy step can be discretized to show an optimal decarbonization pathway based on the minimum cost of carbon abatement.

These measures translate to new decision variables in the EPLANoptMAC model. Meanwhile, the starting point considers the “Reference scenario” described in Step 1 in the previous section, and the end-values take the capacities and fuel substitutions from the “Smart Energy Chile” scenario.

3. Results and discussion

Here, the results of the different analyses are presented. First, key operational indicators are showcased for the Smart Energy Chile scenario steps, and the MAC-curve generated results.

These include primary energy mix, CO₂ emissions, electricity supply, demands, and curtailment. Then, these results are compared to the PELP scenarios, including their total system costs.

3.1. Towards a Smart Energy Chile scenarios

Based on the scenario design principles and assumptions mentioned in Section 2.4., a series of scenario steps were developed, leading toward a Smart Energy Chile scenario. These steps – shown in Figure 2 – lead toward a 100% renewable and decarbonized energy system.

In the reference scenario, some consensus non-controversial actions are already in place; for example, coal phase-out for power production, electrification of private and public road transport, and energy efficiency measures in buildings.

In the second step, the implementation of district heating solutions and electrification of the heating sector similar to those proposed in [23,50] are introduced and curb biomass and fossil fuel consumption. This is largely facilitated by integrating VRES – already present in the system – into the heat supply through both individual and large-scale heat pumps and moving away from individual fossil-based fuel boilers. Furthermore, coupling this electrified heat supply with district heating infrastructure enables the possibility of using thermal storages; thereby providing additional system flexibility. At the same time, the district heating infrastructure introduced in this step allows for the diversification of heat supply options, with the integration of otherwise wasted excess heat from both power production (combined heat and power – CHP – plants) and industry.

In step three, the production of alternative fuels for transport adds a modest increase in biomass consumption as well as new electricity demands. This is mostly driven by one-to-one substitutions of oil fuels with biomass-derived fuels and ammonia, which is also introduced to cover maritime demands, along with related electrolyzer and air separation capacities. Correspondingly, new VRES capacities have to be introduced. Due to the additional capacities and fluctuating supply, the amount of curtailment will also increase. Meanwhile, the introduction of these new fuel production processes also acts as new heat supply options since these produce large amounts of recoverable heat as a by-product, which can be integrated into the district heating supply. Overall, the changes introduced in this step lead to a considerable reduction in carbon emissions: more than half relative to the reference.

Following this, step four sees a larger increase in biomass consumption compared to previous steps, mostly due to the replacement of natural gas with gasified biomass, as well as a modest increase in electricity demand. Meanwhile, step five sees a more substantial change in the primary energy supply mix, with the substitution of the remaining fossil fuels in the transport sector with e-fuels from CO₂ hydrogenation. Similar to previous steps, this requires new buildup of hydrogen production and VRES and new carbon capture capacity. Despite the increase in electricity production, the increase in demand and flexibility from the technologies introduced in this step translate to relatively lower curtailment levels than in the previous two steps. Moreover, the fuel production processes also further the supply of recoverable excess heat. In all, this step also significantly reduces CO₂ emissions, with only about 10% of emissions compared to the reference.

Finally, in the last step – constituting the Smart Energy Chile scenario – a full transition is undertaken in which all the remaining fuels for heat and power production are replaced with green fuels. More specifically, the remaining natural gas consumption is replaced by gasified biomass and biogas. This final step sees a primary energy supply shares of about 80% and 20% for VRES and biomass, respectively. This represents almost a twofold increase in the VRES supply compared to the reference scenario, while the quantity of primary biomass supply remains comparably less than today, amounting to an approximated consumption of 17 GJ per capita. As a result, this final step presents a fully decarbonized fossil-free energy system scenario.

