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Article

The potential of simulating energy systems: the Multi Energy Systems Simulator model

Luigi Bottecchia [1,2,†]*, Pietro Lubello [3,†]*, Pietro Zambelli[1], Carlo Carcasci [3] and Lukas Kranzl[2]

1 Institute of Renewable Energy - Eurac Research, Via A.Volta 13/A, 39100 Bozen/Bolzano, Italy
2 Energy Economics Group, Institute of Energy Systems and Electrical Drives - Technische Universität Wien, Gusshausstraße 25-29/370-3 A-1040 Vienna, Austria
3 Department of Industrial Engineering - University of Florence, Via Santa Marta 3, 50139 Firenze, Italy
* Correspondence: luigi.bottecchia@eurac.edu, pietro.lubello@unifi.it
† These authors contributed equally to this work.

Abstract: Energy system modelling is an essential practice to assist a set of heterogeneous stakeholders in the process of defining an effective and efficient energy transition. From the analysis of a set of open source energy system models, it has emerged that most models employ an approach directed at finding the optimal solution for a given set of constraints. On the contrary, a simulation model is a representation of a system that is used to reproduce and understand its behaviour under given conditions, without seeking an optimal solution. Given the lack of simulation models that are also fully open source, in this paper a new open source energy system model is presented. The developed tool, called Multi Energy Systems Simulator (MESS), is a modular, multi-node model that allows to investigate non optimal solutions by simulating the energy system. The model has been built having in mind urban level analyses. However, each node can represent larger regions allowing wider spatial scales to be be represented as well. MESS is capable of performing analysis on systems composed by multiple energy carriers (e.g. electricity, heat, fuels). In this work, the tool's features will be presented by a comparison between MESS itself and an optimization model, in order to analyze and highlight the differences between the two approaches, the potentialities of a simulation tool and possible areas for further development.

Keywords: Energy System Modelling; Energy Optimization; Energy Simulation; Multi Energy Systems Simulator (MESS)

1. Introduction

The decarbonization of the energy sector is one of the major challenges in confronting the climate emergency. In order to meet the Paris Agreement goals [1], the energy system will have to undergo a profound transformation, shifting from being predominantly fossil fuel-based to relying on clean renewable energy sources, while guaranteeing sustainability, fairness and security of supply [2]. In this context, energy system modelling represents a valid support in the process of planning and decision making for the energy transition. Numerous tools have been developed and employed in the last years and are continuously updated to face new emerging challenges and consider innovative technologies being developed. Several works can be found in the literature reviewing trends and existing solutions [3,4].

1.1. Background

One of the main issues in energy system modelling is guaranteeing a high degree of transparency to allow a complete understanding of how models work [3,4]. This can be translated in the need of providing full access to the code and the data used trough an open source approach. Nonetheless, clarifying the boundary conditions and the definitions adopted can substantially improve the clarity of how a certain model works, hence, a brief background is outlined in this subsection.

In the Fifth Assessment Report of the IPCC [5] an energy system is defined as a system comprehending all components related to the production, conversion, delivery and use of energy. Similarly, Jaccard [6] refers to an energy system as the combined processes of acquiring and using energy in a given society or economy.

Building on these two definitions and following also the terminology used by Pfenninger et al. [7], in this work an energy system will be considered as the combination of processes and technologies related to the production, consumption, conversion and transmission of energy in a given society, economy or location. A location can be considered as a site that contains multiple technologies but also other locations. In this way, an energy system is not only seen from a mere technical point of view, but including also the spatial and socio-economic dimensions.

Analysing energy systems often translates in developing models for their investigation. Rosen [8] considers a model as the formalized representation of a natural system with its own rules. Developing this concept further, Keirstead et al. [9] added that, within the energy and engineering fields, the formalization is to be intended in the form of mathematical models and computer codes. Hence, we will here refer to a model as the representation of a system with its own rules through the use of a mathematical formulation.

In the context of energy system modelling, multiple approaches can been considered. One of the main distinctions that can be made is between is between optimization and simulation models. Building on the definition given by Wurbs [10], Lund et al. [11] consider an optimization approach as the one that makes use of a mathematical formulation to find the optimal solution of a given problem. The problem is generally defined by an objective function subject to multiple constraints. Both the objective function and the constraints are dependant on a set of decision variables whose values are set during the optimization process. The objective function can be related to emissions, system costs or other aspects related to the system. On the contrary, both Wurbs and Lund et al. define a simulation model as the representation of a system used to forecast its behaviour under certain given conditions. Both works highlight that simulation models are meant to be used to understand the performance of a certain system under a given set of assumptions. For the purpose of this work, the authors slightly reviewed this definition and considered a simulation model as the representation of a system used to reproduce and understand its behaviour, under given conditions, without looking for an optimal solution. The slight difference stands in the fact that the authors believe that the first purpose of simulation tools should be to reproduce the behaviour of a given system rather than to forecast it. Indeed, forecasting can be thought as a subsequent step, to be performed through scenario analysis or similar approaches. In this regard, the model could be used to evaluate the consequences of a given choice whether it is technical, political or social.

Lastly, the definition of *urban scale* has been considered. Eurostat provides common definitions for the European geographical areas starting from the concept of *degree of urbanisation*. According to this definition, the degree of urbanisation provides a classification for local administrative units (LAUs) obtained from the combination of geographical proximity and population density [12]. The classification is made by considering a raster cell of 1 km^2. LAUs can then be: Cities (densely populated areas), Town and suburbs (intermediate density areas) or Rural areas (thinly populated areas).Urban areas are represented by the first two classes: Cities and Towns and suburbs [13]. At this point, the non-trivial aspect to consider is the integration of the "urban" concept in the energy system definition. Both Keirstead et al. and Alhamwi et al. [9,14] exploited the approach used by Ramaswami et al. [15], called *"geographic-plus"*, which does not only consider the energy flows but also the geopolitical boundaries of a system. Hence, in the current work, and more in general in the context of energy system modelling, an urban scale is considered the resolution incorporating districts and cities, while an urban area is an area with an intermediate or high density of population. In this way, a energy system model

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is considered to be able to perform analysis at urban scale when it has a spatial resolution that goes down to the district level, allowing to consider urban areas composed by small, medium and large cities.

1.2. Models review

Having clarified what simulating an urban energy system means, a review of different models has been conducted. The review focuses on 40 different open source tools, mostly obtained from the Open Energy Modelling (openmod) initiative [16] list. The models have been compared and evaluated based on three main categories: sectors covered by the model, type of model (optimization or simulation) and whether they allow modelling of urban scale systems or not.

Firstly, the 40 starting models were clustered based on the sectors covered. Particular attention was given to models covering both electricity and heat sectors or to models allowing the definition of user-dependent carriers. Out of the 40 models analyzed only 17 met these requirements. In parallel, another subset was defined by considering all the models allowing to model urban scale energy systems.In this case, only 12 models made the cut. The intersection between this two subsets allowed to identify which models satisfy both requirements: operating with multiple sectors, at an urban scale. The list of the resulting models is shown in Table 1. For the complete list of the investigated models, see Table A1 in Appendix A.

Table 1: List of models that allows modelling of multiple sectors and at urban scale.

Model	Sectors	Model Type	Urban Scale
Calliope [7]	User-dependent	Optimization	Y
OMEGAlpes [17]	Electricity, Heat	Optimization	Y
Oemof [18]	El., Heat, Transport	Optimization, Simulation	Y
PyPSA [19]	El., Heat, Transport	Optimization, Simulation	Y
REopt [20]	Electricity, Heat	Optimization	Y
URBS [21]	User-dependent	Optimization	Y
CEA [22]	Electricity, Heat	Optimization, Simulation	Y
Backbone [23]	All	Optimization	Y

Among the remaining models, none performs simulations according to the definition given in Subsection 1.1. In conclusion, despite the possibility to find well-known simulation tools for the analysis of urban energy systems (e.g. EnergyPLAN [24], HOMER Energy [25]), to the authors knowledge, there are no open source simulation tools meeting the criteria aforementioned, suggesting a niche for the development of such models in the field of energy system modelling.

1.3. Aim and structure of the paper

As pointed out by Chang et al. [4], current trends in modelling the energy transition are related to the increase of cross-sectoral synergies, a growing attention to open access and open source publications and the improvement of the temporal resolution. The key challenges identified in modelling energy systems are in line with what was already mentioned by Pfenninger et al. [3]: the openness and accessibility of the models, the integration of different models and the level of engagement between developers and policy/decision-makers.

Considering this context of development and the existing models, the authors decided to develop an open source model, called Multi Energy System Simulator (MESS) [26]. The model aims at giving its contribution in filling the identified gap among the existing models while participating in the effort to overcome the challenges of the energy system modelling sector. Thus, the aim of this paper can be summarized by the following research questions:

1. What is the potential of simulating an energy system rather than optimizing it?
2. How can MESS contribute in tackling the challenges of modelling the energy transition?

The paper is structured in the following way. Section 2 introduces the main characteristics of the developed tool (MESS) going into the details of how it works. In the same section, the rationale behind the comparison between MESS and an existing optimization tool (Calliope [7]) is introduced. Section 3 illustrates the results of such comparison while Section 4 builds on the results of the previous section to discuss them in the lights of the research questions. Finally, Section 5 summarizes the main findings as well as presenting areas of future developments on the topic.

