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Deliverable D3.6
EINSTEIN Tool:
General Demonstration of Functionality

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Executive Summary

This report gives an overview and a general demonstration of the functionality of the EINSTEIN software tool, summarising the results of the work of WP3 within the i-ThERM project. EINSTEIN is a tool for optimisation of energy performance heating and cooling supply in industrial plants and other large scale applications in the non-industrial sector. Use cases for the enhanced EINSTEIN tool as developed within the i-ThERM project can be subdivided into:

- **use case system *design***: the **detail design and optimisation of heat and cooling supply systems** is the main use case for which EINSTEIN has been initially designed. Design optimisation may be done either for the design of a new plant on the green field or as an improvement of the system within an existing plant (energy audit). EINSTEIN is conceived as a holistic tool providing tools and valuable outputs at all stages of the design process: data collection, creation of alternative proposals, comparing performance and selection of the best option, and generating a report in order to convince decision makers.

- **use case system *operation***: the new EINSTEIN as developed within i-ThERM can also be used during system operation for the **continuous supervision of the system performance** and for **model-based optimisation of system control** parameters.

An illustrative **show case** highlights and demonstrates some of the most relevant features of the tool: a **heat to power conversion system using a low temperature waste heat stream** is compared to possible alternative technologies for reuse of waste heat, such as direct heat recovery or high temperature heat pumps. The main functionalities are demonstrated both at the stage of system design (importing of monitoring data and parameter fitting, pinch analysis, creation of alternative proposals using design assistants) and at the stage of system operation (real time simulation).

Within i-ThERM new functionality for the EINSTEIN tool has been developed and a significant amount of work has been dedicated also to improvements with regard to user friendliness, robustness and documentation. The **fully revised version V3.0*plus* of the EINSTEIN software** tool forms part of this deliverable. The most relevant new features and improvements are:

- The algorithm for **automatic design and optimisation of heat exchanger networks** has been fully revised and improved. More flexibility has been added to the **pinch analysis module** giving now the possibility for selecting / unselecting a subset of hot and cold streams.
- Now also (waste-) **heat to power conversion equipment** can be modelled by EINSTEIN, including the innovative technologies being developed within I-Therm (sCO2-turbines and TFC systems) and also other market available technologies such as ORC (organic Rankine cycle) and steam turbines.
- modelling of an **electricity grid with variable indexes** (tariffs and environmental parameters) for an appropriate assessment of power generation equipment connected to a grid with an increasing fraction of renewable energy sources with fluctuating availability (wind, PV, etc.).
- **Historical monitoring data can be automatically analysed** within the EINSTEIN consistency and completeness check function. With this algorithm the EINSTEIN model parameters can be calibrated in order to match (historical) real performance. Schedules of processes within the EINSTEIN model

can be derived automatically from monitoring data. By **scaling data** appropriately in order to forecast the expected future evolution (e.g. production volumes, …) a **baseline scenario for future energy consumption** and system performance can easily be generated.

- The capability for carrying out **real-time simulations** has been implemented. In this mode data on real operating conditions are imported via a data base and simulations are carried out in parallel to real operation. Simulation results can be compared to measured real performance and so be used either for a calibration of model parameters or for detecting eventual failures in system operation.
- **Forecast and Model-Based Optimisation of System Control:** based on forecasting system simulations system control parameters can be optimised "on-the-run". The optimised parameter set then is sent to data hub and can then be processed by the system control unit.
- **User friendliness, robustness and documentation of the software** have been significantly improved, in order to reduce the "entry barriers" and the required learning effort for getting started with the software, and also to make the work with the software in general more simple and intuitive, so that the tool will be used by a wider target group. Major new developments in this context are:

  a) the **graphical system editor** is now the main interface for the user in order to set-up and edit the system model and interconnect its components, complemented by a new **editor for viewing and editing heat exchanger networks**. A **graphical editor for system mass flows** (production flow chart) allows for defining mass balances within the system including both process streams and other flows such as raw materials and (intermediate and final) products.

  b) a special effort has been dedicated in order to **make editors for component parameters more intuitive** specially for new users of the software. This has been done very carefully for the most frequently used editors (processes, pipes and ducts, equipment), but also all other component editors and the editors for EINSTEIN data bases (e.g. fluids, fuels, equipment) have been revised.

  c) improved output of detailed simulation results: a plot of hourly results (including the option to export to a data file) has been added to the graphical user interface, where all instantaneous energy flows within the system can be visualised.

  d) documentation and tutorial: the user and technical manuals have been appropriately updated and completed in order to reflect the new features within the tool. *A* more comprehensive description on how to use the examples described in the EINSTEIN Audit Guide is given in the user manual for getting started with the tool. Furthermore, additional example cases are provided together with a video tutorial.

  e) Structure, robustness and testing procedure of the software structure has been improved: "*model – view – controller*" structure, use of standardised and reusable modules (objects) in the new GUI, many new standard test cases included in the standard testing procedure.

A validation of the EINSTEIN model for heat to power conversion equipment has been carried out. In order to compensate the lack of real measurement data virtual data from detailed simulations with a more complex model have been used. As a result it has been concluded that the constant exergy efficiency model used within EINSTEIN gives a good approximation of the results from detailed simulations. Further research is necessary in order to (a) determine the reasons for deviations in some ranges of operating conditions and (b) to check whether an operation in these (extreme) parameter ranges is of practical relevance.

1 Objectives and Contents of the D3.6 Package

This report gives an overview and a general demonstration of the functionality of the EINSTEIN software tool, summarising the results of the work of WP3 within the i-ThERM project.

In first place the general functionality of the EINSTEIN tool is summarised and put into the context of the typical use cases. A show case has been designed in order to demonstrate the tool capabilities (Chapter 2).

The major developments carried out within the i-ThERM are described and summarised. Chapter 3 summarised the major functionalities added to the tool, and Chapter 4 describes the improvements in user friendliness, robustness and testing procedure. The details of the work regarding heat recovery, heat to power conversion equipment, and the processing of monitoring data here only a summary highlighting the most relevant aspects is included for completeness. Details of this work are described within the corresponding deliverables D3.2 – D3.4.

In Chapter 5 a validation of the EINSTEIN model for two of the i-ThERM pilot plants is presented.

1.1 Update of EINSTEIN Software: Version 3.0plus

The main result part of the Deliverable D3.6 is a new major release (V3.0plus) of the EINSTEIN software tool[1] with a fully redesigned user interface. A free demo version is available for download at the EINSTEIN web site:

http://www.einstein-energy.net/index.php/software/download

The new release of the software contains also updated user and technical manuals (accesible online at einstein.sourceforge.net).

1.2 Show Case

The D3.6 package is completed by the EINSTEIN model (project xml-file) for the show case described in chapter 2.3. This example project can be opened and processed with the new EINSTEIN software tool.

1 *This release combines the results of ongoing work within the i-Therm project with additional own developments of energyXperts.NET. Together with the finalisation of this report, in June 2019 a beta-Version of the software will be published (EINSTEIN V3.0beta.01plus). The stable version V3.0plus will be released August/September 2019 after concluding an exhaustive final testing period.*

2 General Overview

In this section a general overview is given on the functionality of the EINSTEIN tool:

- what are the typical *use cases* for which EINSTEIN has been developed and who may use it ?
- what are the *outputs and results* generated ?
- a show case illustrates how working with EINSTEIN looks like in practice.

2.1 Use Cases

EINSTEIN is a tool for optimisation of energy performance in industrial heating and cooling supply. In practice, use cases for the enhanced EINSTEIN tool as developed within the i-ThERM project can be subdivided into the following two categories:

- use at the stage of system *design*: design and optimisation of the system
- use at the stage of system *operation*: supervision of performance and optimisation of system control

2.1.1 Use Case System Design

The use case "*system design*" deals with the design and optimisation of the heat and cooling supply system within a plant, where *design* refers to the selection of appropriate energy sources, utilities (equipment, heat exchangers, storage, etc.), their interconnections and control, and *optimisation* means optimisation from an energy, environmental or economic point of view or a combination of those, i.e. a target function to be defined by the user.

The use cases "system design" can be furthermore subdivided by level of effort, frequency and detail level into (a) a one spot detailed design and (b) a periodic quick energy audit (Table 1).

Table 1. Comparison of one-spot detailed design and periodic quick energy audit.

	one-spot detailed design	**periodic quick energy audit**
stage of project development	both green field design and retrofit	retrofit
typical frequency	every 2 – 5 years	once a year
effort / detail level	high	low (high degree of automatic processing)
result	catalogue of measures for a structural change within the system (installation of new or change of equipment, ...)	detection of the need (or not) for a change / update in the system measures for incremental adaptation of the system (e.g. increase of size of an existing heat exchanger, ...)

a) one-spot detailed design

The main use case for which EINSTEIN has been developed is the detail design and optimisation of heat and cooling supply systems in industrial plants and other large scale applications in the non-industrial sector.

Design optimisation may be done in one of the two stages of development of a plant:

- design of a new plant on the green field
- improvement of the system within an existing plant (energy audit)

The basic methodology and the requirements for a supporting software tool in both cases are very similar. Some differences are in the way of obtaining the base data and in the definition of the reference case.

While in greenfield design all base data (boundary conditions, such as e.g. heat and cooling demand, etc.) necessarily have to be estimated, in the energy audit of an existing plant measured data from past experience are available and can be used as a basis for estimating the expected future boundary conditions.

The reference case or base case scenario in an energy audit is “business as usual” without a change in the existing system. In green field design some solution (e.g. the one based on conventional standard technologies) may be used as a reference scenario against which other potential options are compared.

Once the expected future boundary conditions and the reference case are defined, the tasks for design optimisation as supported by EINSTEIN is as follows:

- build a model of the base case scenario
- develop possible alternative proposals (usually installation of new energy saving equipment)
- carry out an energy, environmental and economic evaluation
- summarise one (or some of) the most promising option(s) in a report as a basis for taking the corresponding investment decisions

Table 2 summarises the main tasks in the design process and the support given by the EINSTEIN tool to each of them.

Table 2. The main tasks for system design and optimisation and how EINSTEIN supports each of these tasks.

	main tasks	**support by EINSTEIN tool**
collect data: build a model of the base case scenario	collect available data: • inventory of utilities • operating and boundary conditions (e.g. production volumes, etc.) check for consistency and completeness forecast future evolution	automatic import of monitoring data (e.g. hourly data, monthly data) fully automatic processing algorithms for data estimation (up-/down-) scaling of data
create proposals: generate ideas and develop (several) alternative proposals for energy saving	analysis and detailed breakdown of present state performance as a starting point design of several saving options and their combinations: qualitative (e.g. selection of types of new equipment) and quantitative (selection of appropriate equipment size)	EINSTEIN automatically provides a lot of tables and graphs EINSTEIN design assistants provide tools for (semi-) automatic pre-design EINSTEIN system editor allows for any manual modifications of the system model
compare and select the best: carry out an energy, environmental and economic evaluation and select the best option	predict energy performance economic and financial analysis environmental analysis comparative analysis	EINSTEIN dynamic system simulation tool EINSTEIN economic module EINSTEIN module and data base for determination of environmental parameters: CO_2, nuclear waste and water consumption EINSTEIN provides several graphs and tables with the most relevant aggregate results, providing a comparative study of possible options and the base case scenario
convince the decision makers: generate a report	write a comprehensible audit report	automatic report generation in EINSTEIN with possibility for manual fine-tuning

b) periodic quick energy-audit: check for need of system adaptation

Once an EINSTEIN model for a given plant has been set-up in some initial audit as described in the previous section, this model can be re-used in order to periodically (e.g. once a year) adapt the energy assessment to a continuously changing real situation. The incremental effort and, therefore, cost of each new assessment in this case will be much less than that of the initial audit, as the basic set-up is already done and only changes that may have occurred (e.g. installation of new equipment, production lines, …) have to be introduced into an already existing model.

The *automatic import of monitoring data*, an EINSTEIN feature developed within I-ThERM Task 3.3, helps to semi-automatically generate an updated reference case (base case scenario) and to calibrate the model of

the system. Monitoring data representing the (recent) past can be extrapolated to the future by scaling appropriately up or down, reflecting so the expectations on the future evolution of e.g. production volumes.

Once the new model (base case scenario) is built and calibrated, *semi-automatic design assistants* within EINSTEIN allow for developing a quick and low-cost assessment for potential energy savings, in order to answer the question: Is the existing system still optimum also under the changed future conditions ? Even fully automatic processing (the EINSTEIN "auto-pilot") may give valuable insights in many cases.

Figure 1 shows a typical sequence of periodic model calibration, system optimisation (modelling) and changes in the real system. For more details see the D3.4 report [6]:

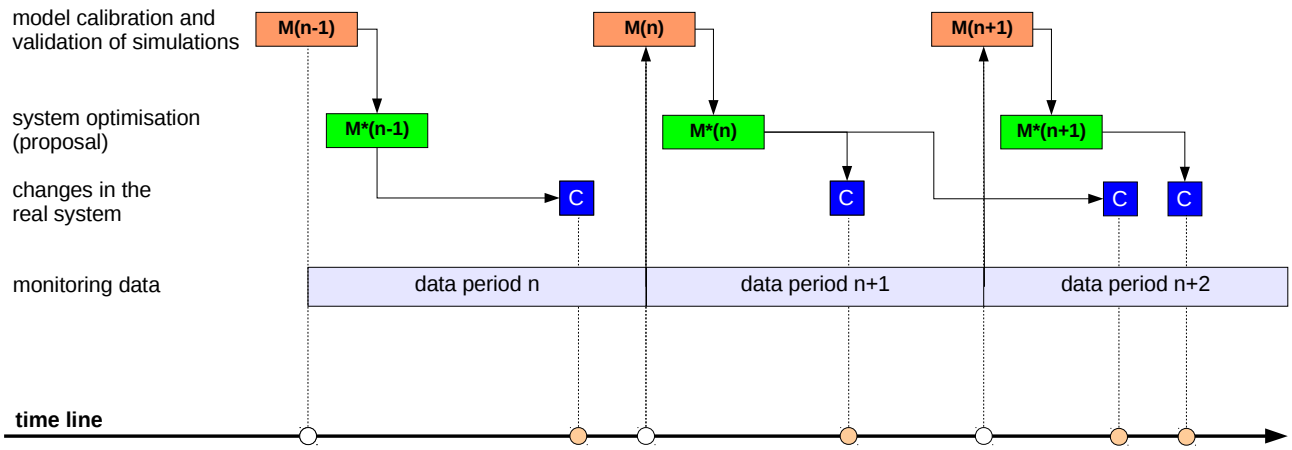


Figure 1. Sequence of model calibration, system optimisation and changes in the real system.

