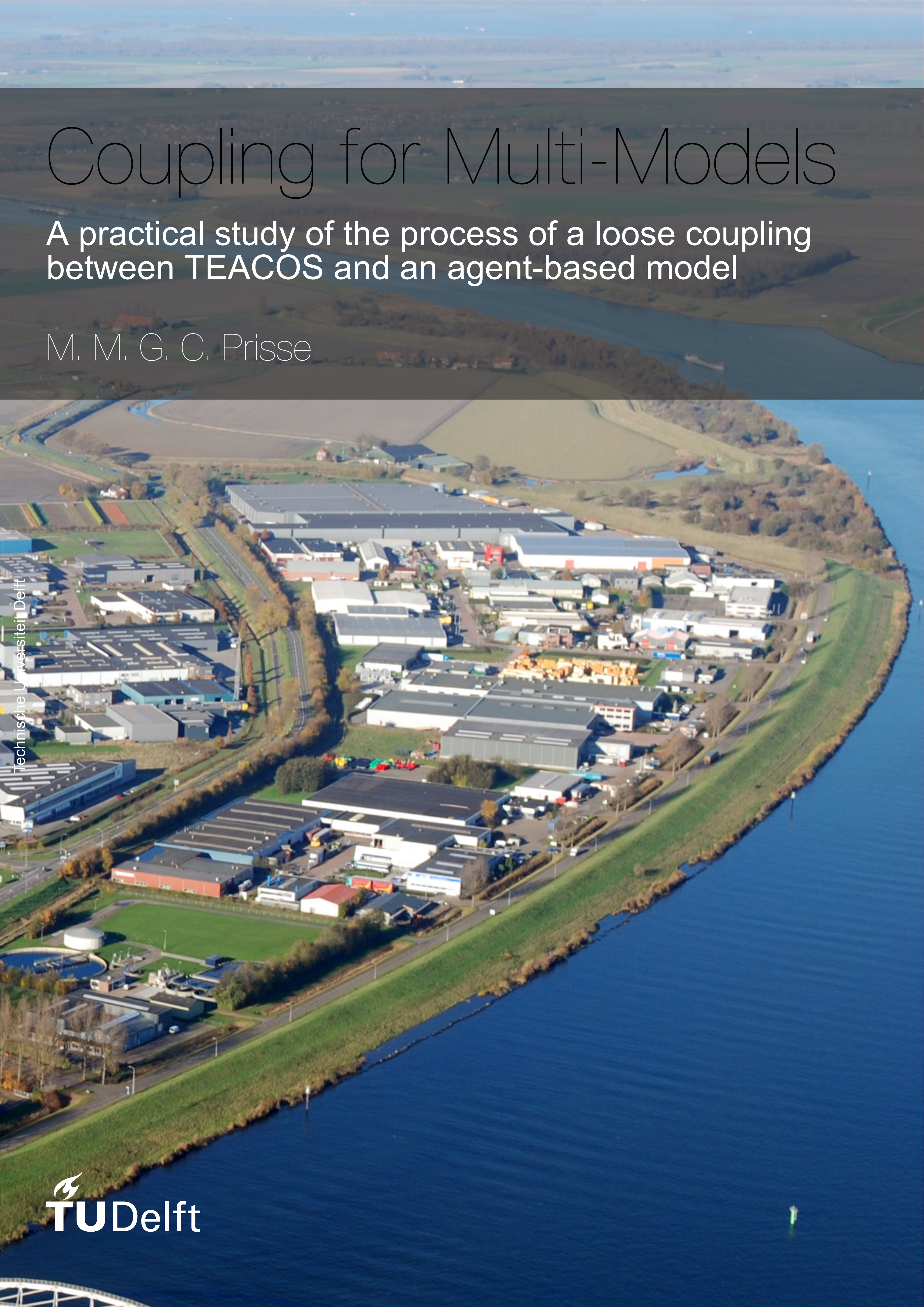

Coupling for Multi-Models

A practical study of the process of a loose coupling between TEACOS and an agent-based model

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TUDelft

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by

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Preface

With this research I am not only completing my Master's Degree, but I'm also ending my time as a student. It is the end of an era, and I have been able to get so much out of my time at TU Delft – it will be hard to pay for public transport from now on. Jokes aside, Delft has given me the room to learn so much as a student while also growing as a person. There are some people that I have met along this journey without whom this would not have been possible, that I would like to thank.

First, my thesis committee for their insights and guidance throughout this entire process, as well as keeping me motivated to finish my thesis. You believed when I did not. Without my first supervisor, Yilin, this would not have been possible. Our useful discussions and your ability to make me see the problem with a fresh set of eyes were truly invaluable. But besides that, thank you so much for your compassion, kind words and asking me how my weekend was. Igor, I had no idea what I was getting into when I knocked on your door but thank you for all your faith in me and the cups of good tea. Willem, thank you so much for keeping me sharp on my writing and getting straight to the point with your feedback.

Outside of my committee, I am incredibly grateful to Stijn from Quo Mare. Your quick replies to all my questions were my light in the dark of this thesis sometimes. Without your hard work on the TEACOS adaptor and willingness to help, this would have been a lot harder. Edwin from TNO, thank you for your input (even when you were on holiday!). Massive shout out to the rest of the "MMvIB micro case bi-weekly" meeting attendees, Charlotte, Vincent, and Gregor. I only dipped my toes into the task you are undertaking, and you have my eternal respect for what you are doing. I hope you guys get to enjoy your holidays.

I also can't express in words how much I adore my friends that I made on my first day of the TPM Bachelor's in 2016. It's been some unreal years together. From the TB Café escalations and desperate last minute study sessions in 2016 to proofreading each other's theses and planning holidays together in 2023. I couldn't imagine my time at TPM without my "study friends", joe.

Big thanks to Ad Doppenberg for proofreading and making time for this. It meant a lot to me.

I also want to express gratitude to my family, but especially my brother, Willem, and mum, Xiaoling, for their unwavering support. You gave me the freedom and security to make the most of my student years, to figure out who I wanted to be, and you were always there to help me up when I fell down. I hope I made you proud!

Finally, Wouter, thanks for being all the clichés in the world. My rock, my cheerleader, and now, my favourite roommate. Your constant support through the ups and (especially) downs of this thesis have meant the world to me. I can't wait to start our next adventure together without me thinking about my multi-models.

M. M. G. C. Prisse
Amsterdam, June 2023

Executive Summary

Multi-models, formed through the coupling of individual models, can serve as powerful tools in addressing complex problems. These systems are able to capture the strengths of individual models and save modelers considerable time by allowing for model reuse. However, the creation of multi-models is not without its challenges, ranging from technical challenges such as aligning different model resolutions to non-technical challenges concerning licensing and the proprietary rights of models. Above all, a multi-model fundamentally depends on the successful coupling of the models.

Delft University of Technology has formed a consortium with other parties to study the set up, coupling and application of multi-models. This research is conducted together with the consortium's micro use case, which aims to combine energy models to study how multi-models can play a role in decision making for the energy transition. The models all communicate using Energy System Description Language (ESDL) files, which ensure syntactic alignment. An industrial area in Tholen, the Netherlands, is used a subject matter for this micro use case.

Literature concerning multi-models contains significant theoretical knowledge about the challenges of coupling two models, but there is little practice-based discussion concerning the coupling models for a multi-model, especially with regards to model reuse. In order to examine these aspects, it's necessary to first establish a coupling that reveals the impact of the models on each other. Within the micro use case of this consortium, this research was tasked to research coupling a simulation model to an existing optimisation model, TEACOS. Therefore, this research tries to answer the following research question: ”What is the effect of coupling an agent-based model to an existing optimisation model, TEACOS, given the case study of Tholen?”

This research proposed three methodological steps to answer this question. First, to conduct research into the manners of coupling that are possible through a literature review. Secondly, to find out what options of coupling are meaningful between TEACOS and an agent-based model (ABM) and implement it. TEACOS is an existing optimisation model, developed by Quo Mare, and calculates the optimal investment paths for an energy system. The ABM simulates human investment behaviour and is developed for the purpose of this research. Thirdly, to establish to study the outcomes from the multi-model, applied to a case study of an industrial area in Tholen, The Netherlands.

In setting up the coupling between the ABM and TEACOS, two things stand out. First, there were a great deal of challenges in each phase - understanding the case context, conceptualising the coupling, formalising the coupling and attaining results - that had to be dealt with, for example, ensuring that these models are using the same units when they are dealing with the same number. In this case, TEACOS could not process gigajoules and defaulted to megajoules, which needed to be accommodated for within the ESDL-file and the ABM. This is important for consistency and to allow for accurate comparisons and integration between different models. Second, in the coupling structure used in this research, attributing specific behaviors to their respective sources within the interconnected models proved to be difficult. This was mainly because it does not become clear which model causes what, since they are constantly communicating and altering the ESDL-file exchanged between them. This complexity is exacerbated by the opaque use of TEACOS. After considerable trial and error, the coupling was successful.

Findings from the model outcomes show that the coupling of the models allow for the integration of human behaviour through the ABM into the search for an investment path by TEACOS and the lowering of uncertainty within the multi-model trajectory for investments. Using the case study of Tholen, it was found that the decisions made by the agents did not coincide with the outcome generated by TEACOS alone. Overall, the number of investments done by the agents always fell short of the number of investments suggested by TEACOS. Therefore, when the runs of the combined models were compared with a base run, it was found that the multi-model was slower to reach the inflection point of model behaviour than the base case. Since the ABM simulates a lower number of solar panels bought, these

constrain TEACOS for the following run, where it starts with a different set of starting conditions than it would have initially optimised for. Effectively, the ABM gives a different set of starting conditions each run than TEACOS would do for itself, adjusting the trajectory found by TEACOS over multiple iterations.

This research has formulated several lessons learnt with regards to the coupling of models for the purpose of a multi model, categorised by organisational and methodological nature. From an organisational standpoint, the importance of organisational interoperability in multi-model projects was highlighted for when analysing the process of the coupling, it was found that while the literature addressed the technical challenges, organisational challenges were understated. More than a third of the challenges met during the coupling were related to (a lack of) organisational interoperability between the models. Organisational interoperability signifies the ability of organisations to effectively communicate and share data across different platforms. During this research, scarce model documentation and disuse of a centralised file storage had a slight negative impact on the project process. On the other hand, the direct and effective communication channels employed within the micro use case had a very positive influence. These examples both highlight the effect of organisational interoperability when working with multiple models and stakeholders. Implementing robust documentation practices from the outset is crucial, and establishing open communication lines should be prioritised.

From a methodological standpoint, the choice for a loose coupling works to maintain model independence, although working with a model that cannot be accessed is undesirable. Furthermore, the choice to communicate through the chosen data format could have been conceptualised more efficiently, since this manner is convoluted and does not allows for an easy post-processing of the outcomes. Since all the desired outcomes are embedded somewhere in the ESDL-file, it is difficult to retrieve them in an easy fashion, let alone make quick analyses of model runs. Finally, the methodological approach to multi-model construction should not only focus on quantitative methods. Quantitative methods alone may not be comprehensive enough to capture knowledge and the organisational aspects of coupling models with multiple stakeholders. The inclusion of qualitative techniques like stakeholder interviews could enhance understanding and enable rapid knowledge transfer in the earlier stages of such a project.

In conclusion, multi-models hold great promise and this research would like to add to the body of knowledge with lessons for modelers attempting a similar coupling. It has become apparent how complex the task of coupling two models are, especially when one of them is an existing black box model, but it has also shown that once the coupling is formalised, the multi-model outcome is different. Should such a similar coupling be done in the future, this research has three takeaways from the process. Firstly, when constructing a model for a multi-model, a trade-off between the cohesion and interdependence of the models occurs which may affect the ease of a coupling. When considering this trade-off, several factors such as the time available, expertise and purpose of the coupling should be kept in mind. Secondly, troubleshooting a multi-model should first be done according to first three levels of interoperability, followed by conformance testing and studying model in- and output. Finally, the advice to future research involving collaborative multi-modeling is to consider a more balanced methodology, merging quantitative and qualitative techniques. This enables a quicker comprehensive understanding of involved models and organisation and fosters a collaborative, holistic approach to the research process.

Furthermore, it was found that while the literature provides a theoretical foundation for this process and its core concepts, the practical challenges may be understated. In light of the findings from the process of this research, it becomes apparent that a more robust and comprehensive approach to organisational interoperability is more conducive to facilitate the successful creation and use of multi-model systems. This research proposes that constant communication between involved parties, comprehensive documentation of the models involved and choices made, combined with some level of standardisation for model reuse, can benefit multi-modeling. A holistic approach would alleviate the burden of organisational challenges and streamline the process for future construction of multi-models. That way, the advantages of the multi-model can be unlocked.

Contents

1

Introduction

1.1. Background

Models are ubiquitous in our daily lives. We interact with them in various ways, from mental models that help us make sense of the world (Senge, 1990) to the complex weather models that help us decide what to wear that day. Models are used across all fields and disciplines with the general purpose of providing a representation and understanding of reality. Models can take various forms, from a physical architectural blueprint that translates and abstract idea into a concrete object to mathematical equations and algorithms that make up a simulation. The primary goal of models and modelling is to reduce the complexity of the real-world and facilitate human understanding of that world.

There are several advantages to using models. Firstly, they may allow for the testing of hypotheses and predictions about complex systems, an otherwise intractable task. Secondly, models support the communication of complex ideas and information, enabling knowledge exchange or aiding decision making processes. Besides this, models are not only functional in their use, but even the construction of a model can be of value for stakeholders and modellers, such as in participatory modeling. This involves collectively building a model with various actors and stimulates the integration of various sources of knowledge and different points of view, creating a shared vision by building a common model (Jones et al., 2009).

However, there's a downside to these models, too. Firstly, one should always remember that models are merely an approximation of reality and can never completely capture all the nuances of a real-world system. Secondly, models are only as good as the assumptions and data used to build them, and any errors or biases in these inputs can lead to faulty models, predictions and conclusions. Finally, models can be time consuming and expensive to develop and their complexity can make them difficult to understand and interpret, especially for non-experts. Another big disadvantages is that using a single model to tackle a complex issue that a large model may come close to the limits of a single model, in terms of computation and complexity.

An alternative to a single model reaching those limits is combining models into a multi-model, also sometimes referred as hybrid or integrated models. It has been found that complex issues are better addressed when using a multi-model in comparison to a single model, due to the combination of the strength of each individual model (Duboz et al., 2003; Quesnel et al., 2009). Multi-models also facilitate the exploration of complex system dynamics from multiple perspectives and definitions (Bollinger et al., 2018). Furthermore, a multi-model addresses the issue of single-source results containing bias because multiple perspectives (represented by the multiple models) coalesce and the multi-model may cover blind spots that the individual models may have had (Heikkila, 2017). Finally, a multi-model has the benefit of fully using the previous investments done in the constructing of independent models, saving time and money (Brandmeyer & Karimi, 2000).

There are various challenges yet to be solved due to the novelty of multi-modelling (Nikolic et al., 2019). The most relevant challenges can be split into two categories, the technical and non-technical challenges. Firstly, the technical challenges are system design and alignment of the models that are to be combined. Multi-model system design concerns itself with the relationship between the models and the coupling of the models. The alignment of the models can be on several topics, but the three most common barriers in terms of alignment are formalism, resolution and scale. A difference in formalism is the most common blocker for multi-models and occurs when the models have an underlying difference in the fundamental mathematical or algorithmic presentation used (Vangheluwe, 2000). Resolution is about the level of detail used in the models. Scale is about the spatial misalignment of the models, where certain model entities have to be (dis)aggregated to construct a multi-model (Schmitz et al., 2013).

There are two non-technical challenges that present themselves most frequently. Firstly, multi-models quickly approach the “model comprehension barrier” (Nikolic et al., 2019). This means that when a multi-model becomes bigger and, consequently, more complex, it becomes increasingly difficult to understand and interpret the meaning of the numbers and outcomes within the multi-model. The second and last major challenge to overcome is that some models require a (sometimes expensive) license to use if they are not open source, while other models may have restrictions on the modification (Pfenninger, 2018). This doesn’t even consider the models that won’t be shared, even with a license. This could prevent the realisation of a multi-model with a specific model before any technical issue could stop the modeller(s).

1.2. Multi-Modeling for the Tholen Business Park: A Case Study

It is the ambition of a consortium of parties to construct working and usable multi-models. The Technical University of Delft is a part of this consortium, joined by a whole plethora of other players on the topic of energy (models). This consortium includes other academic instutes University of Leiden and University of Applied Sciences Groningen, network operator Stedin, Alliander and gasunie with support from companies Kalavasta, Quo Mare, Quintel and DNV. This multi-model project was started in 2020 and is being carried out across three use cases with a different aggregation level: the micro-, meso- and macro use cases. This research is conducted within the boundaries of the existing project progress of the micro use case, a study wherein an existing multi-period, multi-objective optimisation model, the Techno-Economic Analysis Of Complex Option Spaces and is a Long-Term Optimization Tool (TEACOS) is used to study the optimal investment paths for an industrial and business park. The purpose of the multi-model of the micro use case is to be able to aid in the transition to low-carbon energy systems. However, the first step of micro case is to couple models of various resolutions together and ensure that meaningful couplings can be established so the multi-model becomes a possibility. To test the feasibility of such a multi-model, they have selected an industrial area as a case study. The chosen industrial area is the industrial area of Tholen, Zeeland. This thesis will use the same case study as input.

One of the goals of the consortium is to study how to couple a simulation to the existing optimisation model. In this case, it is proposed to incorporate an agent-based model that interacts with the optimisation model, TEACOS. This is proposed to find out if, primarily, how such a coupling can be realised and secondarily, what the effect is of such a coupling. The purpose of this study is not to recreate realistic investment behaviour, which costs significant time and resources as proven by Sachs et al. (2019) in the case of residential areas. This thesis will study this type of coupling, between TEACOS and an agent-based model. Because this research was started as a piece for the micro use case, this research will only operate within that scope and also be constrained by the micro use case. The two most important constraints are that the optimisation model that is chosen to couple has already been selected - the TEACOS model mentioned earlier - and that TEACOS is not open source, meaning that this coupling will have to be done with a black box model.

This thesis acts as an exploration of coupling these types of models, not only hoping to provide the micro case with more information on model coupling, but also to add to the body of knowledge on this novel topic for the larger modeling community. For other modellers attempting a similar coupling, this thesis will offer lessons learnt. Finally, the societal relevance is reflected by the aspiration that one day, multi-models may be used as support to address the wicked problems that society faces. An example is that through the micro case, the multi-model hopes to better support decision making for the energy transition, an urgent topic on the Dutch national agenda. This research hopes to add to the novel topic of multi-models for future modelers seeking to couple these types of models.

1.3. Research Objective

In the context of modelling and for the remainder of this thesis, the definition of a model is a representation of a real-world system or phenomenon that captures its essential features and allows us to make predictions, test hypotheses, and gain insight into the underlying mechanisms of that system or phenomenon.

To help study complex systems, various models can be combined to form a multi-model. This offers various advantages, such as an all-encompassing framework of knowledge with which the entire system can be analysed and not just parts of it. This also reduces the need to develop new models for each situation and allows for the capturing of each models' individual strength. However, this is a considerable undertaking with many challenges. TU Delft and her consortium are willing to tackle the challenges. One of the key challenges for multi-models is the coupling of the individual models and studying how the coupled models may affect the outcome. The focus of his thesis will therefore be to study which interaction structures exist for coupling optimisation and simulation models and how the choices might affect the workings of the multi-model within the scope of the case study.

Therefore, the main research question is formulated as follows:

"What is the effect of coupling an agent-based model to an existing optimisation model, TEACOS, given the case study of Tholen?"

To answer the main question, there are three sub questions that have been formulated. The question specific method will be briefly discussed following each question. An in-depth plan for the method used in this research is found in Chapter 2.

Sub question one: *What interaction structures exist with regards to linking a simulation and an optimisation model?*

To gain insight into coupling, coupling tightness for models and their interaction structures, especially simulations and optimisations, Chapter 2 contains a more in-depth literature review on the core concepts. The answer to this question is used to determine the possibilities for coupling TEACOS, the model from the case study, and the model to be made.

Sub question two: *What is a meaningful coupling of an ABM and the optimisation model to form a multi-model, given the case study?*

There are three steps to this answer. First, the existing models will have to be understood. First, TEACOS will be studied in Chapter 3 and the ABM will be made in Chapter 4. In having the two building blocks for the coupling, the knowledge from the literature study will be applied to conceptualise a meaningful coupling between the models and implement it in Chapter 5 contains an overview of conceptual coupling for the models. The answer to this creates an overview for the multi-model conceptualisation and help understand the model requirements for the agent-based model.

Sub question three: *What are the effects of the chosen interaction structure on the outcome of the multi-model?*

To find out how the outcomes of the multi-model are influenced by the coupling of the models, experiments will be conducted with the multi-model and compared to output generated by TEACOS in Chapter 6.

1.4. Structure of this Research

The first two chapters of this thesis outline the background of the research and the multi-model with its case study. In the third chapter, the method for this research is laid out together with a small literature review of the core concepts. Chapter four, five and six contain the development of the conceptualisation and implementation of the multi-model set up and agent-based model, followed by the results. Finally, chapter seven formulates the conclusions of the research, with a discussion and recommendations for future research.

2

Method & Approach

This chapter will detail the research approach and method applied, identifying the steps taken to answer the research question and starting with a literature review on the core concepts for this research.

2.1. Research Approach

The research approach for the coupling of TEACOS and agent-based model follows a general iterative modeling procedure that has been divided into four methodological phases that align with the sub-questions and finally the main question. These steps include the conceptualisation, formalisation and experimentation of the multi-model. This research will utilise the steps given by Dam et al. (2012) and apply it to the process of constructing a multi-model, starting with the background of both models to be coupled, followed by the conceptualisation, after which the implementation will include verification and it ends with the experimentation, which also will contain the results and validation. An overview of these steps and the related phases is given in Figure 2.1, along with each chapter in which the corresponding steps can be found.

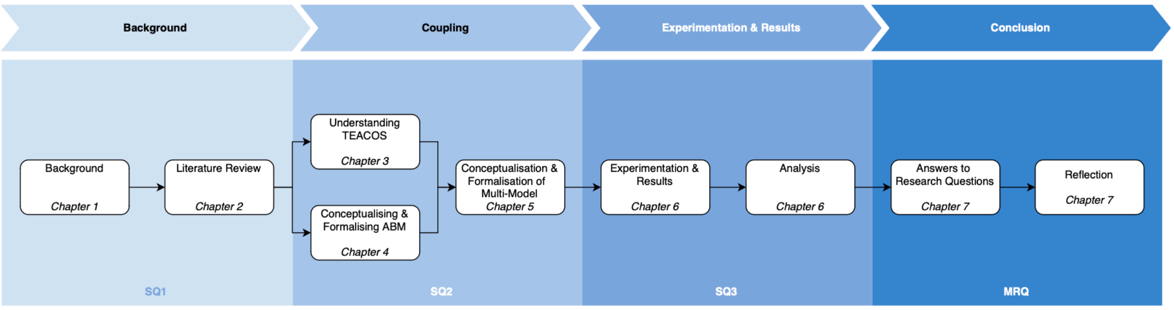


Figure 2.1: Application of the methodological steps for model coupling.

Background

To start, a literature review is conducted on the key topics that were introduced in the introduction, such as coupling tightness of models and interoperability between different systems. This is done in the follow section, Section 2.2. After that, the two models that are to be coupled will have be fully understood. Within the context of this research, it means that existing model, TEACOS, must be studied to the extent that is possible with a black-box. Because this research is a part of the micro case, background will also be given on the micro case since some of the factors that weigh into this research, such as file format and adaptor use. This is done in Chapter 3. For the ABM, this will mean that the construction of the ABM must be complete and that this must adhere to certain requirements set by the multi-model. A detailed methodology for the construction of the ABM is given in subsection 2.1.1. When that has been done, it can be understood in what way a meaningful connection can be established between the two models.

Coupling
For the second step, the coupling is conceptualised and implemented. Following the characteristics of both models and knowledge gained from the literature in the previous phase, an evaluation will be made on several aspects of the coupling, such as the tightness of the coupling and what to look out for in terms technical and syntactic linking of the models. A conceptual design will be formalised for the coupling of the models, detailing the in and output for the models and a hypothesis will be drawn up for what the multi-model outcome may look like. After that, the formalisation will be implemented, using an integrated design environment. Finally, a verification and validation shows that the constructed multi-model is suited for experimentation. This is all done in Chapter 5.

Experimentation
The third step consists of the evaluation of the coupling and the multi-model as a whole by running experiments. These experiments are carried out in various setups that will be detailed by the experimental setup and studying the outcomes of these setups. These can be compared to a ”base case”, which is a scenario in which TEACOS runs on its own. In this way, a comparison can be made of the influence of the ABM on the outcome of the multi-model.