2. Methodology

This section aims first at presenting the model developed and secondly the methodology applied to perform the comparison with an existing optimization tool.

The Multi Energy System Simulator tool (MESS) is a modular, bottom-up, multi-node model that allows to investigate non optimal solutions by simulating the energy system.

In lights of the already mentioned challenges of modelling energy systems ([3,4], MESS was developed with a set of design goals in mind and was deeply inspired by Calliope [7]. This choice was made to try to mitigate the consequences of an additional model in the literature and to improve the interoperability among multiple models. The main design goals in the development of MESS are: *(i)* the model has been built having in mind urban level analyses, while maintaining a certain flexibility in terms of spatial resolution; *(ii)* it should be possible to use the model without the need of coding but just by writing human-readable configuration files; *(iii)* the model should be able to perform analyses on systems composed by multiple energy carriers (e.g., electricity, heat, fuels); *(iv)* the model should have a flexible approach to temporal resolution and timeseries; *(v)* having a free and open source energy system model written in Julia [27].

2.1. How does MESS Work?

In order to use MESS, the user has to set up three configuration files to define the system in analysis and the modelling options. The input files are written in YAML, as to ensure readability and allow the user to intuitively interpret them. Once this step is done it is possible to run the model by using the Julia REPL.

Additionally, MESS offers a library of predefined technologies to be included by the user in the model. Each technology is part of a group of technologies that show similar behaviour in terms of energy fluxes. This categorization has been taken from Calliope and, as in Calliope, the groups are called parents. MESS has six parents: demand, supply, supply_grid, conversion, conversion_plus, storage. A comparison between the parent categories used in Calliope and MESS is given in Table 2.

Table 2: Parent technology groups - Comparison between Calliope and MESS.

Parent	Calliope	MESS	Description
demand	Y	Y	Energy demand for the defined carrier
supply	Y	Y	Supplies energy to a carrier
supply_plus	Y	N	As supply, with additional constraints
supply_grid	N	Y	As supply, energy from national grid
storage	Y	Y	Stores energy
transmission	Y	N	Transmits energy from one location to another
conversion	Y	Y	Converts energy, one carrier to another
conversion_plus	Y	Y	Converts energy, N carriers to M carriers

Demand technologies represent energy sinks. The energy carrier to be considered must be defined and a CSV file detailing the demand for that carrier at each timestep is required. Supply technologies are energy sources. Renewable energy sources as solar photovoltaic or wind turbines are the most evident examples for this parent. The carrier considered and technology-specific parameters should be defined. Different modelling options might be considered for each technology. Supply_grid technologies represent energy sources from distribution grids not modelled in the analysis, as, for example, national distribution grids or district heating grids. The energy carrier of the energy source must be defined in this case as well. Conversion technologies are defined by a single carrier in and a single carrier out (e.g. natural gas-fed boilers), while conversion_plus technologies are defined by multiple energy carriers in and/or out (e.g., combined heat and power technologies). Both categories require the definition of technology-specific parameters. Storage technologies are defined by the same carrier in and out and, depending on the state of charge and the energy balance, might act as energy sink or energy source.

2.1.1. Input files

The general configuration parameters for the simulation are set in a specific file named *model_specs.yaml*. It allows the user to define the name of the model, the timespan and timestep to be used, as well as if the local electricity network is to be solved and the type of solver to be used. The *techs.yaml* file is used to define and set the input parameters of all different technologies that might be included in the model. Each technology is defined by three subsets of parameters: essentials, constraints and monetary, plus the priority index. In the essentials subset, fundamentals parameters are to be declared, as the user-defined technology name, the colour to be used for plotting, the parent and input and/or output carriers. The constraints subset contains the parameters used to set the technical characteristics of the technologies and the ones to be specified are technology dependent. In the monetary category costs related to the technology are to be defined, as CAPEX, OPEX, interest rate etc. The priority parameter is an integer input that sets the priority of each technology i.e., the order in which technologies are to be called by the solver, hence allowing the user to define different ways of solving the model. The *locations.yaml* file describes the nodes composing the network to be studied and which technologies each node hosts. For each technology, additional node specific data can be set, as installed capacity or timeseries files (e.g., demand curves, capacity factor series), or specific parameters can be superscripted on the general ones defined in the *techs.yaml* file. In addition to the configuration files, input files might be needed for demand profiles, non dispatchable power sources generation profiles, energy prices etc.

2.1.2. MESS structure

MESS is divided in four major steps, that are: *(1)* Pre-processor, *(2)* Core, *(3)* Post-processor and *(4)* Plotting.

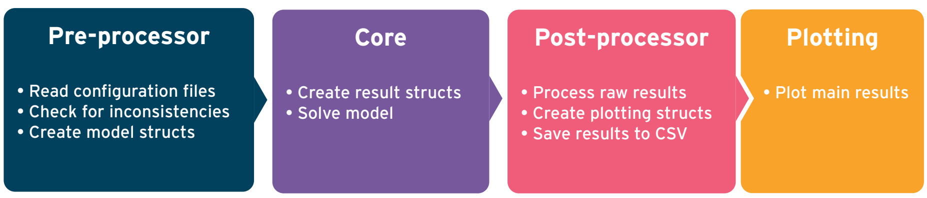

Figure 1. Four steps of MESS.

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Pre-processor

In the pre-processor stage, all the modules required for the execution of the following steps are loaded. This includes loading the exceptions and structures modules. The former module contains all the exceptions that might arise in the program, while the latter all the data structures used. Some of the structures here defined contain the constraints allowed per each category of technology (or, following MESS's and Calliope's terminology, per each parent) as well as the structures that defines the model characteristics. All these information are then combined with the input files in order to create the model structure to be used in the core module.

Core

In the core stage the model is solved. Solving the model is a three-step process. In the first step the single locations are solved at each timestep, in the second step the solutions of each location are considered together and the local network is solved. Finally, in the third step the details of the exchanges with higher level grids (i.e. national grid) are defined. Figure 2 shows a schematic diagram representing the functioning of this phase in MESS.

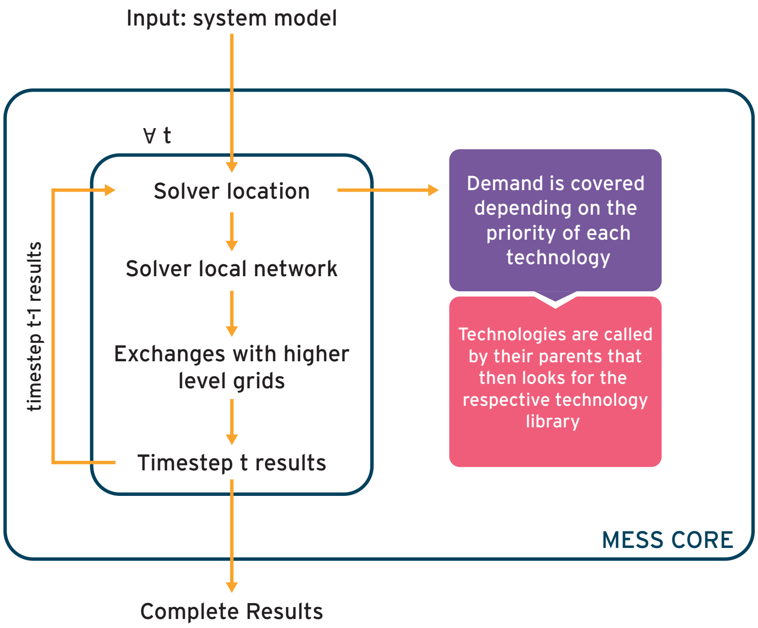

Figure 2. Functioning of the Core phase of MESS.

As briefly introduced, the first step solves each location at each timestep. The energy balance is initialized at zero at each timestep and is progressively updated while the technologies are solved in each location. Generally speaking, demands are the first to be added to the balance and then the different technologies are used to cover the demand based on their priority. This means that the technologies with the highest priority (lower index value) are the first one to be used to cover the demand. Once that the highest priority technology has been called by the solver, it proceeds searching for the second highest one and so on, until the demand is covered. In this phase, using this approach means that non dispatchable renewable energy technologies might lead to an overproduction of energy. This solving strategy adds the possibility of considering counter-intuitive control strategies for each location, expanding the range of scenarios that can be defined and investigated by the user, nonetheless it should be used with caution, since it might lead to unrealistic behaviours. Once that all locations have been individually solved the local network is considered in the second step of the core phase. If there are imbalances in the single locations, and the option of considering the local network has been considered, the local grid is solved. In this second step, the solver does a simple summation of the positive and negative imbalances of the single locations estimating the amount of energy exchanged. In the third and final step of the core phase the exchanges with higher level grids (i.e. national grid) are defined.

Post-processor and Plotting

After having solved the model in the core stage, the generated solution is processed by the post-processor. The objectives of this step are multiple. It allows to process data to obtain aggregated indicators of performance, looking at the whole timespan considered and not only at the timestep resolution (e.g. hourly) imposed. At the same time, it allows to process the data as to proceed with the plotting and to save the results in CSV files that can be used by the user to perform further analyses.