2.1.2 Use Case System Operation

During system operation, and with the new features of EINSTEIN developed within i-ThERM, EINSTEIN can also be used for the continuous supervision of the system performance and for model-based optimisation of system control parameters (giving feed-back to and so interacting with the system control unit).

a) periodic supervision of energy performance

The *real-time simulation capability* of EINSTEIN (see section 3.4) allows for the continuous comparison of actual vs. predicted performance under actual boundary conditions:

Monitoring data of the real system can be imported via a database connection or a data file and define the boundary conditions of a new simulation interval.

Differences between actual and model performance may be an indicator for failures in the system or for a degradation of system performance (e.g. fouling of heat exchangers, leaks in some piping, etc.).

Repeating *ex-post simulations of the system under real boundary conditions* for a certain period, which is possible using the same feature, may help for model calibration by parameter adjustment, fitting model results to real performance.

Initial estimates for some larger period (day, week, month) may be used as *(energy) performance targets* (energy management). Differences between the actual performance and those targets may indicate a

substantial change in the boundary conditions (e.g. expected vs. real production volume) which may be a reason to revise and check the appropriateness of the current system.

Table 3. Use of real-time simulation during system operation

	boundary conditions	**simulation period**	**use of results: differences model vs. real performance**
real-time simulation (in parallel to system operation)	real boundary conditions as from monitoring data	one (or few) time steps (few minutes)	indicate system failure or degradation in system performance of some equipment
ex-post simulation	real boundary conditions as from monitoring data	variable, depending on specific objectives	calibration of model parameters
ex-ante simulation	estimated boundary conditions	day / week / month	may indicate a substantial change in boundary conditions (e.g. expected vs. real production volume)

b) model-based optimisation of system control parameters

Model based optimisation of system control parameters within EINSTEIN relies on the following steps and features:

- *forecast of boundary conditions* for the near future (the next minutes or hours). Relevant boundary conditions that may have an impact on optimum system control can be e.g. the expected evolution of heating, cooling and electricity demands and the availability of waste heat, but also economic and environmental parameters such as the expected evolution of electricity tariffs or the composition of the electricity mix (e.g. availability of renewable electricity). There are lots of different possible methods for forecasting ranging from simple extrapolation of the trend from the (recent) past up to complex algorithms for pattern recognition.
- capability to *forecast system behaviour* for the near future under a given set of system control parameters. This can easily done using the EINSTEIN system simulation kernel (analogous to real-time simulations with real boundary conditions, substituting real input data by virtual forecast data).
- applying a *parameter optimisation algorithm* based on repeated forecast simulations.
- *communicate the desired new values for system control* parameters to the real system control

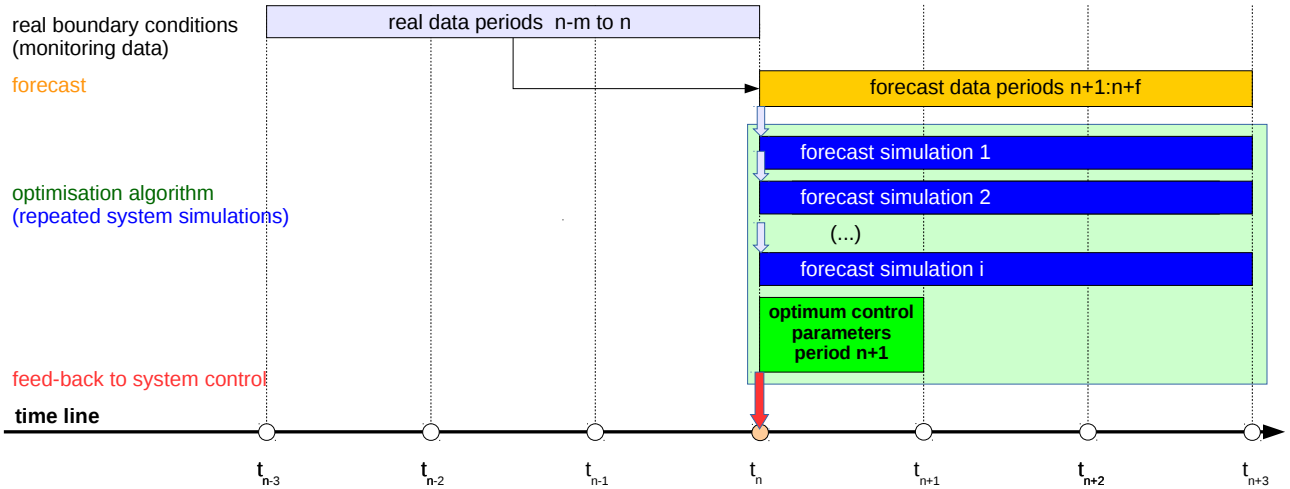


Figure 2. Sequence of operations in model-based optimisation.

2.2 Output and Results Generated

a) consistency and completeness checking of data

The consistency and completeness checking of data is an important operation to be carried out at the stage of data collection.

EINSTEIN has designed so that the format and type of input data is as flexible as possible, so that the user can enter data directly as available without the need for conversion. For giving some examples

- data can be entered in any measurement units. unit conversion is done internally within EINSTEIN
- flow rates can be entered as mass or volume flow rates
- quantities (energy, mass, volume) can be either specified directly or by the corresponding (average) flow rate and the flow duration
- etc.
- time series data can be entered in several different formats, such as hourly data, monthly data, or aggregate data for any other periods specified by the user

This desired flexibility in the data input has two important consequences:

- there may be many white fields in the data entry templates. Data entry in EINSTEIN follows the principle: "*fill in the data You have available, don't worry about the rest*". As from our experience, new users have to get used to this.
- there may be both lack and redundancy of data.

In the case of data redundancy, EINSTEIN automatically tests if data are consistent and emits corresponding warnings if this is not the case.

In the case of lack of data, EINSTEIN disposes of a series of strategies and algorithms to calculate – or if this is not possible – to estimate missing data. For further details on this feature see the corresponding sections in the EINSTEIN Audit Guide [1] and the EINSTEIN Technical Manual [2]. Also here, in case it should not be possible to build a complete data set even using the data estimation algorithms, EINSTEIN emits the corresponding warnings and provides a list of missing data.

b) assisted generation of proposals for energy savings

An arbitrary number of alternative proposals for energy savings may be generated, either manually, semi-automatically using the EINSTEIN design assistants, or a combination of both.

An alternative proposal is a complete model of a new system for the plant, and contains the following information:

- specifications for new equipment: type / model and size, relevant technical data, estimate for investment and O&M costs
- connections for new, and – optionally – changes of connections for existing equipment
- changes in process parameters and system control

As an input and support to both manual and semi-automatic design, EINSTEIN provides an analysis and detailed breakdown of present state energy consumption, e.g. energy demand by fuels, by equipment, by processes, by temperature levels, by time intervals etc. A module for Pinch analysis provides additional information as a basis for heat exchanger network design, but also for implementation of other technologies such as heat pumps or waste heat to power. This information is available both as tables and as graphs.

c) energy performance: dynamic system simulation

Evaluation of energy performance in EINSTEIN is done based on a fully dynamic system simulation. The standard is a one year simulation with 1 h time intervals. Time intervals can be reduced (typical value: about 5 minutes) for real-time simulations.

As an output the state of the system (temperatures, flow rates, powers etc.) at any point within the system (inlet/outlet of each utility, etc.) and at any time interval is obtained.

As for the present state, a detailed breakdown and appropriate aggregate data (e.g. monthly, yearly) are generated in form of tables and graphs.

d) economic and environmental performance

A full detailed economic analysis can be carried out based on yearly cash flows. All economic and cost parameters can be customised by the user, while default values are provided by EINSTEIN. The usual synthetic results such as pay-back, IRR, NPV etc. are generated for each of the alternative proposals

With respect to environmental analysis, values for CO_2 and nuclear waste generation and water consumption are automatically calculated for each of the alternative proposals

e) comparative study

Several graphs and tables with the most relevant aggregate results, providing a comparative study of possible options and the base case scenario are provided (see e.g. Figure 19 and Figure 20. As a synthesis, a graph showing the comparison and trade-off between primary energy saving and cost saving is given (Figure 21). The user can select the best option following his/her own specific optimisation targets (microeconomic, macroeconomic, environmental, ...).

Table 4 summarises the outputs and results generated by EINSTEIN for the use case System Design.

Table 4. The main outputs and results generated by EINSTEIN for the use case System Design

Stage of Design Process	**Outputs**	**Results**
collect data	*consistency and completeness check:* - list of conflicts in data specification - list of missing data, estimated values and error margins	consistent model of the base case scenario: - system configuration and parameters - boundary conditions
create proposals	graphs and tables providing a detailed breakdown of present state performance as a starting point (including pinch analysis) (semi-) automatically generated models for alternative proposals	 models for several alternative proposals
compare and select the best	*energy performance:* - results of dynamic system simulation for any of the alternative proposals. In principle any system parameter (flow rate, power, temperature, etc.) can be obtained as a corresponding time series. - aggregate results and break down of energy consumption are produced analogous to that of the present state *economic and financial analysis* - full detailed economic analysis based on yearly cash flows - usual synthetic results such as pay-back, IRR, NPV etc. for each of the alternative proposals *environmental analysis* calculated values for CO2 and nuclear waste generation and water consumption for each of the alternative proposals *comparative analysis* several graphs and tables with the most relevant aggregate results, providing a comparative study of possible options and the base case scenario	Detailed performance data (energy, economic and environmental) for all alternative proposals Multi-dimensional comparative study of all options as a synthesis (best option selected)
convince the decision makers	automatically generated detailed report (Open/LibreOffice – spreadsheet format). Available in several languages: en, bg, cat, cz, de, es, fr, it, pl, si, sk. Can be edited and customised. User can provide own templates (e.g. with own logos, in other languages, etc.)	proposal for an energy saving investment supported by a detailed audit report

2.3 Show Case

2.3.1 Motivation for the Design of the Show Case

A show case for demonstration of the EINSTEIN functionality has been built around one of the i-ThERM pilot projects for heat to power conversion, as those pilot projects are currently at the most advanced stage.

Waste heat to power conversion with relatively low conversion efficiencies (25 % or less) in most cases is not competitive with direct heat recovery, whenever there is an appropriate demand for heat at sufficiently low temperature and comparable amount of energy (although limit cases may arise due to too large distances between the origin of waste heat and the heat consumer, which would lead to a too high additional investment for piping).

Therefore, in our show case we suppose that there is a waste heat stream appropriate for heat to power conversion (HTP), but no corresponding appropriate and nearby low temperature heat demand. As possible alternative system we consider the use of the waste heat in a high temperature heat pump (HP), for providing saturated steam at a temperature well above the temperature of the available waste heat.

The outcome of a comparative analysis of those systems depends on the relative index (cost, ratio of environmental parameter: primary energy, CO2, etc.) between the fuel saved (e.g. natural gas) and the electricity saved (in the case of waste heat to power) or consumed (in the case of a high temperature heat pump). Following Figure 3 (see Annex 2 for the mathematics behind), and depending on the conversion efficiencies for both technologies, the break-even is between a relative index electricity/fuel of 1,5 (for high efficient HTP and low efficiency HP) and 2,5 (vice versa). Furthermore, economic analysis of course in addition depends on the relative investment costs of both technologies.

In the case of a variable index for cost and environmental parameters in the electricity grid also a combination of both technologies is an option worth being analysed. In this case the control parameters for switching operation between the two systems have to be optimised.

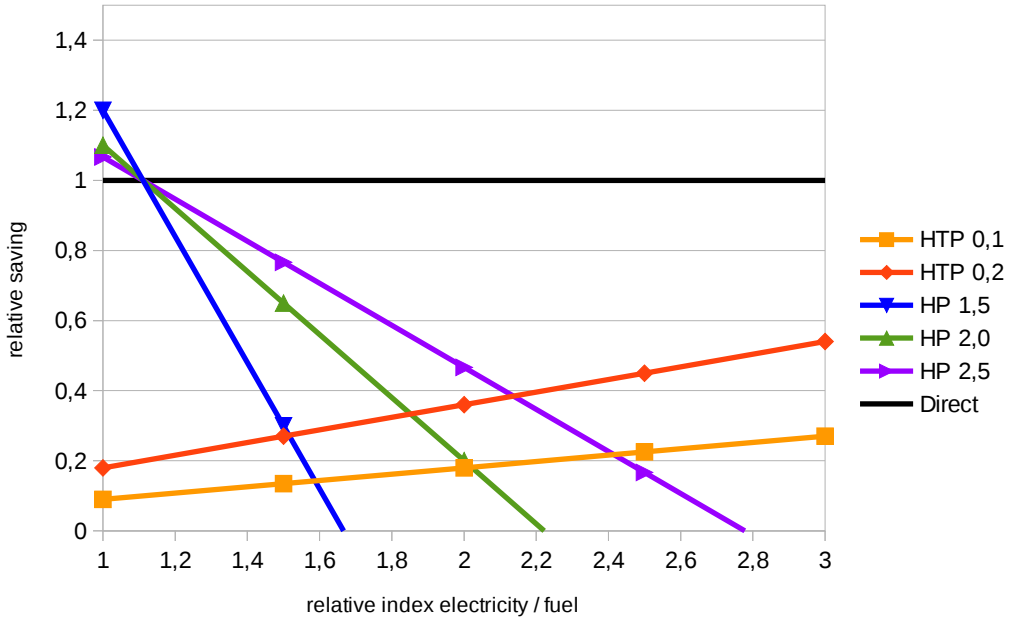


Figure 3. Relative saving (cost, primary energy, CO_2, etc.) per unit of available (waste) heat as a function of the relative index of electricity vs. fuel used. HTP: heat to power conversion with net electric efficiency 0,1 and 0,2. HP: heat pump with effiencies 1,5, 2,0 and 2,5 (COP for heating). Reference conversion efficiency for heat generation: 0,9. Direct heat recovery is used as reference defining the level of relative saving = 1,0.

In the following sections some of the most important tool features are demonstrated for the use case system design (energy audit).

2.3.2 Collect Data: Building a Model for the Base Case Scenario

The first step in energy assessment is the collection of available data:

- an inventory of utilities and processes including all the relevant technical data
- operating and boundary conditions (e.g. production volumes, etc.)

a) an inventory of utilities and processes

The scheme of the base case scenario is shown in Figure 4. In the system there are three heat consuming processes:

- "***process_WH***": a process consuming some high temperature heat at 170 °C and generating waste heat in form of hot cooling water at 90 °C.
- "***steam_LP***": a process consuming low pressure steam at 120 °C (2 bar).
- "***buildings heating***": Space heating demand for buildings

Heat supply is provided by a steam boiler generating high pressure steam at 180 °C and 10 bar, supplying heat to the processes "***process_WH***" and "***steam_LP***", and a hot water boiler providing hot water for space heating. Both boilers are fired by natural gas. The full data set (list of input parameters) describing this base case is given in Table 6.