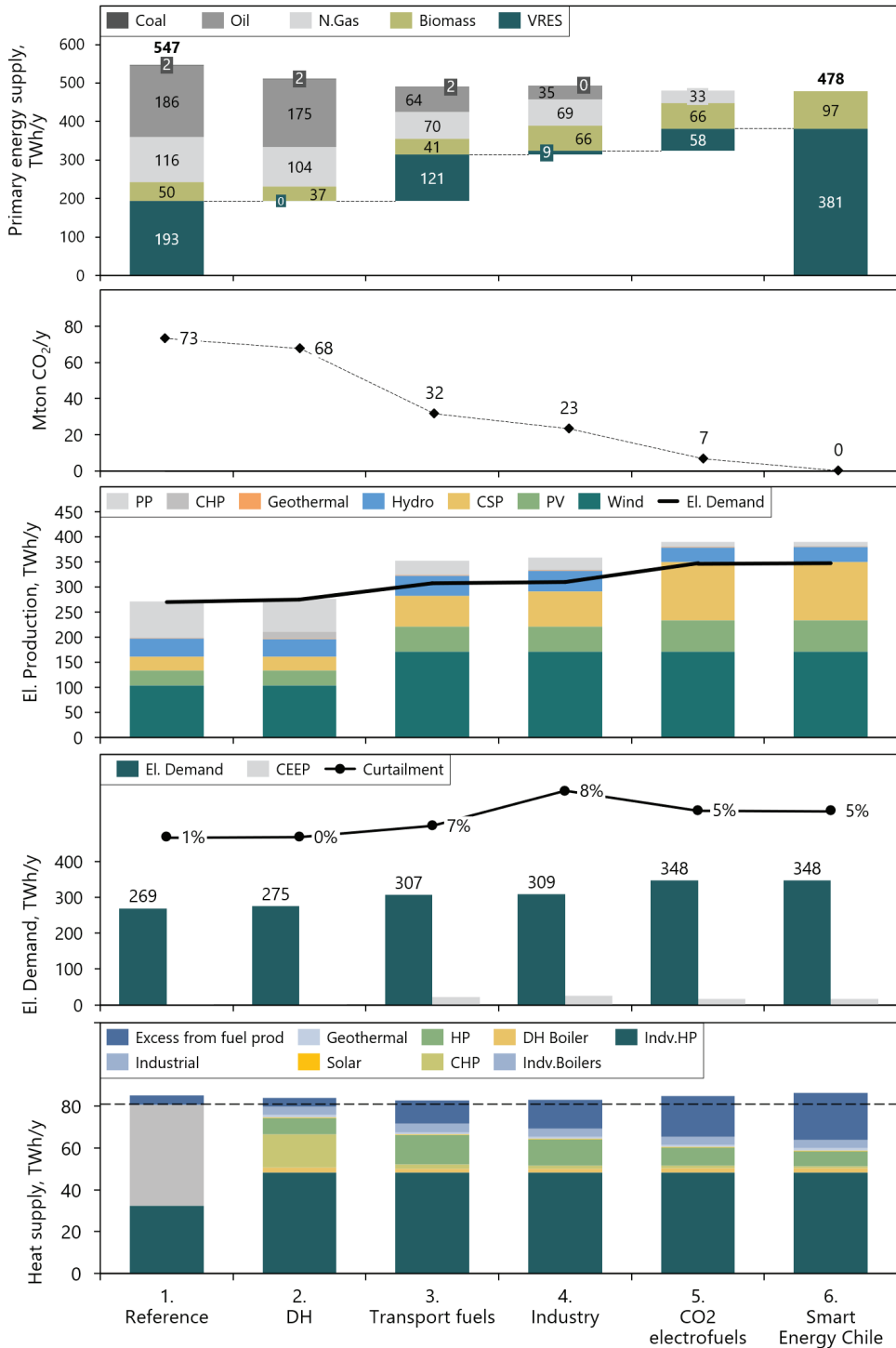


Figure 2. Overview of steps towards a Smart Energy Chile scenario in primary energy supply, total electricity demand, and curtailment throughout the different CO₂ marginal abatement steps.

