Article

Experiences from city scale simulation of thermal grids

Johan Simonsson [1,†,*], Gerald Schweiger [2], Khalid Tourkey Atta [1] and Wolfgang Birk [1]

[1] Luleå University of Technology, Luleå, Sweden
[2] Graz University of Technology, Graz, Austria
* Correspondence: johan.simonsson@ltu.se; johan.simonsson@optimation.se
† Optimation AB, Uppsala, Sweden

Abstract: Dynamic simulation of district heating and cooling networks has an increased importance in the transition towards renewable energy sources and lower temperature district heating grids, as both temporal and spatial behavior need to be considered. Even though a lot and research and development has been performed in the field, there are several pitfalls and challenges towards dynamic district heating and cooling simulation for everyday use. This article presents the experiences from working with district heating and cooling projects, along with relevant research, corresponding research gaps and proposed research directions.

Keywords: Digital twin; Simulation; District heating; District cooling; 4GDH; DHC

1. Introduction

Sustainable energy systems rely on a wide range of energy sources such as biomass, wind, solar energy, combustion of waste fuel and recovered energy from industrial plants and data centers [1,2]. An integral part in the utilization of renewable energy sources is to use the available energy as efficiently as possible. Several reports [3,4] point out that an increased district heating and cooling capacity in the European Union is a key to reduced energy consumption and reduced green house gas emissions, where the goal is a reduction of the energy related CO_2 emissions by 40% in 2030 compared to 1990 levels [5]. Currently half of the total energy consumption in the European Union is for the purpose of district heating and cooling [6], and it is concluded that there is enough excess heat in the European Union to cover the heat demands of all buildings from the service sector and households. Previous research [7,8] has shown that from an economic perspective, the competitiveness of district heating as a mean of decarbonisation is sensitive to the density of the cities. District heating is mainly favourable in high density urban districts, whereas other technologies such as electrical heat pumps can be favourable in rural areas or less dense cities.

With current policies the total energy supplied by district heating is estimated to increase by around 50% by 2050. Within the European Union, in the Nordic countries, Baltic countries and Poland district heating serves more than 50% of the households, and around 12% European Union wide. To meet the demands of an increased utilization of renewable heat sources the 4th Generation District Heating (4GDH) [9] networks include lower supply temperatures with the ability to recycle heat from low temperature sources and forming a smart energy system with integration of e.g. electricity and gas networks. This also has implications for how district heating networks are controlled, where it is shown e.g. in [10] that large energy savings are possible using more advanced control strategies and efficient utilization of thermal storage units and building inertia.

To explore the possibilities and implications of novel types of district heating and cooling networks, the impact of renewable energy sources, and the corresponding control strategies, dynamic simulation of the thermal grid is considered

an important aid in the process. Early results in this area are from 1990's and early 2000's, with examples such as [11] and [12]. More recently several European Union projects have employed district heating and cooling simulation for their use cases, such as OPTi [13] that is used as a case study in this paper, and INDIGO [14] where a simulator is used for district cooling networks. Extensive research and development is also performed within the International Building Performance Simulation Association (IBPSA) [15] aiming to create a complete open source Modelica Framework for building and community energy system design and operation. Furthermore, several articles such as [16–18] deal with the concept of dynamic district heating models and simulation.
Common use cases using simulation of district heating and cooling networks are operational optimization with regards to short term production planning such as [18] considering production rates and scheduling of production units, including optimization of thermal storage. Other examples include [19] where a dynamic simulator is used to explore the impact of supply temperature on a combined heat and power (CHP) plant. Integration and operation, including optimization of operation, of a seasonal storage is examined in [20]. A slightly different use case is [21] where a simulator is used for evaluation of safety risks with regards to safety in case of network failures. Other articles deal with demand response for district heating using district heating simulation tools [22]. In previously mentioned INDIGO the simulator is used for design of district cooling networks.
In this paper the simulator developed within the H2020 OPTi project is presented as a case study, followed by examples, challenges and limitations encountered during the project. On the basis of the case study and references, research gaps and proposed relevant research directions are identified when applicable.
This paper's main contribution is to presents results and lessons learned from a case study on dynamic city-scale district heating modelling and simulation. This includes a thorough discussion on modelling and simulation paradigms, automatic model generation, fidelity, computational performance, validation, and model calibration.

2. Case study: Dynamic city scale district heating simulation

As a practical example used in the article to illustrate the challenges of district heating and cooling simulation, the simulator developed within the OPTi project [13] will be used. The project started in 2015 as an European Union Horizon 2020 project and was coordinated by Luleå University of Technology, Sweden. The project objective was to analyze and rethink the way district heating and cooling systems are architected and controlled. Within the project, OPTi-Sim, a dynamic city scale district heating grid simulator was developed to explore the use cases, ranging from:

- Validation of optimization-based control methods
- Design of automated demand response schemes
- Exploit the potential of passive-heat storage

From the width of the scope, the size of the district heating grid and the lack of measurements available it was determined that a first principle model building on known physical relations was needed. Due to many different stakeholders in the project this was also seen as an aid to facilitate mutual understanding. This choice had large implications with regards to choice of methods and tools, accuracy, computational performance and validation, where the specific challenges encountered are presented in the following sections.
To put things in perspective, the International Renewable Energy Agency (IREA) categorizes power grid models using five different hierarchical levels [23], depending on time resolution, detail and width of scope. The levels are originally aimed at electrical power grids but can be easily adapted to the district heating and cooling context. A summary with some minor adaptions is found in Table 1.

Hierarchical level	Time resolution
Planning and design models	Seasons-Years
Economic models	Hours-Seasons
Static grid models	Single point
Dynamic thermal grid models	Minutes-Hours
Dynamic hydraulic and electrical grid models	Milliseconds-Minutes

Table 1: District heating and cooling grid modeling levels, based on IREA power grid modeling levels.

The case study is, using the defined levels, a dynamic grid model. The experiences drawn from the case study relates mainly to this particular level of modeling, whereas other levels are touched more briefly. The simulator was validated by replicating real life scenarios, where the main use was exploring the use cases by running alternative production and demand control strategies. Modelica was used as the model language, with industrial process components such as pumps and valves provided by commercial simulation libraries.