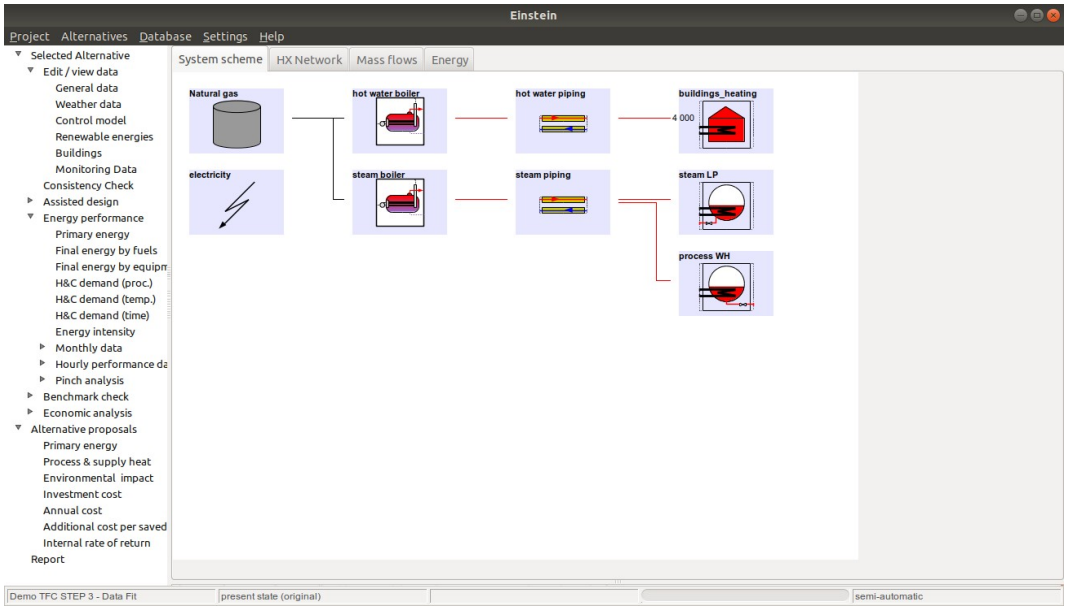


Figure 4. Scheme of the system (base case scenario)

Table 5. Listing of input parameters for the EINSTEIN model.

Parameter	**Unit**	**Value**
Processes		
Process WH (process generating waste heat)		
heat demand (maintenance)	kW	2 649
process temperature	°C	170
minimum temperature difference for heat supply	K	0
residual heat: cooling water	medium	water
cooling water flow rate	kg/h	30 347
cooling water outlet temperature	°C	90
Steam LP (process consuming low pressure steam)		
heat demand (maintenance)	kW	1 600
process temperature	°C	120.5
minimum temperature difference for heat supply	K	0
heat demand (inflow of feed water)	medium	water
feed water flow rate	kg/h	2617
feed water inlet temperature	°C	60
Building		
yearly heating demand for space heating	MWh	4 000
yearly demand for cooling and air conditionning	MWh	0
daily demand for domestic hot water	m3	0
period for space heating		from 01.10 to 31.03
required temperature level for heat supply	°C	55
indoor temperature	°C	20
Heat supply and distribution		
High pressure steam	medium	steam_10bar
type of boiler / fuel		steam boiler / natural gas
nominal power (heat output)	kW	10 000
boiler efficiency	%	90
steam temperature (forward / return)	°C	180.0 / 80.0
rate of recirculation of condensate	%	100
piping length (one way)	m	800

Table 6. (continued)

Parameter	**Unit**	**Value**
Hot water (space heating)	medium	water
type of boiler / fuel		hot water boiler / natural gas
nominal power (heat output)	kW	4 000
boiler efficiency	%	90
hot water temperature (forward / return)	°C	70.0 / 55.0
rate of recirculation	%	100
piping length (one way)	m	10 000
Other information		
Fuel and electricity tariff		water
Natural Gas	€/MWh	40.0
Electricity (purchase / sales)	€/MWh	100.0 / 100.0
Products		water
Some product	t	n/a
Period of operation of the plant		water
Days per year	d	365
Hours per day	h	12.0

b) operating and boundary conditions

In the present show case it is supposed that the only available information on the schedules of processes in time are available monitoring data, which nevertheless are not directly monitoring the processes' operation. The available monitored data are:

- the steam generation in the steam boiler supplying both processes
- the hourly production volume of the final product

The latter one can be correlated to the cooling water flow of process "***process_WH***".

In order to build a base case scenario it is furthermore supposed that production will increase by about 25 %.

Monitoring data are available in form of a csv-data file and can be automatically imported and scaled up, accounting for the expected growth rate.

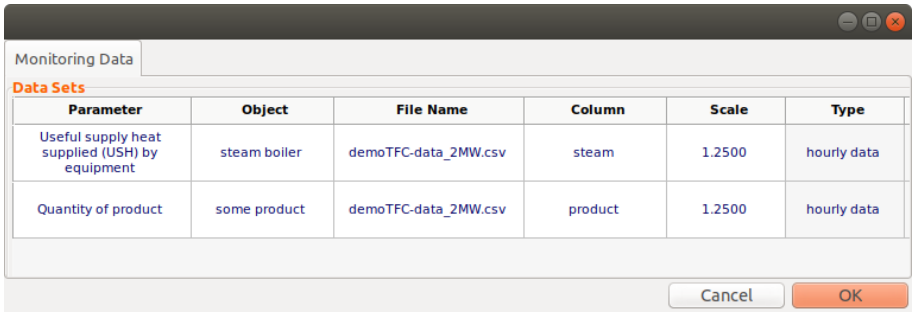


Figure 5. Association between monitoring data and the corresponding quantities in the system model as defined in the EINSTEIN GUI: steam flow rate provided by the steam boiler and quantity of product "some_product" produced. A scaling factor of 1,25 is applied in order to account for an increase in production volume in the future.

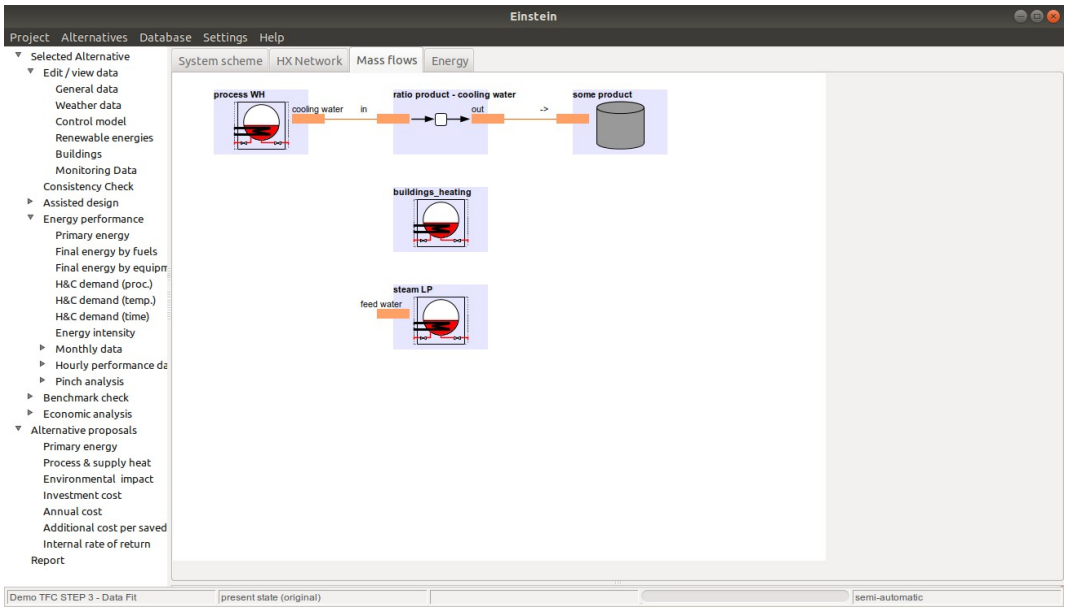


Figure 6. Correlation between cooling water flow (output of process_WH) and quantity of product "some_product" in the mass flow editor within EINSTEIN.

Operation schedules of the processes are then calculated by automatic parameter fitting. The estimation of the time schedule of process "process_WH" in this example is trivial, as the process heat demand is proportional to the production quantity specified within the data.

$$UPH_{process\,WH}(t) = c * m_{some_{product}}(t) \qquad (2.3.1)$$

The estimation of the time schedule of process "steam_LP" nevertheless even in this simple example is more complex, as it is related to the 2 data sets and – in addition – to the heat losses in the steam piping defining the distribution efficiency η_{dist} with some degree of uncertainty:

$$USH(t) = \eta_{dist} * (UPH_{process\,WH}(t) + UPH_{steam\,LP}(t)) \qquad (2.3.2)$$

With Eq. 2.3.1 for $UPH_{process_WH}$ this gives

$$UPH_{steam\,LP}(t) = \frac{USH(t)}{\eta_{dist}} - c * m_{some\ product}(t) \qquad (2.3.3)$$

The resulting time schedule for the heating demands can be seen in Figure 7.

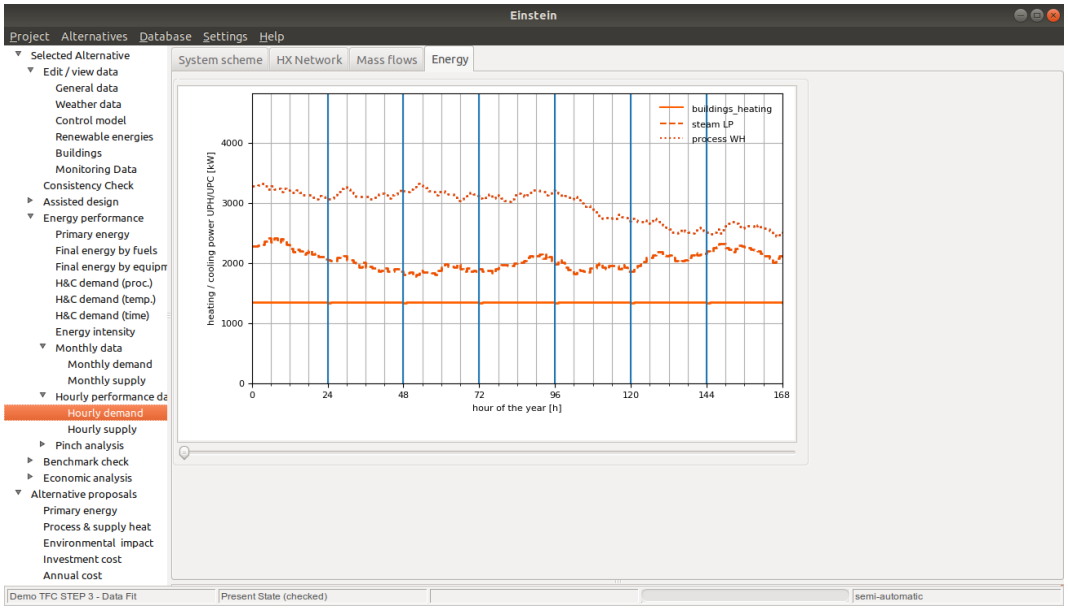


Figure 7. Hourly heating demand for the three processes as a result of data fitting. Shown for the first week (168 hours) of the year.

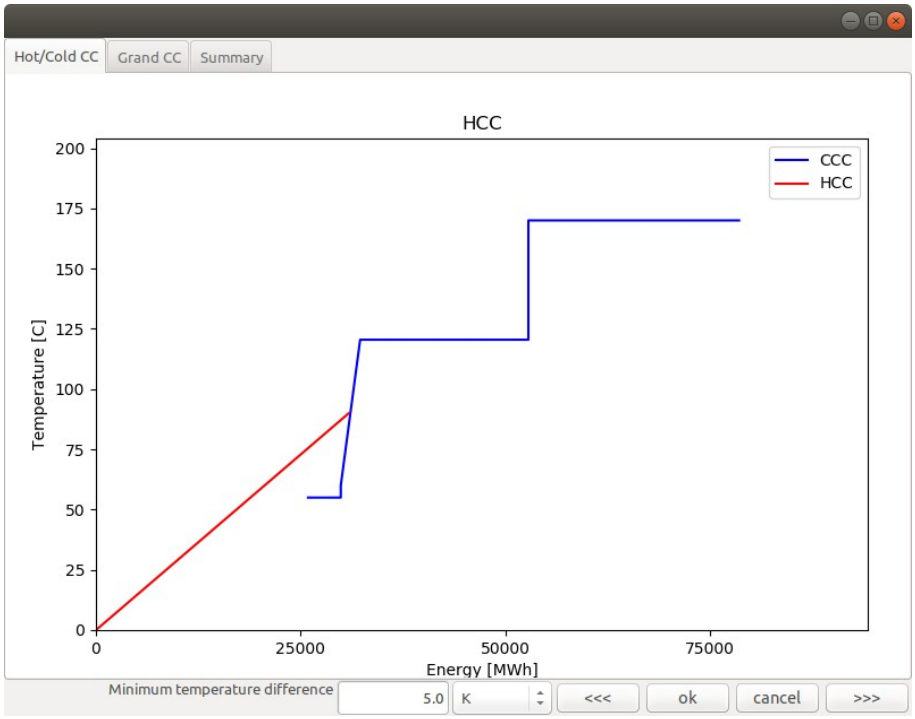
2.3.3 Proposal for Heat Exchanger Network

a) analysis and detailed breakdown of present state

One of the most important data to be used as starting point for evaluation the potential for heat recovery and designing a heat exchanger network is carrying out pinch analysis for the present state situation. This is done automatically by EINSTEIN once the model for the base case scenario is completed (Figure 8).

From Figure 8a a theoretical heat recovery potential for covering all heat demands below 85 °C can be seen, this is part of the preheating demand for process “steam_LP” and the building heating demand. The lower part of the Grand composite curve in Figure 8b shows the amount and quality (temperature level) of waste heat which would still be available even after all the heat recovery potential has been exploited.