2.1.1. Agent-Based Model Methodology

As described in the previous section, to study the coupling between TEACOS and an agent-based model, an agent-based model is to be made that will simulate human behaviour. Agent-based modeling is suited to model complex socio-technical systems (Dam et al., 2012). To construct an agent-based model (ABM), Dam et al. (2012) provides ten steps that are used within this report as a guideline. These are:

1. Problem Formulation and Actor Identification
2. System Identification and Decomposition
3. Concept Formalisation
4. Model Formalisation
5. Software Implementation
6. Model Verification
7. Experimentation
8. Data Analysis
9. Model Validation
10. Model Use

Steps one and two are given by the case context in Chapter 3, starting with a detailed explanation of the micro case and the selected case study, providing context for the problem and system to be studied. The remaining steps will be present in Chapter 4. This wills start with a more detailed explanation on the purpose of the model for the multi-model. This continues with the identification of the concepts that will be identified translated into agents, their networks and the environment. This is supported by a UML diagram, flow diagrams concerning agent behaviour and schematics adapted from Dam et al. (2012) to represent the agent-based model within the environment. Implementation is done within a modeling framework suited for ABMs, which has already been selected in subsection 4.1. The verification, step six, functions as a check to see whether the model functions as imagined in the conceptualisation. Steps seven through nine will decide whether the model is fit to be used for the multi-model, which is done through simple tests and validation. After this, the model can be used for to complete the ”Coupling” phase of the method.

2.2. Literature Review

To give more background and better understanding into the coupling of models a literature review is conducted on the core concepts. For this thesis, these are firstly, an overview of model coupling following by levels of interoperability. Then interaction structures and the specific case of simulation optimisation models are discussed. Key terms such as coupling tightness are interoperability are defined and discussed using the literature.

The papers are found using keywords associated to the topics and by snowballing forwards and backwards from relevant papers. The criteria for choosing a paper to cite is threefold: They have to be peer-reviewed, cited, and published in an academic journal. The preference is given to more recent papers, as the field of modelling has seen a lot of change in recent years. All papers were found using Scopus or Google Scholar.

2.2.1. Coupling & Coupling Tightness

The need for integrated modelling to gain insight into complex problems has widely been recognised (Bulatewicz et al., 2013; Knapen et al., 2013), however, there are some issues when it comes to integration of models. One of the main issues that one may encounter is the interoperability (Bollinger et al., 2018; Nikolic et al., 2019; Rezaeiahari & Khasawneh, 2020). Interoperability means how easily the models align with each other and factors that complicate this include different programming languages, different formalisms and a lack of documentation (Bulatewicz et al., 2010). All these issues are applicable when making a multi-model. When diving into the topic of interoperability, there is one decisive factor which is determined by the conceptualisation of model coupling which affects the interoperability of the models. This is the coupling tightness of the models, which is frequently found in the literature (Brandmeyer & Karimi, 2000; Robineau et al., 2022; Shrestha et al., 2013).

Coupling tightness refers to the fundamental concept of interdependence between models, the manner of which they are connected, and their variables intertwined. Brandmeyer and Karimi (2000) present an interesting synthesis in the form of a framework for coupling methodologies, showcasing the levels of tightness most commonly found. This starts at the base layer with the loosest coupling and builds upwards in “tightness” with each layer incorporating the features of the layer below it while also adding new ones which further intertwine the models. This framework can be seen in Figure 2.2.

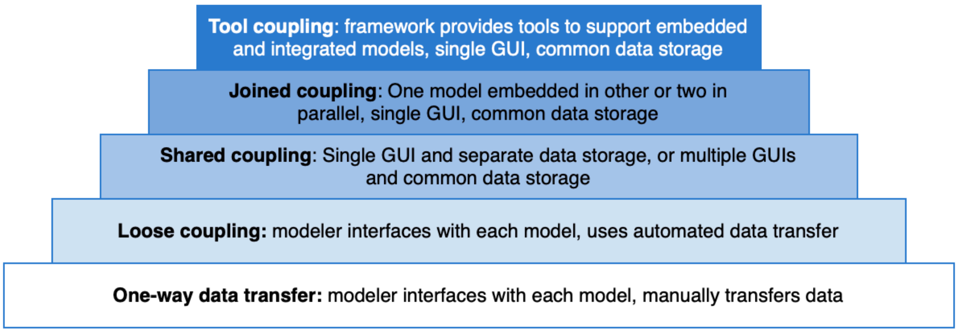


Figure 2.2: Framework of coupling tightness, as taken from Brandmeyer and Karimi (2000)

Within the framework, a division can be made between the looser method of coupling and the tight couplings, in which the bottom two tiers are examples of loose coupling and the top three tiers are examples of tight coupling. Loose model coupling refers to a situation where the models are relatively independent of each other, and the information exchange between them is minimal. Each model can operate on its own data and makes its own decisions independently of the other models (Goodall et al., 2011). The models may be executed sequentially or in parallel, and the coupling between them may be achieved through the exchange of input and output data or through some other means such as messaging or event-driven systems. The looser methods of coupling allow room for model reusability and independence. The one-way data transfer seen in at the bottom in Figure 2.2 is currently most commonly done when using multiple models (Zhang et al., 2020), because pre-processing the in- and output of models is often required as the models are often not directly compatible with each other (Shrestha et al., 2013). This method, however, is time consuming and error prone (Reußner et al., 2009).

Tight model coupling, on the other hand, refers to a situation where the models are highly interconnected and the models surrender some autonomy, such as their format autonomy and platform autonomy (Ceniceros et al., 2021). Brandmeyer and Karimi (2000)’s framework shows that within tightly coupled models, the ”tightness” ranges from sharing a GUI or data storage, seen at the third tier, to being fully embedded in one another until they become one model, seen at the topmost tier. The models may be executed concurrently or parallel and communication between them may be achieved through shared memory, message passing, or other means. Tight coupling is often used in situations where the models are simpler and computationally less intensive, as fixing the internal semantics of the models makes it harder with more complex models and it may exclude models that do not conform to certain conventions (Goodall et al., 2011).

Between the two methods, a key difference is that the models being coupled are developed independently from each other and they remain independent during this coupling. In both instances, the models do not know that the other model exists, however they do share or make use of the same definitions (Kaye, 2003).

The choice of model coupling depends on several factors such as the problem complexity, the computational resources available, and the desired level of accuracy and fidelity. While loose coupling may be appropriate for complex models that require significant computational resources, tight coupling may be necessary for models that require high levels of accuracy and fidelity or for real-time applications where the models must operate in a coordinated manner.

2.2.2. Interoperability

Interoperability between models is essential for addressing the challenge of getting models to communicate and exchange data efficiently. The ability of systems to exchange information (interoperate) plays a big role in the quality and effectiveness of the connecting models and platforms (Rehm et al., 2020). However, when speaking of interoperability, there are various different kinds of interoperability that fall under this umbrella term. The term also holds various meaning across different sectors, but within this research the definition will be defined through the use of a framework from the literature.

Currently, there is no community-wide consensus when it comes to the definitions of the kinds of interoperability, although there are various proposals for the levels of interoperability (Adebesin et al., 2013; Santos et al., 2021). There are two frameworks that are most used in the literature when speaking of the levels of interoperability. Firstly, the The Levels of Conceptual Interoperablity Model (LCIM) that has evolved since its conception to now identify seven levels of interoperability (Tolk et al., 2007; Tolk & Muguira, 2003) and secondly, a framework that proposes four levels of interoperability as proposed by the European Telecommunications Standards Institute's (ETSI) (Van der Veer & Wiles, 2008; Whitman & Panetto, 2006). Tn their review of the LCIM, Santos et al. (2021) find that while the understanding first four levels are mostly stabilised, the other levels lack a common understanding. These first four levels correspond with the four proposed by the other framework. Therefore, this research will use the second framework, with the four levels seen in Figure 2.3

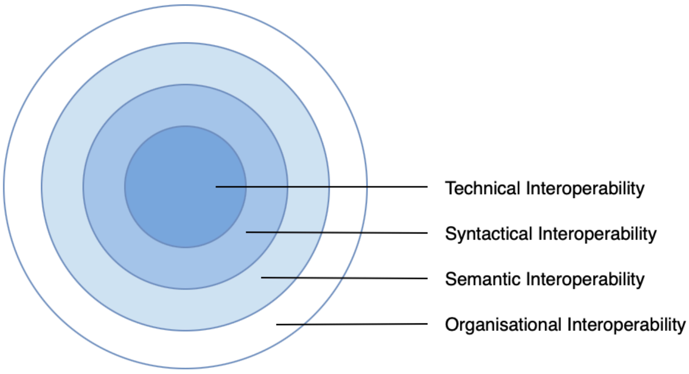


Figure 2.3: Framework for the levels of interoperability, as taken from Van der Veer and Wiles (2008)

The four levels are explained in order of importance. Without the first level, the second one is rendered obsolete, and so on. The first and foremost, is technical interoperability, enabling systems to exchange data. This does not guarantee that the receiving system can read the data, merely the act of communication. Syntactic interoperability guarantees that the format for data exchange is accepted by both systems while semantic interoperability enables the systems to understand the content of the data exchange in the same way. Finally, organisational (or pragmatic, as Whitman and Panetto (2006) calls it) interoperability refers to the ability of organisations and people to communicate and transfer (meaningful) data effectively, even across diverse information systems, geographies and infrastructures. (Van der Veer & Wiles, 2008)

These terminologies and four subdivisions give us the tools to better understand the process of achieving interoperability as well as assessing which part of creating the multi-model is the most tough. It is evident that when constructing a multi-model, achieving these levels of interoperability are a necessity.

2.2.3. Interaction structures

Understanding model interaction is essential for developing accurate and reliable models of complex systems. When talking about interaction structures for the multi-model, the manner in which the models communicate and with which ”hierarchy” is meant. One way to understand model interaction and hierarchy is to think of models as elements, or something that is more visually descriptive, a chain link. Each model represents a particular aspect or step of the system being studied and together, they form a chain of models that describe the entire system. Following this analogy, when speaking of model interaction we speak of the method the chains are linked. Of course, the model interaction is closely related to the coupling tightness. Some types of model interaction are not possible with certain degrees of tightness and vice versa. When looking in the literature, the manners most frequently discussed and used in practice are a feedback loop an direct communication, which can be considered a subset of a feedback loop.

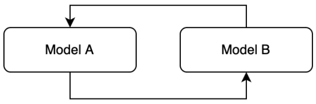


Figure 2.4: A feedback loop between Model A and B

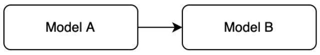


Figure 2.5: Subset one: A one directional link from model A to B

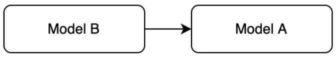


Figure 2.6: Subset two: A one directional link from model B to A

One-way direct model linking occurs when the output of one model is used as the input for another model, but there is no feedback loop between the two models. This approach can be useful when the models are designed to represent different aspects of the same system, but there is no direct interaction between them. For example, one model may simulate the physical environment of a region, while another model simulates the behaviour of the human population in that region. By linking these models together where the physical environment is used as input for the simulation, researchers can gain insights into how the physical environment influences human behaviour.

One advantage of one-way direct model linking is that it can be computationally efficient. Because there is no feedback loop between the models, each model can be run independently, which can reduce the computational resources required to simulate the system as a whole. This can be particularly important when modelling large or complex systems, where the full effects of the feedback loop may not be entirely clear.

Another method of interaction is the feedback loop. Feedback loops are an integral part of the idea of systems and can help to capture the complex behaviour of many natural and social systems (Bertalanffy, 1968). As described by Capra (1997), ”A feedback loop is a circular arrangement of causally connected elements, so that each elements has an affect on the next until the last ”feeds back” into the first element of the cycle”. When applied to the multi-model, that means that a feedback loop occurs when the output of one model is used as input to another model and so forth until the output of the last model is then fed back into the first model. This creates a cycle of information flow, where changes in one model can have a cascading effect on the output of other models in the system. Feedback loops can be positive or negative, depending on whether they amplify or dampen the effects of changes in the system being studied (Walby, 2007). However, feedback loops can also be difficult to manage and interpret, especially when it comes to the multi-model. Changes in one model can have a cascading effect on the output of other models in the system, making it difficult to pinpoint the source of unexpected behaviour within the multi-model.

2.2.4. Simulation Optimisation

A lot of choices have to be made when integrating models, of which the first is with which coupling tightness and with which interaction structure models are linked. Figueira and Almada-Lobo (2014) give a comprehensive summary of the hierarchies available when it comes to simulation and optimisation and their four configurations for model integration can be seen in Figure 2.7

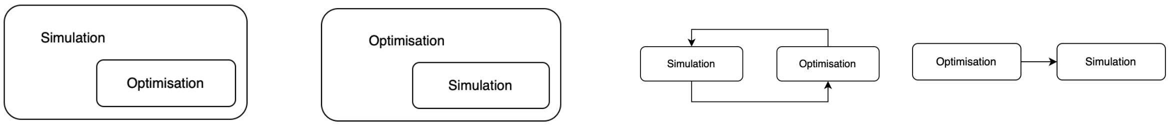


Figure 2.7: Configurations of simulation-optimisation integration, adapted from Figueira and Almada-Lobo (2014)

The first two configurations are a tight coupling, wherein one model is fully integrated into the other as a part of that model. They are not independent models anymore. In the third and fourth configuration, the models are loosely coupled, retain their independence and communicate either through a feedback loop or a one-way directional data flow, in the case of Figueira and Almada-Lobo (2014)'s paper, only from the optimisation to the simulation as input.

Integrated simulation-based optimisation involves using a simulation model of a system to optimise its performance. The simulation model is used to test different scenarios and determine the best set of input parameters that will maximise the output or minimise the cost. This approach is often used in engineering, operations research, and other fields where the system being optimised is too complex or expensive to test in the real world. Optimisation-based simulation, on the other hand, involves using optimisation techniques to improve the accuracy and efficiency of a simulation model. The goal is to find the best set of model parameters that will produce results that match real-world data.

However, for the purpose of this research we will adjust these configurations to three options. We will call the direct, one-way link a subset of the feedback loop, leaving us with the set of options when coupling the ABM and TEACOS that can be seen in Figure 2.8, that we can consider for the purpose of this study.

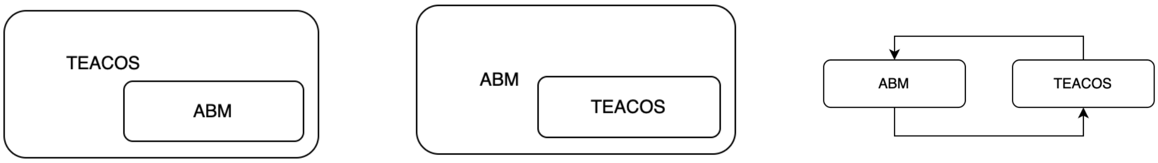


Figure 2.8: Model coupling methods for the case study of Tholen.

3

The Micro Case Background: Tholen Case Study

This chapter will provide background information of the micro use case multi-model and the first building block of the multi-model, TEACOS. The multi-model is explained to lay give more context for the study and explain key aspects, such as ESDL-files and model adaptors. Afterwards, a detailed explanation is given for TEACOS, discussing its purpose, in and output and how it works followed by the explanation for the case study of the micro use case.

3.1. Purpose of the Multi-Model

The purpose of the multi-model developed for the micro case is to allow a user from any industrial area to gain insight into the (future) behaviour of the energy system of the industrial area as well as forecast the optimal investment strategy of assets over time. In this case, assets are as the collective term for sustainable alternatives such as solar panel installations and batteries to make the industrial area more sustainable. Using the multi-model, the end-user will be able to see how the energy system acts across different scenarios. These scenarios can include variations in, for example, future energy costs.

The end user will be able to access the multi-model through an orchestrator. The models in the orchestrator will feel and act as one model for the end users. For example, the user they need to configure the optional assets and select the scenarios, after which they merely have to press “start” to run all models. By doing so, all the processes within the orchestrator will be executed, returning output to the end user, showing the behaviour of the energy system, local energy production, the flows of energy, CO2 emissions and the energy costs, after which the end-user can interpret the results to make their decisions.

A prerequisite for the micro case is that the models are used as independent models. This is because this is an important driver of the maintainability of multi-models, but also due to legal reasons. Certain models proposed for the micro case are property of their respective companies and cannot be fully given up and integrated. The specific research question that drives the micro case is to test the feasibility of combining models that work on different time resolutions. This means that one model may run on time steps of a year, while another may use hourly time steps.

So in terms of coupling tightness, the models will not be tightly coupled to become a singular model. Full integration is not an option when making the multi-model. Instead, all models are used as ”black-boxes”, where they run their course just as they would outside of the multi-model, albeit in an pre-coordinated fashion. It will need to be determined which data exchanges occur when and what the sequence it for the models to run in. Following Brandmeyer and Karimi (2000), that means that a loose coupling is used for the micro case multi-model.

3.2. Multi-Model Setup

To construct the multi-model for the micro case, five models are proposed to cover all purpose of the micro case, along with another piece of software. These models already exist and have been fully developed prior to the multi-model project. They are listed below with a brief description:

- The Energy Transition Model (ETM) is an open-source interactive tool that simulates and analyses the energy system of a country or region. It allows the modeler to build and explore scenarios based on energy demand, supply, and infrastructure as well as policy and technology choices. It helps create insights into the future of an energy system while also supporting the comprehension of the complexity of that energy system. The ETM uses a bottom-up approach, which means that it simulated the behaviour of individual energy technologies and infrastructures at a granular level, and then aggregates them to provide a comprehensive overview of the entire energy system.
- The Energy Potential Scan (EPS) is used to assess the potential for renewable energy generation for buildings for industrial areas. This is done by evaluating the technical, economic, and environmental feasibility of different energy technologies.
- The Techno-Economic Analysis of Complex Option Spaces (TEACOS), a model that can evaluate the feasibility and economic viability of investments towards low-carbon energy systems over multiple periods. TEACOS is based on a Mixed-Integer Linear Programming (MILP) algorithm in AIMMS. It optimises for the best transition pathways for the energy transition and returns the optimal investments for the actors in the energy system.
- The Energy System Simulator (ESSIM) simulates an interconnected energy system over a period of time and checks whether the profile of demand and supply match based on the schedule of flexible energy producers. ESSIM does this by analysing the effects of the schedule in terms of emissions, costs, network, load, and so forth.
- The MapEditor is a tool developed by TNO to either construct an energy system from scratch or edit an existing energy system. It gives 2D visual representation of an energy system and allows for changes to be made to the energy network through a user-friendly GUI. The ESDL MapEditor allows users to make changes by just dragging and dropping energy system components on a map.

Another important part of the multi-model is the Energy System Description Language (ESDL). ESDL is an open-source standard language for describing energy systems in a standardised, machine-readable format. It was developed by TNO with the purpose of facilitating the exchange of energy modeling data between various tools and making it easier to compare the results of different analyses. This can be considered the Rosetta's stone for the micro case models. All files transferred between the models use this language and each model adapts to either work with it or translate it into something the model can work it.

The language is based on XML and the principles of object-oriented programming, allowing for energy systems of all sizes to be represented as a network of interconnected components, such as power plants, storage facilities, and buildings. Each component is defined by a set of attributes, such as their capacity, efficiency and location. They are linked to other components in the energy system through connector type assets which can carry electricity or gas, for example. Because it was developed in the Eclipse Modeling Framework, it is easily compatible with other modeling languages and tools, such as Python and MATLAB.

In the micro case, this standardised format of describing energy systems allows for the ease of sharing data between the models and enables more transparent and reproducible analyses for decision making. The downside is that all models have to be 'adapted' to be able to read and produce ESDL-files. For example, TEACOS is built using AIMMS software and cannot directly read input from an ESDL-file. To accommodate for the use of ESDL-files in TEACOS, an adaptor is needed to translate the ESDL-file to input for TEACOS and once the model has run, translate the output of TEACOS back to an ESDL-file.

A system design for the multi-model has long existed, but has been subject to change over the course of the micro case. Figure 3.1 contains an adapted system diagram based on a working version made by TNO in February 2023. This show the manner of which these models are coupled and which input and data streams are envisioned.

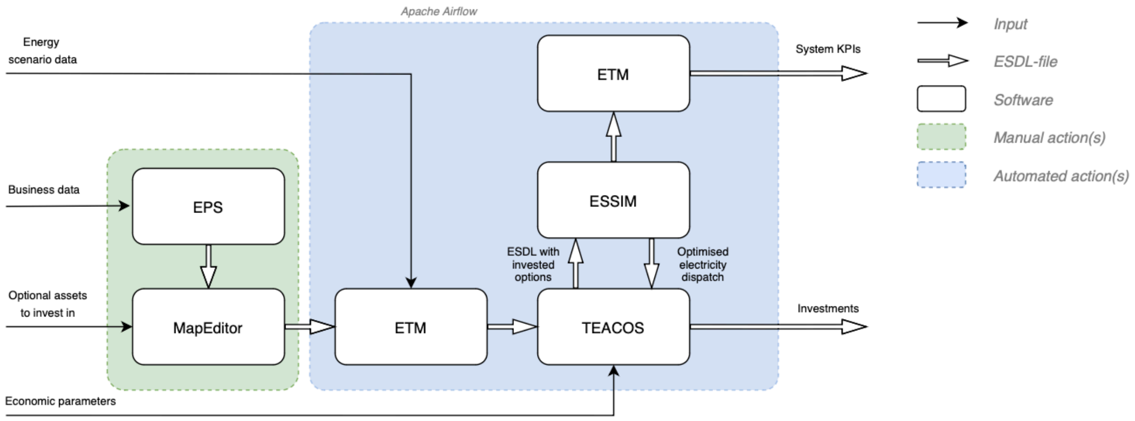


Figure 3.1: The Multi-Model system diagram for the micro case

Using Figure 3.1, the process of the multi-model can be explained in two phases. The first phase still occurs with a manual action, where the outcome of the EPS is combined into an ESDL-file with optional assets, using the MapEditor. This phase requires user input on which assets are to be studied by the remainder of the models, which the user adds as optional assets to the ESDL-file. The file with user input is then used as input for the second phase. The second phase happens in an automated workflow environment, too, containing three models. In this phase, TEACOS optimises for the energy system, seeking the best path forward in terms of optional assets and ESSIM checks whether the solution generated by TEACOS is feasible. If ESSIM declares it infeasible, it goes back to TEACOS for another loop. Once they agree, the resulting ESDL is sent to the ETM to calculate certain KPIs determined for the micro case and TEACOS returns which assets have been invested in.

For this case study, Apache Airflow is used, an open-source platform that facilitates the construction of these automated workflows. In this case, the workflow is the sequence of the models being used. The order in which the models are called upon is decided by Directed Acyclic Graphs (DAGs). A DAG contains information on which model should be called at what time, along with where data is retrieved and subsequently stored. Each run of the multi-model will call upon a DAG, which decides the sequence and dictates which data file goes were, either as input or output.

Another key part in the multi-model is the usage of model adaptor. They ensure that models of any language can be used in the multi-model. A model adaptor works by encoding the data file used by the multi-model to fit as input for the respective model, allowing it run as it normally would. Think of a model adaptor as a translator. After the model has run as it normally would, the model adaptor proceeds to decode the output, transforming it back into the original format with any adjustments made by the model. This way, the data file can be read again by other models in the multi-model. An abstract schematic for model interaction with an adaptor can be seen in Figure 3.2.

In the micro case, the models use an ESDL-file as the common language denominator. An example of an energy system as an ESDL-file, as seen in the MapEditor can be seen in Figure 3.3. It can be seen that the energy system is made up out of energy assets, which stand at the heart of an ESDL system description.

Energy assets can be divided into five different subtypes, which have been represented in Table 3.1 with an example per asset type. Each asset type has a different colour code.