Three main data sources were used for the models:

1. Models based on Geographic Information System (GIS) data
2. Models based on Piping and Instrumentation (P&I) diagrams and design data
3. Models based on historical measurement data (data driven models)

The piping of the thermal grid was automatically generated from GIS data, whereas production units and pumping stations were manually modeled and configured from P&I diagrams and data. Data driven models for heat load of consumers were generated from historical data. The GIS data of the DHC grid of Luleå spans over > 9000 consumers and > 22000 pipes.

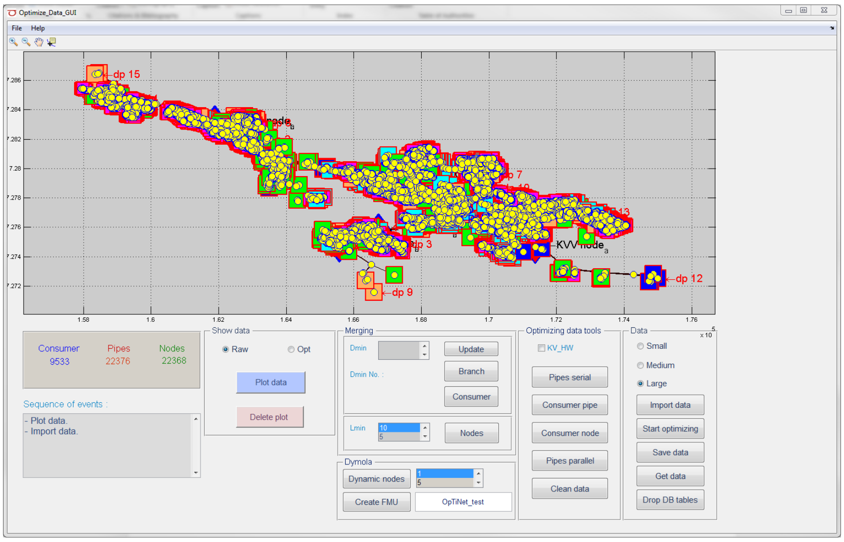

Figure 1. The graphical user interface made using MATLAB.

To enhance the computational performance a topological optimization, known as aggregation, of the grid was performed based on the so called German method described in [24]. The complete topological optimization procedure for the case study consisted of a pre-processing by pruning of erroneous data such as empty nodes or singular pipes, combined with several aggregation steps of merging nearby nodes and consumers, merging serial pipes, and merging of branches. Notably, this part of the case study consumed a large portion of the development resources.

To control the preprocessing and aggregation process a graphical user interface (GUI) in MATLAB was developed, as seen in Figure 1. In the GUI the thermal grid is represented as a network plot where the effect of the preprocessing is visualized. With the topological optimization steps and preprocessing described above, the full Luleå grid consisting of 44752 pipes and 9533 consumers was aggregated down to 3149 pipes and 494 customers before simulation. The total number of simulated components was reduced by around 90%. After optimization the full city scale grid could be simulated on a Core i7 Gen 5 laptop computer at around 2-3 times real time speed.

Examples of the automatically generated grid can be seen in Figure 2, and an example of a production unit can be seen in Figure 3.

The buildings were clustered into seven building categories by size and type of building, validated by measurements for each building category, for simulation of the consumer heat load. Due to the large amount of buildings and lack of measurements it was deemed unfeasible to model each building separately.

The manual and automatic control of e.g the power plant, pump stations and feed forward supply temperature was replicated from available diagrams and measurements. As an example, the pump control for the pump station consists mainly of safety and regulation. The safety part ensures that the pump operational pressures do not violate the limits. The control system ensures that the pressure before the pump will not become below a certain limit and the pressure after the pump will not be higher than a threshold limit. This is performed through the upper two PID controller shown in Figure 4. Also, the safety part will switch off the pump if the speed reaches the lowest allowed speed. The tracking of optimal differential pressure of a selected critical point in the grid is performed by the regulation part.

To highlight some of the challenges encountered during the validation process, a period of 10 days in January exhibiting an outdoor temperature drop from -5°C to -30° and a rebound to -15°C, is used. Large temperature changes during winter, when the space heating demand is high, can be seen as a worst case scenario with regards to model validation,

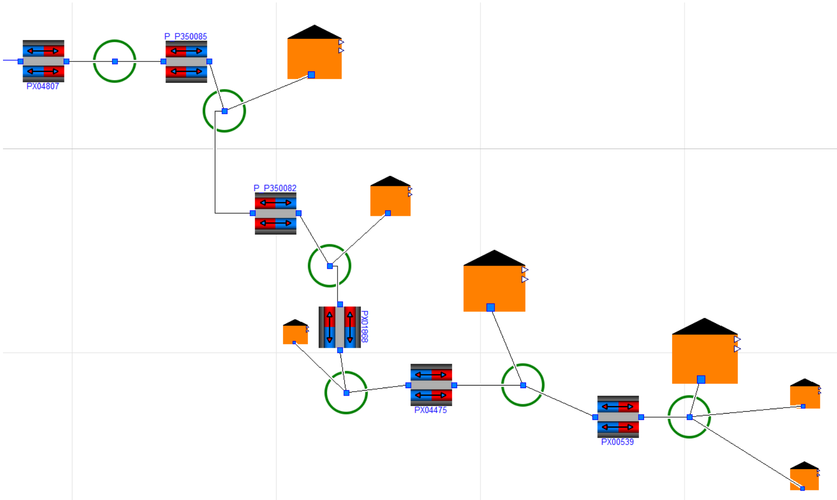

Figure 2. Graphical view of a a Dymola model, featuring a branch of the district heating grid. The model is automatically generated from GIS data, including district heating pipes, nodes and consumers, where the size of the consumer reflects the annual heat load.