3.2. Marginal abatement costs (MAC) curves

2.2.1. Abatement of CO₂ emissions

To generate the marginal abatement cost curves, the set of decarbonization measures leading to the Smart Energy Chile scenarios has to be considered in a separate manner, discretizing them into incremental deployment steps. These steps are applied in EPLANoptMAC, resulting in the optimized MAC curve presented in Figure 3 and 4.

As illustrated in Figure 3, the expansion of PV and onshore wind capacity takes a prominent role early on in Chile's energy system decarbonization, as it provides a cost-effective and carbon-free supply of electricity. At an intermediate stage of decarbonization, some fuel replacements can already be realized by introducing biofuels in the transport sector and considering some related and required infrastructures like hydrogen electrolyzers.

At around this intermediate stage of the transition, the sequence of abatement measures can already reach the nationally determined carbon abatement emission target for 2050, which equates to CO₂ emissions of about 38.3 Mton per year, or a reduction of about 56% relative to 2018. Moreover, implementing the respective abatement measures up to this point yields a system design with the lowest total system costs along the transition.

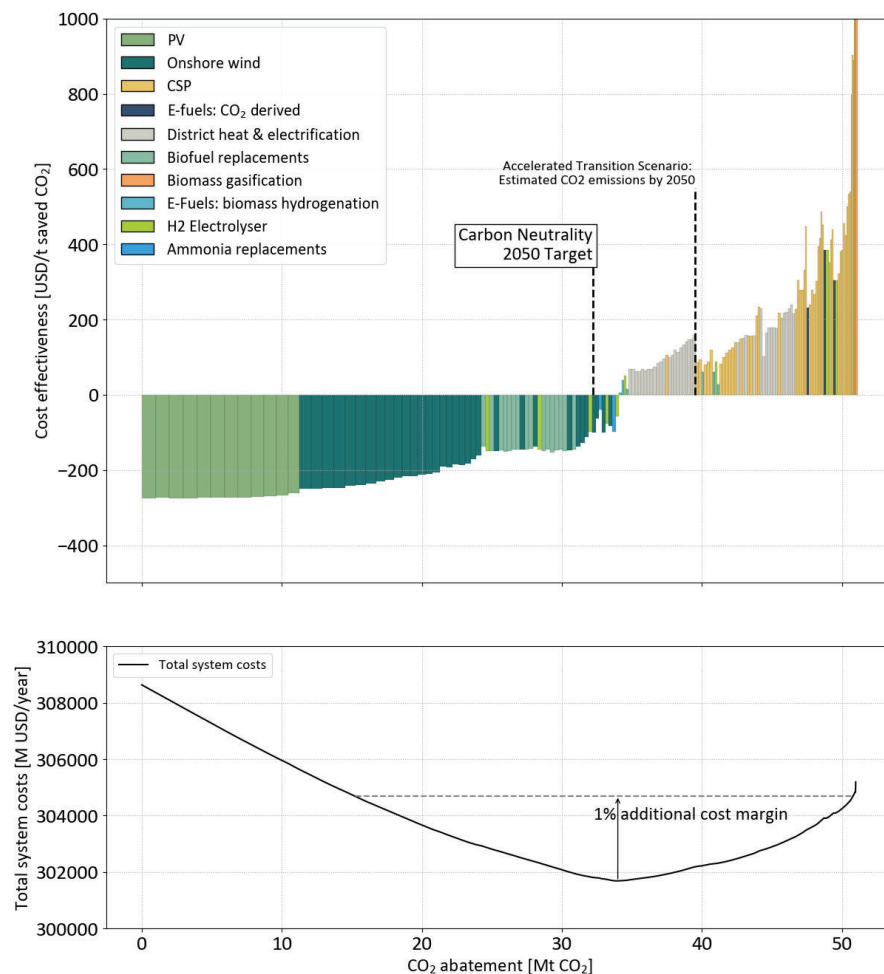


Figure 3. Marginal abatement cost curve with different Smart Energy technologies and CO₂ reductions in a 2050 Chile scenario, and total system cost trends.