One colour that is not an ESDL asset type but is used frequently within the micro case is the grey icon, which represents *group of assets*, depicting for instance a building that is a host to various energy assets within them. This type of grouping is useful to create an simple overview on a higher aggregation level, depicting that there are various buildings with their own energy assets. When wanting to study

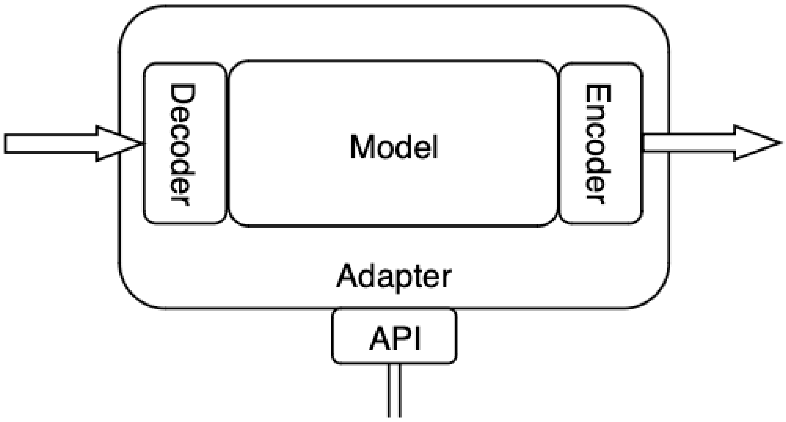
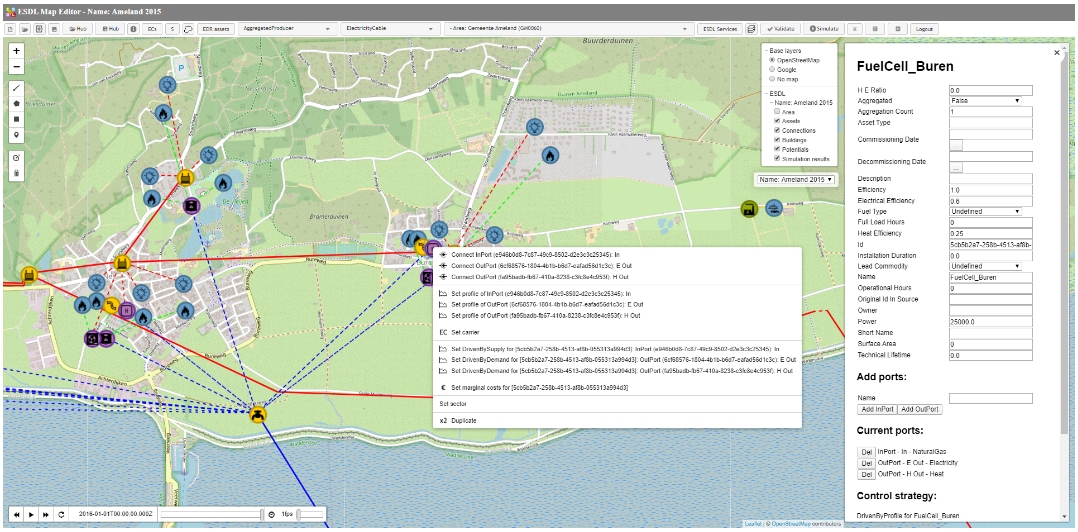


Figure 3.2: High level schematic of the adaptor IT architecture



Connect InPort (e946b0d8-7c87-49c9-8502-d2e3c3c25345): In
Connect OutPort (6cf68576-1804-4b1b-b6d7-eafad56d1c3c): E Out
Connect OutPort (fa95badb-fb67-410a-8238-c3fc8e4c953f): H Out
Set profile of InPort (e946b0d8-7c87-49c9-8502-d2e3c3c25345): In
Set profile of OutPort (6cf68576-1804-4b1b-b6d7-eafad56d1c3c): E Out
Set profile of OutPort (fa95badb-fb67-410a-8238-c3fc8e4c953f): H Out
EC Set carrier
Set DrivenBySupply for [5cb5b2a7-258b-4513-af8b-055313a994d3]: InPort (e946b0d8-7c87-49c9-8502-d2e3c3c25345): In
Set DrivenByDemand for [5cb5b2a7-258b-4513-af8b-055313a994d3]: OutPort (6cf68576-1804-4b1b-b6d7-eafad56d1c3c): E Out
Set DrivenByDemand for [5cb5b2a7-258b-4513-af8b-055313a994d3]: OutPort (fa95badb-fb67-410a-8238-c3fc8e4c953f): H Out
€ Set marginal costs for [5cb5b2a7-258b-4513-af8b-055313a994d3]
Set sector
x2 Duplicate

FuelCell_Buren

H E Ratio	0.0
Aggregated	False
Aggregation Count	1
Asset Type	
Commissioning Date	
Decommissioning Date	
Description	
Efficiency	1.0
Electrical Efficiency	0.6
Fuel Type	Undefined
Full Load Hours	0
Heat Efficiency	0.25
Id	5cb5b2a7-258b-4513-af8b-
Installation Duration	0.0
Lead Commodity	Undefined
Name	FuelCell_Buren
Operational Hours	0
Original Id In Source	
Owner	
Power	25000.0
Short Name	
Surface Area	0
Technical Lifetime	0.0

Add ports:

Name

Current ports:

InPort - In - NaturalGas
OutPort - E Out - Electricity
OutPort - H Out - Heat

Control strategy:

DrivenByProfile for FuelCell_Buren

2016-01-01T00:00:00.000Z 1fps

Figure 3.3: The Online MapEditor for ESDL-files while working on an energy system of Ameland, retrieved from ESDL documentation (TNO, n.d.)

Table 3.1: List of ESDL Asset Types with example included

ESDL Asset Types	Icon Example	ESDL Asset Example
Producer	●	Wind Turbine
Consumer	●	Electricity Demand
Conversion	●	Powerplant
Storage	●	Battery
Transport	⚠	Electricity Cable

the buildings in detail that can be done by clicking on them in the MapEditor. This ability to create a building is used for the energy system of the industrial area of Tholen for all 112 buildings, which aids in a straightforward representation of the complex energy system. This way, the energy system contains all aspects of the network and the demand of the buildings while keeping it comprehensive to study in the MapEditor. This will be further explained in Chapter 5.1 where the ESDL-file for the industrial area of Tholen is discussed.

3.3. TEACOS

This section will go into detail on the workings of TEACOS, describing the purpose and workflow of the model and adaptor, the in- and output and which characteristics or model behaviour are important for the rest of this research, ending with a KPI that will be used to measure the output of the coupled models.

TEACOS, short for Techno-Economic Analysis Of Complex Option Spaces, is a powerful long-term optimisation tool designed to facilitate the transition towards low-carbon energy systems written in the AIMMS language. The tool identifies the most profitable investments while adhering to predefined supply/demand scenarios and potential environmental constraints set by the modeler. It does this using a Mixed Integer Linear Programming (MILP) Algorithm that optimised the Net Present Value of an energy system using the investments as the options of the algorithm. The solver that TEACOS uses is the IBM ILOG CPLEX Optimiser (often simply called CPLEX), a software tool for optimizing linear programming, mixed integer programming, and quadratic programming problems. CPLEX is widely used in both industry and academia for a range of applications, including operations research, supply chain management, logistics, and more.

When applying TEACOS to an energy system, is needs to consider options, also referred to as optional assets within the micro use case. These are, when speaking of the energy system, the investments for low carbon energy systems, such as solar panels or wind mills. Each investment has their own characteristics, such as life expectancy, acquisition and installation costs and marginal costs once installed that are by TEACOS. These optional assets are all taken into consideration by TEACOS when it is run, but TEACOS starts by calculating a base case. The base case is a scenario where none of the optional assets are selected and business goes on as usual. In this base case, business as usual means that, for instance, electricity is sourced from the electricity grid or any sustainable alternative that *already* exist. All costs for the base case are calculated by TEACOS and afterwards, TEACOS tries all combinations of the optional assets that can fulfill the demand of the energy system, calculating the costs for all these scenarios as well. In the end, the scenario with the lowest cost is selected. This can be the base case if, for instance, the optional assets are too expensive. However, oftentimes the output is a selection of the optional assets that should be invested in.

Since TEACOS is written in the AIMMS language, this cannot be directly incorporated into the multi-model as it cannot read ESDL-files. Furthermore, TEACOS is not open source, so a wrapper has to be made to be able to incorporate the model into any kind of multi-model. Therefore, to ensure syntactical alignment and to facilitate the use of TEACOS, an adaptor that will be able to en- and decode ESDL-files has been made by Quo Mare. This adaptor is able to receive an ESDL-file as input and translate it to AIMMS parameters for TEACOS and vice versa for the output. The adaptor has been made available, but this means that TEACOS cannot be accessed directly, merely called upon through an API that calls the adaptor. TEACOS' inner workings are not directly available and any parameters will have to be communicated through the ESDL-file that is used as input. TEACOS is being used a black-box for this research. As explained, TEACOS identifies the most profitable investments by considering optional assets. TEACOS cannot think of these optional assets by itself, so the task of the modeler is to design and input all optional assets for it to consider. These optional assets are currently manually input in the ESDL-file. Within an ESDL-file, these optional assets have three states. These are 'optional', 'enabled' and 'disabled'. The state of an optional asset influences how TEACOS considers the asset as input for a model run *and* after a the model has run, contain TEACOS' decision on whether or not to include the asset for the optimal strategy.

To show how TEACOS considers the optional assets and what the output looks like, an abstract diagram of how TEACOS would work in a hypothetical situation has been made which can be seen in Figure 3.4. In this diagram, it can be seen that TEACOS considers the status quo and also all optional assets with possible configurations.

Now, this image shows how TEACOS behaves in a hypothetical situation where TEACOS with fixed assets. However, in reality, TEACOS is smarter at solving these scenario and does not manually consider each exact potential scenario but which ones the algorithm estimates are better than the base case.

To provide a more detailed explanation of how TEACOS handles optional assets and incorporates a

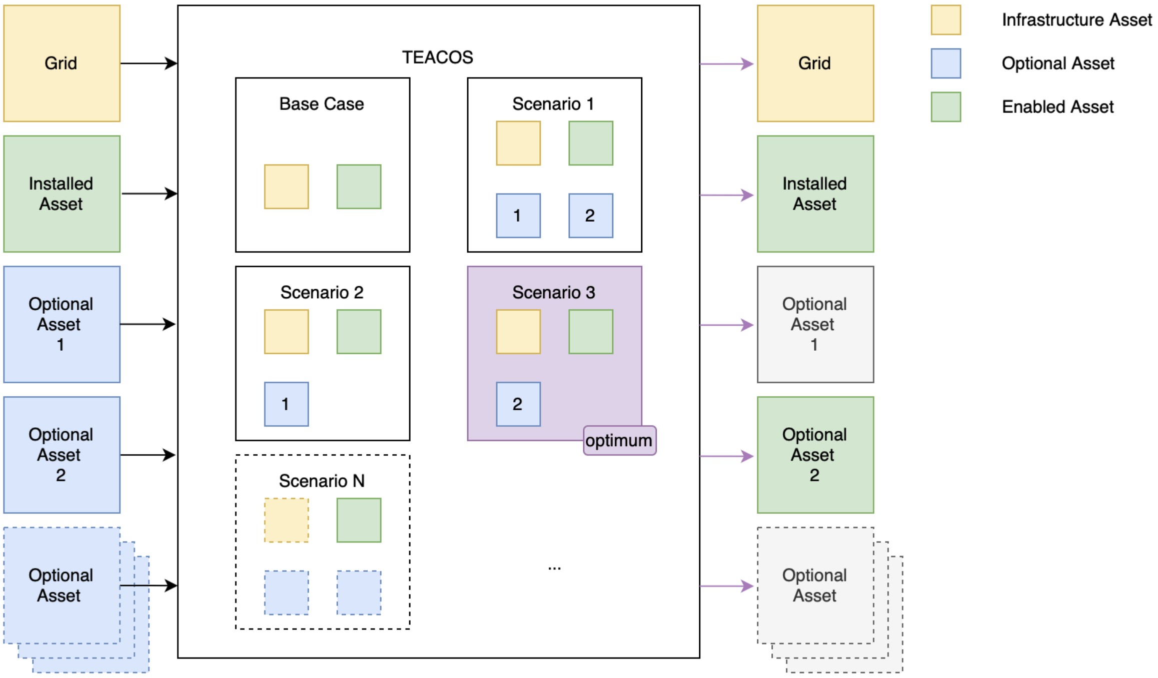


Figure 3.4: Schematic of TEACOS behaviour

range of possibilities, let's consider the example of a photovoltaic (PV) installation. In Figure 3.5, the PV installation is labeled as 'optional' and currently does not contribute any power. This designation indicates that TEACOS will consider this asset as optional in its next run.

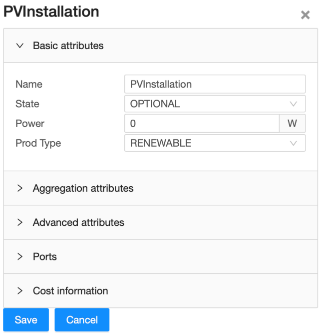
Figure 3.6 illustrates an enabled asset. The interpretation of an enabled asset depends on whether it is an input or output of TEACOS. If it is an input, it signifies that the solar panel already exists and should be included as part of the base case. On the other hand, if it is an output, it indicates that TEACOS considers this asset as a component of the optimal strategy.

In contrast, Figure 3.7 demonstrates a disabled asset. If an asset is disabled, it should not be considered for scenarios if it has been deactivated as an input. If TEACOS disables the asset and it appears as an output, it implies that the asset is not part of the optimal strategy.

TEACOS records its decisions in the ESDL-file by adjusting the status of the assets according to its optimum. Additionally, if a range is given for the asset - for example, a range of one to a hundred PV panels - TEACOS is able to specify the energy demand from the asset, expressed in watts. In the example depicted in Figure 3.6, the solar panel has an energy demand of 16700W for the optimum solution.

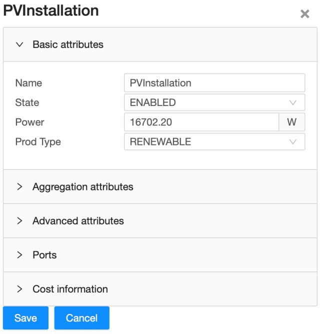
There are two results from the initial studies with TEACOS that are important to note. Firstly, it was found that the models were not aligned on the semantic level at this point, although it has been assumed to be so. Firstly, TEACOS contained a unit issue in which the unit that was used to describe the energy demand, terajoule, could not be read by the adaptor. The unit misalignment was solved by adjusting the energy demand downwards with a factor 100. Secondly, it was found that TEACOS would only give all-or-nothing solutions, which were influenced by three factors, these were the costs of the optional asset, the marginal costs of electricity drawn through that asset and a potential constraint placed upon the capacity of the optional asset. Through testing, a working setup for the optional asset to run experiments was drawn up that can be seen in Figure 3.2.

It must be made clear that the workings of TEACOS are opaque. Due to the chosen setup, there is no direct access to the model and the optimisation happens Quo Mare's internal servers. Hypotheses can be constructed and tested through adjusting the ESDL-file used as input, which can afterwards be discussed and validated with experts, topical or from Quo Mare. However, further verification of



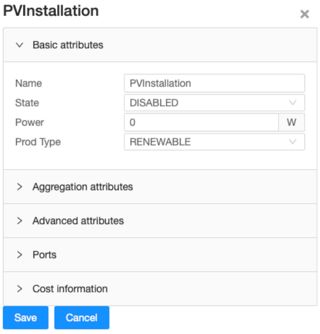
Name PVInstallation
State OPTIONAL
Power 0 W
Prod Type RENEWABLE

Figure 3.5: Example of an optional PV installation asset



Name PVInstallation
State ENABLED
Power 16702.20 W
Prod Type RENEWABLE

Figure 3.6: Example of an enabled PV installation asset



Name PVInstallation
State DISABLED
Power 0 W
Prod Type RENEWABLE

Figure 3.7: Example of a disabled PV installation asset

Table 3.2

Factor	Value	Unit
Fixed costs	500	€
Marginal costs	0.50	€/kWh
Ranged Constraint	50000	W

TEACOS output is very difficult and any hypotheses cannot be directly be confirmed since the model logs and logic are not available.

Finally, it is important to note that in the original conceptualisation for the micro use case, TEACOS is conceptualised as a multi-period model. While this is still the end goal, it was found that making an adaptor for TEACOS as a multi-period optimisation model proved harder than expected. Therefore, the first prototype of the adaptor that is used in this research does not optimise over multiple years, but optimises over one year. To simulate multiple years, it can be possible to propagate TEACOS with itself, using the single-period optimisation in a loop. This means that multiple years can be simulated by running the TEACOS model or the multi model for multiple iterations.

3.4. Case Study: Tholen

The micro case is aimed at the transition for business parks and industrial areas. A case study was chosen to be able to use real data and and illustrate the potential use or challenges. This also allows for communication and input from with the envisioned end user. Several industrial terrains within reasonable range were considered for the micro case, and eventually a choice was made for the industrial area Slabbecoornpolder and Welgelegen of Tholen, in the province of Zeeland, the Netherlands, hereafter referred to as Tholen.

This industrial area Tholen was selected based on its desire to transition towards low-carbon energy systems. In recent years, Tholen has already made steps towards becoming more sustainable, looking towards renewable sources of energy and energy storage. The industrial area does this with a majority of those located on the terrain, working together under the banner of the foundation Renewable Energy Community (REC) Tholen. For this case study of the micro case, contact has been established with REC Tholen.

Furthermore, for this case study, the optional assets implemented in TEACOS are limited to solar panels, also referred to as PV installations within the Energy System Description Language. Although Tholen is considering options such as energy storage with batteries, these will not be considered. Within the micro case it was decided that starting with one optional asset would be enough to test the feasibility of the multi-model within micro case. Therefore, when speaking of optional assets, this research will be referring to solar panels that companies can buy and install on their roofs.

4

Agent-Based Model

This chapter will present the constructed Agent-Based Model, which is the second building block of the multi-model. This chapter will first explain the choice for using Mesa instead of other Agent-Based Modeling frameworks, discussing characteristics and which best fit the purpose of this research. Afterwards, the model is presented based on steps of Dam et al. (2012). This is first detailing the purpose of the model and its conceptualisation, followed by implementation, verification and validation.

4.1. Choice of ABM Framework

To simulate the buying behaviour of companies of an industrial area, an agent-based model (ABM) method is used. Several ABM environments exist, each with their own strong points. This section will compare three environments and, in the end, detail why the python library Mesa was chosen.

Open-source software is an important driver of research. It allows for cost-cutting and faster development and most importantly, for future work to build upon what already exists (Hegemann, 2017). This is in line with the purpose of the multi-model, and therefore all chosen environments to study are open-source software.

Through prior experience with ABMs and desk research, the following three environments are considered: Mesa and AgentPy are python libraries targeted at simulating agent behaviour (Foramitti, 2021; Kazil et al., 2020) and NetLogo, a Scala-based environment made for the simulation of agents (Wilensky, 1999). To compare the options, there are four criteria that are important for this specific project. These are the programming language used, ESDL interaction, experimental setup, and documentation. The comparison of these environments along these criteria can be seen below.

Table 4.1: Comparison of agent-based modelling environments

	Mesa	**AgentPy**	**NetLogo**
Language	Python	Python	Scala and Java
ESDL interaction	Direct, using pyesdl package	Direct, using pyesdl package	Indirect
Experimentation	Existing EMA workbench connection	Existing EMA workbench connection	Existing EMA workbench connection
Documentation	Moderate, still in progress	Limited	Extensive

Considering these criteria, Mesa is the best fit in this case. This is because NetLogo does not meet the ESDL interaction criteria. Being able to interact with ESDLs is one of the requirements that follows from the multi-model setup, as explained in Section **??**. Pyesdl, a python package for interacting with ESDL-files through python, accommodates for easy integration through AgentPy or Mesa. This does not mean that using NetLogo is impossible, however due to the time limit on this research project, a direct, established interaction method is heavily preferred. Both remaining environments are very similar, but differ in a key criteria. When choosing between Mesa and AgentPy, Mesa was chosen due to AgentPy's limited documentation. Not only that, but Mesa's documentation and software updates still frequently occur, with the latest being in the same month of writing, February 2023, and AgentPy's last update was over a year ago.

However, choosing Mesa is not without its downsides. The first, main downside is the lack of experience with the library of Mesa. Furthermore, although Mesa's documentation is more extensive than AgentPy's, it is not as extensive as NetLogo's documentation and user base. This means that coding progress may be slower than expected and needs to be kept in mind.

4.2. Model Purpose & Requirements

This section is centred around the purpose and the requirements of the Mesa Agent-Based Model, stipulating what to keep in mind during the conceptualisation. The goal of the ABM is to simulate investment decisions, particularly their decisions to invest in the optional assets that are selected by TEACOS. This means that only the optional assets that are considered by TEACOS will also be considered by the ABM, which makes it so that the focus is on investments in solar panels. The geographic scope for this model is the industrial area of Tholen, a part of the Tholen municipality located across the highway from the town of Tholen itself. As shown in Figure 4.1, the area of interest that is marked in red is quite large and spans roughly one square kilometre according to measurements made in Google Maps. This area, which can be seen better in Figure 4.2 can be seen to house a lot of buildings that house a variety of businesses, ranging from driving schools to building material suppliers.

Data from the micro case allows for the ease of using this as a case study as it enhances the model's realism. This data already includes the buildings and their locations, including a simple breakdown of their electricity demand, categorised into electricity intended for building-related purposes, such as lighting and computers, and electricity used for process-related tasks, like manufacturing machines and servers.

The key outcome this model aims to represent is the number and distribution of solar panels that are purchased by agents in a single simulation run. The Mesa Model aims to replicate the decision-making processes that influence the acquisition of solar panels in an abstract manner while using the output from TEACOS as an upper limit.

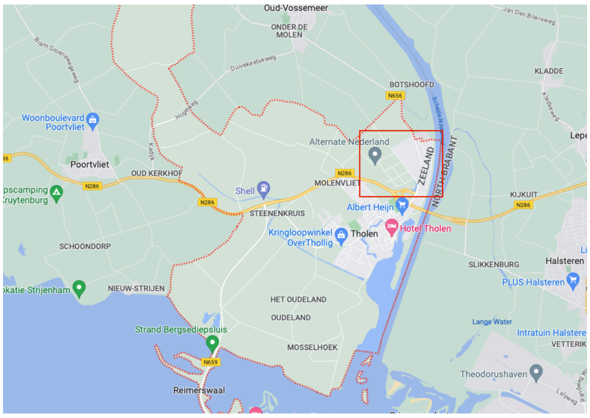


Figure 4.1: Model target area marked in red, located in Gemeente Tholen, the Netherlands

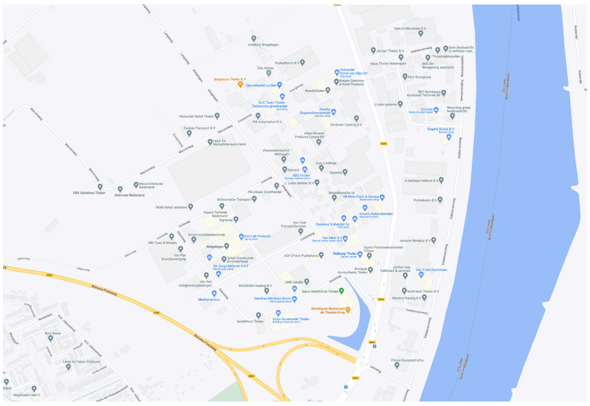


Figure 4.2: Detailed model area

Following the knowledge from the literature review which detail what to watch out for, a list of technical requirements has been made. These requirements refer to the necessary conditions for the models to interact as conceptualised and stem from the levels of interoperability proposed by Whitman and Panetto (2006) and Van der Veer and Wiles (2008).

General requirements

1. **Technical interoperability:** The models are able to communicate at all, making use of a similar

modeling environment. In this case, the choice been to use Python because of three things: Firstly, the adaptor for TEACOS is written in Python. Secondly, Python packages exist to work with ESDL-files and allow for the editing of these files and thirdly, Python offers several packages to create Agent-Based Models, such as Mesa as explained in Subsection 4.1.

2. **Syntactic interoperability:** Semantic alignment between the models is essential and entails that the files used as input and output of the ABM match that of the other model(s). Firstly, this allows for easier communication with the multi-model. This way, the output does not need to be transformed to be read by the ABM. Secondly, in this case, this allows for easier future integration of the ABM into the multi-model pipeline. For the Tholen case study, the ABM needs to be able to read the ESDL-file and save any adjustments made into the same structure.
3. **Semantic Interoperability** The ABM should be able to recognise the TEACOS' output. In this case, the ABM should be able to find the investment strategy within any ESDL-file Only the asset(s) of which the state has been enabled by TEACOS should be considered by the ABM.
4. **Time Step Synchronisation:** The ABM should run for the same time span as the other model(s). In this case, TEACOS optimises for a year, which means the ABM should at least be able to accommodate running for that same duration of time.

There is also one design aspect of the ABM which requires more thought due to the fact that it will be positioned within a multi-model. This is the issue of identifying the correct agent aggregation level. The scale at which agents are made should be the smallest concept that fits to the purpose of the optimisation. This means that when considering how to make the agents in the ABM, the modeler should consider the purpose of the optimisation and which mapping fits the purpose of the multi-model. A tool to support this decision is looking at the structure of the used data file. When agents are made based on the data file instead of being hard coded, the ABM can be fitted to many different projects instead of only one. Not only does this make it more future-proof, but it also eases the process of dealing with changes in the original data-file.