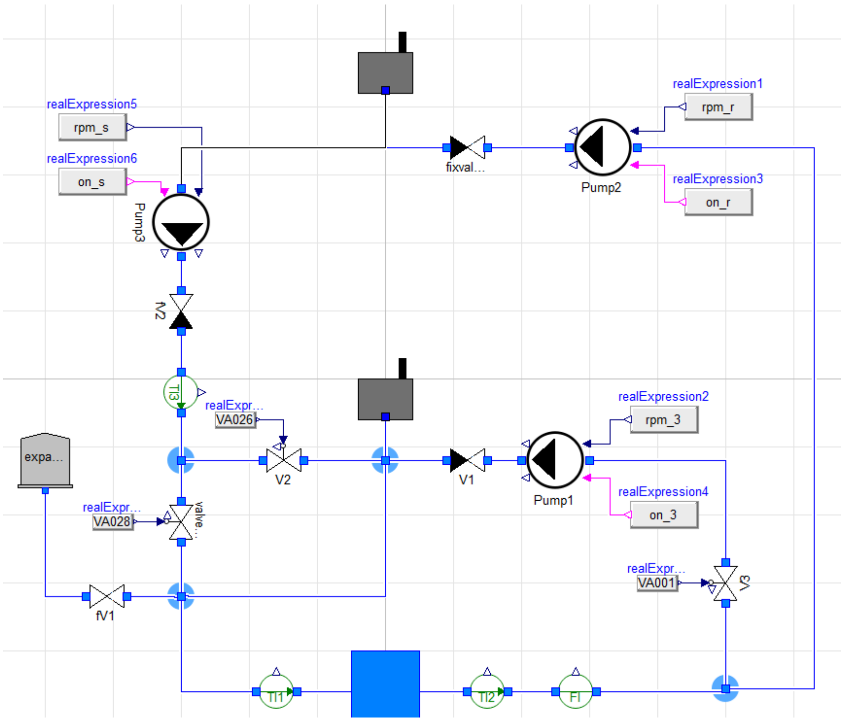

Figure 3. Graphical view of Dymola model of a production unit. The model is manually modeled from P&I diagram and includes components such as pumps, valves and boilers.

exhibiting dynamic behavior of space heating demand and possibly exciting unmodeled behavior at the production side. Notably, due to the limited computational performance simulating more than a 10 calendar days was impractical.
The validation process was based on measurements from the Luleå district heating network. The validation example is focused on the required generated power, collected from time series from the plant data acquisition system. The total power equals the power supplied to the grid from the main combined heating and power plant, plus auxiliary energy units that are sometimes used during the winter months. The inputs to the simulation were the outdoor temperature and time, that are used in the consumer simulation. In Figure 5 the outdoor temperature, the actual total power, and the simulated total power is shown.
As apparent from the figure, for long periods of time there is a good correspondence between measured and simulated power, whereas for other time periods the deviation can be quite large. This raises several important issues, such as

1. What is the needed fidelity for the use case?

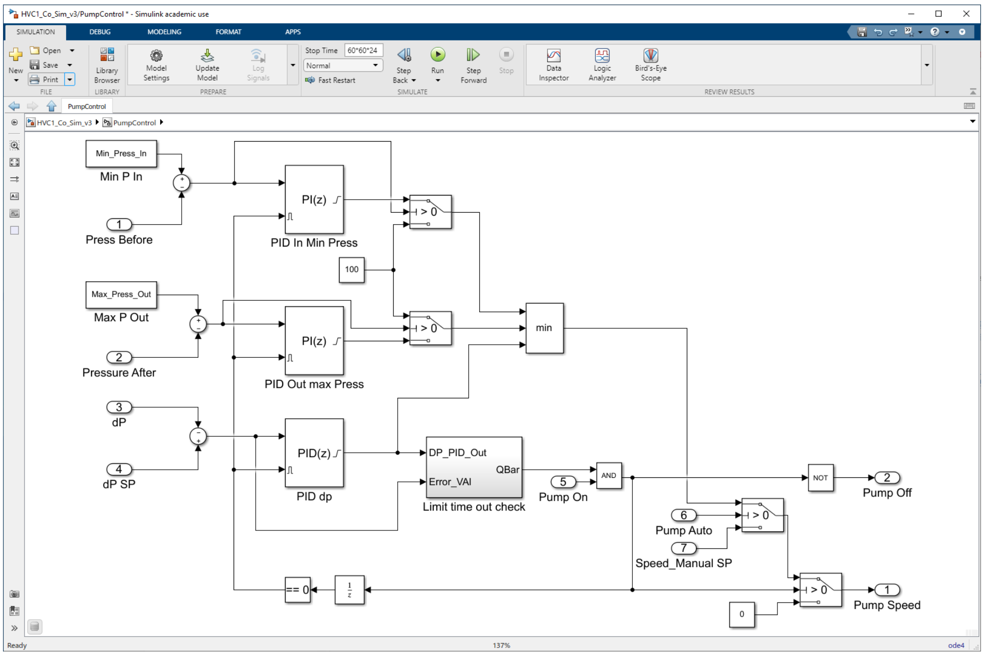

Figure 4. Automatic control structure for pump station in Simulink, recreated from diagrams.

2. What is a good metric to evaluate the accuracy?
3. How can we account for human behavior such as manual control of production units?
4. How can we ensure that the model is up to date with the real process?

These questions do not have simple answers and largely depend on the use-case, which means that the needed fidelity and the used metrics have to be defined in relation to the use-case. It is directly related to the model validation and model update. In section 5, the validation and update aspects are discussed and which methods can be employed. For this particular case it is hypothesized that the deviation stems mainly from the building models being too coarsely modeled, as not all buildings have measurements available for data driven modeling or grey-box modeling, or are only part of an aggregated building set. Thus, identifying the root cause of such a deviation is non-trivial – especially since there are relatively few measurements available in the grid.
The following sections concludes the experiences from modeling and simulation of the Luleå grid, including discussion and proposed research directions with regards to the challenges encountered during the process.

3. Modeling and simulation

For any simulation project there are several important decisions regarding modeling and simulation that needs to be made. Here, the main choices are presented along with experiences, appropriate references and proposed research directions.

3.1. Co-simulation

The general approach to modelling and simulation of large scale systems can be distinguished between monolithic and co- simulation approaches [25]. In a monolithic simulation the entire system is modelled and simulated in a single tool, where as in the co-simulaton approach separate tools for the respective subsystems are coupled together. The proceedings in co-simulation, mostly using the Functional Mockup Interface (FMI) standard [26], has greatly increased the capability of using separate tools for interconnecting models with each other and external tools.
For the case study, the grid model was compiled as a so called Functional Mockup Unit (FMU) according to the FMI standard and used seamlessly in conjunction with automatic control and user behavior simulation in MATLAB. This approach was considered essential for the project due to many stakeholders with different backgrounds and areas of expertise. Integration of components was mostly straight forward, but some care needs to be taken - especially with regards to strongly physically coupled components. For the case study these were avoided by compiling strongly physically coupled components, such as the district heating grid, to a single FMU. Otherwise, methods such as Transmission Line Modelling [27] (TLM) might need to be used.