The plotting phase has been considered as a separate step from the post-processing one, even though the two being highly interlinked. Plotting in MESS is handled using the PlotlyJS package [28] that creates interactive HTML files allowing the user to analyze the generated plots by zooming in and out and highlighting the single values navigating on the plot. At the current status, the plotting phase automatically generates two different kind of plots. The first one shows the overall results at each timestep, for each location, in terms of electricity, heat and gas balance. The second one uses the aggregated results for each location to show how demand is covered in percentage by each technology available in the different locations.

2.2. MESS vs Calliope

Developing and presenting a new model requires a comparison with an existing tool in order to identify its peculiar characteristics and different usage purposes with respect to a renowned standard. Therefore, a comparison between MESS and Calliope [7] has been conducted. Calliope is an energy system model that allows to investigate energy systems with high spatial and temporal resolution. It permits to analyse different scenarios from urban scale to countries. The choice of Calliope as benchmark model was made due to several reasons. Calliope has proven to be a largely utilised tool, with high standards of code testing and with an approach that is both user friendly, since no coding is required by the user, and rigorous. At the same time, Calliope is an optimizer and comparing MESS with it allows to evaluate what is the potential of simulating against optimizing a system. Indeed, as mentioned by [11] these two approaches have different strengths and purposes. Optimization tends to be more indicated for bottom-up models with a high level of technical details and for being used by planners and engineers. Nonetheless, due to its characteristics and the long computational times that are usually required, it might show some limitations in certain applications. Using a simulation approach results in lower computational times - due to its simpler approach - and might allows a more dynamic and productive interaction with policy makers.

Calliope offers three different modelling options: *(i)* planning mode allows to perform an investment decision analysis to find the optimal configuration of a system in terms of installed capacity via the minimization of an objective function, *(ii* dispatch mode is meant to perform an optimization on the economic dispatch of the model. In this case, installed capacities of the different technologies are fixed and the model finds the optimal way of satisfying the demand while minimising the objective function. Last, *(iii)* SPORES mode allows to investigate sub-optimal solutions around the optimal one. In this work, the first two modes have been employed, while the SPORES one has not been considered.

The comparison between MESS and Calliope has been performed as follows. A case study has been considered and energy demands have been defined for a system composed by three locations. The demand profiles considered have been obtained from consumption data of three monitored multi-apartment buildings from the Sinfonia Project [29] in Bolzano, Italy. The load profile of the PV panels has been obtained from

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the Renewable.ninja website [30,31] setting Bolzano as location. According to MESS network simulation capabilities, all locations have been considered able to exchange electricity with the others. A different mix of technologies has been considered for each location. Figure 3 shows the case study considered.

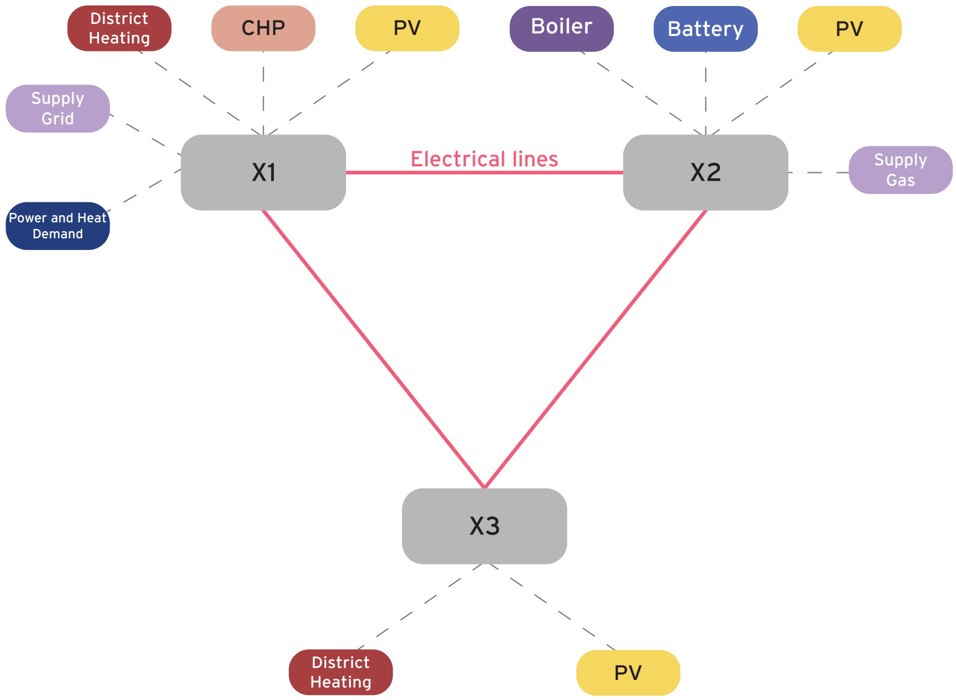

Figure 3. Case study example

First, the model has been run in planning mode to obtain the optimal capacities of the different components considering a year-long period. Then, the dispatching mode has been considered. In this case, capacities are fixed, and the model employs a receding horizon control algorithm. The results of the former modelling mode have been used as an input for the operational mode and for the simulation in MESS and the results of the two different approaches have then been compared.

3. Results

In this section, the results obtained from Calliope and MESS are reported. Calliope has been used both in planning (Subsection 3.1) and operational modes, while MESS has been compared to the results obtained from the latter approach (Subsection 3.2). Table 3 lists the execution times of the three simulations with a timespan of 1 year and a hourly timestep, which have been conducted on a Linux machine running Ubuntu 18.04 with the 15 GB of RAM, and a Intel ® Core i7-8565U CPU @ 1.8GHz 64bit.

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Table 3: Execution times for a three node system for a timespan of 1 year with a hourly timestep resolution. The time reported in the table have been derived from a single-run, and include all the phases from pre-processing to plotting.

Location	Execution time
Calliope - Planning	∼45 min
Calliope - Operational	∼11 min
MESS	∼1 min

3.1. Calliope - Planning mode

Planning mode has been employed to obtain the optimal capacities to be used as inputs for each technology for the following simulations. The obtained capacities are shown in Table 4. Given the costs imposed, the optimized results would tend not to include photovoltaic panels and batteries in the technology mix, hence a lower bound on their capacity to be installed has been imposed. Given the constraints, locations X1, X2 and X3 result having respectively 5.0 kW, 10.0 kW and 7.0 kW installed of PV, while an energy storage system of 5.0 kWh has been imposed in location X2 as well. Locations X1 and X3 mainly rely on district heating to cover their thermal demand, with a minor contribution from CHP in X1, while a boiler unit is supplying thermal energy to X2.

Table 4: Calliope planning mode results, used as inputs for Calliope operational mode and MESS

Location	Technology	Installed capacity
X1	CHP	9.1 kW
X1	District heating	183.1 kW
X1	PV	5.0 kW
X1	Supply gas	22.5 kW
X1	Supply grid power	20.9 kW
X2	Battery	5.0 kWh
X2	Boiler	50.8 kW
X2	PV	10.0 kW
X2	Supply gas	59.8 kW
X3	District heating	131.4 kW
X3	PV	7.0 kW

3.2. Calliope - Operational mode and MESS

Given the capacities obtained from the investment planning optimization, the operational mode in Calliope and the MESS simulation have been run. In this subsection the results obtained are presented.

Annual aggregated results

Figures 4 and 5 show the results aggregated for the whole timespan considered (8760 hours, 1 year). Each bar in Figure 4 shows the total amount of electricity obtained from each technology: blue bars represent Calliope's results, while the green ones MESS'. The energy produced by the PV panels is exactly the same in all three locations, this should not be surprising given the straightforward functioning of a non-dispatchable technology and the simple models employed. Differences can be noted both for the CHP (∼16%) in location X1 and for the battery in location X2 (∼35%). In the former case, such a difference might be ascribed to the CHP producing electricity not only for location X1, but for the other locations as well, in the case of Calliope. Indeed, this possibility is yet to be implemented in MESS: dispatchable technologies can only be controlled by the demand of the location where the technology is installed. In the case of the battery, in Calliope its usage depends on a economic optimization of the system as a whole, while

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in MESS it only tends to maximize the electricity self-consumption of the location where it is installed. Finally, the most evident difference is in the electrical energy imported from the national grid. Looking at Calliope's results, electricity is only imported in location X1: this is because the connection to the grid is placed there, and electricity is then distributed to X2 and X3 from X1. In the case of MESS, no electricity is imported in X1 since the location is self-sufficient, while substantial imports are present in X2 and X3, since all locations are supposed to be connected to the grid.