4.3. Conceptualisation

The conceptual model describes all the elements that are present within the model and the relationship between these elements. An agent-based model consists of physical and social entities that are present in the system as well as the links between them (Dam et al., 2012). Based on Dam et al. (2012), all agent-based models contain agents, a network and an environment. The model, as the name suggest, contains agents that interact with each other with behaviour that is determined by a set of rules. Each agent also has states which influence their behaviour. The environment of an agent-based model is the part of the system with which the agent interacts and is influenced by. The following decomposition can be made of the agent-based model:

- **Environment:** The industrial area of Tholen
- **Agents:** Buildings situated in the industrial area of Tholen
- **Time:** the model runs for a year, with each tick being a month

The environment is that of the industrial area of Tholen. A simple schematic representation layout of the agent based model is made according to the style of Dam et al. (2012), and can be seen below in Figure 4.3.

From the environment, the result from TEACOS is given and the users can interact with the environment by buying their solar panels from it. Each solar panel has several attributes which the agents will consider. The environment interacts with the agents by selling them solar panels in exchange for money and acting as a potential limit for how many they can buy when they have reached the global optimum.

4.3.1. Agents

Agents are the main component within the agent-based model. As the primary elements of the model, the agents' design influences their behaviour, which in turn dictates the model's overall performance and possible emergent behaviour. The agent's behaviour is specifically based on their state and certain

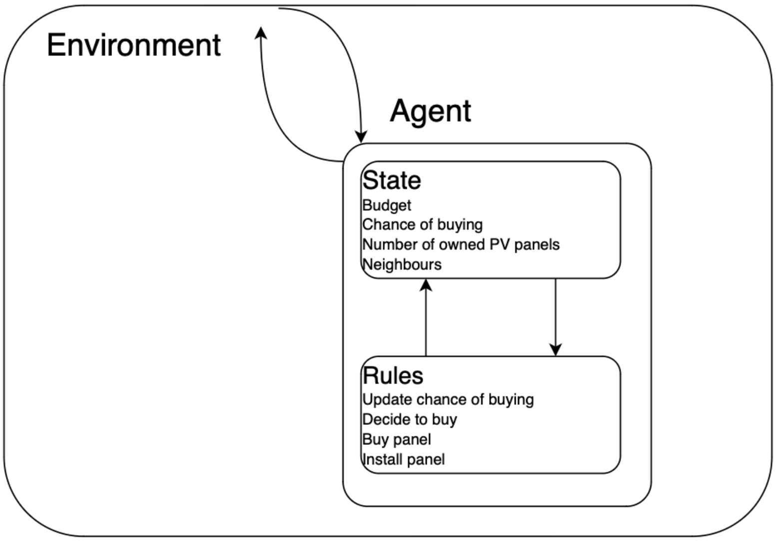


Figure 4.3: Schematic layout of agent-based model, style adapted from Dam et al. (2012).

rules that they follow. The first step of the agent conceptualisation it will need to be decided what entity will make up an agent in the ABM, followed by those entity's states and decision logic, which will be done iteratively.

Agent aggregation level is usually derived from the problem formulation and context. For instance, in a building fire alarm simulation, all agents are the people leaving the building. Due to the extra complexity of the multi-model, however, this step poses a challenge. In the case of Tholen, the agent aggregation level has been set with a upper limit in that they should not be bigger than buildings. This is done because of the semantic alignment for the multi-model and that energy decision making most likely occurs at a building level. The building aggregation level in the energy system in the ESDL-file means that the energy demand is set per building and not individual companies that may be situated in the building. Because of that, TEACOS works using this mapping with regards to energy demand and does not make a distinction between individual companies. Having said this, it is important to stress that such considerations should be individually evaluated for each case and a more in-depth consideration of this challenge and others that affected the conceptualisation can be found in Appendix D.

To aid in the design of agents, a tool commonly used is the Unified Modeling Language (UML). UML is a standardised visual language used for modeling software systems, including agent-based models. It provides a set of diagrams and notation for representing the structure and behaviour of the agents. In Figure 4.4, the UML made for the conceptualisation of the agents is depicted.

In the UML diagram it can be seen that agents can be structured based on the inheritance principle, using the ESDL-file. In this case, it is conceptualised that the agents inherit specific attributes from a class in the ESDL-file transferred from TEACOS. This is made possible by the the object-oriented nature of the multi-model's ESDL-file and that way, the agents can be created as subclasses of the existing PyESDL class. This approach not only helps in saving time for the construction of the agents and the definition of their attributes, such as geometry, but it also adds to the ABM's scalability. By preventing the hard-coding of agents into the model, the ABM can hopefully be applied to other ESDLs with relative ease. A detailed explanation of the attributes shown in Figure 4.4 can be found in the Appendix A.

Agents behave in a way dictated by their state and rules implemented by the modeler. Within this research, this behaviour is kept simple. Nonetheless, a small literature study is conducted to find out on which factors support the decision making of companies investing in sustainable energy solutions, which is validated with information given by RECTholen.

It was found that investment costs come first in all evaluation criteria when it comes to sustainable

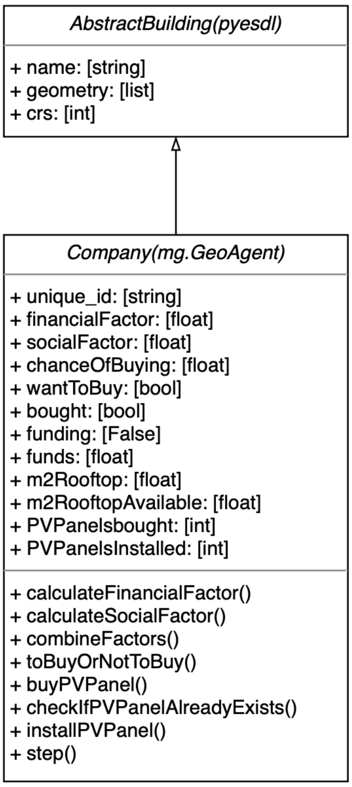


Figure 4.4: UML of a company.

energy (Strantzali & Aravossis, 2016). This financial motivation is underscored by SMEs' decisions mostly being taken based on immediate investment return when compared to other various criteria (Gveroski & Risteka, 2017; Urbano et al., 2021). However, Masurel (2007) points out that in corporate sustainable decision making, external factors play a large role, too. An example used it that companies are conscious of what the rest of the market is doing. This matches with what was mentioned in conversation with REC Tholen, where they found that the companies situated together in an industrial area tended to follow what the others were doing, although to varying degrees. This means that both finance and social factors play a role in the investment decisions of companies. These two factors together decide the chance that a company will invest, however not to the same extent. According to Strantzali and Aravossis (2016), the financial factor is twice as important as the social factor.

Therefore, agents calculate a financial factor based on a disaggregrated ROI for solar panels and a social factor that takes into account how many of the surrounding buildings have invested, which in turn influences them. These factors are combined to make up the chance that a building will invest in solar panels.

Finally, the limitations to whether or not agents can buy a panel is their available funds and the square meters of rooftop available, sticking to the two most basic requirements for acquiring a solar panel. The resulting logic for an agent for the duration of one step can be seen in Figure 4.5. A full-page version can be seen in Appendix A.

4.3.2. Time

To ensure alignment with TEACOS, a run time of one year was chosen. Furthermore is was decided that the ticks would be in months, giving a run only twelve ticks to complete its cycle. Originally, it has been planned to run the agent-based model for the number of years the entire multi-model would run, from 2023 to 2050, with twelve ticks each year but this idea had to be adjusted to accommodate for temporal alignment with TEACOS as single-period model.

The conceptual design for the ABM is formalised and implemented, following steps four and five of the agent-based modeling approach written out by Dam et al. (2012). To do this, the conceptual model will first have to be translated to a Python model through parametrization. Finally, the implemented model will be verified for step six in Section 4.4.1.

4.4. Implementation

Model implementation is done through Python scripts using two main agent-based libraries, Mesa, which can be found on Github[1] This section will cover how the conceptual model is translated to work in the Python environment with this open source library. The Mesa Library allows for the implementation of the agents with easy syntax, especially given the simplicity of the conceptualised model.

The model does not have a model interface for user interaction, with everything happening in the modeller's choice of coding program. No visual was needed for the model to work either, however, to gain a visual understanding one was made either way. This is not an interactive visualisation that runs like the one Mesa has built in, instead, these are static images of the Tholen business park. This was done because seeing as the agents cannot move, the added effort of implementing Mesa's interactive visualisation would not tell the user more than the static images. An example of what the ABM looks like can be seen in Figure 4.6.

The parameterization determines the values for the parameters in the conceptual model. The parameters are divided into variables attributed to the model (environment) or the agents. An overview of the chosen model parameters can be found in Appendix B.

4.4.1. Verification

The goal of the verification of the ABM is to check whether the model behaves as it is intended to. Therefore, while making the model and after the completion of it, several steps were taken to verify this for step six of the agent-based modeling approach (Dam et al., 2012). Firstly, code walk-through to analyse the Python code in depth. Second, recording and tracking agent behaviour along with multi-agent testing were done according to the rules of Dam et al. (2012). Finally, multi-agent testing is done to monitor the behaviour of all agents for the duration of a single run. Appendix C contains a detailed account of the three verification methods used.

Overall, the model was found to have been implemented successfully based on the verification steps and any subsequent adjusting that has been done.

4.4.2. Sensitivity Analysis

Sensitivity analysis is a common technique used to determine how different values of an independent variable will impact a particular dependent variable under a given set of assumptions. In the context of an Agent-Based Model, it is often used to see how changing parameters of the model can influence the results.

A global sensitivity analysis was performed on the ABM using the EMA workbench, a python package. 800 experiments were run with 10 model replications per experiment. Figure 4.7 shows the found Sobol indices for the number of solar panels bought by agents.

S1 indices denote first order effects, which means the variance in the target value directly caused by the parameter. ST indices indicate a combination of all interaction effects in the model. Confidence intervals are indicated by the vertical lines, and it can be seen in Figure 4.7 that the confidence interview wasn't very high, which may suggest that the indices did not stabilise. Overall, it was found that the agents' budget had the most impact on the number of investments done, which makes a lot of sense, given that without budget, they can't make the investments. After that, it was the cost and lastly, it is the radius.

What is most interesting to note is that all parameters have a very high interaction effect on the outcome. This suggests that the output of the ABM isn't solely or primarily influenced by individual parameters changing, but instead is heavily influenced by the interaction of multiple parameters. In other words, changing two or more parameters at the same time has a greater effect on the output than changing each of those parameters independently.

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[1] https://github.com/mmgcp/teacos-adapter.git

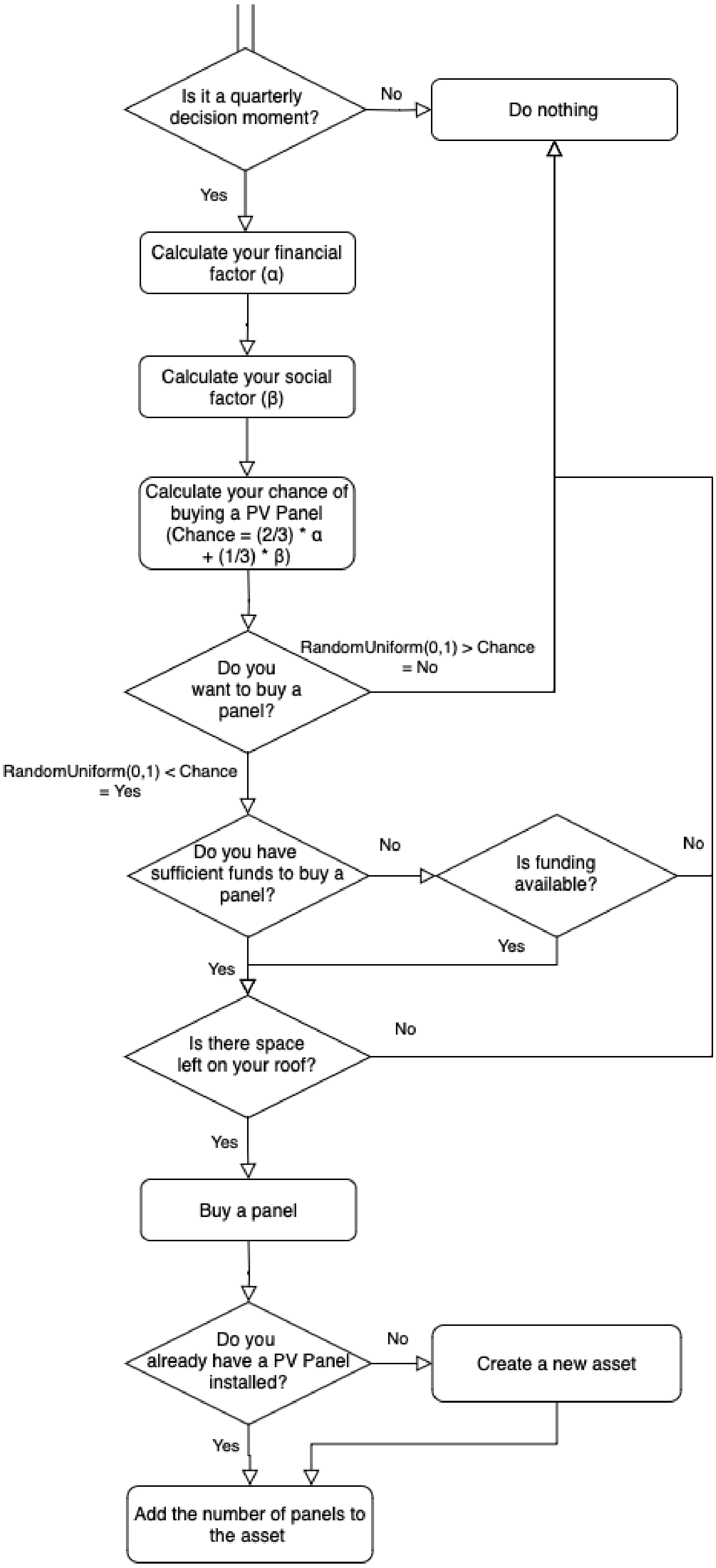


Figure 4.5: Agent decision logic for buying PV panels.

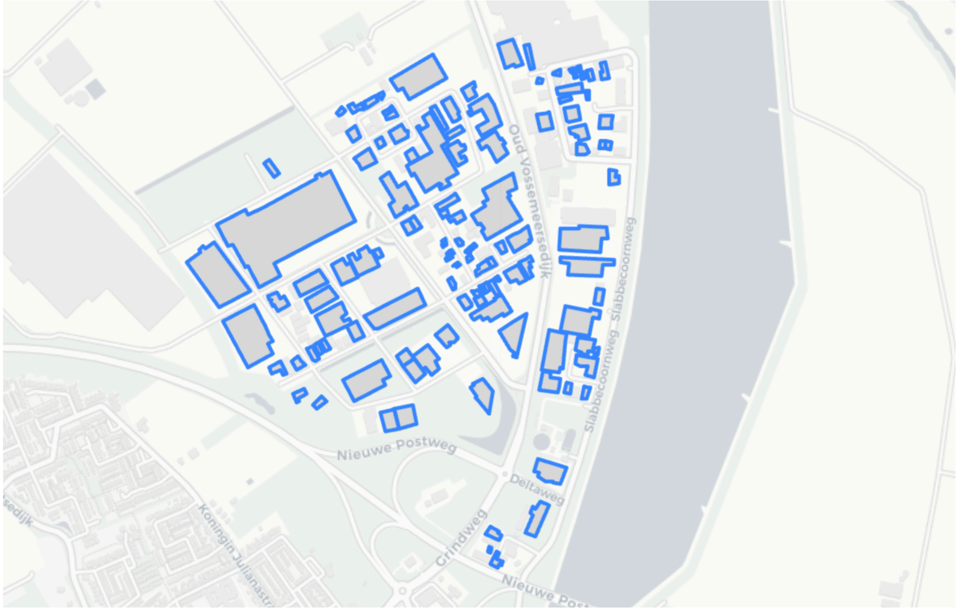


Figure 4.6: A static image of the ABM in Mesa, using the python package folium for the map.

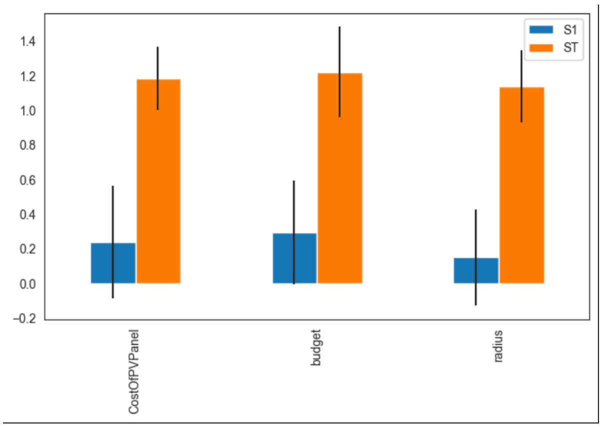


Figure 4.7: The results from a Sobol Sensitivity Analysis performed using the EMA workbench.

5

The Multi-Model

This chapter focuses on the conceptual design and implementation of the multi-model of the TEACOS and the ABM, thereby answers the second research question: *"What is a meaningful coupling of the ABM and the optimisation model, given the case?"*. Following the knowledge from the literature review, this chapter will apply this to the coupling for these two models. The first step of the approach for creating a meaningful interface, facilitating communication between the two models, is a short overview of each model's characteristics that are important for the coupling, outlining their main functions, capabilities, and underlying principles. These will then be related back to the literature and what options there are for a meaningful connextion. Next, the proposed design for the model adaptor is presented, explaining the reasoning behind design choices and how these will enable successful model integration. The conceptualisation concludes with a hypothesis for what the multi-model output may look like and how this would benefit to answer the research question. The chapter concludes by presenting the implementation of the multi-model, with its verification and validation.

5.1. Conceptualisation

When deciding how to couple models, one considers many factors. To make a decision on what manner of connection is meaningful and in what way that connection can be realised, a short summary of important characteristics to consider has been made in Table 5.1.

Table 5.1: Model characteristics summary

	ABM	**TEACOS**
Purpose	Simulate building investment behaviour in solar panels	Generate an optimum number of solar panels to invest in on a yearly basis
Input	Optimum number of solar panels to invest in	Investments made per building
Output	Investments made per building	Optimum number of solar panels to invest in
Data-file	ESDL-files	Adaptor uses ESDL-files
Programming language	Python	TEACOS uses AIMMS, the adaptor uses Python
Accessibility	Full access	No access to TEACOS, full access to adaptor

When deciding on what manner of coupling and which interaction structure to apply to these two models, two things need to be considered, which is which level of coupling tightness is feasible and also how interoperability - at least on the technical, syntactical and semantic - can be realised.

In the literature, it was found that there are three options. A tight integration, which is either the ABM is fully integrated into TEACOS or vice versa and a loose coupling. The tight integration where ABM is completely enveloped by TEACOS is not an option given the accessibility trait of TEACOS. Without access to the source code, it is simply impossible to do. In terms of a tight integration where TEACOS would be integrated within the ABM, this would be technically feasible. However, in the words coined by (Yourdon & Constantine, 1979), this would raise the *coupling* of the models - that is to say, the interdependence of the models. Should an adjustment be made to TEACOS, it would most definitely warrant a change in the ABM and perhaps the other way around too. This would also result in a higher instability of the multi-model (Martin, 1994).

Therefore, to keep the interdependence between the models low, a loose style coupling was chosen. But not so loose that manual steps are to be taken in between, what is proposed in for example the loosest coupling proposed by Brandmeyer and Karimi (2000). Finally, within the loose coupling, one needs to fulfill the requirements to allow the systems to communicate with each other.

As seen in the ETSI whitepaper (Van der Veer & Wiles, 2008), there are three stages in getting the models to communicate, which are technical, syntactic and semantic. For merely *a* coupling, only the first is necessary, since technical interoperability means the models are able to send each other data. This can easily be accomplished by conceptualising the coupling in their shared programming language, which is Python. However, the attainment of the other two levels of interoperability contribute to a meaningful coupling, since it is only then that they can understand what is being communicated and what it means. This motivates the choice for conceptualising the data exchange between the two models as being done through the ESDL-files, since both models (the adaptor, in TEACOS' case) are able to use this type of file.

Finally, when considering the interaction structure between the models, a feedback loop is chosen. It is precisely the cascading effects mentioned by Walby (2007) that are interesting in this scenario. Although this may add more complexity to understanding model behaviour, a feedback loop allows for the studying of continuous interaction between two nonlinear systems.

5.1.1. System Diagram

TEACOS and ABM will be loosely coupled, each model working individually, not knowing that the other model exists. Because the two models will communicate through ESDL-files that are being exchanged, the envisioned input and output of the multi-model are therefore also ESDL-files. Both models are called upon using one script that dictates the interaction and order of model use. For the user, this makes the two models act like one model. A conceptual system diagram for the model coupling can be seen in Figure 5.1.

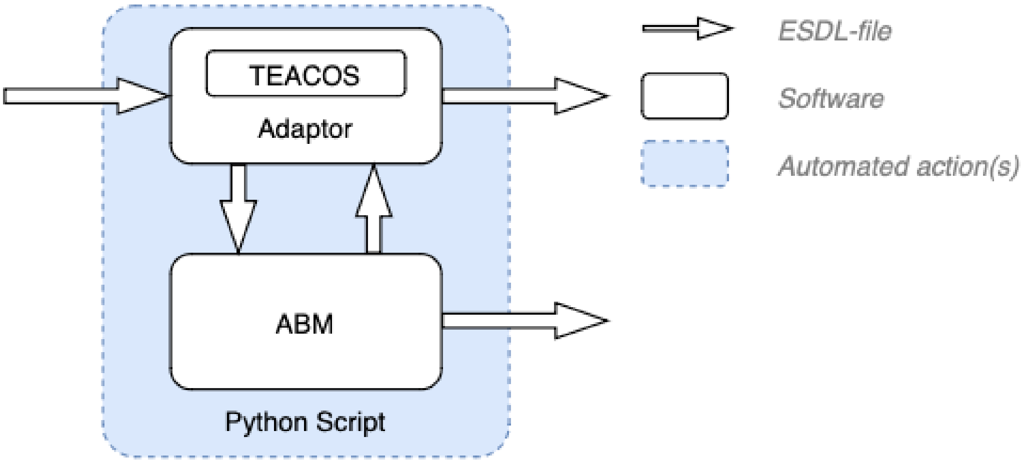


Figure 5.1: Conceptual schematic for the linking of TEACOS and the ABM

In the proposed model coupling, the coupling is executed through a Python script that calls TEACOS and the ABM for a number of iterations. The reason we start with the TEACOS is because the input of the ABM is not required while the other way around it is. This way, the effect of incorporating the output

Its purpose is to allow for the investigation into the effects that the ABM may have on the outcome of TEACOS. The script will walk through several steps for each iteration that are depicted in Figure 5.2.

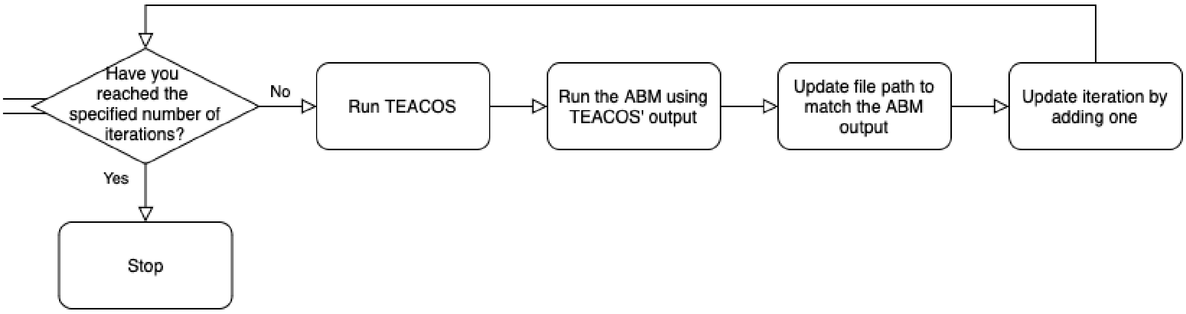


Figure 5.2: Schematic for the decision logic followed for the coupling of TEACOS and the ABM.

5.1.2. Output Hypothesis

With this setup, the user sets the number of iterations in the script. This was decided because this adds flexibility to the number of iterations that will be run during the experimentation phase. It can be seen that the models communicate in a continuous loop, wherein the output from the ABM is used as input for TEACOS and vice versa. This means that the simulated investment behaviour from the ABM may affect the starting conditions for TEACOS each run. The hypothesis is that this means that the ABM will affect the factors that are considered by TEACOS. By doing this, the ABM affect the degrees of freedom TEACOS has to come to an optimum. A concept design for their hypothetical interaction has been made with dummy numbers and can be seen in Figure 5.3.