After this point, a few additional no-regret measures can still be realized, namely some transport fuel substitutions with ammonia and additional electrolyzer and onshore wind capacities. As seen in Figure 4, the trend in curtailment levels resulting from the early and mid-stage introduction of VRES capacities also starts slowly stalling relative to the total electricity demand due to the flexibility provided by the introduction of new measures.

From there, the changes in the heating sector with higher penetration of district heating and electrification with individual heat pumps become a viable, albeit more expensive option. This early redesign of the heating sector allows the system to reach similar decarbonization levels to those projected under the PELP's "*accelerated transition*" scenario. At this level the expansion of district heating comes to about 20% of the space heating market, and individual heating is mostly electrified, displacing inefficient fuel boilers. Moreover, as presented in Figure 4, these measures also introduce further reductions in the total primary energy supply, and provide additional flexibility to the system, allowing for curtailment to decrease.

Interestingly, the abatement potentials of certain measures starting at the mid-phase of the transition do not necessarily follow a linear increase. Rather, certain consecutive measures present discontinuities in their cost of carbon abatement potentials. This is partly due to the system effects of introducing certain technologies. For example, by implementing a given flexibility measure (e.g. storages, electrolyzers), the subsequent increase in generation capacity can become competitive again. Nevertheless, the resulting system designs for most of the measures past the mid-stages of the transition yield total system costs within a 1% margin of the minimum cost configuration.

In the final stages, the decarbonization relies on expensive or less mature technologies and measures, including sequentially increasing capacities of CSP (including storage), additional flexibility with electrolyzers, and e-fuel production with CO₂ hydrogenation for transport fuel replacements. In these stages, CSP will increase curtailment while new hydrogen and e-fuel production will act as counteractive flexibility measures. Considering a system scenario where all these measures are realized, would lead to system emissions of about 17.3 Mton per year.