(a)



(b)

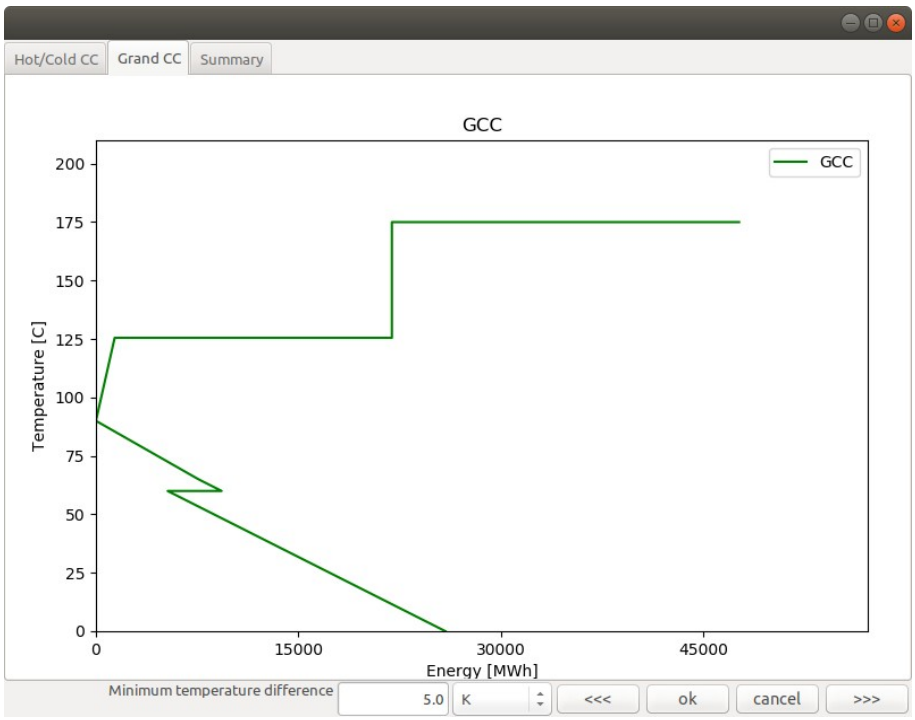


Figure 8a

Figure 8. Results of pinch analysis. (a) Hot and cold composite curves; (b) Grand composite curve. ΔT = 5K.

b) first approach: automatic design of HX network

EINSTEIN design assistants provide tools for (semi-) automatic pre-design of energy saving options. In this case the automatic pre-design of a heat exchanger network is demonstrated.

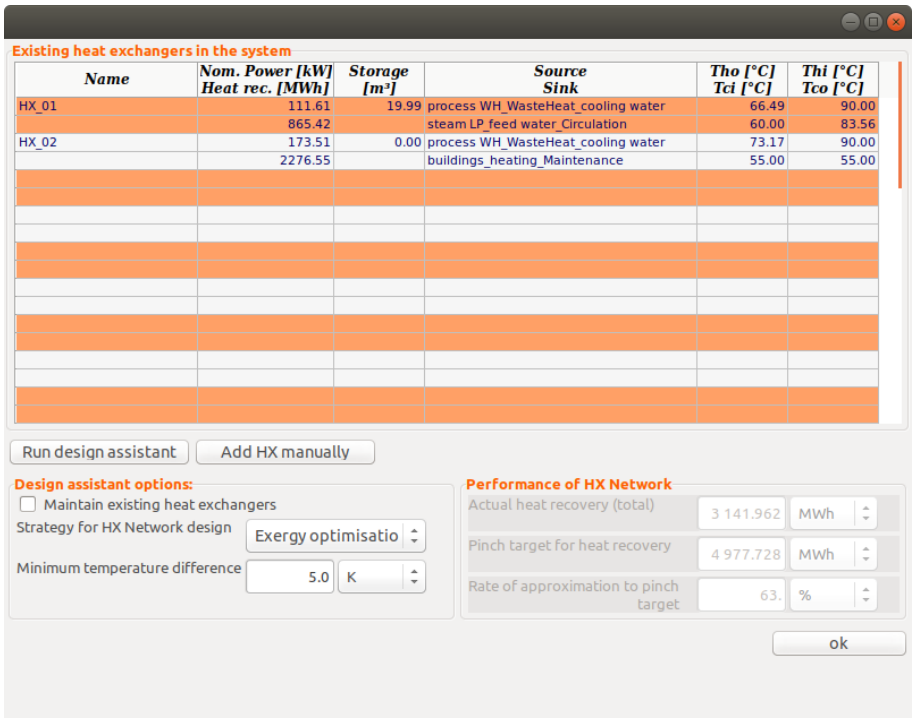


Figure 9. EINSTEIN design assistant showing results of the automatic pre-design of a heat exchanger network.

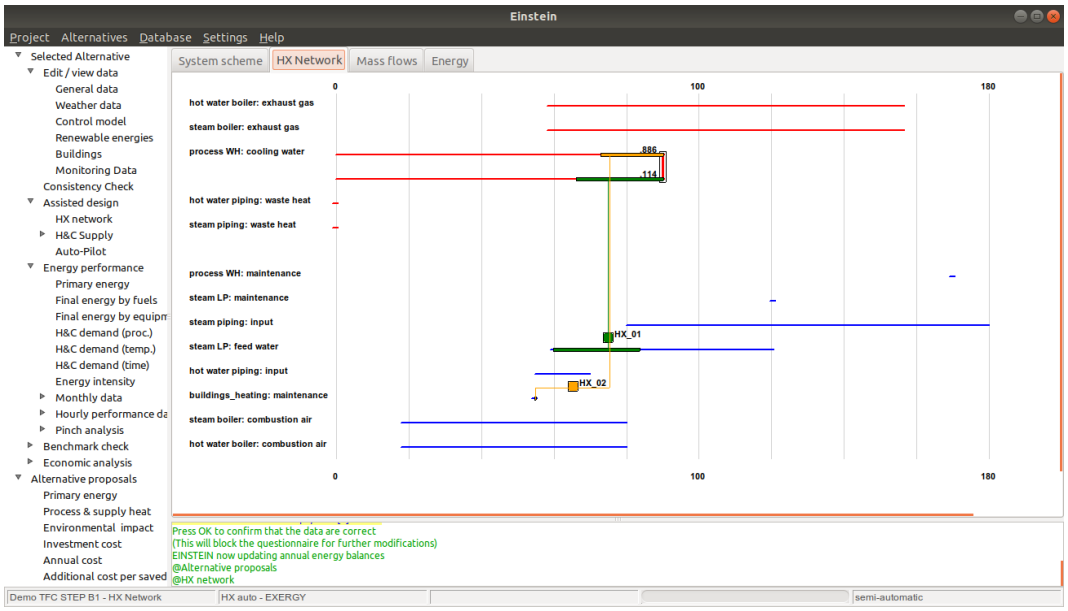


Figure 10. Scheme of the resulting heat exchanger network

c) manual fine tuning

Supposing that – e.g. due to non technical reasons, such as cost of piping, contractual issues, etc. - feeding recovered heat for providing space heating in buildings is not possible, the corresponding heat exchanger can be manually deleted from the system, maintaining only the proposed heat exchanger for feed water preheating.

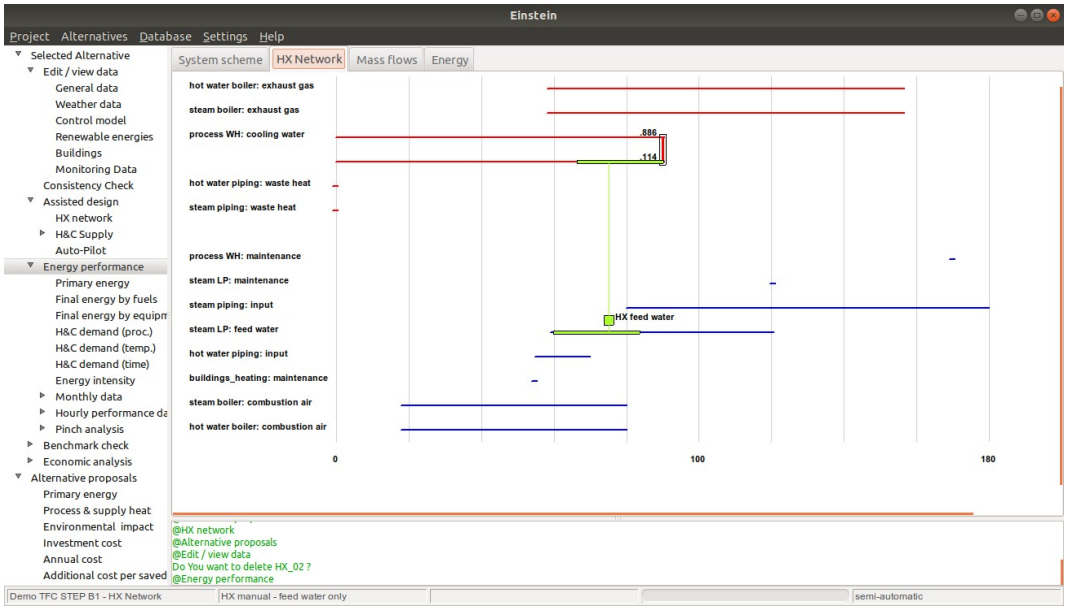


Figure 11. Scheme of the remaining heat recovery after manual fine tuning

2.3.4 Proposal for Waste Heat to Power Conversion

a) design of the alternative scenario and analysis of energy performance

In a new alternative scenario, a waste heat to power (HTP) conversion unit using a low temperature heat source can be manually added to the system (Figure 12). Figure 13 and Figure 14 show the points of operation of the system (electric efficiency as a function of driving tempearture and part load behaviour).

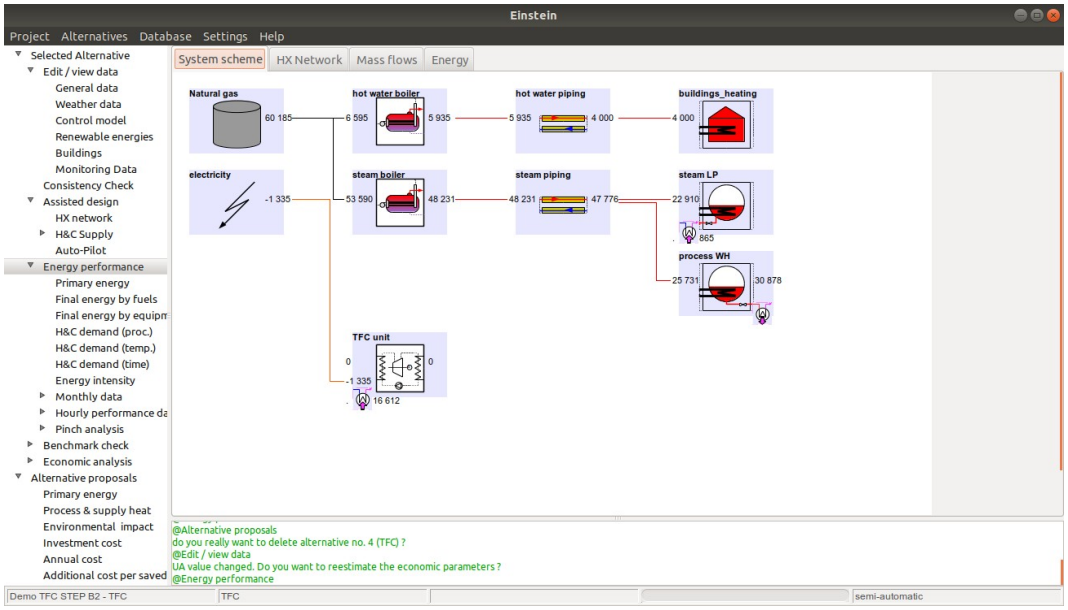


Figure 12. Scheme of the new system including a HTP unit

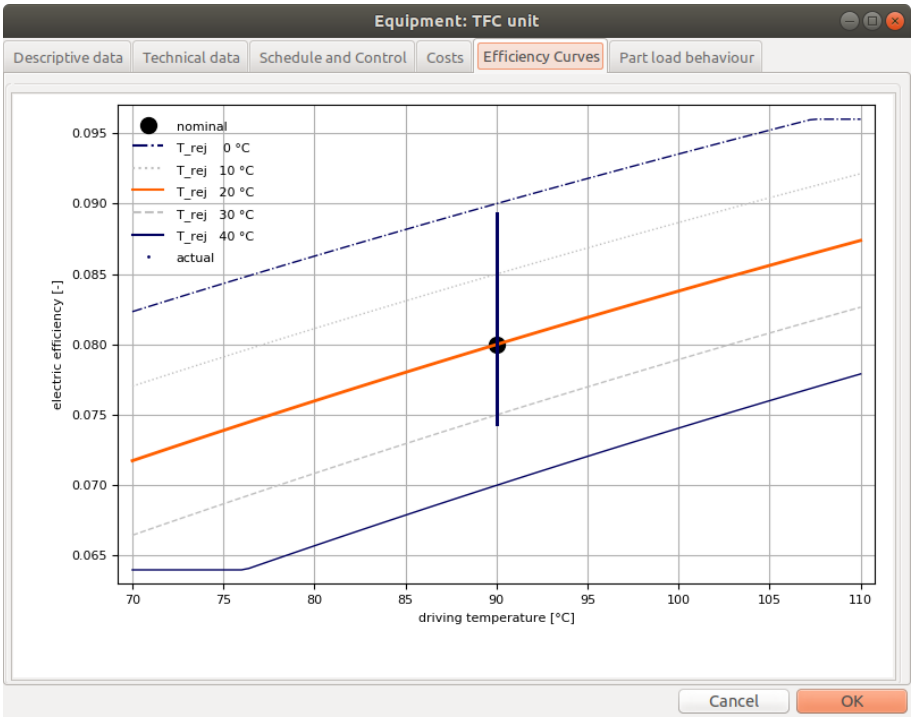


Figure 13. TFC unit. Electric efficiency as a function of the driving temperature. Region of operating temperatures in the example.

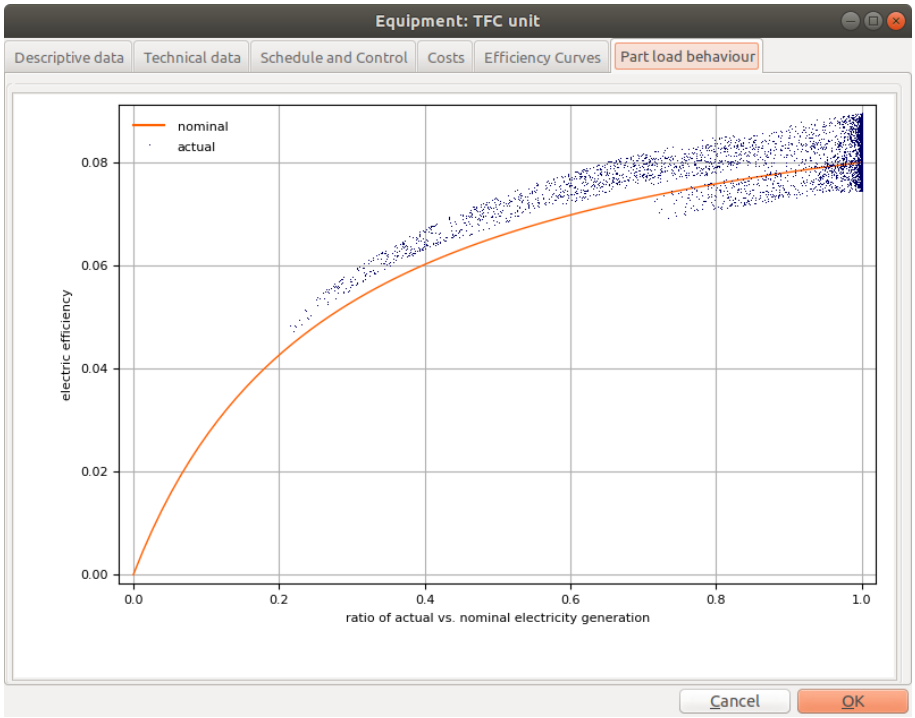


Figure 14. Electric efficiency as a function of the part load ratio. Dots indicate the range of actual operating conditions in the example.

b) economic analysis

EINSTEIN allows also for economic analysis. Some details for the given example are shown in the following figures. Figure 15 shows some of the cost details (here: investment cost and subsidies, energy costs) for the alternative scenario with a TFC unit. The resulting summary of economic performance is given in Figure 16.