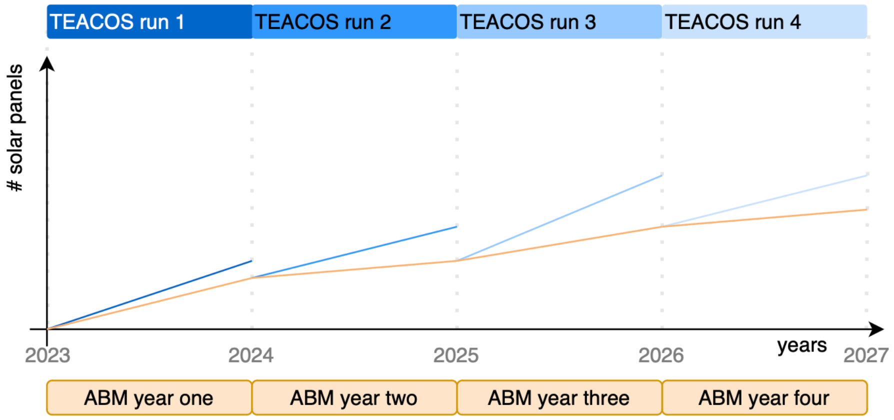


Figure 5.3: Schematic for the linking of single-period TEACOS and the ABM

In this setup, the models exchange data with each other after each run. The ABM recognises the output of TEACOS as the global optimum and runs it own simulation with certain investment decisions made by the agents. This is then returned as the new starting point for TEACOS' next run. It can be seen in this hypothetical case that the ABM does not reach the proposed optimum that TEACOS returns, which means that the second TEACOS run does not start from the ”optimal” point, but instead, by a point decided by the ABM.

5.2. Implementation

The implementation was done in Python through a singular script. Just as was chosen for the Agent-based Model, this script does not offer a model interface for the coupled models. Instead, everything happens within the modeler's integrated development environment (IDE) of choice. The script has been written in such a way that the user is required to at least two key elements: the file path for the input ESDL-file and the number of iterations that is desired. Using Python, technical alignment was easily achieved and the models could communicate with each other.

Using the file path specified by the user, the coupled models retrieve the file from its location. Using the ESDL-file assured for syntactic interoperability between the models, and if this was the input file then TEACOS would run first. This is followed by a run of the ABM for the first loop, with n iterations following after, as specified by the user. Besides the two required variables, there are also input parameters that are optional parameters. These are the parameters for the ABM. If they are not specified, the ABM runs with a set of predetermined parameters. However, to allow for the testing of other scenarios, these can be overwritten when running the coupled models. However, it was hard to specify the correct pathing for the coupled model, making sure that for each iteration the correct file was selected. This is a software engineering issue exacerbated by lack of experience in this field.

Finally, after the models were able to exchange and read each new output ESDL-file, it was found that there were some semantic irregularities between the models. For example, where the ABM would make use of Gigajoules, the adaptor would not be able to process that unit. In the end, through small pilot runs with manual checking of the results and intermediate results, it was found that the models could understand each other's output fully.

All in all, coupling the models successfully was very time consuming and by far the most issues and challenges were encountered during this step. These issues included difficulties running the model adaptor locally, and the aforementioned semantic issues between the models. A comprehensive overview of all issues encountered during this phase can be found in Appendix D with an in-depth documentation on the nature of the issue as well as the measures taken to overcome it. It is worth noting that some issues were not resolved, such as the issue connecting from the TU Delft IP address, but instead a workaround was found, such as whitelisting other IP addresses that did allow access.

5.3. Verification & Validation

The development of a reliable multi-model involves procedures aimed at ensuring that the developed model is made correctly and does what it is meant to do. To check these, verification and validation will be performed on the multi-model. Verification refers to the process of determining whether the developed multi-models accurately represent the conceptual design and specifications decided prior. This step answers the question, ”Are we building the model right?” On the other hand, validation is the process of assessing whether the multi-model, once verified, correctly represent the process under investigation. It answers the question, ”Are we building the right model?” The answers to these questions will give insight into the appropriateness of the multi-model and its applicability for research. Wallace and Fujii, 1989

5.3.1. Verification

To verify the model coupling, there are three verification tests that will be done to confirm that the multi-model is built correctly. These are conformance testing, which is done before coupling the models. This will test the individual models and their performance to ensure that the models being used are fit for the multi-model. Secondly, during the coupling, code checking will be done and continuous testing of the code to ensure that the coupling is implemented as intended. Finally a comparison of manually executed runs with the runs done by the coupled models will verify that the coupling exhibits the same behaviour as manual runs.

Conformance testing has already been done extensively in Chapters 3 and 4. The individual components of this multi-model have been studied and do what they're supposed to do. Code walkthrough was both done with experts throughout the coupling process as well as in the same manner as code walkthrough with the ABM. Using the python package Logger, statements would keep track of the status of the coupling. For a more in-depth explanation of the code walkthrough can be found in Appendix C.

Finally, a comparison has been made of the manual runs and the automated runs. Due to the effort a manual run costs, this has only been done twice to account for the stochasticity of the ABM. This was deemed an acceptable amount since this steps only checks whether the general model behaviour exhibited was the same. It was found that the manual runs consistently exhibited the same behaviour as the automated runs, from which the conclusion is drawn that the coupling was successful. To support this conclusion, a comparison is made between the streams of the electricity systems of the manual and automated runs and the numbers are compared for the first five iterations. The Sankey diagram comparing the energy systems with each other can be seen in Figure 5.5, where the flows of the automated run look like the manually done runs.

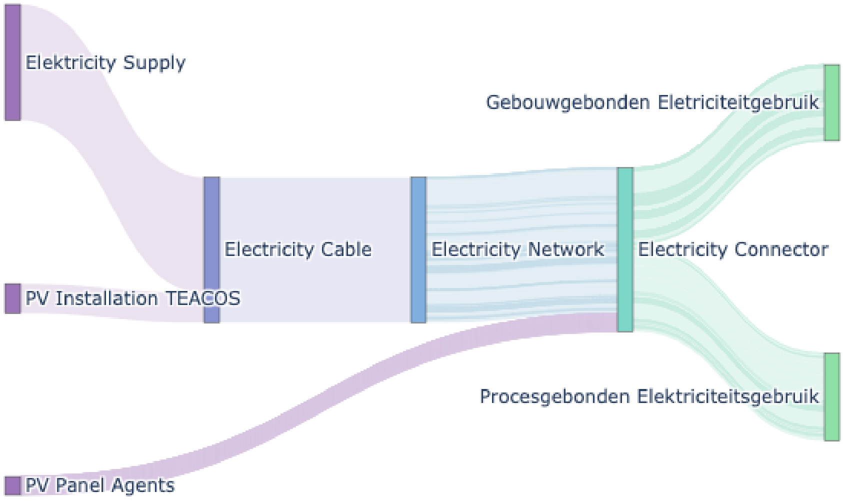


Figure 5.4: Result of example automated third full iteration.

5.3.2. Validation

The multi-modal research study used face validation as a primary technique to test the validity of the model. It's vital to remember that face validity is intrinsically a subjective approach to determining validity, rather than being grounded in empirical or statistical data as other validation methods might be, such as historical data validation or train/test split validation. Instead, face validity relies on input from an expert or a panel of experts who evaluate whether the model seems plausible and suitable based on their expert judgment.

In this research study, two forms of face validation were conducted. The first form was a continuous validation approach implemented during the process of model coupling, particularly during the pilot runs. Secondly, a final validation was executed with a panel of experts once the model had been fully developed and implemented.

As the first steps of the model coupling process were initiated, the results from the pilot runs were critically analyzed every week in consultation with a TEACOS expert. The aim was not only to validate the intermediate results but also to gain an in-depth understanding of the model's outcomes.

The research study also followed a three-step process for face validation, which included: (1) a presentation of the goal and conceptualization of the multi-model, (2) a live demonstration of the multi-model and its various functionalities, and (3) a thorough review of the multi-model. These steps were carried out with the assistance of a panel of multi-model experts who were part of the micro case. Among these experts, two had an extensive understanding of the TEACOS model.

The panel first reviewed and approved the conceptual design and feasibility of the multi-model. Then, they were presented with a live demonstration of the coupled models, which also included a comprehensive walkthrough of the model's code. The experts examined the model's run time and outcomes,

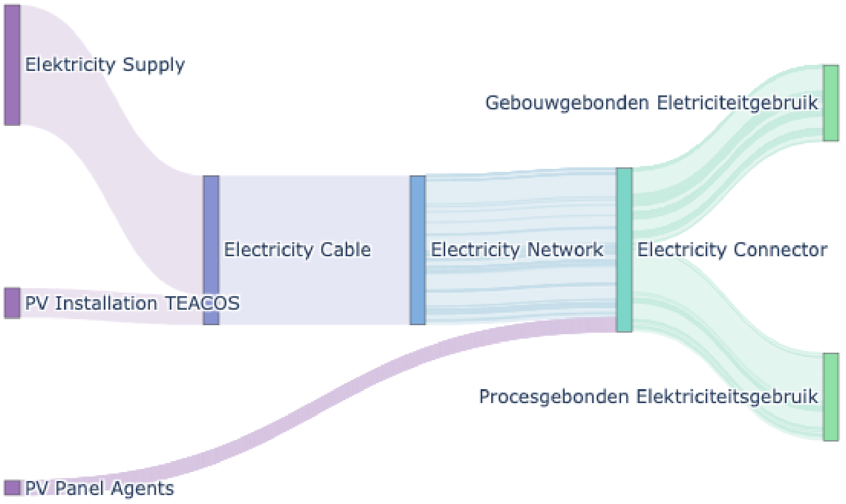


Figure 5.5: Result of manual third full iteration.

and they asked detailed questions about the model's coupling process, specifically how the ABM used the output of TEACOS. Once all their inquiries were addressed, they provided their review and feedback on both the model coupling process and the outcomes of the pilot runs.

The experts' feedback primarily emphasized enhancing the transparency of the multi-model coupling outcomes. They suggested that the process and the data being shared between the models should be more visible and easily accessible, as the current process seemed opaque and required extensive labor to search through the output files for comprehension. They also noted that despite the pilot runs suggesting an all-or-nothing strategy between TEACOS and the multi-model, the setup with the ranged constraint should also enable more varied outputs. It was deemed that the cost research was insufficient to fully map the cost strategy for TEACOS, but it was passable for the purpose of this research, since it is not output-focused.

5.4. Data for Implementation

After the implementation of the model coupling, what remains is to prepare an ESDL-file to be exchanged between the coupled models. This ESDL-file should contain the entire energy system, defined as the buildings and their energy data, the energy network and it should also include one optional asset for solar panels, as decided by the case context.

A version of the industrial area of Tholen as an ESDL-file had already been made by the micro case participants. A representation of this draft version from January 2023 can be seen in Figure 5.6. In this representation, a representation of the general electricity grid has already been implemented, along with all buildings in the industrial area and their energy demand. Two optional assets had already been implemented as well. Several steps were undertaken to prepare the ESDL for this research. This meant a ”cleaning” of the file and ensuring that the implementation of the optional asset is done correctly. The reason it was chosen to ”clean” the existing draft version and not start from scratch is due to the effort required to create an ESDL from scratch.

The cleaning of the ESDL consisted getting rid of the areas that fell out of scope. The EPS model of the multi-model had added certain paths, which consisted of ‘internal’ PV installations in all buildings.

However, not all buildings own solar panels and the inclusion of them fall out of scope for this research. The removal of these internal assets can be done through a python script using PyESDL.

To be able to use TEACOS and the ABM as desired, the optional asset proposed is important. In this case, the two optional assets are replaced by one asset with the same characteristics except for the three factors that were decided during component testing, which is explained in subsection 5.3. Finally, some assets were moved to the centre for optics, changing nothing but the visual representation. A visual representation of the ESDL-file in the MapEditor can be seen in Figure 5.7.

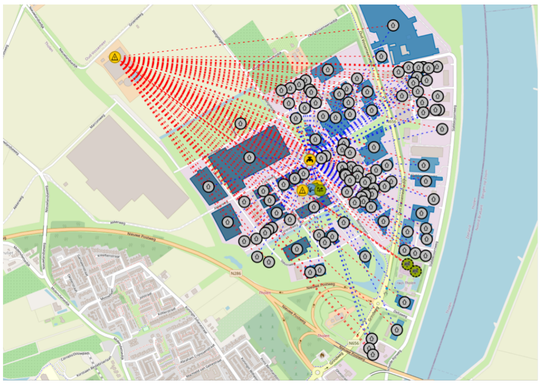


Figure 5.6: The original version of Tholen in the ESDL-file, visualised by the MapEditor.

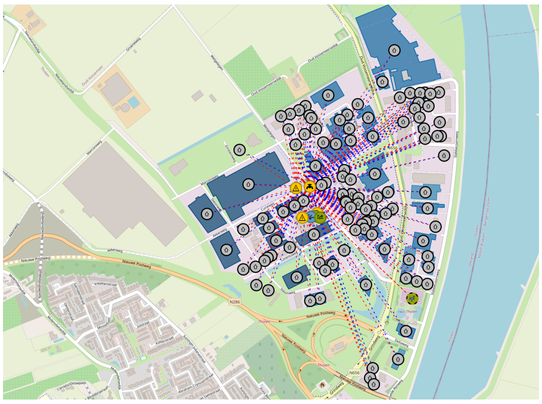


Figure 5.7: The final version of Tholen in the ESDL-file, visualised by the MapEditor.

6

Results

This chapter contains the results that can be found from the formalised coupling between TEACOS and the ABM. Attaining these results has been done with an dynamic experimental setup that will first be explained. Following that, the results will be presented and analysed.

6.1. Experimental Setup

The purpose of the experimental setup was to examine the multi-model behaviour and compare it with only TEACOS' behaviour. To facilitate this investigation, two key performance indicators (KPIs) were devised for the multi-model. The first KPI is the investment trajectory returned by the multi-model. As discussed in Chapter 3, TEACOS provides a range of electricity to be sourced from the optional assets in the shape of a trajectory within multiple iterations. However, an all-or-nothing strategy was observed to be employed by TEACOS when deciding the optimum, which signifies that TEACOS would recommend either the maximum range of solar panels or none at all, meaning the value of this KPI would either be the same number or zero. No midway could be found with the current setup, although this should be theoretically possible. As a result, a second KPI is proposed to investigate the multi-model behaviour with the experimental setup.

The *inflection point KPI* is the iteration at which the suggested optimum trajectory of investments alters. During conformance testing in Chapter 3, it was observed that TEACOS sometimes shifts its strategy to maintaining the status quo. In terms of the energy system, this KPI signifies the moment at which, according to TEACOS, further investment in optional assets becomes more costly than maintaining the status quo, thereby denoting the current situation as ”optimal”. Therefore, the inflection point KPI can also be interpreted as the moment at which the optimal situation is achieved, as per TEACOS' perspective.

When making the experimental setup, there are two limiting factors that need to be kept in mind. These are computational limits of the model as well as the limit enforced by Quo Mare, the owners of TEACOS. The former is due to the fact that a run with the multi-model of five iterations (five times the TEACOS-ABM sequence) costs roughly five minutes. The latter has to do with the fact that the TEACOS model is hosted in such a way that each run is computed through an external servery and costs money. Therefore, the number of runs expended to this research are limited.

Therefore, this research proposes to use a dynamic experimental setup. A dynamic experimental setup means that the experimental setup will adopt a cyclical, adaptive approach to conducting experiments. In this manner, initial experiments are conducted and areas of interest are found, such as significant findings, anomalies, or aspects that warrant deeper investigation. These areas of interest are then used to set up the next cycle of experiments. The dynamic setup ensures a continuous refinement of experimental focus, reducing unnecessary iterations and allowing the multi-model system to generate interesting behavior with minimum required experimentation How this decision is made will be explained after the structure for the dynamic hypothesis has been given.

The dynamic setup is divided into two rounds. The first round will be explorative and determine the number replications needed and also include making the base case to compare the rest of the models with. The second round will be used to explore different configurations of the model to study the effects on the KPIs, using the number of replications decided in the first round.

6.2. Model Outcomes

The first, explorative round of experiments is done to get a general idea of model outcomes as well as to research the number of replications to be conducted. Given a fixed time frame for experiments, limited computational capacity and the limit imposed on runs by Quo Mare, keeping the number of replications to the minimum is desired. However, when conducting experiments, it is essential to account for the inherent stochasticity of the system under investigation. For the multi-model, the ABM contributes stochastic behavior due to its reliance on individual agent interactions. A balance will have to be struck on the number of replications that is within acceptable limits and also deals with the stochasticity of the ABM.

6.2.1. Replication assessment

To decide the minimum number of replications, the coefficient of variation (CV) is calculated and shown. It is a known method for assessing the stability and precision of experimental results for ABMs (Lee et al., 2015). In the context of determining the minimum number of replications required for a study, the coefficient of variation can also assist in estimating the minimum number of replications necessary to achieve reliable results (Omer et al., 2014). By calculating the coefficient of variation from the first round of the dynamic experimental setup, this number can be used for the next round of the experimental setup. In this context, the minimum number of replications required for the research can be identified as the point at which the coefficient of variation reaches a stable state with the progressive increase in replications. The experimental setup to find the minimum number of replications was as follows:

Table 6.1: The first round of the dynamic experimental setup

Experiment	ABM Parameters	Energy System	Iterations	Replications
Explorative	Standard	Tholen	25	15
Base Case	N/A	Tholen	25	1

The parameters of the ABM are those that were decided during implementation in Chapter 4, the energy system stands for which energy system is being studied. The iterations stand for how many loops of model interaction are chosen for the multi-model. The number of replications stand for how often the experiment is run. It would have been more desirable to conduct more replications for this first round of experiments. However, this was not possible because a run with twenty five iterations already requires a runtime of roughly half an hour. Fifteen was deemed an acceptable amount to facilitate this type of exploration of the replications.

Figure 6.1 show the result. The point where the coefficient of variation stabilises with an increasing number of replications is considered the minimum number of replications. The inflection point KPI was chosen as well as the number of investments simulated by the ABM. Observations have been made that suggest a stabilisation of the indicators occurs after approximately six to eight iterations, and they stabilise around a CV of 0.15. An acceptable number for the CV has to be assessed per project and case, but a general rule of thumb is that lower is better. According to Brown (1998) a CV of 0.30 is the maximum and since stabiliations of 0.15 is far lower than that, this coefficient is deemed acceptable. Nevertheless, an increase in the number of replications would typically be recommended from a statistical standpoint to improve reliability and precision, in the context of this particular study, adherence to the minimum requisite number of eight replications has been deemed sufficient.

The decision for this is supported by the research objective, since the primary emphasis of this study is not an in-depth analysis of model outputs, nor is statistical significance in the outcomes a key priority, but instead the goal is to enable explorative modeling and to study the methodology for coupling. Therefore, the usage of the absolute minimum number of replications is not expected to undermine the validity of the study's findings significantly. Preference has been given to the ability to conduct more exploratory experiments, even though fewer replications are involved. This decision acknowledges a potential

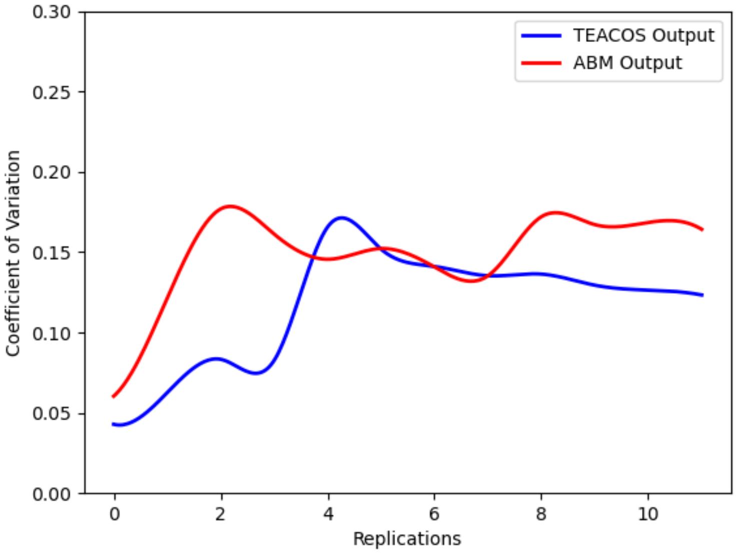


Figure 6.1: Coefficient of variation for outcomes

trade-off between statistical robustness and the opportunity to explore a wider range of hypotheses or concepts within the study. It should be noted that larger replication counts could potentially enhance future research, particularly in the areas of model testing and usage when wanting to practically apply the multi-model.

6.2.2. Tholen Energy System

When analysing the results from the explorative experiments, several interesting things can be found. Figure 6.2 provides a clear picture of how electricity is distributed throughout the industrial area and helps identify the flows within the energy system. This type of flow diagram represents the various components of the electrical grid, including power generation sources on the left, and two categorised purposes of electricity use, on the right. The lines connecting these nodes symbolize the flow of electricity. The width of each line corresponds to the volume of electricity transferred, with wider lines indicating larger quantities. The direction of the electricity if from left to right, from generation to consumption. The relative thickness of the lines allows for an at-a-glance understanding of the proportional distribution of electricity within the industrial area.

Figure 6.2 demonstrates two things: the desired activity by the multi-model and placing it within the context of the energy system. First, an investment trajectory is returned by the multi-model, with the initial year of that trajectory being specifically shown, as the middle left node ”PV Installation TEACOS” and finally, the outcome of simulated investments is shown by the bottom left node ”PV Panel Agents”. Second, it shows that within the energy system, the investment trajectory for the first year only satisfies a small portion of the total electricity demand and that the remainder of the demand is sourced from the electricity grid.

However, to see the progression of multi-model behaviour, an envelope plot, depicted in Figure 6.3 is made with both model outputs, per iteration. An envelope plot is a type of data visualization that is often used to present the range of possible outcomes, and in this case the envelope will show the range that TEACOS returns as a possible range for investments, with the top of the range being the optimum. The outcome of the ABM stands for the investment done by the agents. The reason it ends after 21 iterations is because all replications have reached the inflection points KPI by 21 iterations.

It can be seen that the simulation output never reaches the optimum amount within the range of TEACOS.

When comparing the output of the multi-model compared to the base case as visualised in 6.4, it can

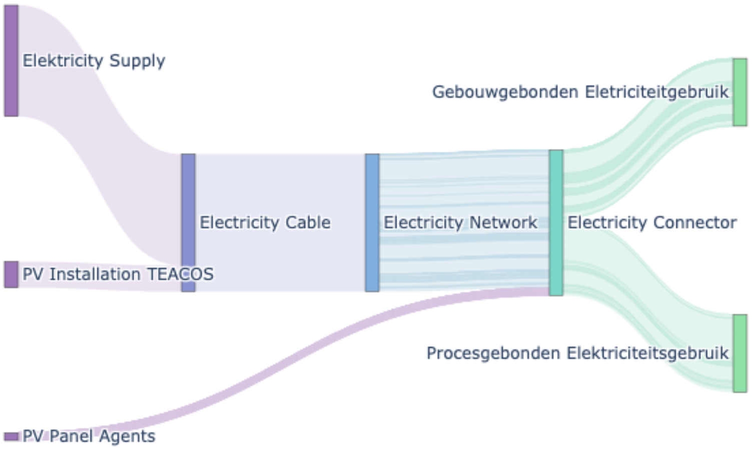


Figure 6.2: Sankey diagram of Tholen energy system for the first iteration

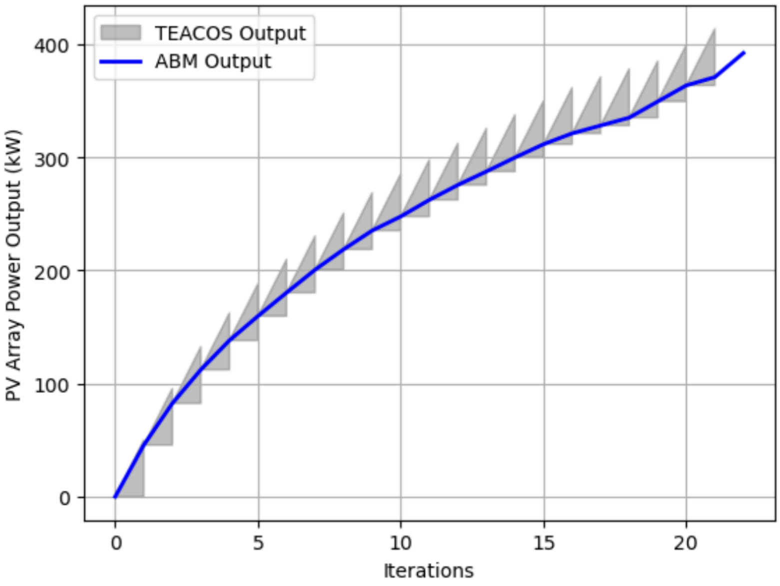


Figure 6.3: Envelope plot of TEACOS and ABM outcomes within the multi-model

be seen that they diverge and that the base case reaches the inflection point far earlier than the multi-model output. This means that in the base case of TEACOS, the model behaviour changes after seven years, whereas is takes the multi model more iterations to reach the same point.