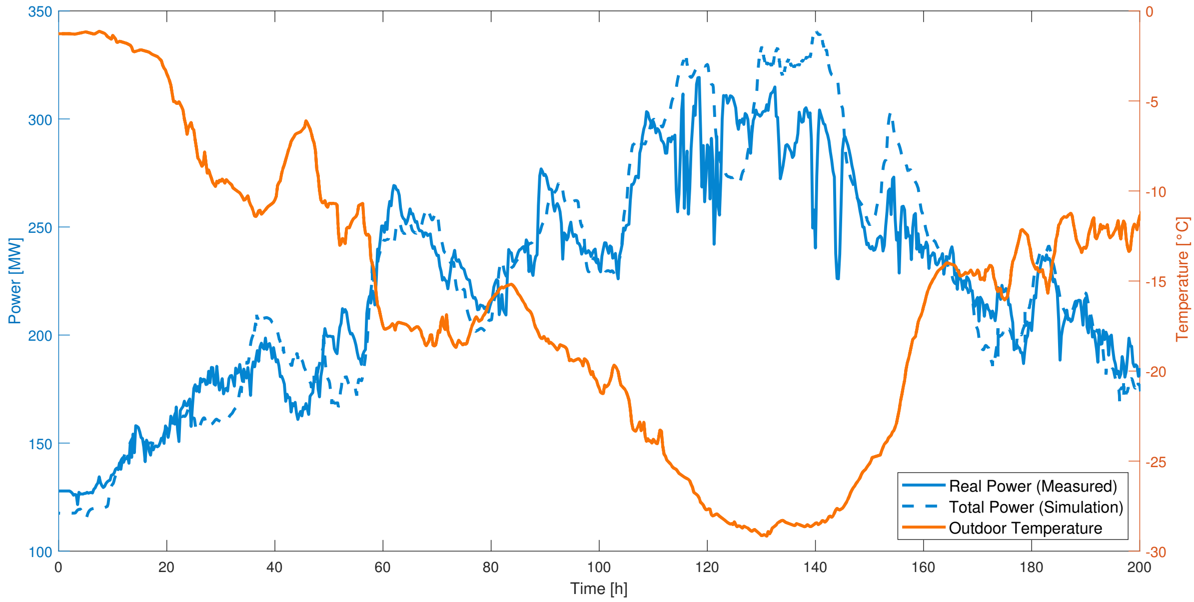

Figure 5. Simulation of the Luleå grid over 10 days in January for a temperature scenario going from -5°C to -30°C and return in the end to -15°C.

The cost of multiple software licenses provided a large hurdle with regards to prolonged use of the simulator outside of academia. Novel business models might be needed to deal with this issue when co-simulation gets a wider adoption.

3.2. Physical or data driven models

Recently data driven machine learning (ML) models such as Artificial Neural Networks (ANN) has gained a lot of popularity and attention. With an application to district heating most machine learning models have been used for forecasting of heat demand, e.g [28]. For simulation and prediction of complex large scale systems such a district heating and cooling network there are several limitations of the most popular machine learning approaches that needs to be addressed to make the models fit for purpose, such as the interpretability of results, how to train a model for scenarios or designs that have not yet been realized, and how persistent excitation properties can be guaranteed for proper identification of the system. A lack of measurements in the grid, as in the case study, will also limit the feasibility of a data driven approach.
A middle ground is to use so called gray box models, where a data driven model can be used to complement a physics based model. Yet another interesting option is to use the physics based model as a reference to train a data driven model, for cases where the data driven model has desirable properties such as propagation of uncertainties or fast execution time [29]. Needless to say, this requires that the physics based model is in place and correct in the first place.
For the case study, a physics based grid model was used. There were few measurements available in the grid, and therefore scarce data available, while the physics of water flow is well studied. The model was also used as an aid to augment the understanding of the physical process. On the consumer side, a mix of physics based, gray box and data driven models was used.
To summarize, the data driven approach provides interesting methods that are often used e.g for heat load prediction, but to the authors knowledge there is no feasible way to model a whole district heating or cooling grid without explicitly using the known physics.

3.3. Acausal and causal modelling

Another important choice of modeling paradigms is between acausal and causal modelling. For causal modelling, such as e.g Simulink [30], there is always a direct causality so that the models are functions with predefined outputs and inputs. For acausal modeling however, there are also *relations*, such as the relation between pressure drop and flow rate in a pipe. Equation based models are expressed in a way that is relatively easily interpretable for domain experts and engineers. Acausal and causal modeling for district heating simulation are thoroughly described and compared in [25].

For the case study, using acausal first principle methods was considered crucial by the participants, providing a common ground for discussions and interoperability of tools. By using acausal equation based modeling, reusability, adaptability and extendability of models is increased compared to causal modeling of dynamical systems.
It is the authors belief that equation based acausal modelling will continue to play an important role in the world of district heating and cooling simulation. There is however times when a causal model is a better choice, such as for the control system, being causal in its nature, or when high quality causal models are readily available for some parts of a system. Notably, combining acausal and causal models from different modeling tools is enabled by a co-simulation approach.

3.4. District heating simulation tools

The Modelica model language is widely used within both industry and the scientific community for modeling of district heating and cooling networks. Other non domain specific tools such as MATLAB/Simulink [30] can also be used for district heating simulations, but are limited to causal modelling. Using Julia [31] for simulation has recently gained popularity due to its performance focused approach, where Modia [32] provides a Modelica-like domain specific extension of Julia for modeling and simulation of physical systems, although in an early phase of development. The tool IDA ICE [33] has also been used for district heating simulation with better scalability performance than Modelica and Simulink for the presented use case in [34], but is lacking support for FMI. A comparison of tools can be found in [25].
There are also several domain specific tools for district heating simulation, where a comprehensive overview of available simulation tools within district heating, and their features and limitations, can be found in [35] and [36]. Tools such as Termis [37], PSS SINCAL [38], TRNSYS [39] and Netsim [40] are widely used for simulation of DHC networks. Most available domain specific tools are at the time of writing either (i) static, i.e. do not provide a representation of the dynamic behaviour of the DHC system (ii) specialized for a limited amount of use cases or (iii) do not allow for co-simulation/interfacing with other software.
For the case study, the choice of the Modelica model language was motivated by co-simulation capabilities and well established and validated model libraries. While Modelica has been the go-to language for modelling of district heating and cooling networks for some time, the engineer and researcher of tomorrow will have a wider array of interesting choices.
It is often mentioned that fully dynamic simulations are needed for simulation of 4GDH systems, with a larger proportion of renewable and highly fluctuating energy sources [35]. However this and other accuracy and fidelity related questions should not be assumed, but chosen in accordance to the project requirements – static models might well be appropriate in many cases. Comparisons between static and dynamic models for different scenarios, and time and spatial resolutions, would provide a valuable contribution to the scientific community.