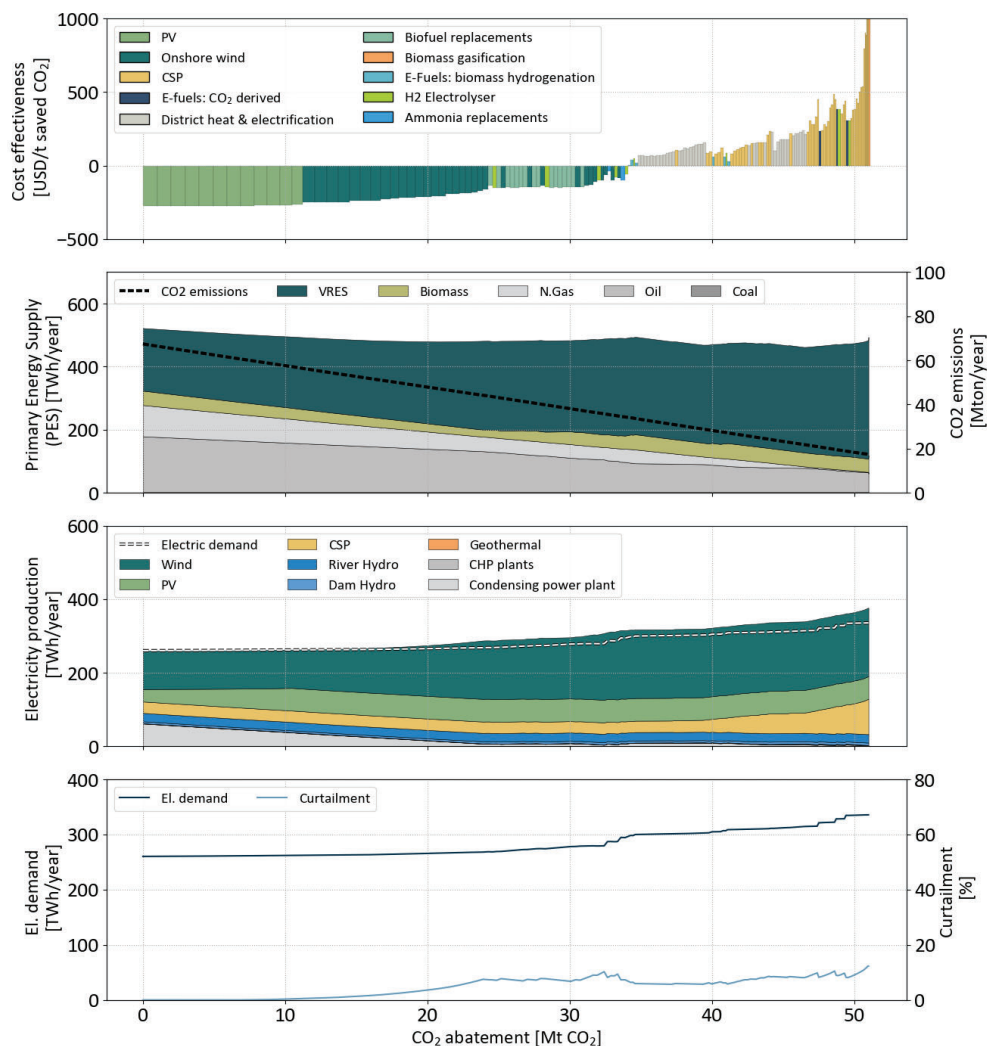


Figure 4. Trends in primary energy supply, total electricity demand, and curtailment throughout the different CO₂ marginal abatement steps.

3.3. Comparison across abatement scenarios

To illustrate the different abatement alternatives, the results from the Smart Energy Scenario steps and the MAC curve generation are compared to the PELP scenarios, replicated for this study. This comparison, presented in Figure 5, provides a view of the performance of these scenarios based on primary energy supply, CO₂ emissions, and total system costs.

In terms of primary energy supply, the PELP scenarios (namely the “Carbon Neutrality” and “Accelerated Transition”) present higher energy consumption than the other observed scenarios. This is driven by the high input assumptions concerning hydrogen production for exports, which activate power production for power plants when considering the hourly fluctuations of demand and production during a year, which is not captured fully in the original scenario development from the PELP. This also translates into cost differences, as the system

incurs both larger variable costs for fuels and investment costs for additional capacity. Meanwhile, the “*Current trends*” scenario presents relatively similar levels for all indicators to the reference scenario in the Smart Energy steps, which is natural given the methodology used to develop the latter.

Across the different Smart Energy steps, efficiency gains can be observed as well as progressive CO₂ reductions, though at increasing costs relative to the reference in the last stages. Nonetheless, a cheaper system configuration can be observed at Step 4, and the cost increase in the Smart Energy Chile scenario represents less than a 1% increase relative to the reference. At the same time, two scenarios generated from the MAC curve optimization are observed: one with the lowest system costs and one with the highest abatement level. Here, we see that the minimum cost option closely resembles Step 4 from the Smart Energy steps in terms of the energy mix and emissions, however at a lower system cost due to incurring in lower investment costs and low variable costs. Meanwhile, while reaching significantly low emission levels when compared to the reference, the highest abatement option does not reach the same abatement potential compared to Step 5 or to the Smart Energy Chile scenario. However, both of these MAC-generated scenarios present lower-cost systems than any of the system configurations from the Smart Energy steps. However, given future cost and price uncertainties this difference is marginal, making it hard to conclude whether one scenario is that much more cost-effective than the other.