Figure 6.4 contains an ”upper limit” for the trajectory, which then results in the inflection point. It seems that there is a general tipping point for the energy system that, when reached, changes the tactic that TEACOS employs. In both cases, the base case and the multi-model case, after reaching a little over 400kW, the trajectory does not increase because TEACOS does not recommend any further investments.

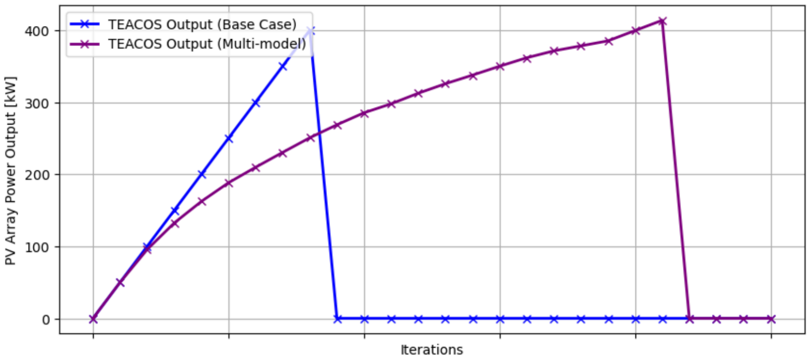


Figure 6.4: Comparison of model outcomes of multi-model versus base case

To better understand the trajectory of the multi-model a more in-depth analysis of the investment behaviour across all replications in the multi-model has been visualised in Figure 6.5. Here, the average trajectory of investments done across all replications has been plotted up until the inflection point. This is because after that point has been reached, the value becomes zero, which would greatly affect the average if included.

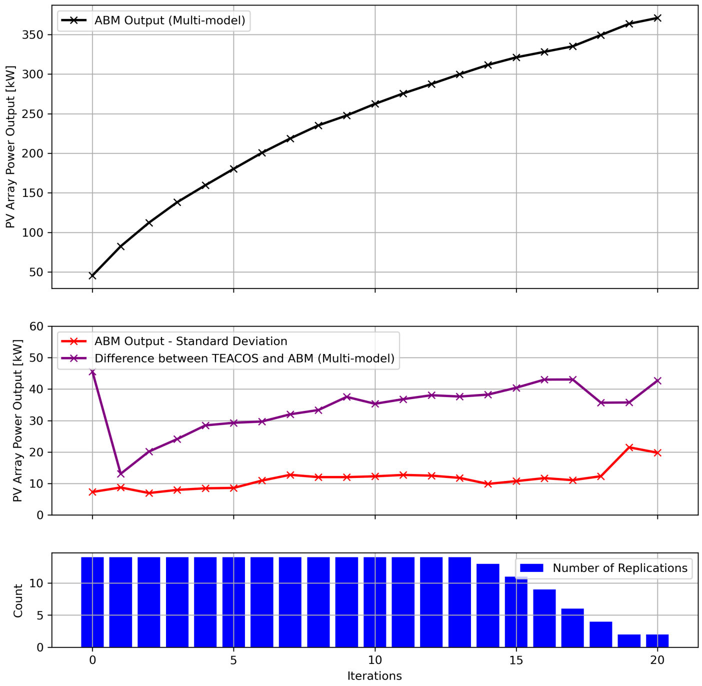


Figure 6.5: Progression of investments

In the first figure, it can be seen that towards the end the line loses some stability and becomes more wobbly. However, the combined display of these graphs provides a nuanced understanding of the results. The second graph showcases the standard deviation, which can be observed to increase towards the end. This increase, however, isn't necessarily a reflection of increased variability in the results but rather the result of a lower count, as illustrated in the third graph.

The diminished count towards the end of the data set is a result of certain runs terminating earlier than others. This early termination is due to these specific runs reaching their inflection point, an event that effectively ends their contribution to the data set. Therefore, as we progress towards the end of the data, fewer runs are contributing to the calculation of the standard deviation. This smaller pool of data increases the likelihood of a higher standard deviation, reflecting less about the variability of the overall results and more about the early termination of certain runs.

6.2.3. Different Configuration Comparison

After this analysis, the second round of the experimental setup was conducted. The second round of experiments in our dynamic experimental setup aims to further assess the consistency of multi-model behaviour under various conditions and to investigate how modifications in the energy system's configuration affect the inflection point KPI. The objective is to understand the outcome of the multi-model with different system configurations, which will hopefully provide insights that may aid in the understanding of the multi-model. In this experimental setup, the juxtaposition of individual agent runs and complete energy system runs will be tested. However this will not be done with all 112 agents because of two reason.

Firstly, the computational time demanded by the multi-model was a major constraint. On average, a run comprising fifteen iterations takes roughly fifteen minutes to complete. Extending this to cover all 112 agents, for eight replications each would necessitate an impractical total of 170 hours of continuous runs. Even if this were possible, the second reason is the limit on the number of runs mentioned earlier in the first round of the experimental setup.

Therefore a selection of five agent is made to study, both individually and together. Five is enough to allow for interaction within the energy system of all five agents together, and not so much that the computational time of running and processing the experiments becomes too big. Finally, five would also for a represents the general topology of the agents in the model. In this case, the decision was made on the size of the building, wherein a small building has a surface area that is less than 2500m^2, a medium sized building has a surface area that is between 2500m^2 and 10000m^2 and a big building is anything over 10000m^2. An overview of the chosen agents can be seen below in Table 6.2.

Table 6.2: Overview of the subset of agents selected for the alternate setup with their size.

Building	**Size**
Building with Agent 1	Big
Building with Agent 2	Medium
Building with Agent 3	Small
Building with Agent 4	Small
Building with Agent 5	Small

Six ESDL-files were constructed for this setup, one containing only each agent within the energy system and one containing all five agents and no other agents. This resulted in the following experimental setup for the second round.

Table 6.3

Experiment	**ABM Parameters**	**Energy System**	**Iterations**	**Replications**
Individual Configuration	Standard	Agent 1	10	8
	Standard	Agent 2	10	8
	Standard	Agent 3	10	8
	Standard	Agent 4	10	8
	Standard	Agent 5	10	8
Five agent configuration	Standard	Five agents - group	10	8

The box plot in Figure 6.6 contains also the previous configuration and shows that that configuration, representing the entire energy system of Tholen, requires the most to reach the inflection point KPI. The mean is 17 iterations - approximately a decade longer than all other configurations. The configurations involving individual agents, on average, take six years to reach this inflection point. This duration is longer than the configurations involving all five agents. This disparity is attributable to the single agents

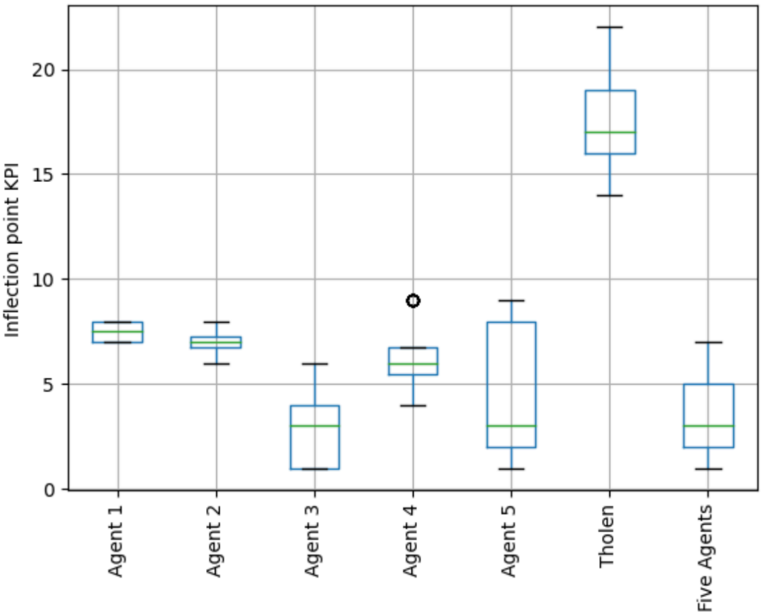


Figure 6.6: Boxplot showing distribution for the inflection point KPI

also having the social factor incorporated into their behaviour. However, as they are the only agents in that energy system for this experiment, this social factor is not activated, and therefore negatively impacts the KPI as their motivation to invest lies lower.

6.3. Process Analysis

To be able to say something about the coupling process, an analysis has also been done on the the process of this research. Several things stand out, and to make them explicit, all challenges faced during this research have been categorised along two axes: The phase of the project in which the challenge occurred and which level of interoperability the challenge is a part of. The level of interoperability refers to the nature of the challenge, which can be any of four categories: a technical, syntactic, semantic of organisational level of interoperability (Van der Veer & Wiles, 2008). Subsection 2.2.2 contains an explanation with examples. In specific cases, a challenge may be multi faceted and be attributed to two levels of interoperability. In all cases, the motivation for the categorisation is given in the in-depth explanation of the challenge. The challenges are divided into sections based on the phase of the project.

Table 6.4: Overview of challenges, subdivided into level interoperability and research phase.

Phase **Interoperability**	**Background**	**Conceptualisation**	**Formalisation**	**Results**	**Total**
Technical	1	1	3	0	5
Syntactical	1	0	0	1	2
Semantic	0	2	1	0	3
Organisational	2	1	2	1	6
Total	4	4	6	2	16

It can be seen that the distribution of challenges on the levels of interoperability is not equal, especially when shown in a bar chart. Figure 6.8 show that both syntactic and semantic interoperability only had two and three challenges, respectively. Striving for technical and organisational interoperability, on the other hand proved to be a more cumbersome task, with five and six challenges addressed during this research. Two histograms show the distribution of challenges per phase and per level of interoperability as well. It can also be seen in Figure 6.7 that during the Formalisation phase of this research, the most challenges were faced.

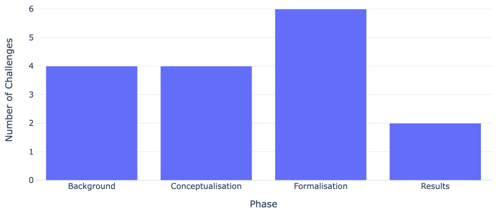


Figure 6.7: Bar chart of the number of challenges per phase

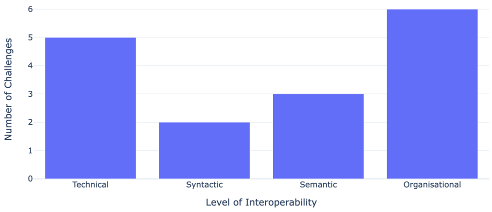


Figure 6.8: Bar chart of the number of challenges per level of interoperability

7

Reflection & Conclusion

This chapter first answers all the subquestions before reflecting upon the methodology and the results obtained in Section 7.1, after which Section 7.2 lays out the lessons learnt in terms of methodology during the research process. Finally, everything comes together in the conclusion in Section 7.3. This chapter and research end with recommendations for future work in Section 7.4.

Starting off, the main research question of this study was as follows:

”What is the effect of coupling an agent-based model to an existing optimisation model, TEACOS, given the case study of Tholen?”

To answer this research question, three subquestions were formulated to allow for the studying of the effects of coupling two models, which resulted in the three proposed methodological phases to be complete to answer them - understanding the two models, coupling them and finally, experimentation - for model-based experimentation to study the coupling of models and therefore, the construction of multi-models. These phases have been applied to a case study of the energy system of Tholen, the Netherlands. To fulfill the three methodological phases, this research has completed several steps.

A comprehensive review of the existing literature was conducted, focusing on the topic of model coupling, specifically simulation optimisation. Findings from previous studies were identified, highlighting essential considerations for conceptualising a model coupling, such as coupling tightness and levels of interoperability. The first subquestion was presented as: ”Which structures of interaction exist when linking a simulation to an optimisation model?” Three common interaction structures were found in literature, which can be divided into two categories based on their coupling tightness. Two of the structures are tightly integrated coupling structures - simulation-based optimisation and optimisation-based simulation. In the former, a simulation model is fully encapsulated by an optimisation, while in the latter, the reverse is true. The third interaction structure is loosely coupled with a feedback loop enabling communication between the models. This loose coupling is further divided into one-directional communication methods.

To address the second subquestion: ”How can a meaningful coupling of an Agent-Based Model (ABM) and the optimisation model be formed to create a multi-model, given the specifics of the case study?”, information from the first subquestion was applied. TEACOS, the optimisation model, was studied, and a simple ABM was constructed using the Mesa platform. The accessibility of the models was the deciding factor which interaction structure to implement, with the black box characteristic

The third interaction structure, a loose coupling, was selected and implemented to facilitate communication between the models and study the influence of the ABM on TEACOS. While the implementation was time-consuming, it was necessary to achieve the desired outcome.

When analysing the results, an answer to the final subquestion ”What are the effects of the chosen interaction structure on the outcome of the multi-model?” was found. Through a dynamic experimental setup that allowed for explorative analysis within the constraints of keeping the runs as low as possible, multi-model behaviour was analysed across several different configurations. In the setup used within this research, the multi-model behaviour is altered due to the fact that the output of the ABM influences the starting conditions for TEACOS. These are the starting conditions TEACOS has to take into mind when deciding its strategy and it can be seen that this influence affects the number of years before TEACOS switches tactics, indicated by the shift in the inflection point KPI. This shift in multi-model outcome between investment behaviour and optimisation cannot be captured by only using the optimisation model.

7.1. Reflection

This section reflects upon the research, structured over the two key parts of this research, the methodological steps taken and the outcomes found.

7.1.1. Methodology

When looking back on the method, there are several things that stand out. Firstly, the non-linear, iterative process of the conceptualisation of the ABM and the multi-model coupling result in a very fit ABM. Following Yourdon and Constantine (1979)'s reasoning, this resulted in a high *cohesion* - semantic relatedness - for the models, but not a very low *interdependence*. As Hellhake et al. (2022) writes, when coupling [software] modules, a high *cohesion* and low *coupling* are desired. In the case of the ABM and TEACOS, cohesion was high due to the fact that the multi-model characteristics were taken into consideration during the conceptualisation of the ABM. For example, using ESDL-files as input for the ABM. A modeller tasked with creating a simple ABM on investment behaviour would most likely not consider using the ESDL-file as a basis - and while this decision does raise the *cohesion* between the models, it lowers the *coupling*.

The iterative manner of conceptualising allowed for a high cohesion between the models and, therefore, an easier coupling as syntactical alignment would have been hard to realise otherwise. Still, to avoid overfitting to a certain case when coupling models, it is proposed to make a generic ABM and construct a wrapper or an adaptor. This is a process that was also encountered during Shahumyan and Moeckel (2015), where initially a tight coupling had been the target, but a more loose coupling through Python wrappers was eventually used.

The trade off between an easy fit or a more robust model needs to be considered for each research depending on the purpose, but there are several things to keep in mind while making this decision, which include the time allocated for the project and what the expertise is of the modelers. The complexity of the models should also be considered. In contrast to this research, a model that is simple and easily syntactically and semantically aligned with is better suited to a low *coupling* model as this is a better choice in the long run.

Furthermore, upon reflecting of the method chosen, a more comprehensive, mixed-methods approach would have better suited this type of research. While the construction of multi-models and coupling of models often heavily relies on quantitative methods, given the collaborative nature of multi-modeling and the multiple stakeholders involved, the research could have been enriched by integrating more qualitative techniques. For instance, interviews with stakeholders could have been conducted early in the research process. These discussions could have facilitated a more profound understanding of the models, hastened the transfer of knowledge, and potentially improved the conceptualisation of the research problem. Furthermore, such qualitative insights might have helped to uncover more subtle or complex dynamics for the multi-model that quantitative analysis alone might not reveal.

7.1.2. Outcomes

To start off, the coupled model results are in line with the conceptualisation of model interaction made in the conceptualisation phase. The loose coupling between TEACOS and the ABM has resulted in an interaction within the multi-model where the behaviour simulated by the ABM affects the optimisation run by TEACOS. Reflecting upon the outcomes, the fact that a meaningful coupling was achieved that was able to generate multi-model outcomes is already considered an achievement.

Through this type of coupling, the agent-based model TEACOS is able to affect the trajectory of TEACOS. A key finding is that the interaction structure affects the multi-model's outcome, demonstrated by the shifting inflection point in TEACOS's investment strategy. This shift is influenced by the output of the Agent-Based Model (ABM), which alters the starting conditions for TEACOS, ultimately influencing the timing of its strategic switch. However, it also becomes clear when combining this with the information learnt during conformance testing of TEACOS, that the current depth of the inflection point is shallow because the shift in the inflection point is caused by TEACOS's cost calculation. This cost calculation determines the optimal investment trajectory. TEACOS balances the cost of installing new assets against the cost of sourcing all electricity from the grid, opting for the least costly total. This decision is informed by the amount of electricity that remains to be sourced. Therefore, a change in tactics occurs when a specific level of remaining demand is reached. In the multi-model, this remaining demand is, in turn, influenced by the outcome of the ABM as the investment made in the simulation are never able to match the optimum proposed. Since the trajectories of the optimal and the ABM diverge, this difference results in a delayed inflection point.

Therefore, it can be concluded that the chosen interaction structure affects the outcome by altering the investment trajectory and delaying the inflection point. In essence, the incorporation of the simulation reduces the range of the output given by TEACOS by proposing a trajectory within the range. This effect comes from the interaction of the agent-based model's output on the initial conditions that TEACOS considers within the multi-model, and reduces uncertainty within the multi-model on the trajectory proposed.

However, in general, this means that in the future, human behaviour can be incorporated into a study of the optimum trajectory using a loose, feedback loop style type of coupling. The outcomes for this specific case are in line with what was expected from the dynamic hypothesis.

Looking on the process outcomes of this research, it became evident that the organisational challenges associated with coupling models play a substantial role in the challenges faced, an aspect somewhat underrepresented in existing literature. While literature provides ample discussion on the technical aspects of model coupling, the organisational hurdles faced in such endeavours often remain unaddressed.

Fuchs et al. (2010) and Larson (2006) propose a framework for multi-model collaboration but these concern themselves only with the software module coupling and pass over the intricacies involved in aligning the organisational aspects of different model owners. Bollinger et al. (2018) and Nikolic et al. (2019) all dive into coupling models and organising principles, yet these principles are primarily concerned with the alignment of ontologies and resolutions and software module coupling. Additionally, while Nikas et al. (2021) highlights the importance of communication between different multi-model consortia and multi-modeling groups, the need for communication *within* these groups is scarcely mentioned. den Boon et al. (2019) is found to mention that it is a 'good practice' to practice thorough model documentation when making multi-models, which this research would support. However, there is no guideline on the communication and organisational principles between modelers or organisations constructing the multi-model.

In the literature, there is a lack of focus on the broader organisational, practical context within which these models operate, particularly when the models belong to different entities. In light of these findings, it becomes clear that the organisational dimension of coupling models warrants further exploration in future research. Understanding and addressing these organisational challenges can significantly enhance the efficiency and effectiveness of model coupling, ultimately leading to more robust and meaningful collaborations in the context of multi-model projects.

7.1.3. Limitations

The main limitation of the model is caused by the simplicity and abstraction of the Agent-Based Model (ABM). The ABM is made with a lot of underlying assumptions and a very basic decision logic for the agents. Such a simplified model, might not fully capture the intricacies of human behaviour. A more detailed ABM could result in emergent human investment behaviour, which could affect TEACOS. However, while this is very true, it is not deemed (overly) significant for this research for two reasons. Yet, this could not have been done any differently due to time and resource constraint. Furthermore, the primary focus of this research was on the process of coupling and the challenges surrounding this task, rather than on a in-depth representation of human behaviour. This aligns with the school of thought that a system's utility primarily depends on its ability to fulfill its primary goal, rather than on the depth of its complexity. In this context, the ABM successfully fulfilled its core function of making decisions, modifying the ESDL-file, and communicating changes to TEACOS. Therefore, the lack of complexity in the ABM is not considered a significant issue for the current research, but it remains a limitation.

One of the constraints encountered in this study was the incomplete development status of the TEACOS adaptor. This situation not only prevented the complete utilisation of TEACOS' capabilities, such as the multi-period aspect of the optimisation, but it also influenced the process due to incomplete or improperly functioning components.

Furthermore, another limitation was the lack of expertise in software engineering. Having had no prior experience with adaptors, orchestrators and coupling models meant that trouble shooting errors was a long and arduous process and required ad-hoc learning of topics. Many technical errors and complicated coding situations took very long to solve and required help from other parties.

7.2. Lessons Learnt

Following the reflection and limitations, several lessons learnt have been formulated, divided by category of organisational and methodological lessons learnt:

The process of this thesis underscored the importance of maintaining clear and consistent communication between team members, particularly when dealing with complex model structures and couplings. Effective coordination and collaboration can significantly streamline the troubleshooting process and the overall research journey.

Organisational Lessons
The importance of prioritising organisational interoperability in multi-model research projects has been underscored, particularly in projects involving multiple stakeholders. It has been observed that the level of organisational or pragmatic interoperability have an influence on the shape and experience of a project and its problem-solving capabilities. Therefore, it needs to be from any multi-model project's start that enough attention is payed to this aspect.

The implementation of robust documentation practices that are used from the start and recognising the role of organisational aspects in multi-model projects - likely involving multiple stakeholders - is crucial. Enhancing the documentation of the process not only smoothens the current project's process, onboarding of future participants but will also aid future endeavors.

For other future projects, establishing open and efficient lines of communication as were had during this research from the outset should be a prerequisite. In a multi-stakeholder environment for multi modeling with various models, the manner of communication between involved parties had a very clear, positive effect on this research. This research was lucky enough to enjoy the willingness and availability of all involved parties for swift, informal contact. These two key aspects - willingness and availability - are often taken for granted when in possession, but were treasured in this case. Most notably, it mitigated the challenges posed by the lack of interoperability — ambiguities due to poor documentation, for instance, were swiftly clarified through direct interaction with knowledgeable stakeholders. Furthermore, in light of the opaque nature of TEACOS, this direct communication facilitated quick consultation and validation of any findings.

Methodological Lessons
For future research that utilise a loose coupling for a new multi-model, the aim for high cohesion and low interdependence is contingent upon the objective of the coupling itself, as well as time allocated for the project and available expertise. If the primary goal is to research and test the feasibility of the coupling, or there is little time and not a lot of expertise, a relatively high interdependence between the models may not be detrimental. On the other hand, if focusing more on model reuse and modular multi-models for practical applications and time and knowledge are abundant, it's better to keep the interdependence low. One potential strategy for achieving the latter could be to develop all models independently, without specific predispositions towards certain characteristics, and to use wrappers or adaptor to couple them.

When establishing a loose coupling or coupling with a black-box model, troubleshooting can be a complex process. As a first step, ensure all levels of interoperability are tested: begin with technical, then syntactical, and finally semantic. The paper by Van der Veer and Wiles (2008) contains question which can be asked to identify non-interoperability across these levels. If these levels are functioning without error, and full communication between the models is feasible, it's likely that the issue lies in the implementation of the coupling design. To identify the source of such a problem, conformance testing is recommended, as it isolates the model and helps identify where the aberrant behaviour occurs. If conformance testing doesn't yield results, the problem probably lies within the coupling or the way the models influence each other. In such cases, it would be prudent to carefully study the inputs and outputs of all involved models, focusing on how the exchanged data files are affected and how these, in turn, influence each subsequent model.

Going forward, it would be beneficial for future research in the spheres of collaborative multi-modeling with multiple stakeholders to integrate a balanced methodological approach that merges quantitative and qualitative techniques. This strategy has the potential to yield a faster, deeper understanding of the models in play and promote a more collaborative and comprehensive perspective in the research process.

7.3. Conclusion

In this study, the research has primarily addressed the coupling of two distinct models: an optimisation model, TEACOS, and an agent-based model (ABM) made specifically for this thesis. Although the construction of a multi-model is not a new concept theoretically, the execution of the coupling of models still faces numerous known technical and non-technical challenges in the literature. In this research, the focus lay on the coupling and interoperability of the models on all levels - technical, syntactic, semantic, and organisational. The complexity of this task is amplified with each additional model that one may add to a multi-model, yet it remains a vital component of the multi-model construction process.

The research question posed at the start of this research was, ”How does the coupling of an agent-based model with an optimisation model affect the outcome generated by the multi-model, given the case study of Tholen?”. This has been explored through three steps: construction of a simple ABM to capture human investment behaviour, coupling the aforementioned ABM with TEACOS, a single-period optimisation model, and running the coupled models. In the results, an intriguing dynamic of interplay between the coupled models was found. The ABM's output notably influenced TEACOS's starting conditions, which in turn impacted its investment strategy generated by the multi-model. Specifically, this influence could be seen in the number of years before a shift in the trajectory occurred, marked by a change in the inflection point KPI. This shift is driven by TEACOS's cost analysis that informs its investment trajectory, balancing the costs of installing new assets against sourcing electricity from the grid. A divergence was observed between the trajectories of the base case and the multi-model, where the multi-model showed a more delayed trajectory to reach the same point. This behaviour of altering investment behaviours and optimisation and lowering the uncertainty of the optimisation illustrates the value-add that multi-models bring to analysis.