3.5. Simulation models

Components such as pipes, pumps and valves are well represented in commercial and open source industrial simulation libraries. While the equations describing these components are well known and verified it should be noted that oversimplification of e.g valve or pump characteristics can have a profound effect on the accuracy of the simulation. For the case study the accuracy of the models was not considered as a limiting factor, instead the computational performance of the simulation was experienced as the major bottleneck.
Research with regards to individual simulation models for use in district heating simulation has been mainly focused on efficient and accurate pipe models, with examples in [41,42]. The pipe is a crucial model in fully dynamic district heating grid simulations, where the long pipe lengths require a spatial distribution, and as a consequence model improvements resulting in increased computational performance or accuracy are highly important for the overall simulation. A comparison of different pipe models and their respective accuracy compared to actual measurements can be found in [43].
For the case study a commercial model library, providing validated models, was used. While this provides convenience, there is also a trade-off between how general or specific the model is with regards to the use case. The scope of simulating a district heating and cooling system is relatively narrow compared to that of a general purpose process industrial model library, and using more specialized models might yield better performance at the cost of increased development time.
It is the authors experience that the accuracy demands need to be carefully investigated with regards to the use cases, with model libraries chosen as a result of the imposed demands.

3.6. Simulation of heat consumption and production

The simulation of heat load consumption and production, including the simulation of produced heat from fluctuating sources that can depend on a multitude of different factors such as wind speed or server utilization, are important for realistic simulation results. There are many published methods for heat load prediction that can be employed for simulation such as [44,45]. Since the patterns are subject to social behavior, individual buildings can show erratic patterns that are hard to predict. Furthermore, specific consumers such as industrial plants are not always possible to predict from known data.

In the case study, both consumers utilizing first principle and data driven methods were used, using seven separate categories of consumers. There was however a significant scaling problem - while it might be possible to accurately predict the heat load of a single building it is challenging to scale up to more than 9000 consumers. Based on this issue the consumer were categorized into seven different types depending on size and type of building.

A less researched area is how to accurately model production units affected by unknown control and safety structures and manual operation. How e.g operators choose to start peak load boilers can have a profound effect on the grid dynamics, but information about these procedures might not be available to the digital twin. While not as straight forward as heat load prediction, research in this direction might provide valuable insights.

3.7. Automatic model generation

Historically most modeling efforts have involved manual efforts of replicating the physical reality from data and diagrams. This quickly becomes inefficient and error prone. The acquisition of relevant data can be a tedious process in itself, and often requires a significant effort of preprocessing or converting the data in order to make it suitable for parameterization the simulation models.

There exists several different formats for the data depending on the domain. Automatic model generation from GIS, as in the case study, and BIM data has been covered in several articles [46–48], with an extension to also generate models from CAD diagrams in [16]. A promising approach, e.g used for forecasting of heating and cooling demands [49], is using CityGML: 3D city models. Native CityGML lacks the representation of energy relevant building parameters [49]. However, CityGML supports specific extensions which are called Application Domain Extension (ADE)[50] that has been applied in various studies to calculate the energy demand on different scales [51].

Despite being an active research area, and that the feasibility of automatic modeling has been shown, the lack of common standards make most solutions specific for the use case. Promising results within standardization of model specification are shown using the metamodel concept such as SysML [52] and AutomationML [53]. In the general case the choice of data format is not a choice for the modeling engineer or researcher, but needs to be dealt with already at the planning and management stage.

Regardless of the data source it can usually be assumed that not all relevant design data can be acquired. This raises an important question – how can the validity of a digital twin be ensured without complete underlying data? This process is called *data enrichment* and is discussed for building models e.g in [54,55]. It should be noted that the methods are dependent on standardized data, might require project specific adaptions, and that there are no model-agnostic answers to the question.

The case study used GIS data for automatic generation of the grid and consumers, whereas production units were modeled manually. It was experienced from the case study as well as other projects that data acquisition and preprocessing of data consumes a large amount of time where the results can seldom be reused. It is considered crucial for future usability and effectiveness with further research and industry adoption of standards, but also sharing of code and algorithms within the scientific community.

3.8. Topological optimization

Before the thermal grid model can be generated the topology is usually optimized for the proposed use case, with regards to the resolution of the grid, as described previously for the case study. This process, called aggregation, of pipes or consumers in the district heating grid also has a profound impact on performance [24], and after a certain level also on the accuracy. The most popular methods for aggregation are the so called Danish and German method respectively. A comparison of both methods and a discussion of potentials and limitations of aggregation methods on 4GDH systems ca be found in [56]. The methods are focused mainly on static simulations, and in the Danish case there is no support for multiple production units. It is also not straight forward to derive any objective properties with regards to the spatial or temporal resolution from the aggregation process for the presented methods.

For the case study the algorithm was loosely based on the German method, where a significant amount of time was consumed for tweaking the algorithm for the use cases and finding a feasible trade-off between performance and accuracy.

It is suggested by the authors that aggregation methods are further researched with respect to the validity for 4GDH networks with fully dynamic simulation and multiple production units. Effective numerical methods can to some extent mitigate the need for aggregation methods from a computational performance standpoint.