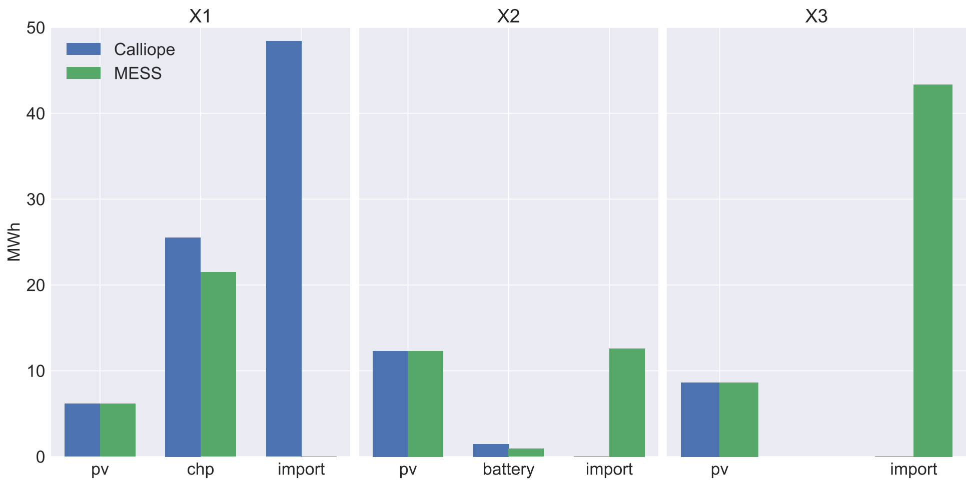

Figure 4. Annual electricity per technology source - Calliope and MESS comparison

Similar considerations can be made for Figure 5. The boiler in X2 and district heating in X3 are the only heat sources for their locations and the results obtained from Calliope and MESS match completely. The differences highlighted for the CHP in the electricity case have repercussions on the heating part for location X1 as well. The CHP is operated in the electrical load following mode, hence the higher quantity of electricity generated in Calliope's solution translates in a higher production of heat as well, which is compensated by MESS with an higher quantity of heat purchased from the district heating grid.

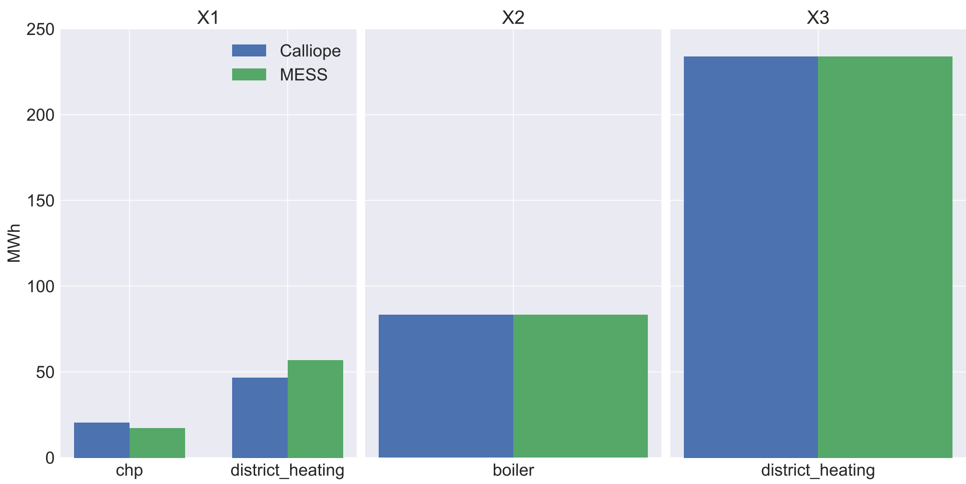

Figure 5. Annual heating per technology source - Calliope and MESS comparison

Monthly aggregated results

Monthly aggregated results are here shown for location X1. The same results for location X2 and X3 can be found in Appendix B.

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Figure 6 shows the monthly amount of energy derived from different technologies for Calliope (left-hand side graph) and MESS (right-hand side graph). As seen in Figure 4, the differences between the two models are in how the CHP works and the reliance on imported energy. Calliope shows a greater utilization of CHP in winter months, while and heavier reliance on electricity import in the summer. This could be ascribed to the higher thermal demand of the winter months: in that case it would make more economic sense to have the CHP running rather then buying electricity from the grid, since the CHP could provide both electrical and thermal energy. On the other hand, MESS shows a more regular behaviour of the CHP throughout the year. As seen in the previous paragraph, the CHP in MESS works in a electrical load following mode, hence its' behaviour is only dictated by the electricity demand and the PV production, resulting in a more even behaviour. Moreover, no electricity is imported from the grid, since the CHP size is enough to cover, together with the PV panels, the electricity demand.

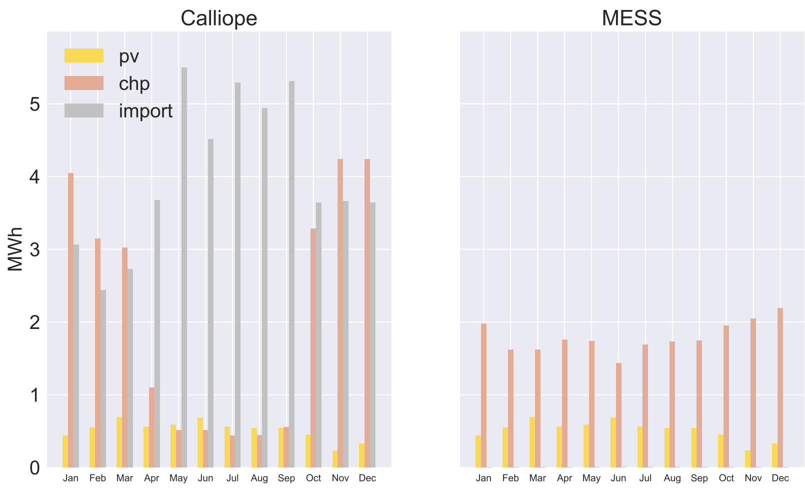

Figure 6. Monthly electricity production per technology source: Location X1 - Calliope and MESS comparison

The graphs in Figure 7 confirm what has been said about Figure 6. Indeed, the results obtained with Calliope show a higher heat production from the CHP in the winter and a way lower production in the summer. Instead, MESS relies more heavily on the district heating in colder months and has an excess production of heat in the warmer ones, heat that hence will be discarded. Details of the monthly behaviour for all the locations are presented in Appendix B.

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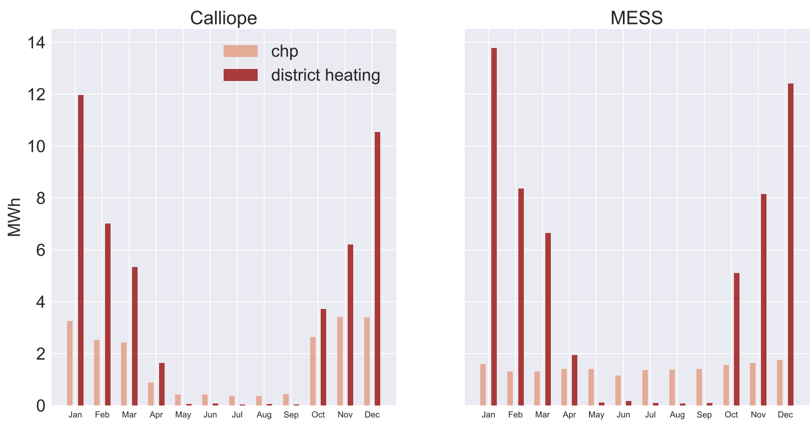

Figure 7. Monthly heating per source: Location X1 - Calliope and MESS comparison

Hourly results - Typical weeks

Finally, the results obtained from the two modelling tools are shown on an hourly basis for four representative weeks of the year. Figure 8 shows the results obtained via Calliope for a week in winter, spring, summer and autumn, while Figure 9 shows the same results for MESS.

Looking at Figure 8 it is possible to notice a similar behaviour for the winter and autumn weeks and for the spring and summer ones. The main difference between the two pairs is the behaviour of the CHP. In the colder seasons the CHP has a major role, since it allows to cover both the electrical and thermal demands, as seen also in the previous paragraphs. The reliance on the grid is much heavier in the warmer seasons, since the contribution of the CHP is almost negligible. The electricity demand is always exceeded by the electrical energy produced or imported from the grid, this is because location X1 acts as a connection point for all three locations to the national grid. In winter and autumn, the CHP tends to reach its peak production and the remaining electricity demand from location X2 and X3 is covered by buying electricity from the grid. In spring and summer, since the thermal demand is lower, it makes more economic sense to buy electricity from the grid and the CHP is used way less. Another thing worth noticing is the unmet demand at the beginning of the spring week. In this case, the electricity demand in X1 is actually met, but not from a combination of the technologies seen so far, but from an excess of PV electricity from the other locations, since it happens in the central hours of the day.

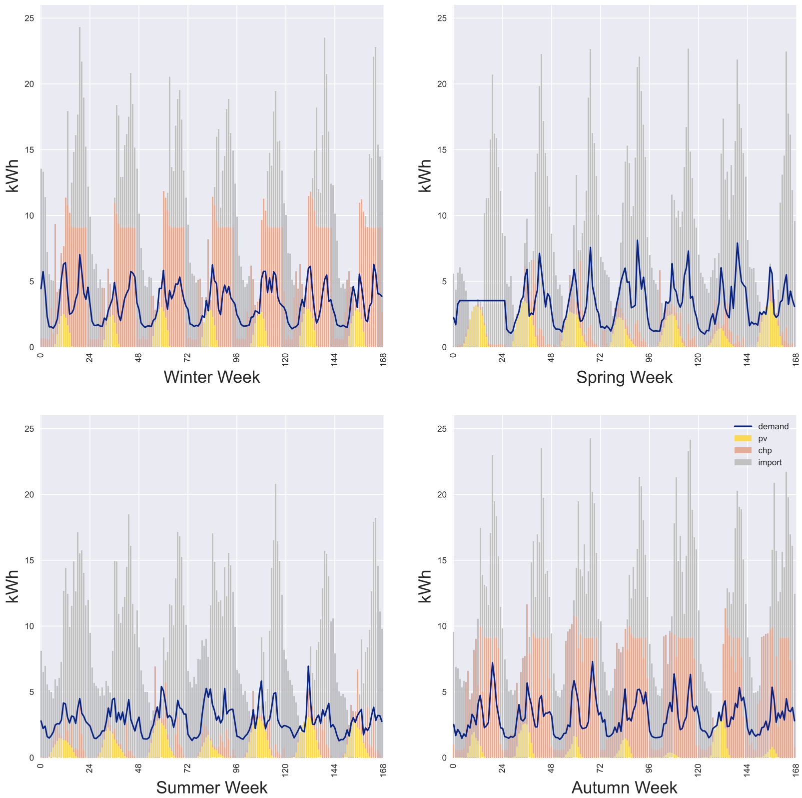

Figure 8. Hourly electricity production of four representative weeks: Location X1 - Calliope

In the case of MESS the interpretation of the results shown in Figure 9 is more straightforward, since each location tends to be more independent and in general less reliance is made on the local grid. In of the considered weeks the demand is completely satisfied by the combination of PV panels and CHP. Priority is here given to the non-dispatchable electricity produced by the PV panels, while the CHP covers the remaining demand. Given a good superposition of production and demand, and the size of the solar panels, almost no excess electricity is produced in the analysed weeks, except for a very few hours in the summer. In that case the excess electricity will be exported to the other locations, if required, or otherwise sold to the grid. In Appendix C it is possible to see the weekly results for the other two locations.