(a)

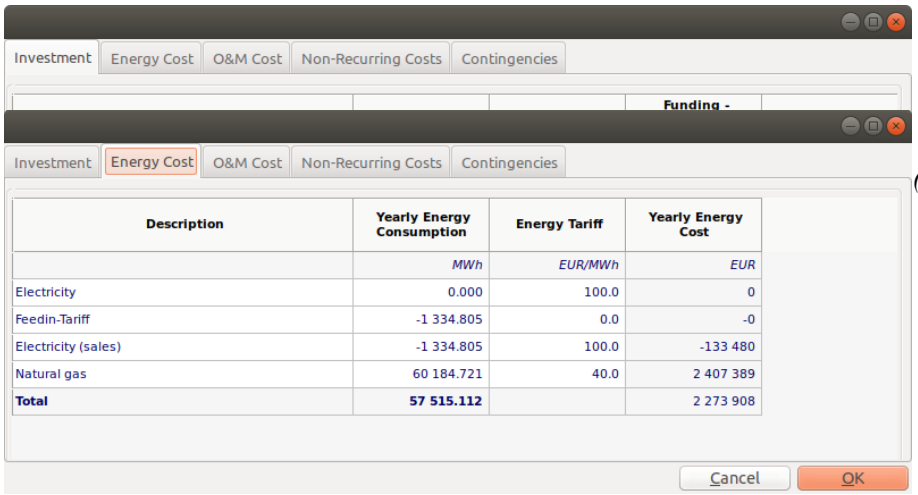


Figure 15. Cost (b) energy costs

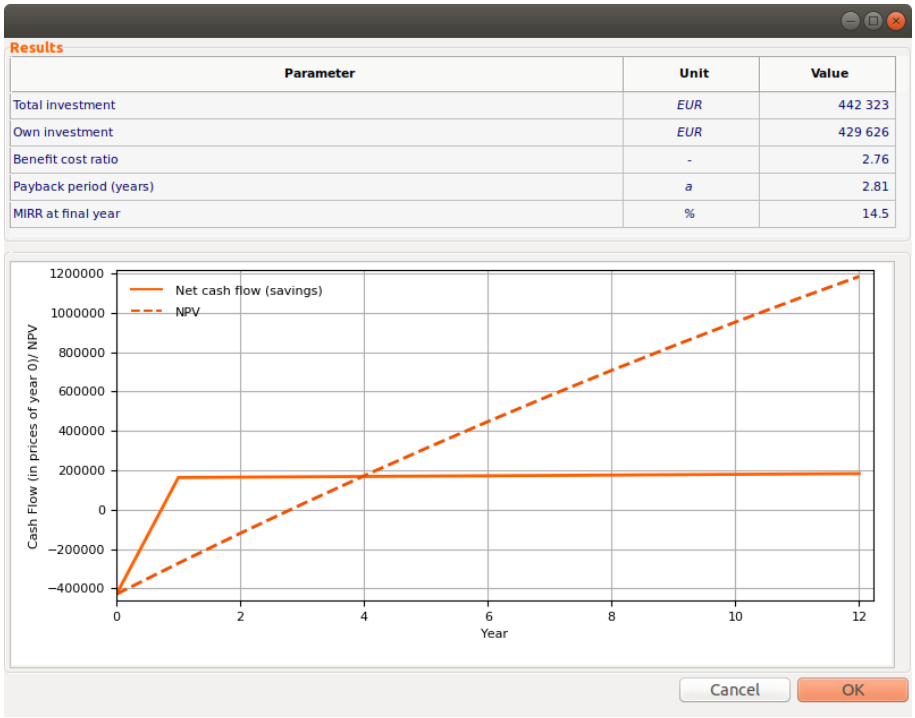


Figure 16. Economic performance for the alternative scenario with TFC unit.

2.3.5 Proposal for a High Temperature Heat Pump

The installation of a high temperature heat pump could be a possible competing technology for the previously proposed heat to power conversion. In this case a heat pump would rise the temperature of the available waste heat from below 90 °C to above 120 °C in order to reuse the energy for process heating.

A preliminary design can be done for example with the semi-automatic design assistant for heat pumps in EINSTEIN. Figure 17 shows the scheme of the new system with heat pump and Figure 18 shows the contribution of the heat supply equipment to the total heat demand.

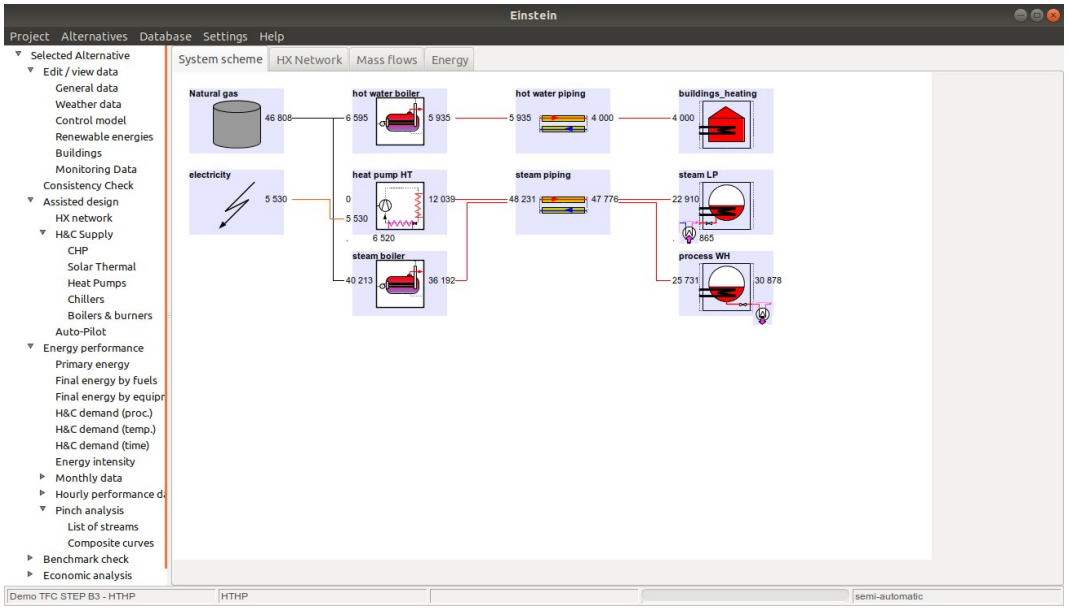


Figure 17. Scheme of the system with high temperature heat pump.

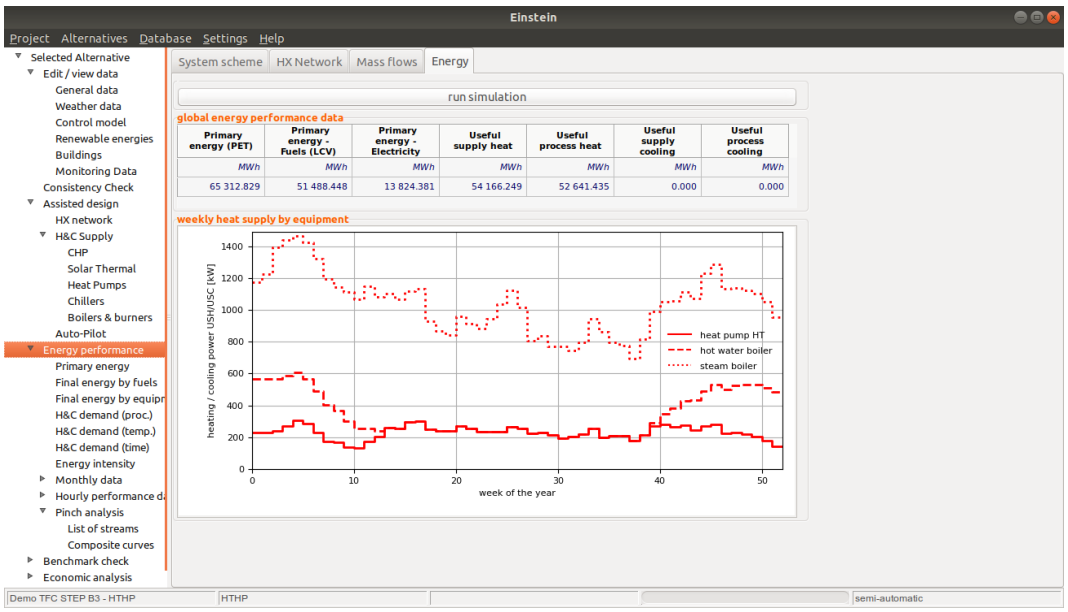


Figure 18. Contribution of equipment to the total heat supply.

2.3.6 Compare and Select the Best

The overall performance of the systems can be compared with regard to energy (Figure 19), environmental and economic (Figure 20) performance. With regard to economic performance, also the influence of a reduced energy tariff (reduction from 100 to 80 EUR/MWh, corresponding to a ratio of 2,5:1 and 2,0:1 of electricity and natural gas tariffs) has been studied. From Figure 21 it can be seen, that in the system with TFC the total yearly energy system costs slightly increase, as revenues from electricity sales are lower. On the contrary, for the system with high temperature heat pump energy costs are significantly lower, as the cost for electricity driving the heat pump is reduced.

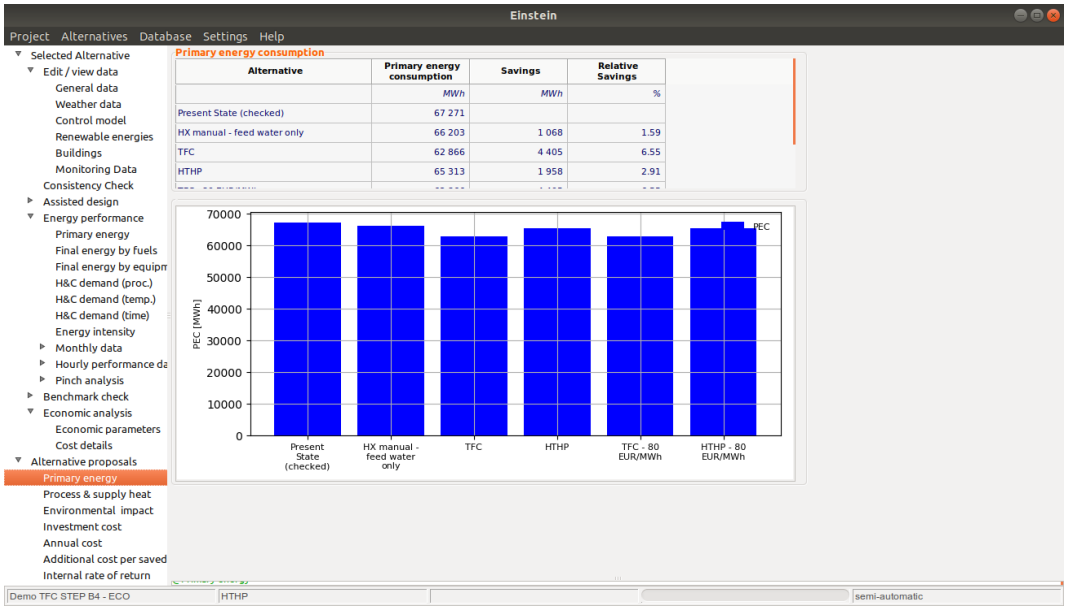


Figure 19. Comparative study: primary energy consumption

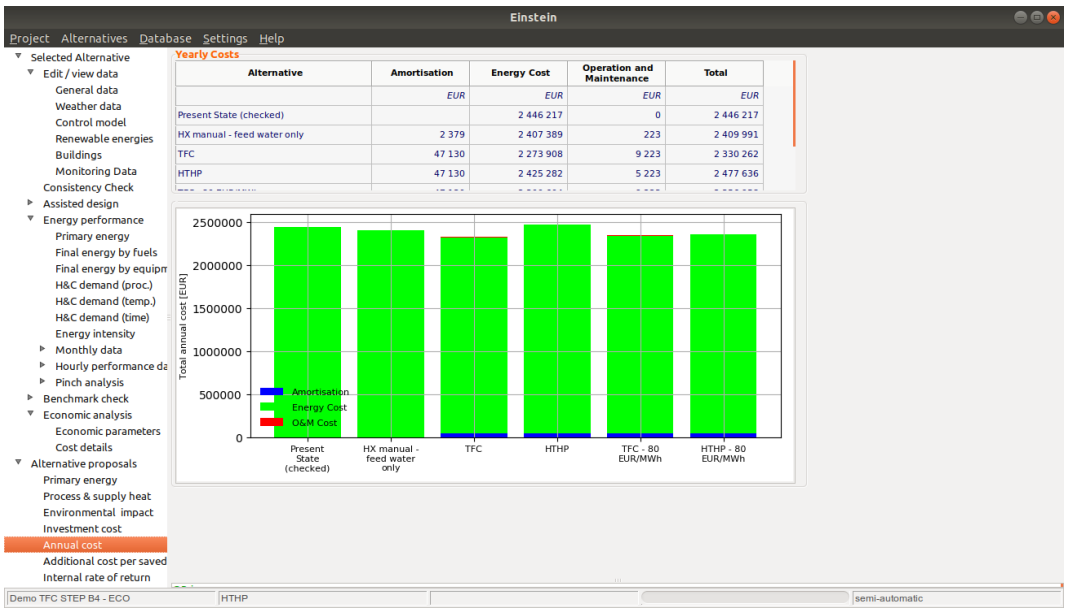


Figure 20. Comparative study: total yearly energy system costs composed by amortisation of initial investment, energy costs and revenues, and O&M costs.