3.9. Fidelity

The fidelity, such as the time scales of interest and the spatial resolution, needed for the use case has large implications on the requirements on the model and simulation related choices. Individual components are usually not specified with regards to fidelity, but rather by what features or simplifications that should be included. Relating these parameters and settings to e.g time scales of interest can be challenging. With appropriate planning and requirement specification these problems can be mitigated for many projects. However, this requires extra work and possibly different simulators for different part of the project.
For the case study it was apparent the different stakeholders of the projects had different and sometimes contradictory requirements. On a substation level for example, dynamics with a time resolution of seconds can be of interest, while the spatial resolution of the grids is relatively unimportant. However, the degrade in computational performance caused by the stiffness of modelling fast dynamics can render the simulator useless for simulation scenarios ranging over long time spans.
Ideally, the same simulator could be used for different phases and stakeholders of the projects. This would require that the model can be automatically adapted to e.g the required spatial and time step resolution. For linear systems different model reduction techniques are well developed [57], where e.g fast dynamics can automatically be reduced to static relationships. Model reduction is far less researched for differential algebraic systems, where the survey in [58] can serve for an introduction. To the authors knowledge there are no implementations for commonly used modelling tools, and it is perceived that more research in this direction would be a valuable contribution.

4. Computational performance

The largest obstacle with regards to usability in the case study was the computational performance. With scenarios possibly spanning over weeks, months or even years, several orders of magnitude of increased simulation performance would have been desirable. Debugging models with regards to computational performance is often a tedious task that requires extensive knowledge from the developer.
As an example to highlight the volatility of computational performance, a grid model with 84 consumers was generated, running a simulation of 10000s within Dymola using the variable step size solver LSODAR. The inputs to the model were the heat load and return temperature of the consumers, varying slowly over time. The consumer model used a simplified approach where the mass flow rate is directly calculated from the inputs.
The first example uses continuous input signals generated within the simulation model. The second examples uses the same signals as in the first example, but sampled with a sampling time of 1s, to emulate how input signals are often provided to the model. The third example is similar to the second example, except that for *one* of the consumers the power input signal is filtered with a first order filter with the time constant $\tau = 3s$, emulating how components with faster dynamics could be introduced to the system.
The results of the simulations are provided in table 2. For the modelling expert or someone well versed in numerical computing this should not come off as a surprise – the second example limits the maximum step size for the variable step size solver, the third example makes the system stiff, causing a severe degradation in computational performance. For the engineer or new practitioner however, this might come off as unpleasant news when small changes (from an engineering perspective) cause a large degrade in performance.

Simulation case	CPU time
Continuous inputs	11.7 seconds
Sampled inputs	41.3 seconds
Sampled inputs and fast dynamics	2.36e+03 seconds

Table 2: Consumed CPU time for simulation of 10000s using the solver LSODAR for three different cases.

4.1. Numerical methods

The nature of problem that a district heating or cooling grid poses several numerical challenges. Fluid networks are non-linear, and the problem is stiff due to the difference in the time constants between the pressure and temperature dynamics, and faster dynamics that might appear on consumer or production level. The model is hard to parallelize due

to the strongly coupled nature of the system. Usually there are also components that are discrete such as the simulation of the distributed control system (DCS).
The choice of solvers is usually limited by the choice of tool for modelling. For the Modelica language using sparse solvers [59], or more efficient compilers as proposed in [60] have been proposed. Using DAE solvers rather than ODE solvers have also been showing large improvements for power grid models [61]. Yet another promising approach is using Quantized State System Solvers (QSS) [62]. The stiffness of the problem can be addressed by using multirate solvers, where a summary of state of the art solvers and tools, including multirate techniques, for the Modelica language has been published in [63]. However, as the article points out, while many of these concepts are promising even with current state of the art tools and solvers the performance is very limited as the model size grows to even moderately large.
Despite promising concepts, from an engineering perspective an integrated approach is needed where all major problems causing numerical problems are addressed to a point where accuracy, robustness and simulation speed is *good enough* for the employed tools and use cases. Using a co-simulation approach provides the possibility for using state of the art solvers and methods from different tools - provided that they support co-simulation and that the co-simulation itself does not introduce other issues. Following up on promising concepts it seems that the step from concept to deployment is large, likely due to the diversity and complex nature of hybrid DAE systems.
For the case study a classic fixed step explicit order 4 Runge-Kutta method as implemented in Dymola was eventually used. Despite many theoretical advantages of variable step size methods, in practice it turned out that the overhead, and in some cases unpredictable behavior, of these methods was too large to provide an acceptable computational performance.
From the case study as well as other projects, and the body of scientific work in this area, it is perceived that a large part of the work from previous projects is not reused, so that the wheel is reinvented again and again. A reference model that could be used for benchmarking numerical methods, aggregation methods and so on, could be one way forward towards better cooperation between projects, and in the longer run towards better performance.

5. Validation

A crucial step in modeling and model calibration is the validation of the resulting model. As stated in literature like e.g. [64], model validation is the process of assessing the eligibility of a model and to what degree it represents the true model for a specific use. The validation data may not have been used in the modeling or the calibration and is in that sense new data for the model.

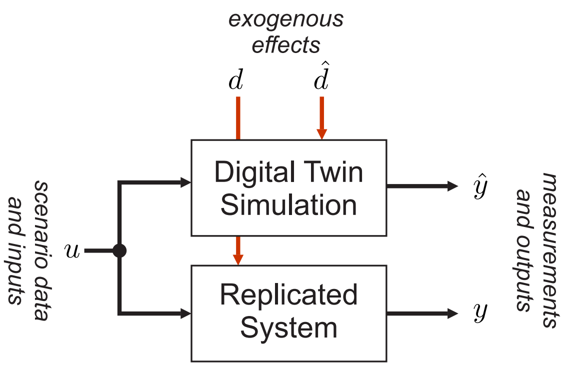

Figure 6. Basic setting for validation and update of a model

The basic setting for model validation is depicted in Fig. 6, where the estimate of the output model can be used to assess the validity of the model. Using a metric on the deviation between the model or deriving a model error model [65] not only provides and understanding of the validity but also a means to characterize the root cause for deviation and to compare different models with each other.
Reflecting back to the case study, validation and model calibration showed to be a time consuming task. It was often experienced that there was a discrepancy between what the engineers considered important, and the accuracy metrics. The accuracy of a simulation is often quantified by metrics such as Root Mean Squared Error (RMSE) and Mean Absolute Percentage Error (MAPE), measuring the deviation of the simulated value compared to the measured value at fixed time instances, namely $y - \hat{y}$. To reach a sufficiently high accuracy for a complex system can in many cases be a difficult task. There exists a multitude of exogenous inputs d and design parameters that affect the dynamic behavior of a district heating network, that can only in part be acquired from data or modeled, denoted as $\hat{d}$. Examples are detailed pipe