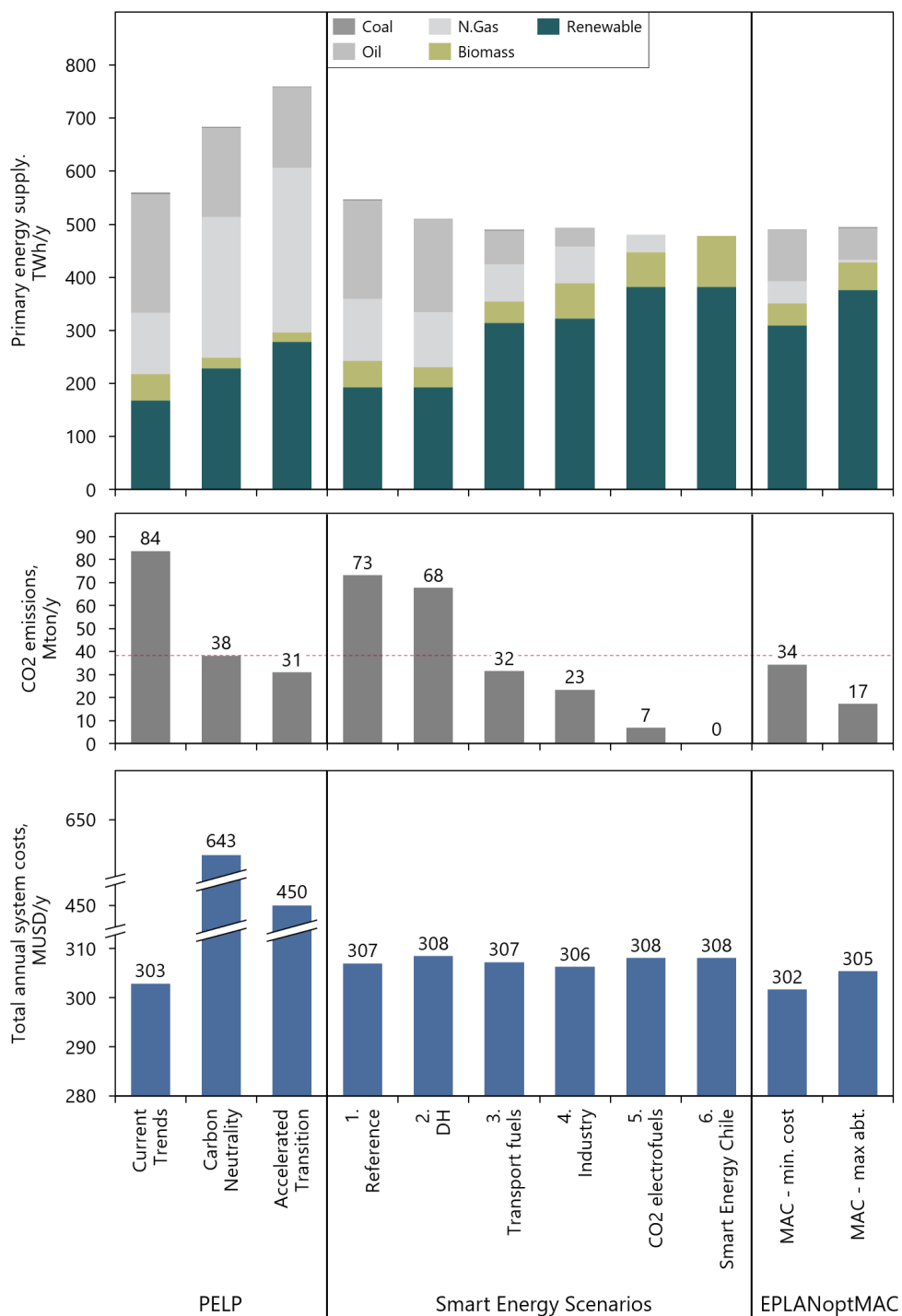


Figure 5. Overview of key indicators across the different abatement scenarios.