Interestingly, the study also exposes a gaps surrounding the discussion around organisational interoperability while constructing multi-models. While most research devotes attention to technical challenges like incompatible ontologies and aligning models' resolution, the aspect of organisational interoperability often remains understated. This is surprising, given how the boons of good organisational interoperability affected this research in a positive way.

This research hopes to showcase both the value that is to be gained by being able to couple an ABM with an existing optimisation model, while also underlining the necessity of organisational interoperability during the construction of multi-models. The main lessons learned regarding organisational interoperability are the importance of thorough documentation and clear and effective communication. The emphasis of the lessons learnt on the methodological side are the necessity of early conformance testing in model coupling, the need for striking a balance between cohesion and coupling based on the goals of the multi-model, and the utility of a systematic, step-by-step troubleshooting process for diagnosing and addressing issues in model coupling. This includes a focus on all levels of interoperability - technical, syntactic, semantic, and organisational - and a meticulous study of the data exchanges between models. Finally, the value of incorporating both quantitative and qualitative methodologies in multi-model construction, such as conducting stakeholder interviews for better model understanding, conceptualisation, and faster knowledge transfer, is highlighted. Together, these methodological lessons add depth and robustness to the multi-modelling process, making it more comprehensive and effective in addressing complex research questions.

7.4. Recommendation for Future Work

This study has looked into loose coupling for agent-based simulation models using a single period optimisation and applying various frameworks to the process. Despite encountering certain complexities, it presents a promising avenue for further exploration. The following three areas have been identified for future work:

Firstly, it’s critical to establish practical multi-model specific frameworks for interoperability. Current frameworks, such as the LCIM and ETSI framework are theoreticaal and not made specifically for the construction of multi-models. Therefore, this research would like to propose that subsequent research could aim to elaborate data from other practically applied multi-model literature and. While this research is the first step towards a more practical approach for such a framework, more operational work can be done towards the topic of interoperability for multi-models.

Secondly, continuing down the path of coupling simulation optimisations in this loose manner, this research has worked with a single-period optimisation. Given the original multi-period nature, a next step would be conducting a similar research with multi-period optimisation.

This research raises a key question: How well does a modeler need to understand a model to use it effectively? While it’s helpful to be able to reuse models or treat them as ”black boxes,” it’s not always easy to combine them or understand the results. Not every model can be fully opened up or made open source, so it’s important to understand the bare minimum a modeler needs to know to use a model successfully. The answers could inform better guidelines for documenting models in multi-modeling, making it easier to use and combine different models in the future.

Bibliography

Adebesin, F., Kotzé, P., Foster, R., & van Greunen, D. (2013). A Review of Interoperability Standards in E-health and Imperatives for their Adoption in Africa. *South African Historical Journal*, *50*. https://doi.org/10.18489/sacj.v50i1.176

Bertalanffy, L. v. (1968). General Systems Theory as Integrating Factor in Contemporary Science. *Akten des XIV. Internationalen Kongresses für Philosophie*, *2*, 335–340. https://doi.org/10.5840/wcp1419682120

Bollinger, L. A., Davis, C. B., Evins, R., Chappin, E. J. L., & Nikolic, I. (2018). Multi-model ecologies for shaping future energy systems: Design patterns and development paths. *Renewable and Sustainable Energy Reviews*, *82*, 3441–3451. https://doi.org/10.1016/j.rser.2017.10.047

Brandmeyer, J. E., & Karimi, H. A. (2000). Coupling methodologies for environmental models. *Environmental Modelling & Software*, *15*(5), 479–488. https://doi.org/10.1016/S1364-8152(00)00027-X

Brown, C. E. (1998). Coefficient of Variation. In C. E. Brown (Ed.), *Applied Multivariate Statistics in Geohydrology and Related Sciences* (pp. 155–157). Springer. https://doi.org/10.1007/978-3-642-80328-4_13

Bulatewicz, T., Allen, A., Peterson, J. M., Staggenborg, S., Welch, S. M., & Steward, D. R. (2013). The Simple Script Wrapper for OpenMI: Enabling interdisciplinary modeling studies. *Environmental Modelling & Software*, *39*, 283–294. https://doi.org/10.1016/j.envsoft.2012.07.006

Bulatewicz, T., Yang, X., Peterson, J. M., Staggenborg, S., Welch, S. M., & Steward, D. R. (2010). Accessible integration of agriculture, groundwater, and economic models using the Open Modeling Interface (OpenMI): Methodology and initial results [Publisher: Copernicus GmbH]. *Hydrology and Earth System Sciences*, *14*(3), 521–534. https://doi.org/10.5194/hess-14-521-2010

Capra, F. (1997). Creativity and Leadership. *Learning Communities*.

Ceniceros, J. A. R., Aguilar-Calderón, J. A., Espinosa, R., & Tripp-Barba, C. (2021). The external and data loose coupling for the integration of software units: A systematic mapping study [Publisher: PeerJ Inc.]. *PeerJ Computer Science*, *7*, e796. https://doi.org/10.7717/peerj-cs.796

Consumentenbond. (2022). Hoeveel zonnepanelen heb ik nodig? | Consumentenbond. Retrieved May 20, 2023, from https://www.consumentenbond.nl/zonnepanelen/hoeveel-zonnepanelen

Dam, K. H. v., Nikolic, I., & Lukszo, Z. (2012). *Agent-Based Modelling of Socio-Technical Systems*. Springer Science & Business Media.

den Boon, S., Jit, M., Brisson, M., Medley, G., Beutels, P., White, R., Flasche, S., Hollingsworth, T. D., Garske, T., Pitzer, V. E., Hoogendoorn, M., Geffen, O., Clark, A., Kim, J., & Hutubessy, R. (2019). Guidelines for multi-model comparisons of the impact of infectious disease interventions. *BMC Medicine*, *17*(1), 163. https://doi.org/10.1186/s12916-019-1403-9

Duboz, R., Ramat, É., & Preux, P. (2003). Scale Transfer Modeling: Using Emergent Computation for Coupling an Ordinary Differential Equation System with a Reactive Agent Model [Publisher: Taylor & Francis _eprint: https://doi.org/10.1080/0232929031000150355]. *Systems Analysis Modelling Simulation*, *43*(6), 793–814. https://doi.org/10.1080/0232929031000150355

Figueira, G., & Almada-Lobo, B. (2014). Hybrid simulation–optimization methods: A taxonomy and discussion. *Simulation Modelling Practice and Theory*, *46*, 118–134. https://doi.org/10.1016/j.simpat.2014.03.007

Foramitti, J. (2021). AgentPy: A package for agent-based modeling in Python. *Journal of Open Source Software*, *6*(62), 3065. https://doi.org/10.21105/joss.03065

Fuchs, S., Katranuschkov, P., & Scherer, R. J. (2010). A framework for multi-model collaboration and visualisation. *Proc. ECPPM*, 115–120.

Gomag. (n.d.). Victron Energy Solar Panel 340W-24V Mono 1956x992x45mm. Retrieved May 20, 2023, from https://www.poweracu.com/photovoltaic/victron-energy-solar-panel-30w-12v-mono-430x545x25mm-689-690-691-692-693-694.html

Goodall, J., Robinson, B., & Castronova, A. (2011). Modeling Water Resource Systems using a Service-Oriented Computing Paradigm. *Environmental Modelling and Software - ENVSOFT*, *26*, 573–582. https://doi.org/10.1016/j.envsoft.2010.11.013

GreenMatch. (n.d.). How Much Do Solar Panels Cost (2023 Prices)? | GreenMatch. Retrieved May 20, 2023, from https://www.greenmatch.co.uk/blog/2014/08/what-is-the-installation-cost-for-solar-panels

Hegemann, J. (2017). Why aren't more researchers using open source? | Opensource.com. Retrieved March 1, 2023, from https://opensource.com/article/17/6/open-source-research

Heikkila, T. (2017). Evidence for Tackling the Complexities of Water Governance [_eprint: https://onlinelibrary.wiley.co *Public Administration Review*, *77*(1), 17–20. https://doi.org/10.1111/puar.12679

Hellhake, D., Bogner, J., Schmid, T., & Wagner, S. (2022). Towards using coupling measures to guide black-box integration testing in component-based systems [_eprint: https://onlinelibrary.wiley.com/doi/pdf/10. *Software Testing, Verification and Reliability*, *32*(4), e1811. https://doi.org/10.1002/stvr.1811

Jones, N. A., Perez, P., Measham, T. G., Kelly, G. J., d'Aquino, P., Daniell, K. A., Dray, A., & Ferrand, N. (2009). Evaluating Participatory Modeling: Developing a Framework for Cross-Case Analysis. *Environmental Management*, *44*(6), 1180–1195. https://doi.org/10.1007/s00267-009-9391-8

Kaye, D. (2003). *Loosely Coupled: The Missing Pieces of Web Services* [Google-Books-ID: 1VzE-QoU1qMQC]. RDS Strategies LLC.

Kazil, J., Masad, D., & Crooks, A. (2020). Utilizing Python for Agent-Based Modeling: The Mesa Framework. In R. Thomson, H. Bisgin, C. Dancy, A. Hyder, & M. Hussain (Eds.), *Social, Cultural, and Behavioral Modeling* (pp. 308–317). Springer International Publishing. https://doi.org/10.1007/978-3-030-61255-9_30

Knapen, R., Janssen, S., Roosenschoon, O., Verweij, P., de Winter, W., Uiterwijk, M., & Wien, J.-E. (2013). Evaluating OpenMI as a model integration platform across disciplines. *Environmental Modelling & Software*, *39*, 274–282. https://doi.org/10.1016/j.envsoft.2012.06.011

Larson, J. W. (2006). Ten organising principles for coupling in multiphysics and multiscale models. *ANZIAM Journal*, *48*, C1090–C1111. https://doi.org/10.21914/anziamj.v48i0.138

Lee, J.-S., Filatova, T., Ligmann-Zielinska, A., Hassani-Mahmooei, B., Stonedahl, F., Lorscheid, I., Voinov, A., Polhill, J. G., Sun, Z., & Parker, D. C. (2015). The complexities of agent-based modeling output analysis [Publisher: Guildford: University of Surrey]. *Journal of Artificial Societies and Social Simulation*, *18*(4). https://doi.org/10.18564/jasss.2897

Martin, R. (1994). OO Design Quality Metrics.

Masurel, E. (2007). Why SMEs invest in environmental measures: Sustainability evidence from small and medium-sized printing firms [_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/bse.478]. *Business Strategy and the Environment*, *16*(3), 190–201. https://doi.org/10.1002/bse.478

Nikas, A., Gambhir, A., Trutnevyte, E., Koasidis, K., Lund, H., Thellufsen, J. Z., Mayer, D., Zachmann, G., Miguel, L. J., Ferreras-Alonso, N., Sognnaes, I., Peters, G. P., Colombo, E., Howells, M., Hawkes, A., van den Broek, M., Van de Ven, D. J., Gonzalez-Eguino, M., Flamos, A., & Doukas, H. (2021). Perspective of comprehensive and comprehensible multi-model energy and climate science in Europe. *Energy*, *215*, 119153. https://doi.org/10.1016/j.energy.2020.119153

Nikolic, I., Warnier, M., Kwakkel, J., Chappin, E., Lukszo, Z., Brazier, F., Verbraeck, A., Cvetkovic, M., & Palensky, P. (2019). *Multi-Model Ecology and Interface for transition models* (tech. rep.). Delft University of Technology. https://doi.org/10.4233/UUID:1AA3D16C-2ACD-40CE-B6B8-0712FD947840

Omer, S., Abdalla, A., Sarker, A., & Singh, M. (2014). Bayesian Determination of the Number of Replications in Crop Trials. *European Journal of Experimental Biology*, *4*, 129–133.

Quesnel, G., Duboz, R., & Ramat, É. (2009). The Virtual Laboratory Environment – An operational framework for multi-modelling, simulation and analysis of complex dynamical systems. *Simulation Modelling Practice and Theory*, *17*(4), 641–653. https://doi.org/10.1016/j.simpat.2008.11.003

Rehm, G., Galanis, D., Labropoulou, P., Piperidis, S., Welß, M., Usbeck, R., Köhler, J., Deligiannis, M., Gkirtzou, K., Fischer, J., Chiarcos, C., Feldhus, N., Moreno-Schneider, J., Kintzel, F., Montiel, E., Doncel, V. R., McCrae, J. P., Laqua, D., Theile, I. P., … Lagzdiņš, A. (2020). Towards an Interoperable Ecosystem of AI and LT Platforms: A Roadmap for the Implementation of Different Levels of Interoperability [arXiv:2004.08355 [cs]]. Retrieved May 8, 2023, from http://arxiv.org/abs/2004.08355

Comment: Proceedings of the 1st International Workshop on Language Technology Platforms (IWLTP 2020). To appear

Reußner, F., Alex, J., Bach, M., Schütze, M., & Muschalla, D. (2009). Basin-wide integrated modelling via OpenMI considering multiple urban catchments. *Water Science and Technology*, *60*(5), 1241–1248. https://doi.org/10.2166/wst.2009.471

Rezaeiahari, M., & Khasawneh, M. T. (2020). Simulation optimization approach for patient scheduling at destination medical centers. *Expert Systems with Applications*, *140*, 112881. https://doi.org/10.1016/j.eswa.2019.112881

Robineau, T., Rodler, A., Morille, B., Ramier, D., Sage, J., Musy, M., Graffin, V., & Berthier, E. (2022). Coupling hydrological and microclimate models to simulate evapotranspiration from urban green areas and air temperature at the district scale. *Urban Climate*, *44*, 101179. https://doi.org/10.1016/j.uclim.2022.101179

Sachs, J., Meng, Y., Giarola, S., & Hawkes, A. (2019). An agent-based model for energy investment decisions in the residential sector. *Energy*, *172*, 752–768. https://doi.org/10.1016/j.energy.2019.01.161
Use for qualitative part of study: In addition to these approaches, many conceptual frameworks have been established to describe the factors that can affect the households' decision on energy use [38,39].

Santos, K. S. S., Pinheiro, L. B. L., & Maciel, R. S. P. (2021). Interoperability Types Classifications: A Tertiary Study. *XVII Brazilian Symposium on Information Systems*, 1–8. https://doi.org/10.1145/3466933.3466952

Schmitz, O., Salvadore, E., Poelmans, L., van der Kwast, J., & Karssenberg, D. (2013). A framework to resolve spatio-temporal misalignment in component-based modelling. *Journal of Hydroinformatics*, *16*(4), 850–871. https://doi.org/10.2166/hydro.2013.180

Senge, P. (1990). *The Fifth Discipline*. Doupleday Currence.

Shahumyan, H., & Moeckel, R. (2015). Integrating Models for Complex Planning Policy Analysis: Challenges and a Solution in Coupling Dissimilar Models [ISBN: 9780692474341 Publisher: Computers in Urban Planning and Urban Management]. *Ferreira, J. Jr. and Goodspeed, R. (eds.) Proceedings of 14th International Conference on Computers in Urban Planning and Urban Management (CUPUM 2015): Planning Support Systems and Smart Cities*. Retrieved June 1, 2023, from http://hdl.handle.net/10197/8267

Shrestha, N. K., Leta, O. T., De Fraine, B., van Griensven, A., & Bauwens, W. (2013). OpenMI-based integrated sediment transport modelling of the river Zenne, Belgium. *Environmental Modelling & Software*, *47*, 193–206. https://doi.org/10.1016/j.envsoft.2013.05.004

Strantzali, E., & Aravossis, K. (2016). Decision making in renewable energy investments: A review. *Renewable and Sustainable Energy Reviews*, *55*, 885–898. https://doi.org/10.1016/j.rser.2015.11.021

TNO. (n.d.). ESDL MapEditor. Retrieved May 1, 2023, from https://energytransition.gitbook.io/esdl/esdl-based-tools/mapeditor

Tolk, A., Diallo, S., & Turnitsa, C. (2007). Applying the Levels of Conceptual Interoperability Model in Support of Integratability, Interoperability, and Composability for System-of-Systems Engineering. *Journal of Systems, Cybernetics, and Informatics*, *5*(5). https://digitalcommons.odu.edu/msve_fac_pubs/27

Tolk, A., & Muguira, J. A. (2003). The Levels of Conceptual Interoperability Model.

Van der Veer, H., & Wiles, A. (2008). Achieving technical interoperability. *European telecommunications standards institute*. Retrieved May 8, 2023, from https://www.etsi.org/images/files/ETSIWhitePapers/IOP%20whitepaper%20Edition%203%20final.pdf

Vangheluwe, H. (2000). DEVS as a common denominator for multi-formalism hybrid systems modelling. *CACSD. Conference Proceedings. IEEE International Symposium on Computer-Aided Control System Design (Cat. No.00TH8537)*, 129–134. https://doi.org/10.1109/CACSD.2000.900199

Walby, S. (2007). Complexity Theory, Systems Theory, and Multiple Intersecting Social Inequalities [Publisher: SAGE Publications Inc]. *Philosophy of the Social Sciences*, *37*(4), 449–470. https://doi.org/10.1177/0048393107307663

Wallace, D., & Fujii, R. (1989). Software verification and validation: An overview [Conference Name: IEEE Software]. *IEEE Software*, *6*(3), 10–17. https://doi.org/10.1109/52.28119

Whitman, L. E., & Panetto, H. (2006). The missing link: Culture and language barriers to interoperability. *Annual Reviews in Control*, *30*(2), 233–241. https://doi.org/10.1016/j.arcontrol.2006.09.008

Wilensky, U. (1999). NetLogo. *Center for Connected Learning and Computer-Based Modeling, Northwestern University. Evanston, IL.*

Yourdon, E., & Constantine, L. L. (1979). *Structured design. Fundamentals of a discipline of computer program and systems design* [Publication Title: Englewood Cliffs: Yourdon Press ADS Bibcode: 1979sdfd.book.....Y]. Retrieved June 1, 2023, from https://ui.adsabs.harvard.edu/abs/1979sdfd.book.....Y

Zhang, Z., Jing, R., Lin, J., Wang, X., van Dam, K. H., Wang, M., Meng, C., Xie, S., & Zhao, Y. (2020). Combining agent-based residential demand modeling with design optimization for integrated energy systems planning and operation. *Applied Energy*, *263*, 114623. https://doi.org/10.1016/j.apenergy.2020.114623

Zonneplan. (n.d.). Afmetingen zonnepanelen | Welke formaten zijn er in 2023? Retrieved May 20, 2023, from https://www.zonneplan.nl/kenniscentrum/zonnepanelen/afmetingen

A

Full-Page Conceptual Diagrams

This appendix contains a full page representation of the UML and decision logic conceptualised for the agents in the ABM. Both are shown on the following pages, starting with the UML in Figure A.1 and the decision logic in Figure A.2.

A.1. UML

ESDL AbstractBuilding attributes

The attributes that are passed on from the Pyesdl file are the name of the building, and two Geographic Information System (GIS) attributes used for the agents and visualisation. These two attributes are the geometry and the crs of a building. The geometry is a polygon, which is very useful when visualising and placing the agents on the map, as the Polygon is constructed based on their exact coordinates. The crs is used to place the Polygon with the correct projection onto the map. These two attributes normally do not work with Mesa, however, a GIS extension exists for Mesa. This extension is called Mesa Geo. It allows for the creation of GIS-based agents. In this case, that means that the polygon from the ESDL-file can be used to outline agents and they *are* that polygon shape, as well as assess their neighbours based on distance or other GIS-like functions that have been implemented. This is also why the class of the agents is a Mesa Geo GeoAgent and not just a Mesa Agent.

ABM Building attributes

All agents have their own unique ID so we can identify them, the factors on which they make their decisions which are financial factor, social factor and the combination of those two, depending on the scenario. These will be explained more in depth in Section **??**. Furthermore, the agents contain a boolean of whether or not they want to buy panels and if they actually have bought panels. The difference here is that some companies may want to buy panels but lack the budget to do that. This is based on the next attribute, which is their funding. Currently this number is randomised for each agent based on a triangular distribution. The minimum value a is half the cost of a solar panel, the peal value c is the price of four solar panels and the maximum value c is defined by eight times the cost of solar panels. This is because solar panels are often sold and installed in batches of at least four, which what was set as the batch size for the ABM. With this triangular distribution, it was not the purpose to model realistic budgets as that data is unavailable. It is merely to set some sort of budget that will enable companies to have a financial limit to what is possible. Furthermore, companies have a number of square meters of rooftop, which is deduced from their polygon. The rooftop size available is how many square meters of rooftop is still free, and this is another constraint for the number of solar panels they can install. Finally each company has a number of PV panels bought and installed. The distinction is made here between panels installed because the latter has to do with how it will be conceptualised for writing the panels back into the ESDL-file.

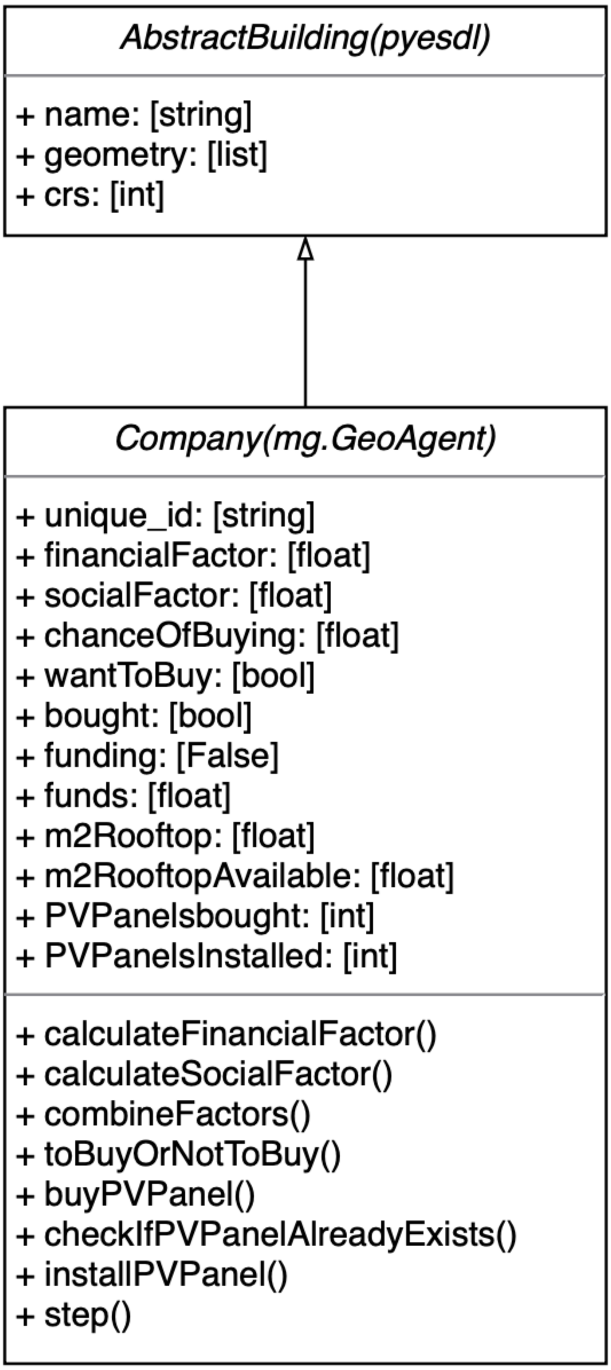


Figure A.1: Full page of the agent UMLs

A.2. Decision Logic Diagram

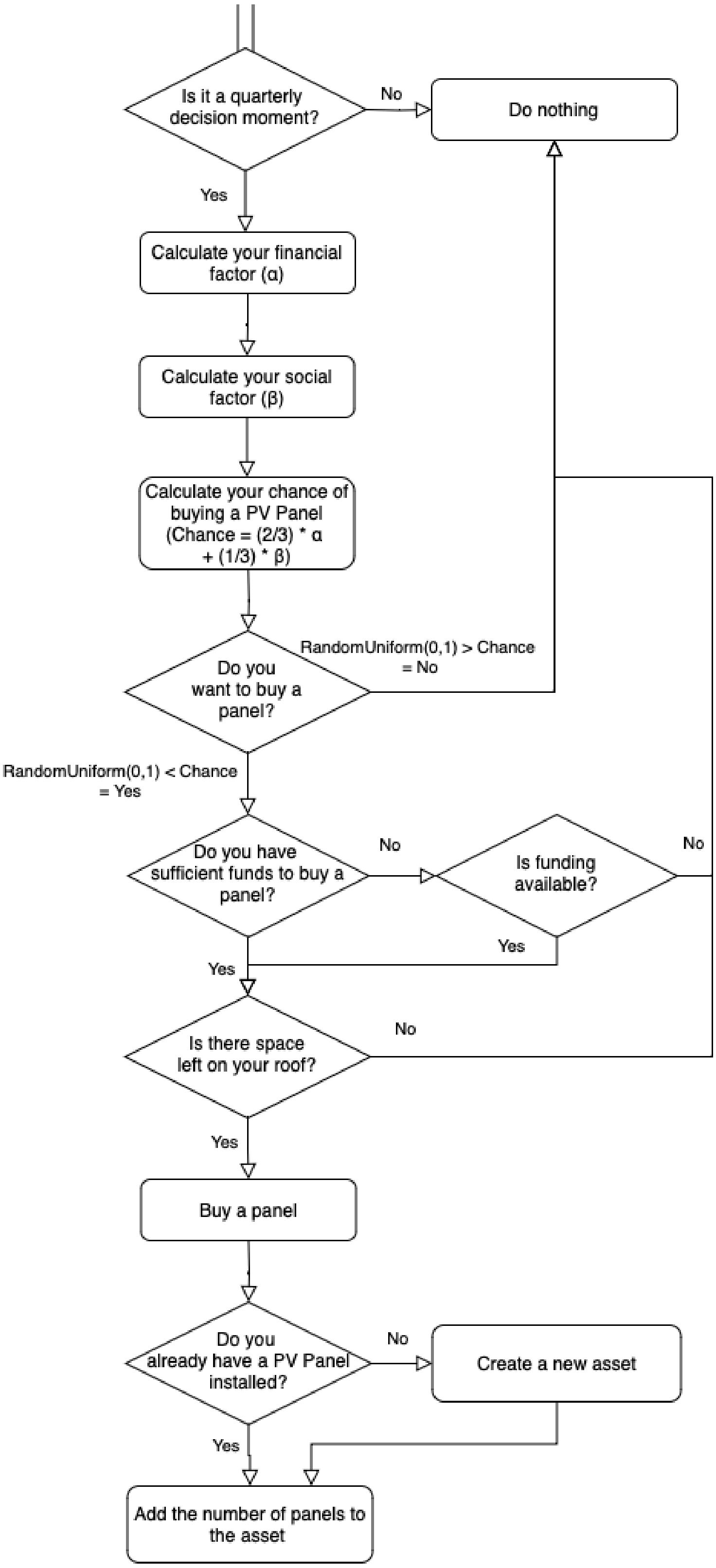


Figure A.2: Full page of agent decision logic for buying PV panels.