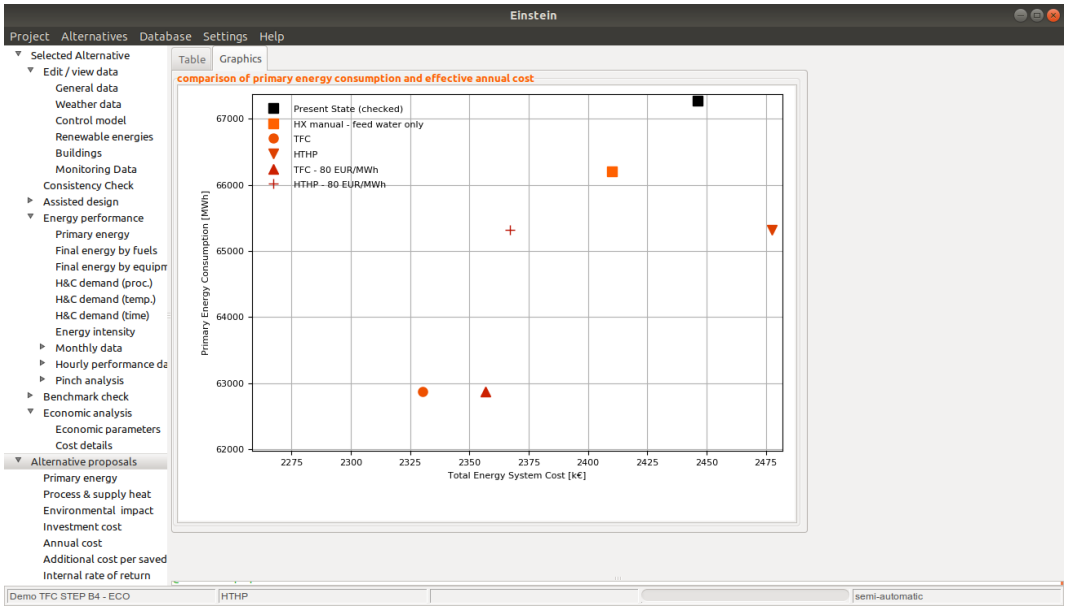


Figure 21. Comparative study: two dimensional graphical comparison of alternative proposals: primary energy and yearly total energy system cost.

2.3.7 Convince Decision Makers: EINSTEIN Audit Report

After concluding the analysis, EINSTEIN automatically generates an exhaustive audit report. As an example the summary of the global results is given in Figure 22.

Show Case Demo TFC

EINSTEIN thermal energy industry audit

Summary

		Present state	Proposed alternative	Savings
Total primary energy consumption (1)				
Total	MWh	67.271	62.866	6,55%
-Total fuels	MWh	67.271	66.203	1,59%
-Total electricity	MWh	0	-3.337	-
Primary energy saving due to renewable energy	MWh			-
CO2 emissions	t/a	15.289	14.379	5,95%
Total annual energy system cost (2)	€	2.446.217	2.330.262	4,74%
Total investment cost(3)	€	-	442.323	-
Pay-back period (4)	a	-	2,8	-

(1) Including primary energy consumption for non-thermal uses
(2) Including energy cost (fuel and electricity bills), operation and maintenance costs and annuity of total investment.
(3) Total investment cost (own investment + subsidies)

Figure 22. Example page of the EINSTEIN audit report

3 Functionality Developed within the i-ThERM Project

3.1 Heat Exchanger Networks for Direct Waste Heat Recovery

A detailed description of this functionality is given in the Deliverable D3.2 report [4]. Here only the most relevant aspects and additional features introduced since then are summarised.

3.1.1 Improvements in Pinch Analysis Module

In the new version V3.0 of EINSTEIN it is possible to manually select / unselect a subset of hot and cold streams for pinch analysis and heat exchanger network optimisation. This gives more flexibility to pinch analysis allowing to include or exclude some of the streams:

- it allows to exclude streams for which heat recovery is not possible for some reasons, such as e.g. large distance between source and sink
- it allows to exclude (or treat separately) heat demands or waste heat streams which are only seasonally available, etc.
- it allows the user to decide whether to include within pinch analysis the heat demands at the process (process streams) or – alternatively – the corresponding heat demand of the heat supply circuit (e.g. steam piping; feed-up water or condensate return as potential cold stream).

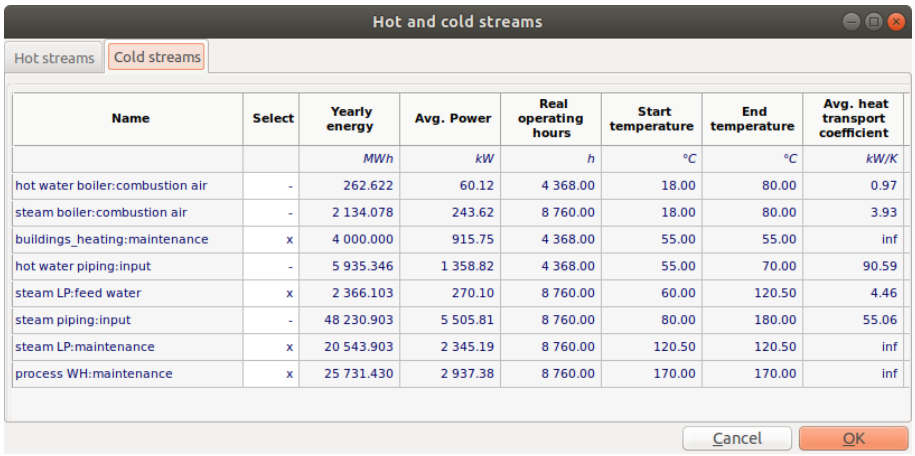


Figure 23. List of cold streams with the possibility to select / unselect streams

3.1.2 Improved Algorithm for Automatic Design of Heat Exchanger Networks

The algorithm for automatic design of heat exchanger networks has been fully revised and improved. A detailed technical description of the new algorithm can be found in the Technical Manual of EINSTEIN [2].

The new algorithm disposes of three modes:

- **Exergy optimisation**: in this mode, a heat exchanger network is proposed which maximises energy recovery but at the same time minimising the requirement of exergy for residual heating / cooling.
- **Minimum size**: in this mode energy recovery is maximised while using a heat exchanger with minimum size (and, therefore, cost).

- **Flow rate matching**: this mode is based on the algoritm used in previous versions of EINSTEIN, resulting in most cases in a simpler heat exchanger network, but with a result further away from the optimum of energy recovery.

3.2 Heat to Power Conversion (HTP)

3.2.1 Models for HTP Equipment

The modelling capability of EINSTEIN has been extended so that now also (waste-) heat to power conversion equipment can be included within the system, including both the innovative technologies being developed within I-Therm (sCO2-turbines and TFC systems) and also other market available technologies such as ORC (organic Rankine cycle) and steam turbines.

The main features of the new module for (waste-) heat to power equipment are described in the technical manual of this software [2, Section 4.4]. Examples and test cases are given in the Deliverable D3.3 report [5].

The heat-to-power equipment can be fed with driving heat either by an active heat supply (boiler, burner, gas turbine, etc.) or by heat recovered from any waste heat stream within the system.

The control of the equipment can be either by the availability of supply heat and/or by an external master control setting the part load ratio.

For simulations within EINSTEIN both systems are treated as a *black box* with an input for the driving hot stream (steam, hot water, other) and the stream for dissipation of the residual heat (cooling water or air), and the generated electricity as an output.

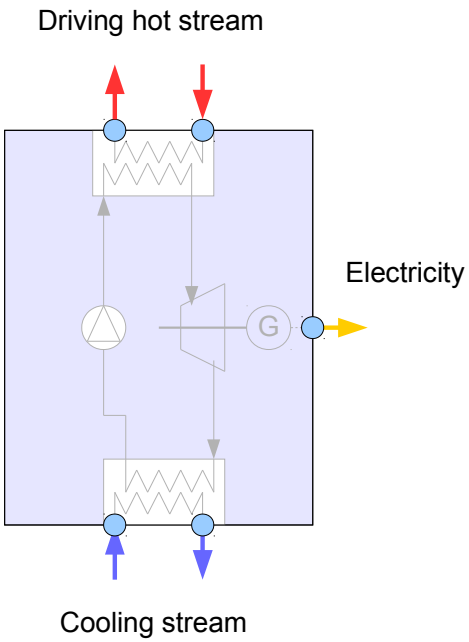


Figure 1. Black box model for waste heat to power generating units (Rankine cycle in the inner of the box only for illustrative purposes; can be substituted by any other cycle).

A specific equipment then is defined by

- nominal operation conditions (nominal power and temperature levels at input and output)
- performance at nominal operation conditions and steady state
- part load behaviour. Within the EINSTEIN model part load correction can be adjusted by a part load correction factor
- performance at off-nominal operation conditions: the equipment efficiency is corrected and adjusted to actual working conditions by using a simple "constant exergy efficiency" model.
- transient operation conditions are not considered relevant in the current EINSTEIN model, as by default one hour simulation time steps are used.

This model has been tested and validated against simulation results with a more detailed model for the TFC turbine developed by project partner Spirax Sarco (see section 5.1)

3.2.2 Grid Integration – Variable Indexes of Electricity Grid

In EINSTEIN V3.0 it is possible to define the relevant economic and environmental parameters of the electricity grid as a function of time:

- cost (electricity tariff, separately for both purchase and sales of electricity)
- environmental parameters (primary energy ratio, CO2 and nuclear waste ratio per kWh of electricity)

By this the interaction of a system with electricity grids with a high fraction of renewable energy sources with fluctuating availability (wind, PV, etc.) can be optimised.

Data can be entered via a data file containing hourly data.

3.3 Processing of Monitoring Data

Monitoring data can be used within EINSTEIN for the following purposes:

- Provide additional information for defining the system configuration in the present state (**calibration of model parameters**)
- Define **boundary conditions** to be used as *input* in system simulations (see section 3.4 on real-time simulations)
- Be used as **reference data** for the validation of the *output* of system simulations

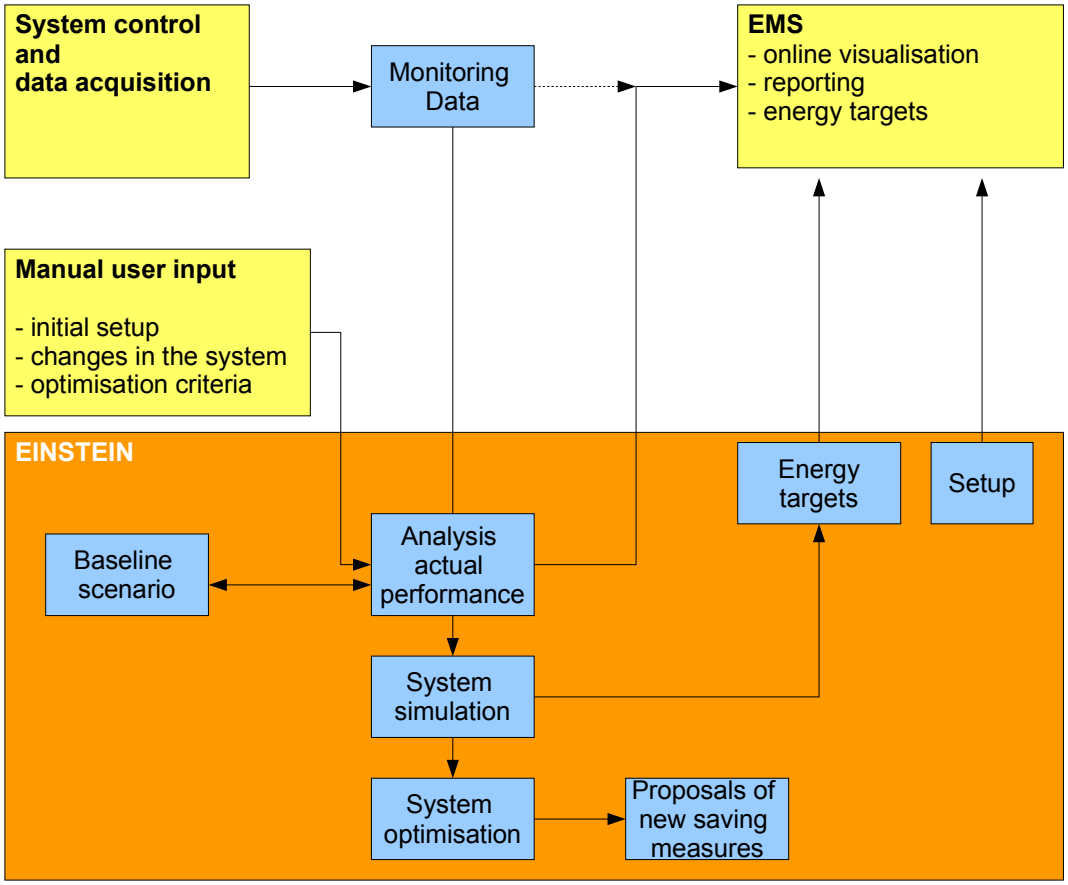


Figure 24 Monitoring data in the data flow between the system control and data acquisition unit, EINSTEIN and an energy management system.

A detailed description of this functionality is given in the Deliverable D3.4 report [6]. Here only the most relevant aspects are summarised.

3.3.1 Type of Monitoring Data

Monitoring data are supplied to EINSTEIN in form of data files in one of the two possible formats:

- time series (hourly data)
- subtotals for periods (e.g. weeks, months, quarters, ...)

Possible quantities to be considered are:

- **energy flows** in any point of the system (e.g. fuel and electricity consumption, heat supply from some equipment or to some distribution piping, heat or cooling consumed in some process, etc.)
- **mass flows** or **product quantities** (e.g. mass flows of any working fluid of some process, quantities of final or intermediate products or raw materials). By correlating process- and energy flows within the system with other parameters, such as **quantities of raw materials and final products**, also monitoring data concerning the latter can be used in the analysis. See also section 4.1.3 (editor and back end calculation module for system mass flows).
- **temperatures** (e.g. temperatures of working fluids at some point of the system, temperature of cooling water or cooling air, etc.)

See section 2.3.2 (Figure 5 and Figure 6) in the show case description as an example for the use of this functionality.

3.3.2 Parameter Fitting using Monitoring Data

Model parameters can be determined to a certain degree of accuracy by parameter fitting: minimisation of the error, defined as the difference between the model outputs and available monitoring data.

Whenever monitoring data are given and associated to some model output of EINSTEIN, this is done automatically during the consistency and completeness check using numerical minimisation algorithms.

Some examples for parameter fitting based on monitoring data (TC-EMS-01 to -03) are described in the D3.4 report [6]. See also section 2.3.

3.4 Real-Time Simulation

The capability of EINSTEIN for carrying out *real-time simulations* has been implemented. Real time simulation with EINSTEIN allows for modelling the system performance at current time and – in consequence - compare the measured real performance with simulation results. This allows for:

- adjustment (calibration) of model parameters
- detection of eventual failures in the operation of the system

For this purpose the major developments introduced into the software have been:

a) protocol for data exchange with the system control

A MySQL database can be used as data hub for transferring data between the system control and EINSTEIN. This allows maximum flexibility, as the data base may be located either on a local computer within the company, or on any remote server in the cloud. At the same time, also EINSTEIN can be run locally or on some remote site (Figure 25).

A protocol for the interface (structure of tables within the data base) has been defined and a default data base for testing has been set-up (see annex 1)

Data transfer can be in both regular and irregular time intervals. Typical time intervals should be in the order of few minutes for practical reasons (compromise between accuracy and volume of data to be transferred and processed).