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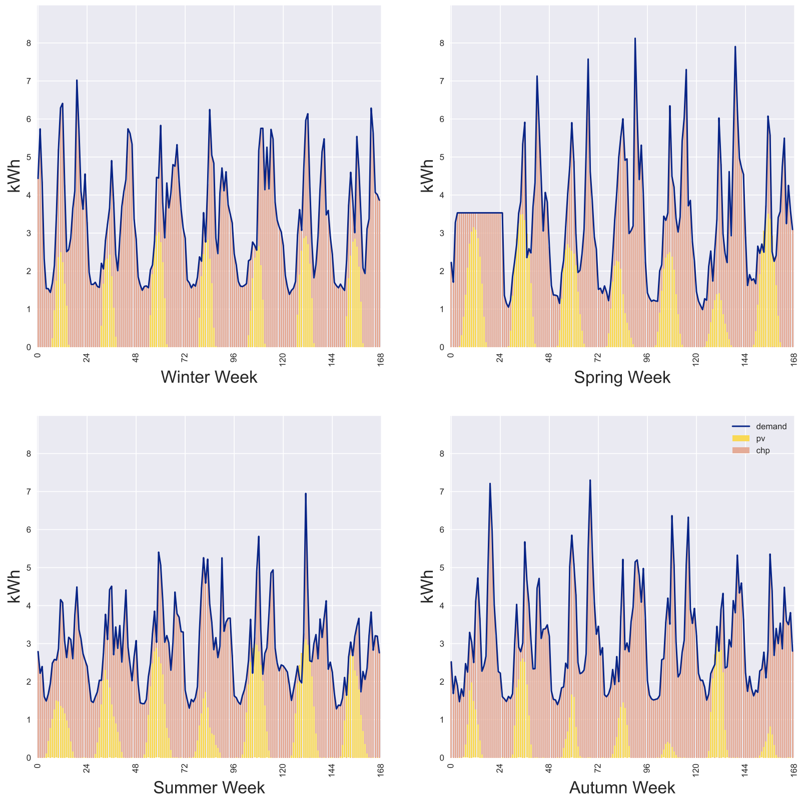

Figure 9. Hourly electricity production of four representative weeks: Location X1 - MESS

4. Discussion

The analysis of the results made it possible to observe some of the differences between MESS and Calliope. The comparison has shown how these differences derive from different principles and strategies adopted by the two models in solving the system. In Calliope, the optimization aims at minimizing whole system running costs, and this is the principle on which the functioning of each component is based. As seen in the previous section, following this principle, CHP is mostly used in the colder parts of the year - when heating demand is high and both electricity and heat are required - while is minimally utilised in the summer, since buying from the grid is more convenient. MESS, on the other hand, follows its own predefined rules and throughout the whole year the CHP runs to help PV panels cover the electricity demand, producing as a byproduct heat, that might be used or not. A similar reasoning applies also to the functioning of other components, such as the battery. Differences are not limited to how single components are solved, but are also on how Calliope solves the network with respect to MESS. Indeed, while MESS gives priority to the self sufficiency of each location, in Calliope technologies can also contribute cover the demand of other locations, always following the principle of whole system running cost minimization. Hence, this contributes as well in explaining the differences in CHP production, and gives an explanation of the differences in total energy import from the grid too.

Given the differences observed, it should be considered that some of the solving principles applied in MESS, despite being simple, are particularly realistic when considering an urban context. To give an example, it might be more likely that in certain areas the majority of owners of a battery will tend to use it to store the excess of production

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from their photovoltaic modules rather than to trade energy with the grid to enhance profits. In this sense, an optimization approach is less flexible and might make it more difficult to represent non-optimal behaviours. Instead in MESS, using a simulation approach makes it easier to implement different solving strategies that might be closer to the optimized ones, e.g., technologies dispatching according to price signals.

Another aspect that emerges from analysing the yearly balances is that the overall differences are not very high. This denotes how a simplified approach like the simulation one, depending on the application considered, could provide results of a satisfactory precision. This result is relevant since suggests that in some situations a simulation approach might be the right choice. As mentioned above, Lund et al. [11] already presented some of the major characteristics of the simulation and optimization approaches. In light of their analysis, the aim of the development of MESS was also to explore the potential of simulating energy systems. The results obtained in this work seem to confirm the idea that while an optimization approach is more indicated for investment planning models and macro energy systems analysis, a simulation approach might be more suitable for quick investigations of numerous scenarios on a smaller scale, making it an interesting option for a wider set of stakeholders in their decision process. Shorter execution times, together with an approach that makes it easier to understand the logic behind the model might contribute to make the modelling process more open and inclusive.

In fact, it might be possible to include modelling process in meeting as well as workshop and information campaign to support the design of new policies and energy strategies. In this way, it would be possible to follow a more transparent and participatory approach.

5. Conclusions

In this work, the authors presented a newly developed model called MESS - Multi Energy System Simulator and compared it to a benchmark optimization model (Calliope) to investigate the potential of simulating energy systems and the advantages and disadvantages with respect to an optimization approach.

Results obtained have shown that, even though there are differences in the way energy demand is covered, mainly due to the logic behind the network solver and the cost minimization approach, the overall yearly results tend to be similar. This reinforced the idea that, despite the simplified approach, simulations can be used to analyse energy systems at an urban scale with satisfactory results. Furthermore, the simplified approach brings advantages in terms of opportunities of investigating multiple alternatives and scenarios in a relatively low amount of time. Simpler models might help address one of the challenges of energy system modelling, which is the need of a higher level of transparency. Indeed, more transparency could contribute to improve the democratisation process of analysing and planning energy systems and, in the end, fostering a fair and just energy transition.

Finally, MESS was developed having in mind a high level of flexibility and modularity. Thus, future area of research and development will be oriented towards the improvement of the library of technologies, including different modelling options for each technology, towards the integration of the spatial dimension, crucial to plan and analyse future energy systems at urban level, and towards the analysis of the effects of different energy policies .

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Data Availability Statement: The data used in this work are publicly available in the following git repository. Here it is possible to find the configuration files used for running models in Calliope (both the Planning and Dispatch one) and MESS.

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Appendix A. Models Review

Table A1. List of model reviewed.