B

ABM Parameterisation

In Table B.1, all values for the parameters in the model are listed with their value and the source for the value used.

Table B.1

Level	Parameter	Value	Source
Model	Size of PV panel	2m2	Gomag (n.d.) and Zonneplan (n.d.)
	Cost of PV panel	€500	Gomag (n.d.) and GreenMatch (n.d.)
	Batchsize of PV Panel	2	Own input
	Capacity PV Panel	350 W	Consumentenbond (2022) and GreenMatch (n.d.)
	Cost of Electricity through PV Panel	0.50 €/kWh	Micro Case
Agent	Funds	np.random.normal(1000)	Own Input
	Radius	0.075	Own Input

The radius was calculated by a test using the Mesa Geo library to see how much agents would be considered with what radius. Using an agent at the edge, this was the result.

Table B.2

Radius value	Number of agents within range
0.00005	2
0.0005	3
0.0025	39
0.0050	78
0.0065	100
0.0070	108
0.0073	111
0.0075	112

The total number of agents is 112, and this can be used when using a radius of 0.0075.

C

Verification

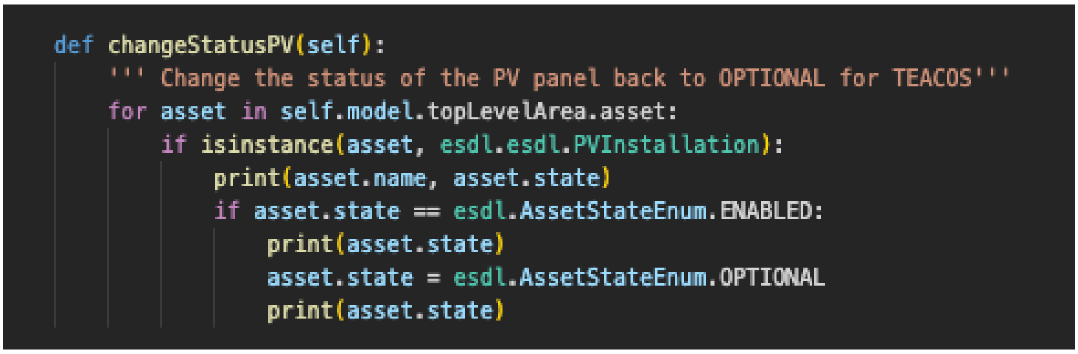
This appendix contains a more in-depth explanation of the verification that have been done for the ABM (Section C.1) and the model coupling (Section C.2).

C.1. ABM Verification

Code Walk-Through

The ABM was implemented iteratively and for each new section, the code was checked and walked through to see whether the code was implemented correctly. This was done by checking the code for errors and whether the implemented behaviour was aligned with the expected, conceptual behaviour.

One of the ways this was consistently done throughout each iteration was through print statements. They were used to check whether or not all actions were being performed and what the states were of the agent at certain times. An example of how these print statements were used to see if an asset's state were properly changed can be seen in Figure C.1.



```python
def changeStatusPV(self):
    ''' Change the status of the PV panel back to OPTIONAL for TEACOS'''
    for asset in self.model.topLevelArea.asset:
        if isinstance(asset, esdl.esdl.PVInstallation):
            print(asset.name, asset.state)
            if asset.state == esdl.AssetStateEnum.ENABLED:
                print(asset.state)
                asset.state = esdl.AssetStateEnum.OPTIONAL
                print(asset.state)
```

Figure C.1: An example of how print statements were used to check the code during the implementation of the ABM.

Recording and tracking agent behaviour

To understand the workings of the model, oftentimes an individual agent was chosen and studied for the duration of a run. This was mainly done towards the end of the implementation after the decision logic had been coded. The agent states and choices were checked each step to see if they corresponded to that of the conceptual design. This was done by looking at an individual agents properties in the dataframe output of Mesa's DataCollector at the end in combination with print statement.

Multi-Agent Testing

Multi-agent testing is done with the base case of the model to monitor behaviour of all agents for the duration of a single run. Overall, correct behaviour was found and no strange instances occurred. An example of the mesa model at the end of a run can be seen in Figure

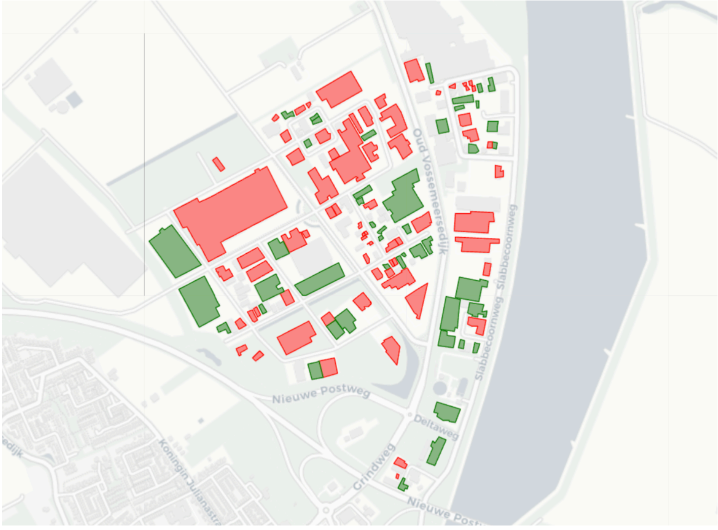


Figure C.2: An example of the model after a run, where red agents have not invested and green agents have invested.

All agents have made a decision, and just as one would expect with social influence, certain clusters have started to emerge with agents that have bought panels and agents that have not bought them.

Besides the verification steps adopted for the purpose of this research to check whether the conceptual model was adapted properly, the code was also constantly being checked by the coding environment. The IDEs used for this research have verification steps of their own built in to check the code. Both PyCharm and Visual Studio Code were used. Both IDEs were used in conjunction with pylint, which is a static code analyser that is able to analyse your code without running it. This way, it is able to catch small errors such as a missing bracket or when a variable is used before it is assigned.

C.2. Model Coupling Verification

Conformance testing

Conformance testing is done to check that the individual components work as proposed. In this case, the ABM has already been tested individually in the previous section and has been verified in subsection 4.4.1. TEACOS cannot be verified in the same way, since access to the source code is prohibited. In that stead, TEACOS is verified through testing and expert input.

It is through this way that is was found that TEACOS only dealt in optima in its current state. Either the optional asset was not selected at all and all electricity would be sourced from the grid or the optional asset was selected to provide *all* the electricity for Tholen. An example of both cases can be seen in the Sankey diagram in Figure XXX, which contains the electricity providers on the left side of each diagram and how these flow to the buildings with their demand on the right side of the diagram.

It was found that this choice could be influenced by three factors, which are the fixed costs, marginal costs and the constraint placed on the optional asset. The fixed costs are the costs for implementing the optional asset, in this case the solar panel, expressed in euros. The marginal costs are how much it would cost to draw electricity from that optional asset, expressed in euros per kWh. And finally, the ranged constraint was a constraint that could be placed on the optional asset for how much electricity could be sourced from the asset. Essentially, it was a user implemented limit on the capacity of the optional asset.

Each of these factors were varied to find out how they might impact TEACOS' behaviour across twelve runs.

It is very clear that TEACOS considers the cost when deciding whether or not to use the optional asset, but the exact manner thereof is not clear. However, several hypotheses have been made and tested through these runs, which have been verified after with model experts. First, it considers the costs and marginal costs together, and there is a tipping point at which the sum of these becomes higher than

Table C.1

Attempt	Costs	Marginal Costs	Ranged Constraint	Optional Asset	Electricity Grid
1	250	0.10	N/A	Yes	No
2	250	0.50	N/A	Yes	No
3	250	1.00	N/A	Yes	No
4	500	0.10	N/A	Yes	No
5	500	0.50	N/A	Yes	No
6	500	1.00	N/A	No	Yes
7	750	0.10	N/A	Yes	No
8	750	0.50	N/A	No	Yes
9	750	1.00	N/A	No	Yes
10	500	0.10	50000	Yes	Yes
11	500	0.50	50000	Yes	Yes
12	500	1.00	50000	No	Yes

simply sourcing electricity from the electricity grid. It is in those cases that it does not select the asset. Attempts six, eight and nine are examples of this. Secondly, the ranged constraint is the only (currently known) way to get a combination result from TEACOS. A combination result refers to an optimal solution wherein TEACOS returns both electricity from the grid *and* from the optional asset. A forceful limit is kept on the optional asset, which is 50k Watts in the examples. In those cases, TEACOS decided to select the optional asset for the maximum available value - it still cannot deal in partial choices - and the rest of the demand is sources from the electricity grid.

Combination results speak much more the imagination than fully one option or the other and allow for better understanding of what is exactly happening within TEACOS. Therefore, in the rest of the research, a ranged contraint of 50000 is chosen, along with the costs of 500 and 0.50, since they are closest to reality and allow TEACOS to make a decision.

Manual runs

Manual runs are done to ensure that the automation is done correctly. This is done by using each model separately, and manually input the file paths for the ESDL-file. After the first TEACOS run, the output from TEACOS is input into the ABM and so forth. This is done for a loop with an iteration within a range of three. Results from the manual run verification shows that the results from the coupled models exhibit the same behaviour as the manual runs.

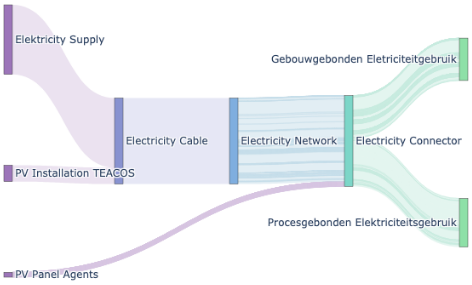


Figure C.3: Result of example automated first full iteration.

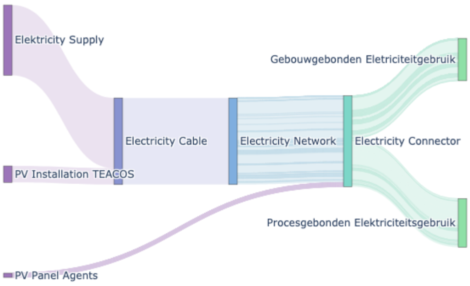


Figure C.4: Result of manual first full iteration.

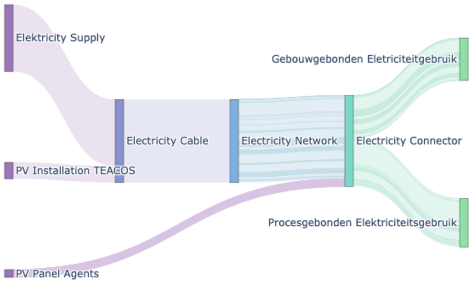


Figure C.5: Result of example automated second full iteration.

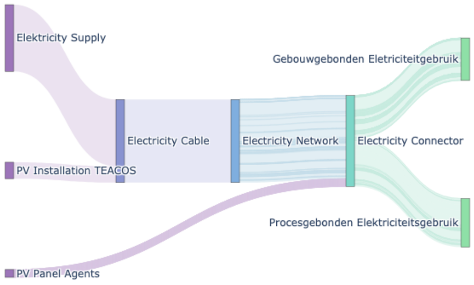


Figure C.6: Result of manual second full iteration.

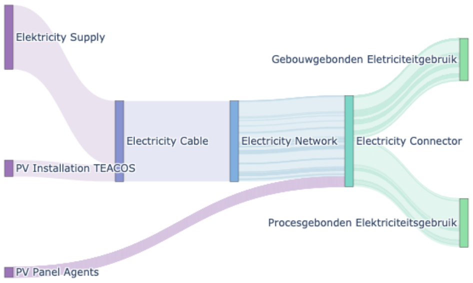


Figure C.7: Result of example automated third full iteration.

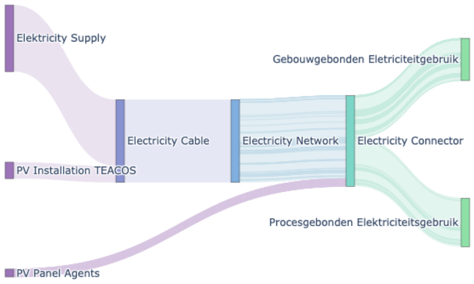


Figure C.8: Result of manual third full iteration.

D

Documentation of challenges

This appendix contains a high level overview and documentation of all the challenges that were dealt with during this research. It is important to note that every project deals with challenge. This research has also seen its fair share of general challenges, which is to say, challenges that would arise in every type of project. When documenting these challenges, from the literature review to the processing of the results, the general challenges have been left out. An effort was made to keep track of the challenges that only arose out of the task of multi-modelling, coupling models and the micro case. Table D.1 contains an overview of the challenges and the level of interoperability. The corresponding challenge can be found in their respective subsection, divided per phase.

Table D.1: Challenge and their phase and the level of interoperability, followed by which subdivision they can be found in.

Challenge	Phase	Interoperability	Subsection
Multi-Model orchestrator timeline	Background	Technical	Subsection D.1.1
Energy System Description Language	Background	Syntactical	Subsection D.1.2
Model understanding	Background	Organisational	Subsection D.1.3
Micro Case Documentation	Background	Organisational	Subsection D.1.4
Single period vs. Multi period	Conceptualisation	Technical	Subsection D.2.1
Agent alignment	Conceptualisation	Semantic	Subsection D.2.2
Semantic alignment between models	Conceptualisation	Semantic	Subsection D.2.3
Getting to know TEACOS	Conceptualisation	Organisational	Subsection D.2.4
Flip Flop Behaviour TEACOS	Formalisation	Syntactic	Subsection D.3.1
Model Run ID Error	Formalisation	Technical	Subsection D.3.2
Connecting to the SQL server	Formalisation	Technical	Subsection D.3.3
Unit inconsistency	Formalisation	Semantic	Subsection D.3.4
Credentials	Formalisation	Organisational	Subsection D.3.5
IP Address	Formalisation	Organisational	Subsection D.3.6
Statelessness of ESDL-file	Results	Technical	Subsection D.4.1
Image rights	Results	Organisational	Subsection D.4.2

D.1. Background: Micro Case

These challenges were experienced during the preparation of this research and intake of all available materials.

D.1.1. The Multi-Model Orchestrator Timeline

This thesis was adapted to fit to the planning of the micro case. In an earlier conceptualisation of this research, the orchestrator had played a bigger role and would have been fully functioning. Getting the orchestrator up and running is a difficult task and took longer than initially thought. Although this research was able to reconceptualise to fit to a feasible project planning within the allotted time, it was still a challenge that took considerable thought and time to work around in a suitable fashion. Getting the orchestrator to work concerns the connection of the models, which is an aspect of the technical level of interoperability.

D.1.2. Energy System Description Language

The micro case uses the Energy System Description Language (ESDL) as the language of the files that are being exchanged between the models. This language and manner of describing energy systems works really well, depending the familiarity of the user. This challenge is categorised as a syntactical error, since it has to do with the exchange of information between the models in a predefined format and structure. It is simply that the chosen data format and structure takes quite a while to understand and, going one step further, easily manipulate. The lack of documentation for the Python ESDL package was a considerable part of this challenge, given that it was hard to understand how to use and therefore, in practice, use it.

D.1.3. Model understanding

The models involved in the micro case are complex, standalone models developed with or by experts on their respective topics. Because not all models are open source, documentation and publications are very limited. Much of the knowledge gained on the models was garnered through speaking with their respective owners. A great proposed document existed wherein the models were classified according to a template, identifying inputs, output et cetera. This challenge was categorised as misalignment on organisational level due to the fact that this has to do with the circumstances surrounding the model.

D.1.4. Micro case documentation

The manner of file sharing for the micro case was not conducive to this research. Up until the point of joining, various files has been shared through the mail. Despite the existence of a cloud file storage, SharePoint, this was rarely used. The size of the micro was between five or six active participants, between which the sharing of files through e-mail had worked up until that point. Later on, when wanting to examine existing ESDL files, these were also not centrally stored. Therefore, when joining the project midway, the lack of accessibility to files that had been shared in the past and an underutilised central storage were major challenges. These challenges were partially overcome by asking around (after which files were emailed) and proposing to store the ESDL files on the SharePoint, which was done for a brief while. This challenge is made more difficult due to the existence of there being two file sharing locations. Many files were present later on in GitHub, however, due to the structure of the GitHub, these were not easily found, either. This challenge is a part of organisational interoperability since it concerns itself with the integration of the coupling beyond the boundaries of a single model.

D.2. Conceptualisation

These challenges were experienced during the conceptualisation phase of this research.

D.2.1. Single period vs. Multi period

During the conceptualisation phase it was found that TEACOS would not function to the full extent of its capabilities. Instead of working with a multi-period period optimisation, it would be a single period optimisation. This was because making an adaptor for TEACOS that could handle multi period optimisation would take considerably more time, and therefore, the decision was made to start with a minimum viable product of TEACOS that was single period.

D.2.2. Agent alignment

In this case, when conceptualising the agents in the model, more thought was required than usual to ensure semantic alignment between the agents. TEACOS does not strictly define agents in the same way the ABM does, but to ensure that the same meaning is given to the entities present in both models, this is addressed by simply spending more time on the conceptualisation.

D.2.3. Semantic alignment between models

The concepts used between the models need to hold the same meaning. However, some terms used by TEACOS were stored in the ESDL-file in such as way that is was not always immediately clear what they would translate to within the ABM. An example of this is the energy demand of the buildings. Within the ESDL-file, this was stored under the name 'multiplier', which does not initially imply that this is the number you are looking for when wanting to know the energy consumption. This is because a multiplier is often applied to the actual number. This was misleading and led to confusion, which was cleared during consultation with the micro case participants. Because this issue concerns the meaning given to words across the coupling, this is on the semantic level of interoperability.

D.2.4. Getting to know TEACOS

When conceptualising, the biggest hurdle was to conceptualise for a model that could only be observed from the outside and any knowledge from the inner workings of the model came second hand or from documentation. This meant conceptualisation took significantly longer and, more importantly, had to be verified with experts on TEACOS. Ideally, this would have been done every step of the way. Due to the fact that the root of this issue is concerns legal characteristics of TEACOS, this is categorised as an organisational challenge.

D.3. Formalisation

These challenges were experienced during the formalisation phase of this research, either when constructing the ABM or the coupling of the models.

D.3.1. Flip Flop Behaviour

During the verification of the results, it was found that the model adaptor could not understand every type of input given by the ESDL-file. In this case, it had do with a ranged constraint being set to number already, which resulted in flip flopping of the outcome of TEACOS, where it would sometimes not make a decision. This was solved by adjusting the input file and accommodating in how the ABM returned the data to TEACOS. This is classified as a technical error because it has to do with the communication with the model.

D.3.2. Model Run Error

Another error that occasionally occurs in a very small portion of the runs, is that during the running of TEACOS, the model run ID is unknown and it does not start the model run. This error could not be solved at the root error and the hypothesis is that the adaptor initializes the model too quickly, before the model run ID has been generated. The only solution to solve this is to run it again, in which case it often does work. This problem can therefore be circumvented with enough runs. Because the nature of this error lies in successfully establishing a communication line with TEACOS, this is categorised as a technical error.

D.3.3. Connecting to external SQL Server

To access TEACOS, the model adaptor has to establish a connection to the SQL server on which the model is hosted. There are two requirements for establishing this connection: Firstly, the credentials of a personalised account generated by Quo Mare, the and secondly,the connection needs to be established through an IP Address that is white listed by Quo Mare. However, every once in a while, a Logging Error will occur when trying to establish this connection. When this error occurs, restarting the adaptor has solved this issue in a 100% of the cases. Because this error has to do with establishing a connection to the SQL server and has to do with model communication, this is categorised as a technical error.

D.3.4. Unit inconsistency

During the conformance testing of TEACOS, it was found that there were some issues with the translation of units from the ESDL-file to TEACOS. Where the ESDL files used terajoules to denote the unit of the energy demand of buildings, this unit could not be read by the TEACOS adaptor (yet). Because of that, the adaptor reverted the unit of the energy demand back to megajoules. This issue was solved by changing how the unit was stored in the ESDL. Sadly, to get it to work, some concessions had to be done in the value of the energy demand. Because this issue has to do with the translation of units between models and how they are interpreted, it is categorised as a semantic issue.

D.3.5. Credentials

This is a challenge that one only encounters when working with a model that is not open source. To use - not access - TEACOS for the purpose this research, credentials are required to access the server on which the model is hosted. This was easily solved by receiving said credentials from Quo Mare, the company that owns TEACOS. Therefore, in this case it did prove to be a substantial challenge, but it is included because when simply constructing one one's model, this would not be a part of the process. This is something that arises specifically when studying a model owned by an outside organisation that is not open source and should be kept in mind when broaching a project that includes models with similar attributes. This is a challenge on the level of organisational interoperability because it has to do with external business processes, unrelated to the models.

D.3.6. IP Address

Initially there was an issue whitelisting the IP-range of the Technical University of Delft. This specific issue still has not been solved, but it was circumvented by whitelisting the author's private IP address. While this resolved the IP address error, a connection with the SQL server still couldn't be established on a reliable basis. Eventually, this issue resolved itself due to unknown reasons. Even through communication with Quo Mare, it could not be discovered what had changed to accommodate. This challenge is attributed to two levels of interoperability. Firstly, the technical level of interoperability, since it has to do with the technical end-to-end exchange of data amongst the models. Secondly, it also has to do with the organisational level of interoperability, since the IP-address issue from the side of TU Delft has to do with their business processes.

D.4. Results

These challenges were experienced after the models had run and have to do with the results from the (coupled) models.

D.4.1. Statelessness of ESDL-file

It was found that when wanting to process the results, the script written to generate the Sankey diagram required information of previous runs. In this case, the ESDL file output by the ABM did not contain the decision made by TEACOS anymore. In essence, it does not and cannot ”remember” what had happened in the past. This static representation of what was happening meant that when processing the results, the script to process the results would sometimes include the asset when TEACOS had *not* chosen it. This was solved by having the models return variables that could be remembered within the script for coupling. This is a challenge that is hard to categorise. However, due to the fact that it has to do with the data format, it has been categorised as a syntactical error.

D.4.2. Image rights

The fact that TEACOS remains intellectual property means that some proprietary functions, such as the automatic generation of diagrams, could not be used for this research. Therefore, many data processing functions and visual representations had to be manually replicated. This challenge arose because of licensing and IP, and therefore it is categorised as a challenge on the level of organisational interoperability.