geometries, soil temperatures around the piping, consumer behavior and operator and automatic control of production units.
An important question raised in [66] is whether a higher accuracy results in a more useful simulator. Higher accuracy also goes hand-in-hand with higher complexity and usually comes with a loss of computational performance, or with additional parameters that require calibration, making the simulator *less* useful from an engineering perspective. Needed accuracy is determined by the purpose or the use-case and from a scientific perspective the law of parsimony should be applied meaning the simplest model for the intended use is also the right one, provided it gives the same answers as a model of higher accuracy and complexity
Accuracy metrics such as RMSE does not take into account dynamic behavior, so that moderately delayed fast dynamics might be considered by the metric as a large deviation. There exists approaches to mitigate these shortcomings such as nonlinear alignment techniques (also referred to as dynamic time warping) [67], although not widely adopted by the scientific community. Furthermore, discrete events for cases like "when A happens, B should happen within a specified time frame" can as well not be captured by just measuring the deviation between the measurement and the simulation. Using other distance measures, such as the Levenshtein distance [68] that can be used to evaluate the order of which events occur, is one option. In the end, the lack of widespread adoption is a problem in itself with using any metric beyond the most common ones. Even when there are methods that are valid for individual components, the question of how to evaluate a complex model such as a district heating grid is largely unanswered.
Another validation related issue is assessment of the need to update the model. The decision on the update can be based on the outcome from a simulation run in relation to the system it replicates, as shown in Fig. 6. There the observations y and $\hat{y}$ can be used to establish a metrics for the validity of the model, like e.g. the root mean squares of $y - \hat{y}$.
While this approach seems straight forward there are a number of factors that drive the deviation $y - \hat{y}$:

- Unknown exogenous effects:
  A minority of the factors that affect the replicated system can be measured or observed meaning that there is a deviation between d and $\hat{d}$, rendering a deviation between y and $\hat{y}$. While there is often a qualitative understanding of these effects, a quantitative description is usually lacking.
- Modelling errors:
  Any model is only valid to a certain degree of accuracy and is therefore not perfectly replicating the real-life system, again rendering a deviation between y and $\hat{y}$.
- Wear and tear:
  Any component operating in a real-life situation will be affected by wear and tear over its life cycle, leading to maintenance action and eventual component replacement. Such degradation phenomena renders similar effects like modelling errors, but occurs gradually.
- Undocumented realisations:
  In line with the modelling errors are undocumented realisations, which means that the real-life system deviates in realisation from its documented specification. Such effects are already present when an initial validation of a model is performed, but will nevertheless affect the monitoring performance.
- Unreported system changes:
  A system update is clearly necessary whenever a change in the real-life system occurs, like e.g. replacement of components. The consequence is similar to the modelling errors.

Referring back to Fig. 5, it can be seen that the overall behaviour on the long term is well replicated but in several instances there are quite large deviations. Applying a typical measure for the fit like the normalized root mean squares error does indicate a poor fit value, less than 90%, as expected. Nevertheless, from an engineering perspective on designing a control strategy for the supply of heat to the grid, the accuracy has been deemed sufficient by practitioners in the field. Some of the reasons for the deviations are model errors in the building models, assuming that individual buildings for a certain category have the same heat load pattern, and assuming a disturbances-free scenario. It is well known that individual buildings heat load pattern do exhibit a stochastic behavior on the short term.
Consequently, a monitoring procedure needs to be resilient to these factors and render an appropriate decision on the update needs. An additional challenge in most actual district heating networks is the fact that there are few measurements available from the grid, often restricted to a handful of temperature and pressure sensors. While there is a tendency in the industry in general is to include more sensors, in line with the vision of Industry 4.0 and the smart sensors concept [69], the current lack of measurements makes model calibration, validation and update a difficult task.
Further complicating the calibration and update is the composition of the real-life system which is replicated. As seen in the principle sketch Fig. 7, the real-life system could be composed of physical system components which are well understood and models are available (white boxes), physical component where partial or no knowledge of the behaviour

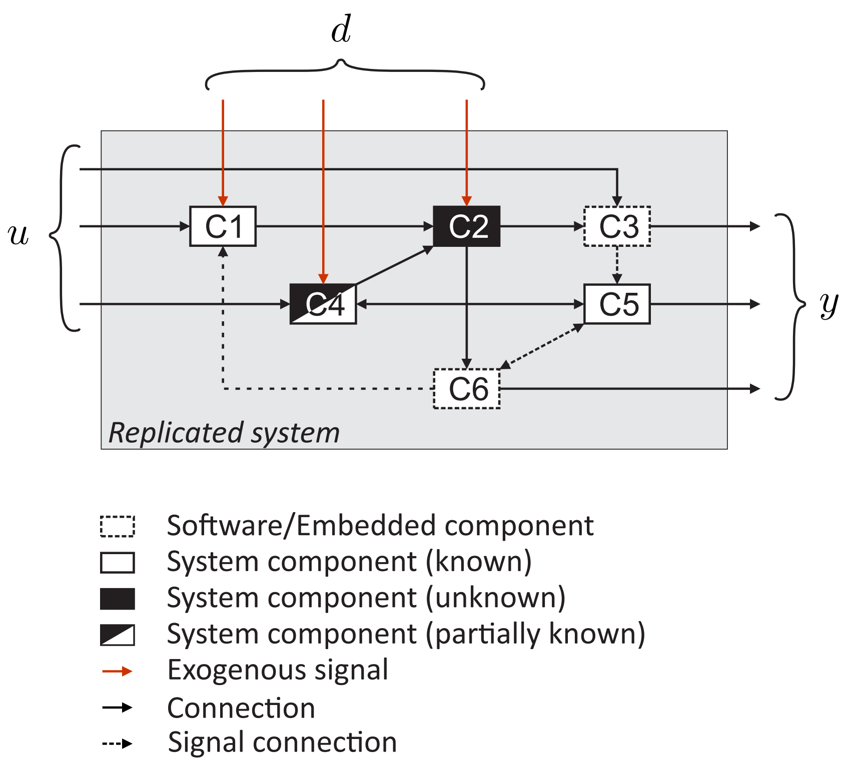

Figure 7. Principle sketch of the composition of the replicated system consisting of both physical and cyber components fully interconnected. Each connection can contain a multitude of physical or signal interconnections that are potentially directed.

is available (gray and black boxes). Naturally, all those will interact and also be connected to software components like a control system. Already when performing model calibration the interconnection between components play a role in the quality of the calibration if it is primarily based on measurement data. Similarly, the interconnections need to be considered in the model update.