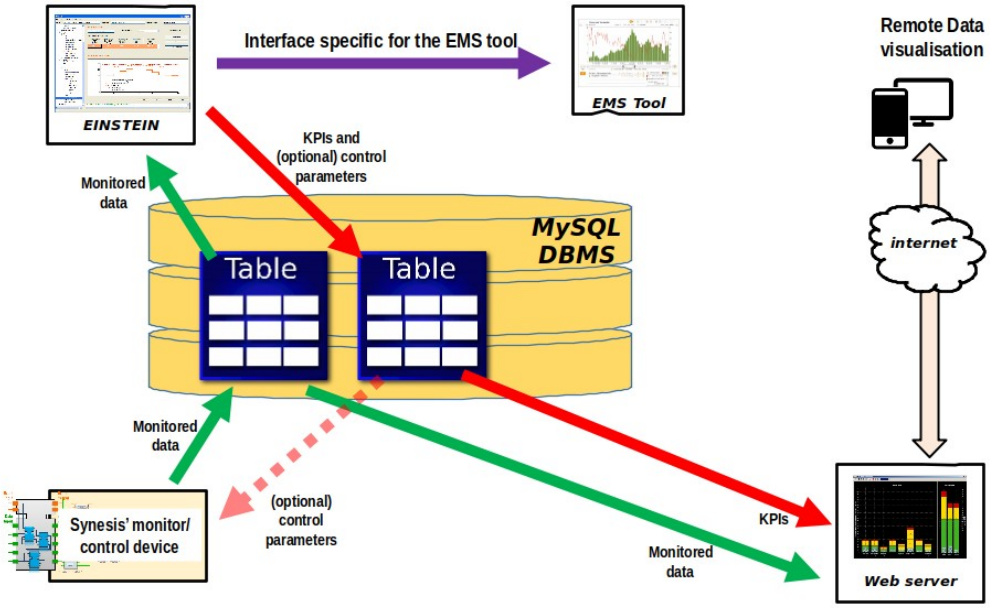


Figure 25. Architecture of system control, EINSTEIN, MySQL data base and web visualisation tools. Source: Andrea Chiodi (Synesis), presentation at i-ThERM project meeting 6 in Uxbridge, London (UK), July 2018.

b) definition of boundary conditions by external data sources

Within the simulation engine of EINSTEIN the possibility to define boundary conditions of the system model by external data sources (data files or data bases) has been added. In the current version the following parameters can be specified externally:

- process heat and cooling demands and waste heat streams (temperature, flow rates, power)
- operating temperatures (driving heat, heat rejection, ambient temperature)
- master control of equipment

Within system simulations, the parameters specified by monitoring data are considered as exogenously given and not recalculated by the simulation algorithm.

The user interface for assigning columns within data sources (data files or data bases) to internal parameters is the same as described above for the processing of monitoring data (section 3.3).

c) simulation with variable time step

EINSTEIN now is able to carry out in variable time steps well below the standard time step of 1 h. The simulation of one (or several) new time steps will be triggered by the availability of new data from the interface with the system monitoring.

The user can define limits (minimum and maximum value) for the simulation time step in EINSTEIN simulations within which the simulation time step automatically adapts to the intervals of data arriving. In principle any simulation time intervals are possible, but for practical purposes (compromise between accuracy and amount of data) simulation and measurement time steps proposed are around 0,1 h (6 minutes).

If the interval between monitoring data is higher than the maximum simulation time step, several time steps are simulated and data for the intermediate times are interpolated. In the other opposite, if monitoring data arrive with a higher frequency than the minimum simulation time step, monitoring data are compressed using sums or average values (Figure 26).

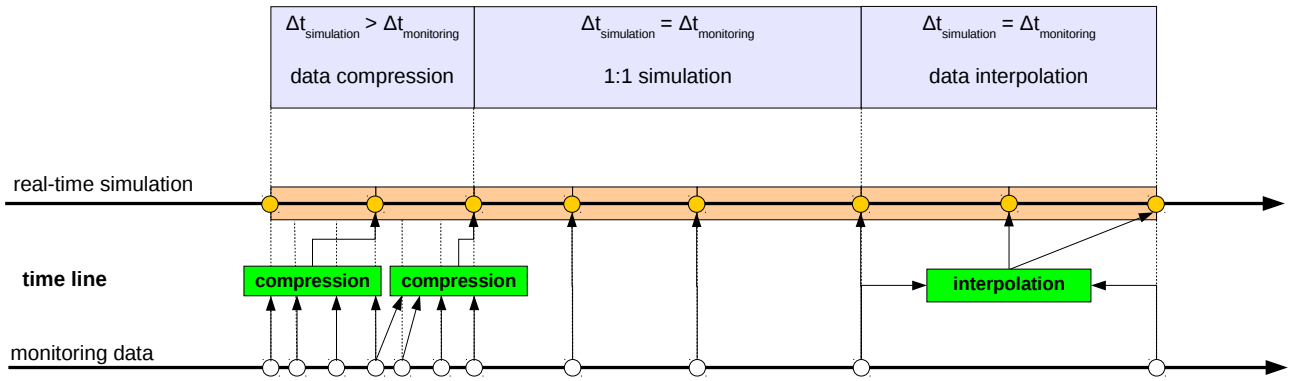


Figure 26. Time step in real-time simulation as a function of the intervals of availability of monitoring data.

d) batch execution from command line

For real-time simulations EINSTEIN is run in the background from the command line without opening a user interface. Simulation results are written into a data file and/or fed back into the MySQL data base and can be accessed there for visualisation or further processing.

3.5 Forecast and Model-Based Optimisation of System Control

System performance can be optimised "on-the-run" based on forecasting system simulations in order to optimise some system control parameters.

In this mode, a new optimisation cycle in EINSTEIN is triggered by the arrival of new monitoring data. Parameter optimisation is carried out by simulating the system under estimated future boundary conditions (forecast) and under variation of a previously defined set of system control parameters. The optimised parameter set then is sent to the data hub and from there then be processed by the system control unit (Figure 2).

The implementation of this feature required the following additional modules and functionalities:

a) adaptation of software structure (data storage, model set-up and calls to simulation kernel)

Some modifications within the internal structure of the software had been necessary in order to allow for parameter variation and repeating simulations under different parameter sets:

- now internally two system models are used: one representing the real system with the real control parameters (1:1 image of the real system), and – in addition – a virtual model where system operation parameters can be changed by the optimisation algorithm
- in each time step two different simulation runs are carried out: one backward looking, simulating the past time step as described in the section on standard real-time simulation, and (n-times repeated) forward looking forecast simulations in order to predict the future performance under different control parameter settings
- some system control parameters have been made accessible for modification by external data sources, instead of being fixed parameters as in standard simulation.

b) implementation of an optimisation algorithm

A module for parameter optimisation has been implemented within EINSTEIN. This module relies mainly on several standard optimisation functions of the python package scipy.optimize [7].

The default method for determining the local optima is *Sequential Least SQuares Programming (SLSQP)* and for global optima the *Brute Force* method. Nevertheless, any other optimisation algorithm available in the scipy.optimize package can be easily implemented, too.

c) forecast of boundary conditions

Model based optimisation builds on forecasting boundary conditions for the near future (typically from few minutes to few hours) based on extrapolation of the past. Currently within EINSTEIN two very simple forecast models are implemented (for a detailed mathematical description see the EINSTEIN Technical Manual [2]. In these simple models the forecasting is done independently for each single variable of the set of boundary conditions:

- *CONST*: boundary conditions are assumed to remain constant at the level of the last time step
- *TREND*: boundary conditions are supposed to start from the last real value (as in CONST) and approach asymptotically to a linear trend. The trend curve itself is (slowly) self-adapting, while the speed of self-adaptation can be configured as one of the parameters of the trend forecast.

More complex models, e.g. based on pattern recognition (cyclical features, etc.), could be added if needed for specific applications.

d) feed-back of optimised parameter values to the real system

The same MySQL data base as used for reading in monitoring data (see above) can be used also for feed-back of optimised system parameters to the real system. For this purpose EINSTEIN writes the results of optimisation into the data base, and the system control can read out there the values recommended by

EINSTEIN and (probably based on additional security checks) implement these new values in the real controller or not.

4 User Friendliness

A major amount of work has been dedicated to the improvement of user friendliness and documentation of the software. The general objective is, in first place, to reduce the "entry barriers" and the required learning effort for getting started with the software, and in second place, also to make the work with the software in general more simple and intuitive, so that the tool can and will be used by a wider target group.

In order to reach this, more specific objectives that have been addressed are:

- to make the model building as self-explaining and intuitive as possible, reducing to a minimum the need for recurring to EINSTEIN manuals or specific EINSTEIN terminology
- where possible give graphical support for model building
- reduce possible confusion for beginners by hiding advanced features and options into a second plane where convenient
- revise and complete the documentation (user and technical manual) where necessary
- improve the tutorial for getting started (based on the already existing beginners' cases described in the EINSTEIN Audit Guide)

4.1 Visual Editing of the Model

4.1.1 Graphical System Editor

Within a fully re-designed EINSTEIN user interface, the graphical system editor, which in earlier versions has been used only for visualisation of energy flows, now is the main interface for the user in order to set-up and edit the system model (see e.g. Figure 4). Components of the system model, such as utilities or processes can be added to the model via this graphical interface. Component parameters can be read and edited by simply clicking on the corresponding symbol, and connections between the components can be established by simple mouse clicks.

A large amount of specific icons has been created in order to visually distinguish different types of equipment, piping and processes.

Furthermore, also heat exchangers are now visualised and can be edited within this graphical system editor

4.1.2 New Editor for Heat Exchanger Networks and Visualisation of Hot and Cold Streams

A new editor has been added for viewing and editing heat exchanger networks. Heat exchangers can be added by simply clicking on the corresponding source and sink streams.

Parameters of heat exchangers can be edited by clicking on the corresponding heat exchanger symbol

The editor offers three different types of view:

- matrix view: heat exchangers are plotted equidistant and ordered by upstream / downstream.
- linear temperature scale: heat exchangers are plotted on their place corresponding to source and sink tempeatures on a linear temperature scale

- logarithmic temperature scale: as above, but using a logarithmic instead of a linear temperature scale.

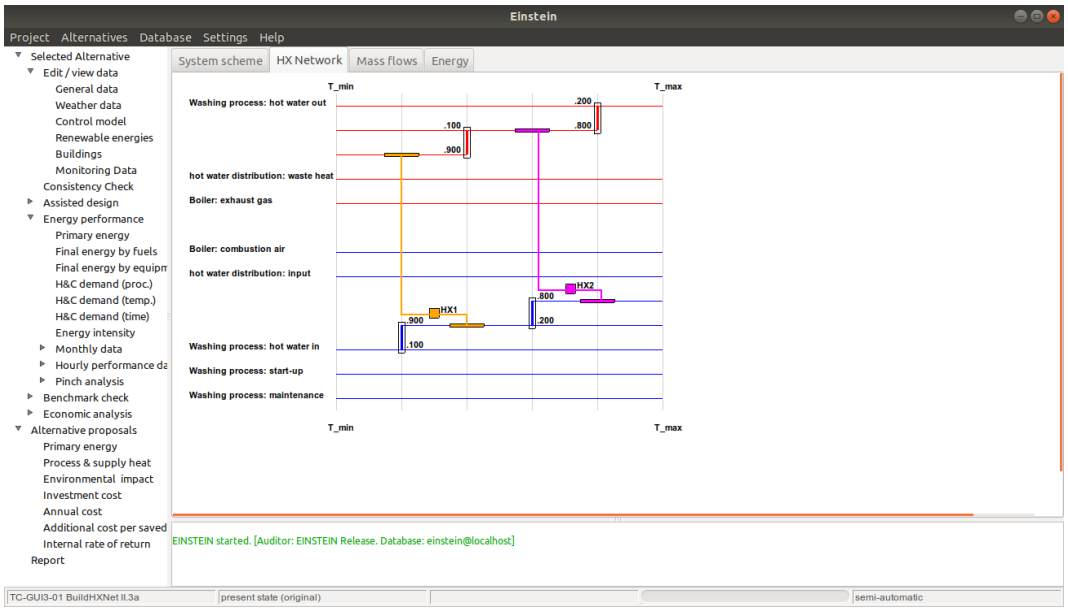


Figure 27. Editor for heat exchanger networks (matrix view).

4.1.3 Editor for System Mass Flows (Production Flow Chart)

The mass flows in different points of the system can be correlated in different ways:

- *direct (input-output) correlation*: e.g. the output of one process may be used (fully or partially) as an input to another process

- *indirect correlation (available information y = f(x))*: the quantity of working fluid to be processed in some process may be correlated to some other quantity in the system, e.g. it may be know from experience that for painting one car (in the average) a certain amount of solvent has to be processed in thermal post-combustion within the paintry section, etc.

EINSTEIN disposes of a graphical editor for mass flows within the system where both types of correlations can be defined (Figure 28; solid lines are input-output connections, whereas dashed lines represent "information flows"), complemented by the corresponding back end module for the calculation and checking of mass balances.

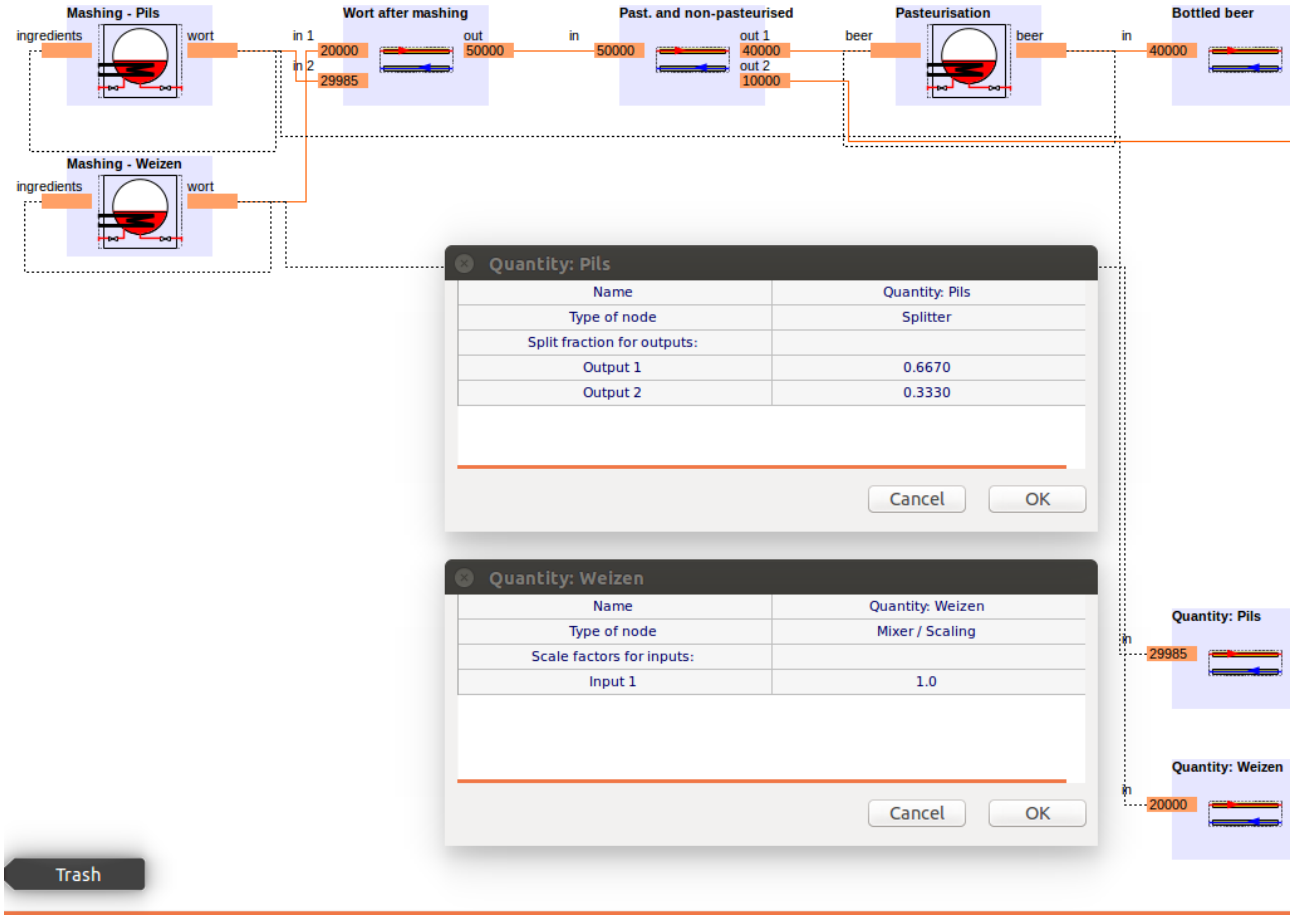


Figure 28 EINSTEIN editor for the mass flow network

Correlations between system mass flows can be used to simplify the data entry for the project. E.g. if the same medium is processed in several processing steps, the corresponding quantity or flow rate has to be defined only once.