Model	Sectors	Math modeltype	Timeresolution	Georesolution	Urban Scale	Modelling Software
Backbone	All	Optimization	Hour	Depends on user	Y	GAMS
Balmorel	Electricity, Heat	Optimization	Hour	NUTS3	N	GAMS
CAPOW	Electricity	Simulation	Hour	Zonal	N	PYTHON - PYOMO
Calliope	User-dependent	Optimization	Hour	User-dependent	Y	PYTHON - PYOMO
DESSTinEE	Electricity	Simulation	Hour	National	N	EXCEL - VBA
DIETER	El. and Sector Coupling	Optimization	Hour	Node	N	GAMS - CPLEX
Dispa-SET	Electricity	Optimization	Hour	NUTS1	N	PYTHON - PYOMO, GAMS
ELMOD	Electricity, Heat	Optimization	Hour	Network	N	GAMS
EMLab-Generation	Electricity, Carbon	Simulation	Year	Zones	N	JAVA
EMMA	Electricity	Optimization	Hour	Country	N	GAMS
ESO-X	Electricity	Optimization	Hour	Node	N	GAMS - CPLEX
Energy Transition Model	El., Heat, Transport	Simulation	Year	Country	N	RUBY - RAILS
EnergyNumbers-Balancing	Electricity	Simulation	Hour	National	N	FORTRAN
EnergyRt		Optimization			N	GAMS - CPLEX
EnergyScope	El., Heat, Transport	Optimization	Hour	Country	N	GLPK - CPLEX
Ficus	Electricity, Heat	Optimization	15 Minute			PYTHON - PYOMO
FlexiGIS	Electricity	Opti., Simulation	15 Minute	Urban	Y	
Genesys	Electricity	Opti., Simulation	Hour	EUMENA, 21 regions	N	C++
GridCal	Electricity	Opti., Simulation				PYTHON
MEDEAS	Electricity, Heat	Other	Year	global, continents, nations	N	PYTHON
NEMO		Opti., Simulation	Hour	NEM regions	N	PYTHON
OMEGAlpes	Electricity, Heat	Optimization			Y	PYTHON
OSeMOSYS	All	Optimization	Day	Country	N	PYTHON
Oemof	El., Heat, Transport	Opti., Simulation	Hour	Depends on user	Y	PYTHON - PYOMO
OnSSET		Optimization	Multi year	1 km to 10 km	Y	PYTHON
PowNet	Electricity	Opti., Simulation	Hour	High-voltage substation	N	PYTHON - PYOMO
PowerMatcher						JAVA
PyPSA	El., Heat, Transport	Opti., Simulation	Hour	User dependent	Y	PYTHON - PYOMO
REopt	Electricity, Heat	Optimization	Hour	Site	Y	JULIA - JuMP
Region4FLEX	El. and Sector Coupling	Optimization	15 Minute	Administrative districts	Y	PYTHON
Renpass	Electricity	Opti., Simulation	Hour	Regional (only DE) or Country.	N	R
SIREN	Electricity	Simulation	Hour		N	PYTHON
SciGRID	Electricity, Transmission	Simulation		nodal resolution		PYTHON
SimSES	Electricity	Simulation	Minute		N	MATLAB
StELMOD	Electricity	Optimization	Hour	Nodal resolution		GAMS
Switch	Electricity	Optimization	Hour	buildings, to continental	Y	PYTHON - PYOMO
Temoa	All	Optimization	Multi year	single region	N	PYTHON - PYOMO
TransiEnt	El., Heat, Gas	Simulation	Second	Hamburg	N	MODELICA
URBS	User-dependent	Optimization	Hour	User-dependent	Y	PYTHON - PYOMO
City Energy Analyst	Electricity, Heat	Optimization, Simulation	Hour		Y	PYTHON
Total						40

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Appendix B. Monthly Results

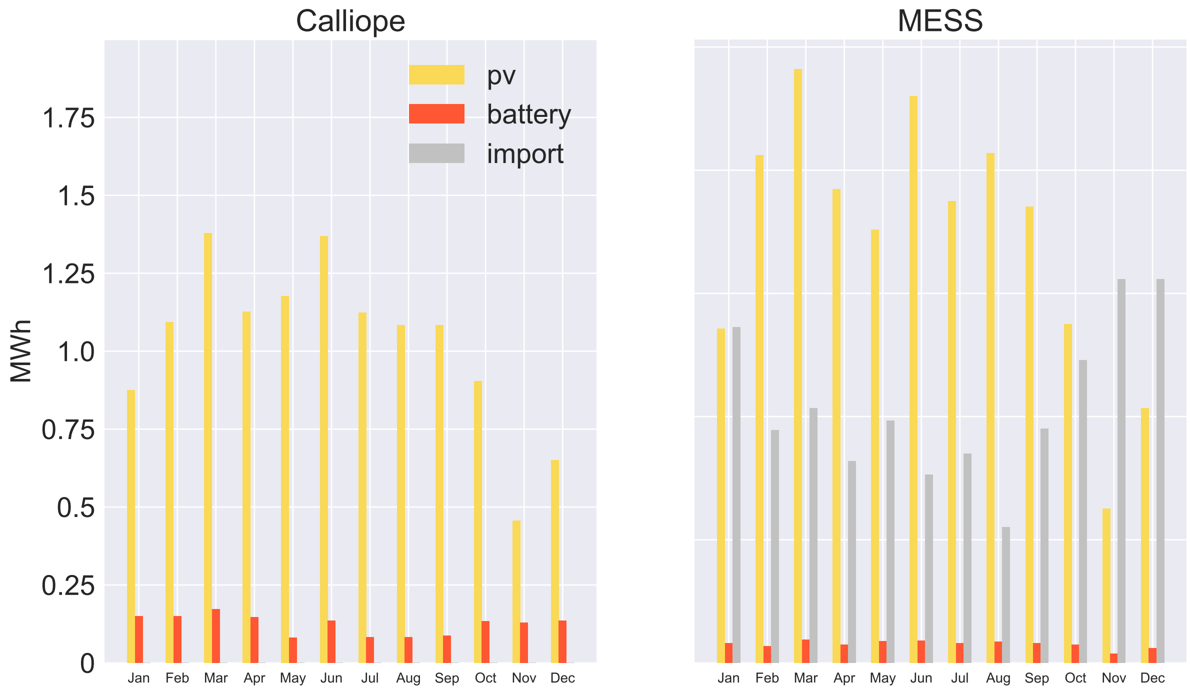

Figure A1. Monthly electricity production per technology source: Location X2 - Calliope and MESS comparison

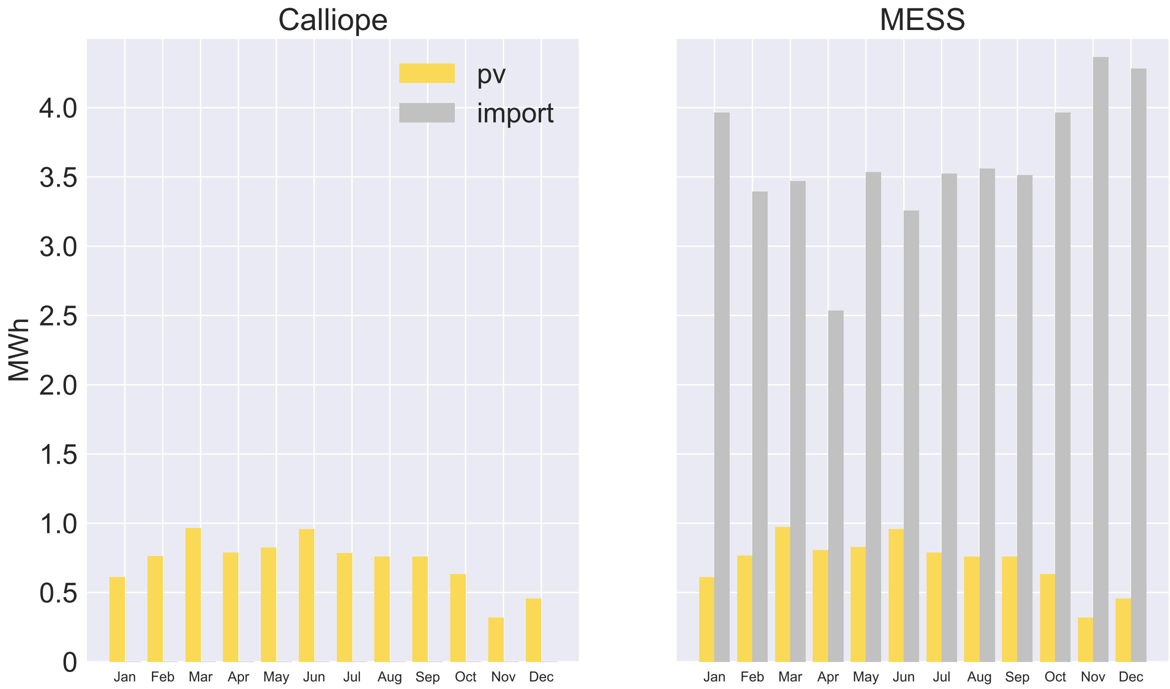

Figure A2. Monthly electricity production per technology source: Location X3 - Calliope and MESS comparison

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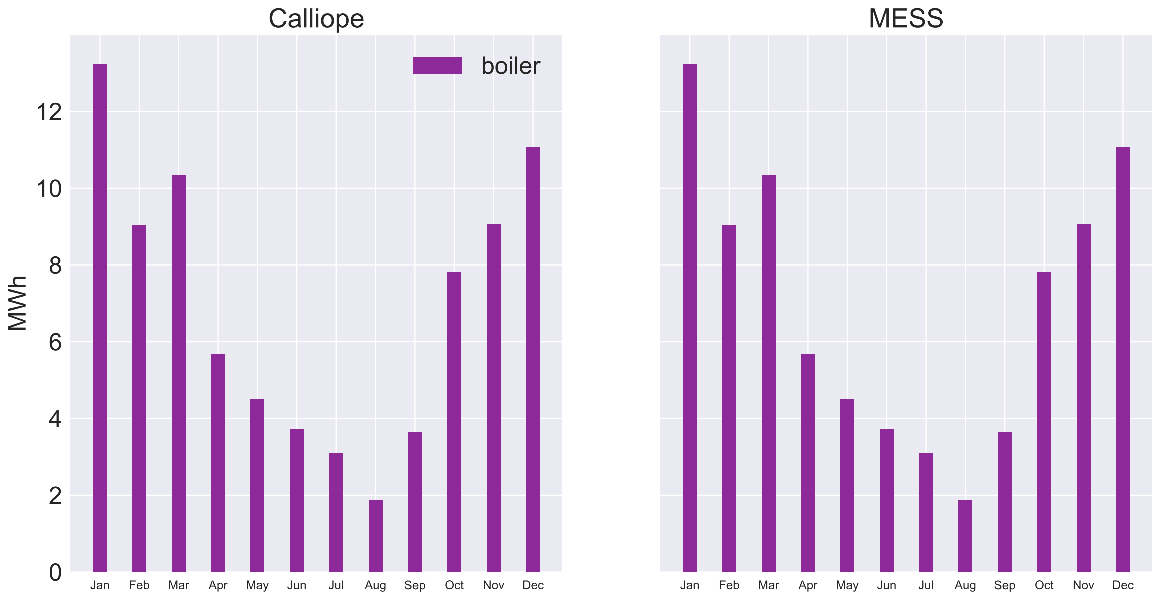