Thus, to be able to update the models with sufficient accuracy, the measurements need to be monitored, and informative data needs to be used to update the model. Data from faulty sensors, equipment under maintenance, and un-modeled modes of operation need to be discarded – a non-trivial data analysis task. Furthermore there are few methods for updating or calibrating DAE models from known data. It can be assumed that without model updates the model accuracy will deteriorate with time due to e.g equipment wear or changes, or new operating procedures. Promising work in this area, using aforementioned AutomationML and FMI, has been conducted in [70].

Methods for model calibration are well established but are often focused on methods for a limited set of specified models (e.g system identification for ARX and state space models) and not suitable for calibration of models on DAE form. Some promising steps has been undertaken by e.g [71] and [72] on model calibration for DAE models. But there is still to little known about the validity of these methods, and possibly research on novel methods, for dynamic model calibration in district heating grids.

While model update can be understood as a model calibration, there are preceding steps before a calibration or better said re-calibration can take place

- The need for a model update has to be determined. Similarly to model validation it is important to understand if the deviation between the models and real-life system is caused by a deprecation of the model. Thus, the current model need to be monitored continuously during the operation and in relation to the real-life system.
- When it is clear that a model update is necessary, the components that need updating have to be identified and located within the large scale system. Clearly, multiple components may need updating simultaneously.
- After identifying the component for updating it need to be determined how an update can occur. The update of parameters in a given model structure is most likely the most straightforward task where system identification or machine learning principles can be used. If the update would require structural changes a pure data driven approach might not be possible and a re-generation of the component including calibration might be required.

Essentially, the model update requires a number of steps where there are a several methodologies available that could be used in combination with each other. Each of these methods are depending on user selections that affect the performance

of the methods. As soon as those methods need to be used in a tool chain the effects on each other need to be understood and quantified. In this respect and as far as the authors are aware, there are no studies that investigate the aggregation of established methods into tool chains automating the model update.
Clearly, there is a need for research in this direction and to propose automated methodologies and tool chains which reliably monitor and update models.

6. The digital twin

The concept of a digital twin is attributed to Michael Grieves in 2003 [73] and was popularized by the inclusion in NASA's Modeling, Simulation, Information Technology & Processing Roadmap [74]. There, the following definition is provided

> "A Digital Twin is an integrated multiphysics, multiscale simulation of a vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its corresponding flying twin. The Digital Twin is ultra-realistic and may consider one or more important and interdependent vehicle systems, including propulsion/energy storage, avionics, life support, vehicle structure, thermal management/TPS, etc."

While this is a useful vision, a more applicable approach for an industrial process is described in [75] comprising the following properties of a digital twin

1. The Digital Twin is the linked collection of the relevant digital artefacts including engineering data, operation data and behaviour descriptions via several simulation models. The simulation models making-up the Digital Twin are specific for their intended use and apply the suitable fidelity for the problem to be solved.
2. The Digital Twin evolves along with the real system along the whole life cycle and integrates the currently available knowledge about it.
3. The Digital Twin is not only used to describe the behaviour but also to derive solutions relevant for the real system, i.e. it provides functionalities for assist systems to optimize operation and service. Thus, the Digital Twin extends the concept of model-based systems engineering (MBSE) from engineering and manufacturing to the operation and service phases.

While not strictly required to fulfill this definition, enabling features to achieve the digital twin are that the model can be automatically *generated* from data, and that the model can be automatically *updated* from data. The evolution of the digital twin can be seen as a way of addressing the weaknesses of many simulators, where the simulator provides a useful tool at a certain stage of a project, but remains underutilized for earlier and later stages. In [76] it is emphasized how data-driven methods used in conjunction with first-principle model techniques can enhance models to adapt to changing dynamics and environmental characteristics. It is also concluded that error quantification and plug and play-functionality in a modular approach are open research subjects that are fundamental for the future of complex systems models.
Based on the definition above we can distinguish three levels of the digital twin: (i) the digital twin that is a snapshot of the real process at a certain stage, (ii) the digital twin that can be regenerated from underlying data when the underlying data changes, and (iii) the digital twin that is continuously updated and regenerated along with the process as it evolves. The main components of the digital twin, including all previously defined levels are

1. Automatic model generation
2. Models of the components, including control and user behavior
3. Numerical methods for simulation
4. Model update functionality

Concerning the current case-study, the simulator fulfills the properties of a digital twin having a focus on analysis and optimization of both control and operation. While the simulator can be understood as one model, there are multiple simulation models for production, distribution and consumer-side present and fully integrated to reflect the complete system behaviour. The models are derived using automated model generation and the models are reflecting all components including the control system, user behaviour and behaviour of the human operators. The implementation of the simulator using FMUs enables the integration of models from different modeling paradigms and simulation of different operating scenario, optimization schemes and climatic conditions. Such a digital twin has the purpose for so-called what-if analysis with a high level of flexibility in terms of the analyzed scenarios.
A lacking functionality is the integrated model update and the ability of the digital twin to track the real-life system properly in parallel during real-time operation. Further, the fidelity of the models varies in relation to the scenarios that can be analysed. To give an example, analysis of the energy used for heating on the overall system level is well replicated by the digital twin, while the energy used for heating at a specific individual building might not.

In order to reach a full city scale digital twin with all the above mentioned properties, several of the identified challenges in the paper still need to be addressed.

7. Conclusions

In this article, experiences from modeling and simulation of district heating and cooling grids are presented, including a case study with practical examples. Research gaps and proposed relevant research directions are presented, drawing from the experiences.
It is shown how the concept of a digital twin is relates to simulation and modeling in general, and that it in its essence is a way to deal with the challenges and limitations identified in the paper.
It is perceived by the authors that while each individual component will need research and development for a simulator suitable for daily use, or a complete digital twin, the integration of the concepts is an equally important issue. The adoption of standards within industry, tool vendors and academia is considered crucial.
While some of the presented research and suggested research directions are strictly from a district heating and cooling perspective, the main body is applicable to process industrial modeling and simulation in general. It is the authors hope that the growing interest in the digital twin will result in moving the industry forward towards both digital and environmental sustainability.

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