4. Summary and conclusions

In this study, different carbon abatement scenarios for the Chilean energy system have been developed and examined. These scenarios include Chile's nationally developed PELP scenarios, newly developed scenarios applying a Smart Energy System approach, and optimized abatement scenarios generated with the EPLANoptMAC tool.

Coupling the latter two methodologies adds great value as it provides different yet complementary perspectives on Chile's potential transition and decarbonization pathways toward 2050. On the one hand, the Smart Energy scenarios benefit from having a more granular view of how the broad measures assessed in each step can be incrementally implemented and which of these should be prioritized at different stages of the transition. For instance, prioritizing renewable capacity with high curtailment in the early and mid stages of the transition, and flexibility options at the latter stages. On the other, the optimized MAC curve generated scenarios are complemented with the analytical approach by getting pre-set targets and by the perspective provided via scenario exploration, which can look beyond the bounds of the given optimization problem. This allows exploring full decarbonization and 100% renewable energy system with key enabling technologies that might, for example, present only marginally higher costs or fail to converge due to particular system dynamics in a highly sector-coupled system.

The results from the analysis show that by following a Smart Energy System approach and the guiding principles outlined in Section 2.1, a fully fossil-free and 100% renewable energy system is technically feasible and, in fact, goes far beyond the current national Carbon Neutrality scenarios. Achieving this will require a heavy redesign of the energy system, with integration across the different sectors in terms of integrating their demands via electrification and utilizing common infrastructures and grids, which – in turn – can also provide additional system flexibility once new capacities and fuel production technologies are introduced. A large expansion in VRES capacity must occur in the initial phases of the transition, consisting of PV and Wind capacities, followed by fuel replacements and, later on, a redesign of the heat supply, including electrification with heat pumps and the expansion of district heating grids. At later stages, balancing technologies will be needed along with deploying CSP capacity to cover new electricity demands. This highlights the importance of enabling infrastructures and interconnections of the sectors to ensure that VRES can be used to their full capacity. Moreover, biomass can also take a prominent role within its available limits, in tandem with e-fuels, to reach the last stages of a transition towards a 100% renewable energy system. This could be achieved at lower costs relative to the PELPs “Carbon Neutrality” scenario, and with less than a 1% increase in systems costs relative to the reference.

Finally, the resulting MAC curve scenarios show that certain technologies with great potential for decarbonization are not yet cost-effective in terms of their costs for carbon reductions. This means that policy and other incentives should be targeted to promote and further develop these measures in the context of Chile. Also, it shows that a less ambitious carbon neutrality could be achieved with fewer technical changes or redesigns than with the Smart Energy Scenarios. Moreover, the results also reveal the value and benefits of capturing system dynamics in generating MAC curves, as it captures the impact of enabling technologies and planning objectives with a granular and holistic approach. This is particularly important in the context of Chile, where MAC curves are used in the assessment of National Determined Contributions (NDCs) and climate action plans [26,29]. Without the system perspective, valuable carbon abatement options might not otherwise show their full benefits.

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APPENDIX: Supplementary material – Scenario data

See attachment.

SUMMARY

Energy system models (ESMs) can serve as valuable tools for representing the energy system and gain insight about the energy transition. In recent years, the analyses conducted with such tools have grown in scope and complexity, leading to more integration of tools across a range of modelling paradigms and disciplines. In this context, this thesis explores the emerging practice of model coupling with ESMs (i.e., linking ESMs together with other tools), discussing its implications from a theoretical, methodological, and analytical perspective. On a theoretical level, aligning domains and models is found to be beneficial to get a broad range of answers from different perspectives, yet – given the context of climate change – this must be managed with urgency by applying purpose-driven model coupling configurations. From a methodological and analytical perspective, the studies presented in this thesis show that extra modeling effort and complexity compound with the increased resolution provided by model coupling. Nonetheless, these applied studies show that model coupling can provide complementary perspectives on the transition of a national energy system, taking Chile as a case.