Figure A3. Monthly heating per technology source: Location X2 - Calliope and MESS comparison

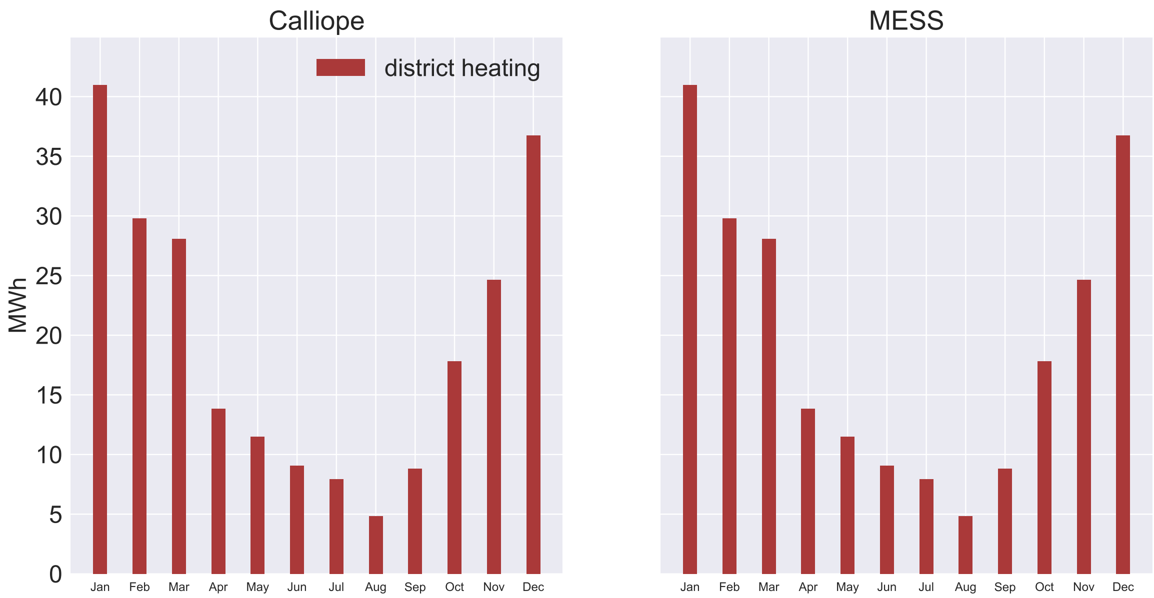

Figure A4. Monthly heating per technology source: Location X3 - Calliope and MESS comparison

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3 ## Appendix C. Weekly Results

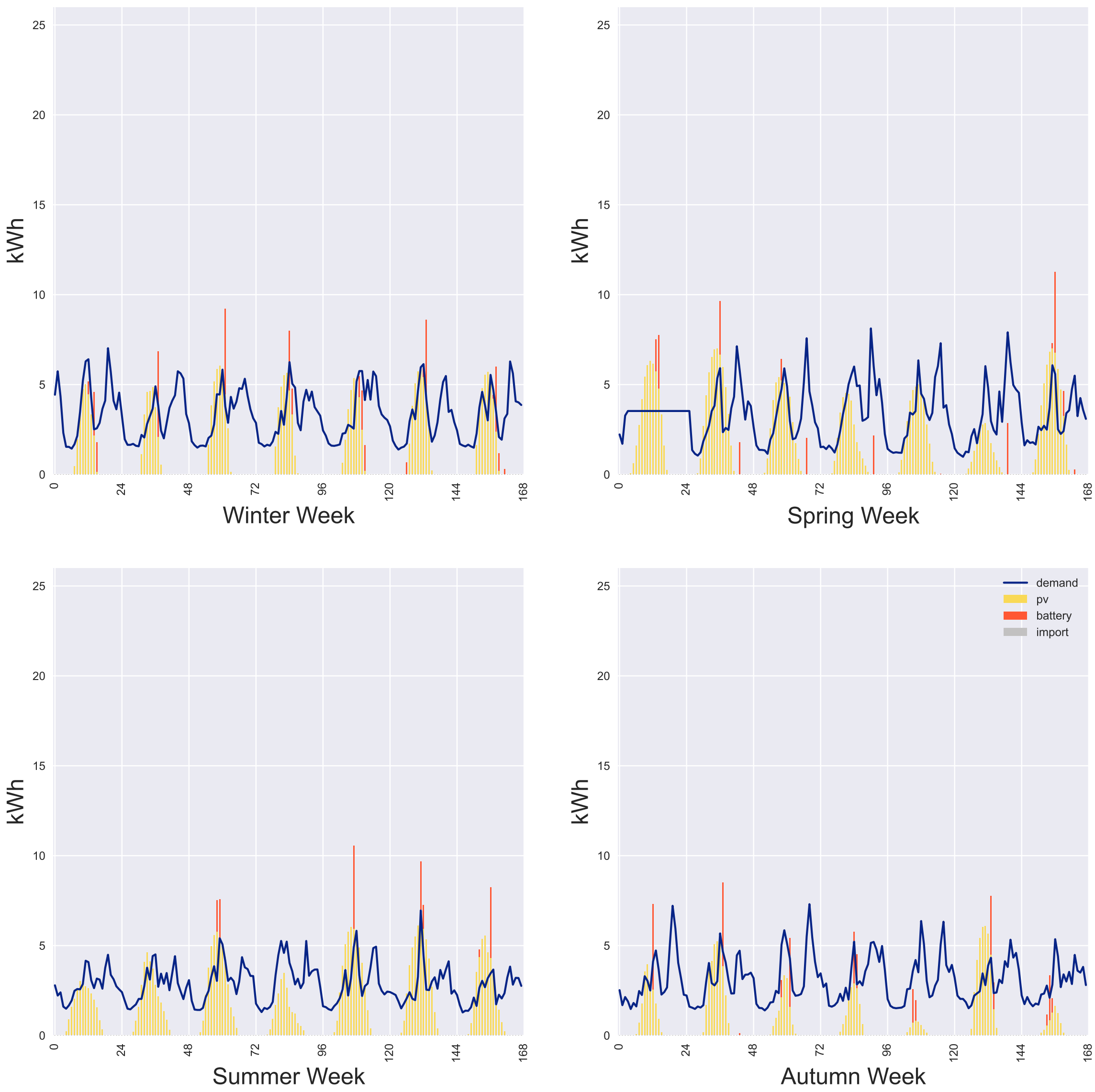

Figure A5. Weekly electricity production per technology source: Location X2 - Calliope

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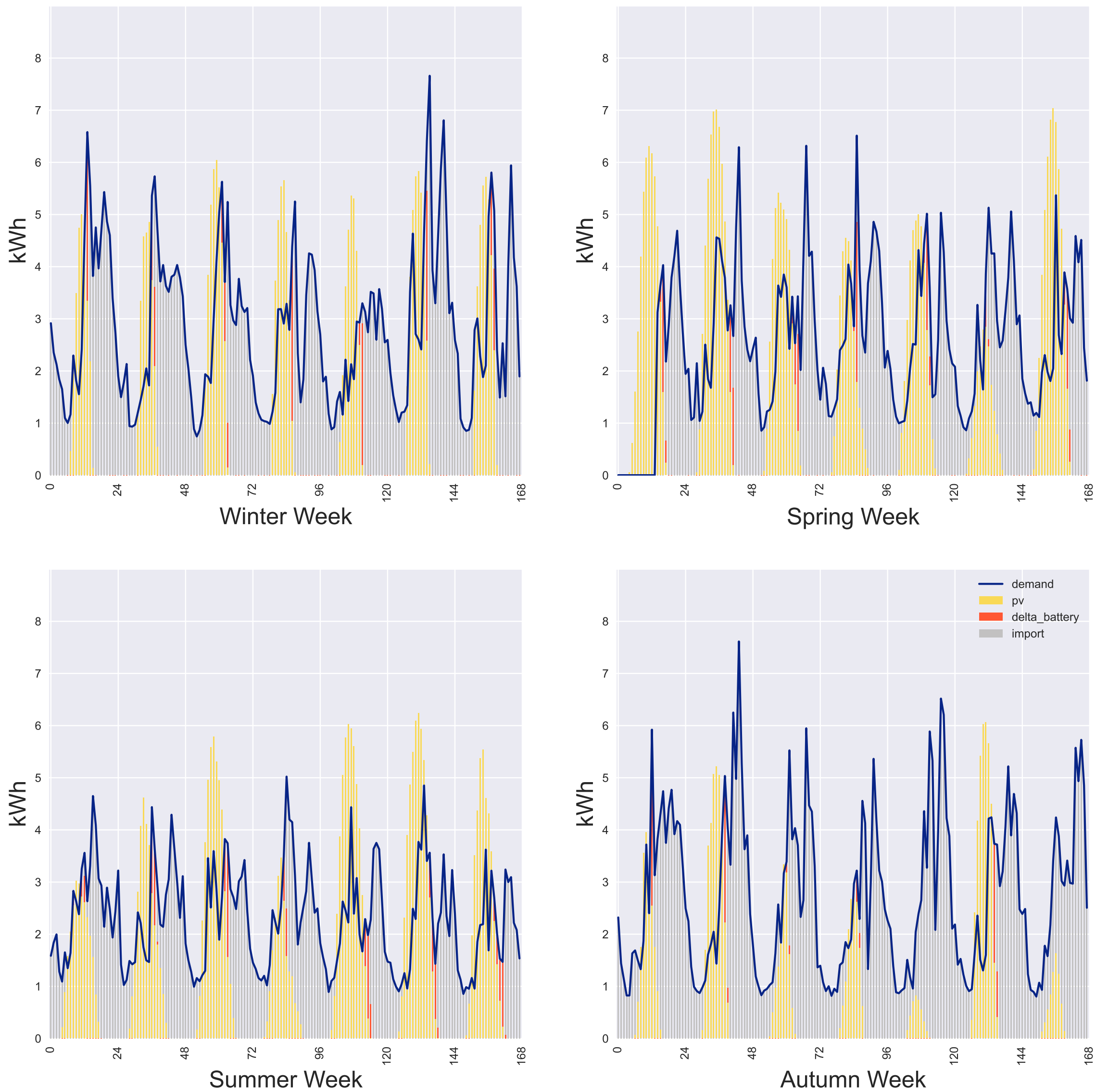

Figure A6. Weekly electricity production per technology source: Location X2 - MESS

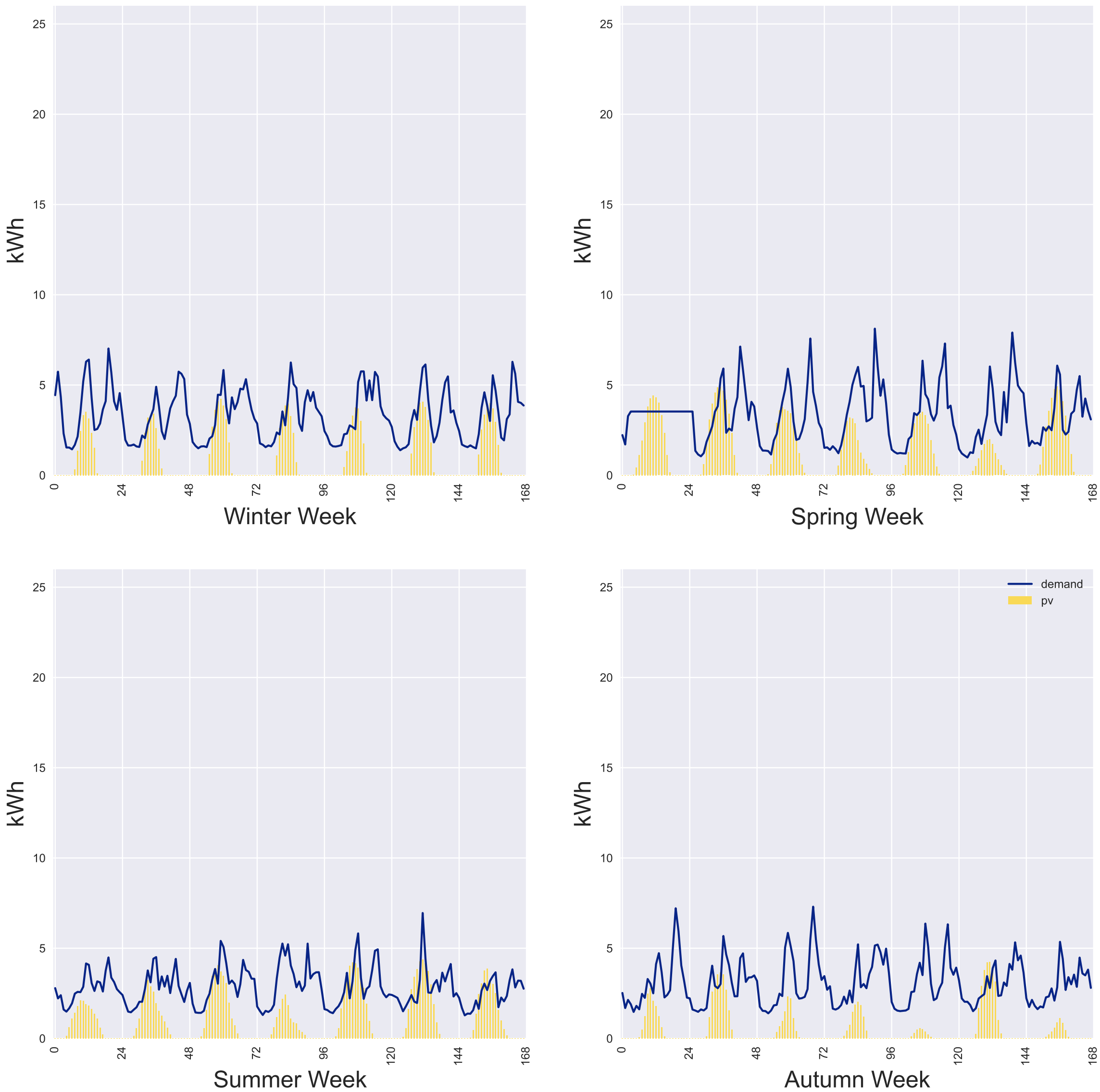

Figure A7. Weekly electricity production per technology source: Location X3 - Calliope

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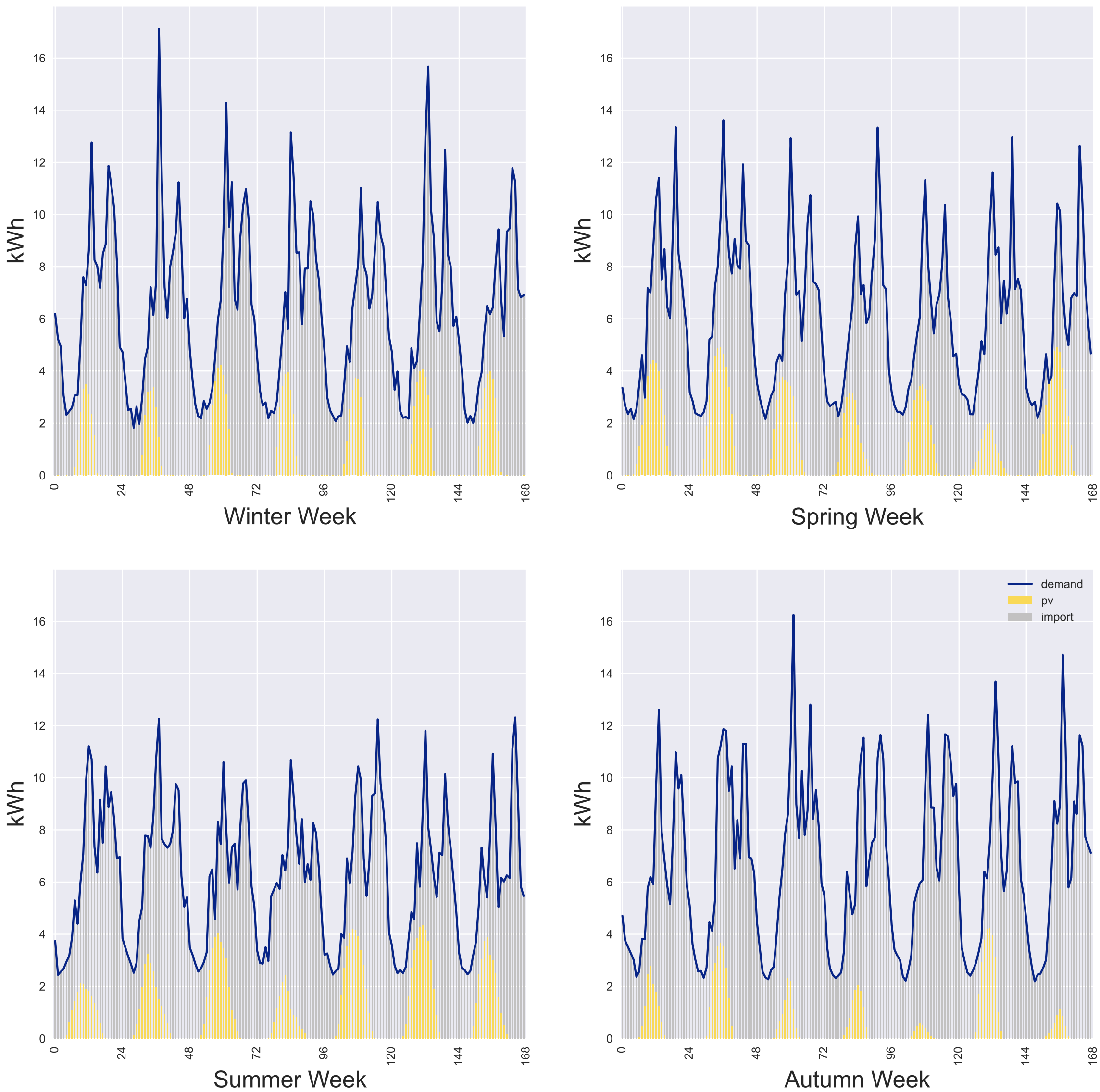

Figure A8. Weekly electricity production per technology source: Location X3 - MESS

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