Furthermore flow rates of some media from/to the processes can be calculated based on information on other quantities such as (final or intermediate) products or raw materials.

4.2 Improvement of Editors for Component Parameters and Data Bases

A special effort has been dedicated in order to make editors for component parameters (processes, equipment, piping, heat exchangers) more intuitive specially for new users of the software by rearranging parameters, and move optional parameters into a second plane in order to be easily accessible by advanced users, but be hidden at first sight in order to not confuse beginners.

Special emphasis has been given to the components relevant for i-ThERM systems (specially waste heat to power equipment).

4.2.1 Process Editor

Following the standard EINSTEIN process model (see Audit Guide, Chapter 2) process heat (or cooling) demand can be composed by 3 components:

- circulation: heating (cooling) of incoming fluids
- maintenance: compensation of heat losses and latent heat (e.g. evaporation)
- start-up: initial heating (or cooling) of reservoirs

In the new process editor only the parameters corresponding to those demand components which are really used (different from 0) are visible. Other demand components can be added only if needed.

A summary table gives a quick overview of all the demand components present for a given process.

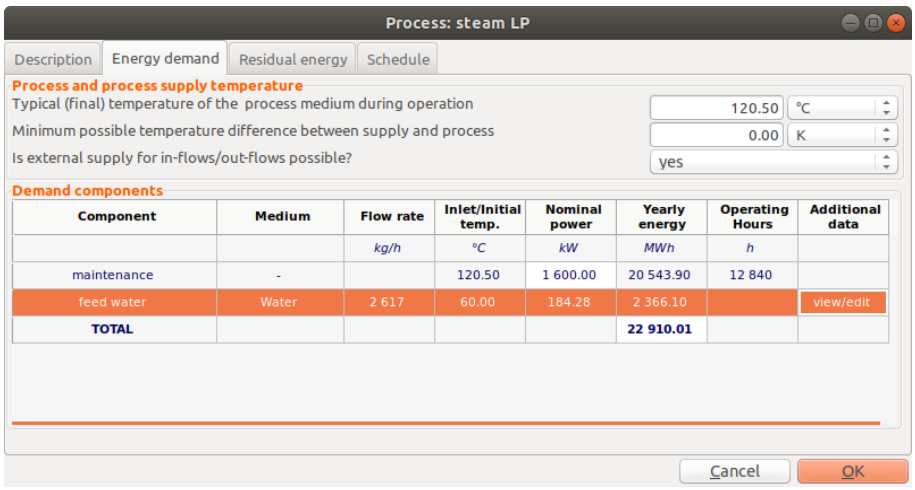


Figure 29 New EINSTEIN process editor

4.2.2 Pipe and Duct Editor

Also the new pipe and duct editor follows the philosophy to make visible only those fields for data entry which are really needed. The user can preselect between a (fully) open circuit, a (fully closed) circuit and a partially closed circuit with recirculation and feed-up, and – depending on this preselection – the editor adapts showing the required fields for data entry.

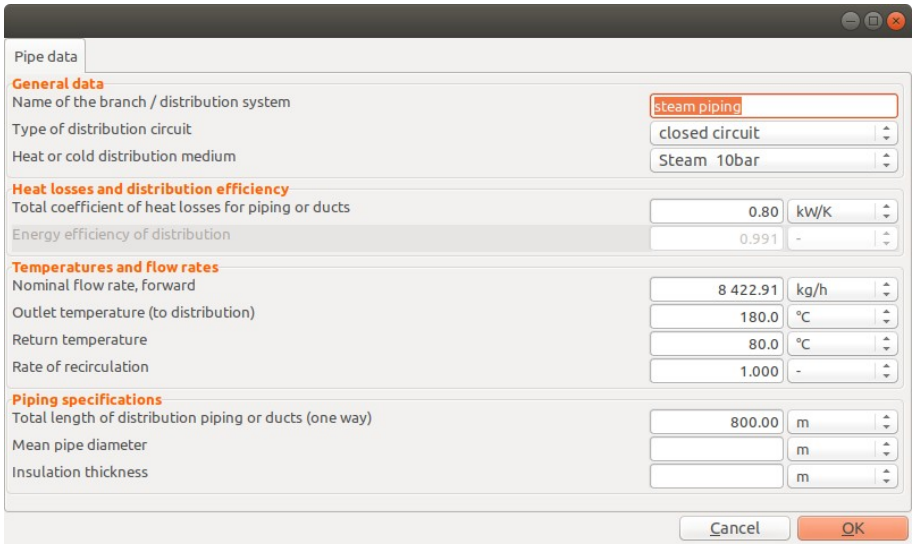


Figure 30 New EINSTEIN editor for ducts and pipings

4.2.3 Equipment Editor

Within the new equipment editor, all technical data are now grouped within a technical data table which is adapted to the specific type of equipment, so that all parameters which are not needed are hidden.

Furthermore, a clear visual distinction between nominal data and real data (average data in real operation conditions) has been introduced by locating the parameters in the corresponding column within the technical data table.

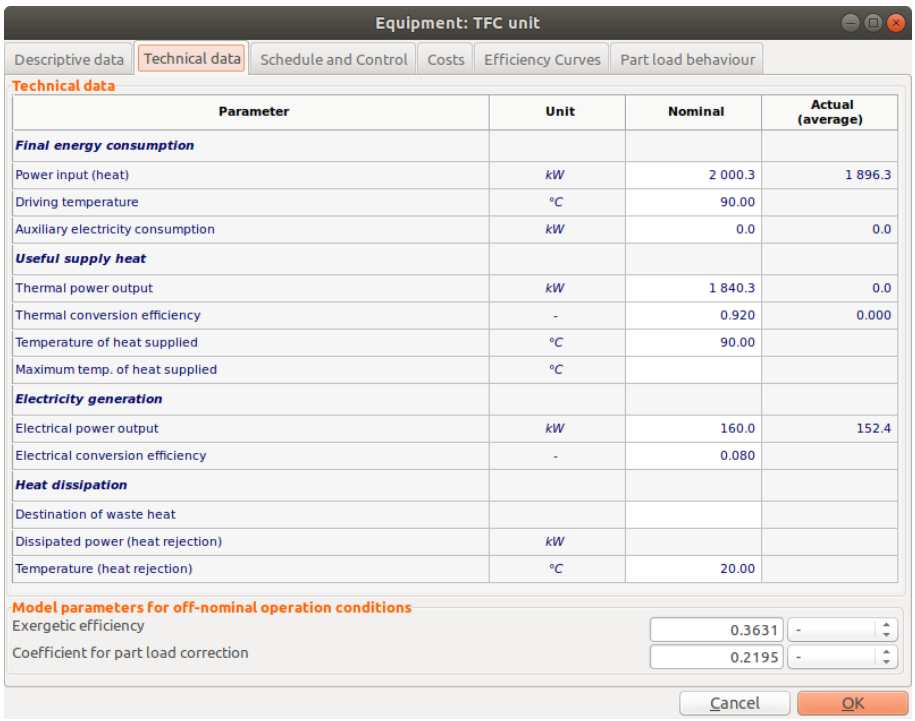


Figure 31 New EINSTEIN editor for equipment.

4.2.4 Other Component Editors

Also all other component editors (heat exchangers, other waste heat sources, etc.) have been revised following the same philosophy.

4.2.5 Editors for Data Bases

EINSTEIN disposes of a series of data bases which are used as background information for the calculations and can (and have to) be modified by the user. The most important data bases are:

- fluid and material properties
- fuel properties
- available equipment models (in separate data bases for different types of equipment)
- profiles (time schedules): as building complex time schedules is time consuming, the schedules can be stored and re-used in other projects

The editors for these data bases have been improved by separating the editor into an overview table, which allows to visualise the whole content of the data base (displaying some of the most relevant parameters for each entry), and an editor for a single data base entry in a separate window.

4.3 Output of Detailed Simulation Results

The possibility for the user to generate output of detail results of simulations has been improved.

4.3.1 Plot of Hourly Simulation Results in the GUI

A plot of hourly results has been added to the graphical user interface, where all energy flows within the system can be visualised (see e.g. Figure 7).

4.3.2 Data File with Hourly Simulation Results as Standard Output

The simulation engine of the tool can be configured by the user in order to generate a data file with the hourly simulation results.

4.4 Documentation

The most relevant supporting documentation for the user is available online in form of the user manual (einstein.sourceforge.net) providing links to the complementary documentation, and under www.einstein-energy.net.

The documentation of EINSTEIN is composed by:

a) the *user manual*, giving all necessary information for using the tool

b) the *technical manual*, describing in detail the meaning of each of the parameters, the algorithms and equations behind the calculation engines, etc.

c) the *EINSTEIN Audit Guide:* Chapters 1 to 3 provide the theoretical background of the EINSTEIN audit methodology and the terminology and accountancy standard of energy flows used within the tool. Chapter 4 provides three example cases for getting started with the tool.

Both user and technical manual have been appropriately updated and completed in order to reflect the new features within the tool.

A special effort has been furthermore dedicated to improving the getting started and FAQ section of the user manual in order to give a better support to new users.

4.5 Tutorial

The examples described in detail within the EINSTEIN Audit Guide Chapter 4 are pre-loaded within the EINSTEIN tool so that they can be directly opened by the user.

The getting started section within the user manual has been revised in order to give a better and more comprehensive description on how to use these examples for getting started with the tool.

Furthermore, some video tutorials have been elaborated and included into the "getting started" section.

The show case described in chapter 2.3 will be included as an additional more complex example case together with a video tutorial (to be included in the user manual for the stable final version V3.0plus)

4.6 Structural Improvement, Robustness and Testing

A series of improvements in the software structure and testing procedure have been introduced, which indirectly help to improve the user friendliness in the following senses:

- improvement of robustness of the code by modularity and a substantially increased number of standard tests
- reduction of manpower required for future updates

4.6.1 Structural Improvement of the Software Kernel

The software kernel has been gradually updated towards a clear "*model – view – controller*" structure, separating clearly the view (mainly the graphical user interface) from the calculation modules, and the latter from the data base (introduction of a database abstraction layer: all data base access is mainly carried out by a set of load and save functions for the different objects.

This evolution towards a clear software structure by itself reduces the possibility of bugs, and, furthermore, helps to increase productivity and reduce required manpower for future developments.

4.6.2 Structural Improvement of the Graphical User Interface

Taking the opportunity of the complete reorganisation of the graphical user interface, all the new and many of the existing elements of the graphical user interface have been reprogrammed based on standardised and reusable modules (objects).

The impact for the user is that, while in previous versions different GUI windows which had been written by different developers, behaved different in many ways, now almost everywhere standard widgets are used and a standard behaviour (e.g. on left/right mouse clicks etc.) of the tool in all windows is widely achieved.

Furthermore, as with the comments above on the structure on the software kernel, also within the GUI modularity helps to minimise the introduction of new and the detection of possibly existing bugs and, therfore, increase the robustness of the code.

4.6.3 Additional Test Cases for New Tool Features

For each of the new features developed during the i-ThERM project a set of standard test cases has been developed which allow for automatic testing (and if necessary bug-fixing) for each new tool release.

These test cases, although designed specially for the new features, act also as a test for many of the commonly used features of the tool and, therefore, increase also the reliability of the standard testing procedure for the standard tool features.

5 Modelling of i-ThERM Demo Plants

At the date when this report is written real measurement data were not yet available for the pilot plants foreseen within the I-ThERM project. Therefore, as an alternative for carrying out a calibration and validation of the EINSTEIN model for these systems, data from detailed simulations using a more complex model and carried out at Brunel University had been provided.

The data represent a parametric variation of the boundary conditions of the waste to power around some nominal design point: flow rates and inlet temperatures of both heat input and cooling water. Furthermore the input power has been calculated in the data.

5.1 Modelling of the TFC plant

5.1.1 Data set and EINSTEIN model

Table 6 shows the base operating conditions used for a parametric study of the plant. In the second column, the nominal parameters of the EINSTEIN model obtained by parameter fitting are shown.

Table 6. Base operating conditions and nominal conditions (result of parameter fit)

		Base operating conditions for parametric study	Nominal conditions EINSTEIN model
Driving heat	kW	1.132,8	1.303,7
inlet temperature	°C	127,8	127,8
inlet flow rate	kg/h	1.620	
Cooling water			
inlet temperature	°C	20	20
inlet flow rate	kg/h	57.960	
Net electricity generation	kW	85,10	102,14
Net electric efficiency	-	7,512%	7,835%
Part load correction (EINSTEIN model)			
Part Load ratio (at input)	-	0,8689	1
Part load correction (electric efficiency)	-	0,9588	1
Part load correction parameter	-	0,2195	

Real time simulations have been carried out with EINSTEIN, with the following parameters specified as input via the virtual monitoring data file:

- flow rates and inlet temperatures for driving heat and heat rejection
- part load ratio (master control) obtained as the ratio of actual driving heat (from input data) and nominal driving heat (as on the right column of Table 6)

In the following sections the net electricity generation and/or the corresponding net electric efficiency as obtained with the EINSTEIN simulations has been compared to the equivalent value from detailed simulations in the data

5.1.2 Results

a) Efficiency as a function of the inlet temperature

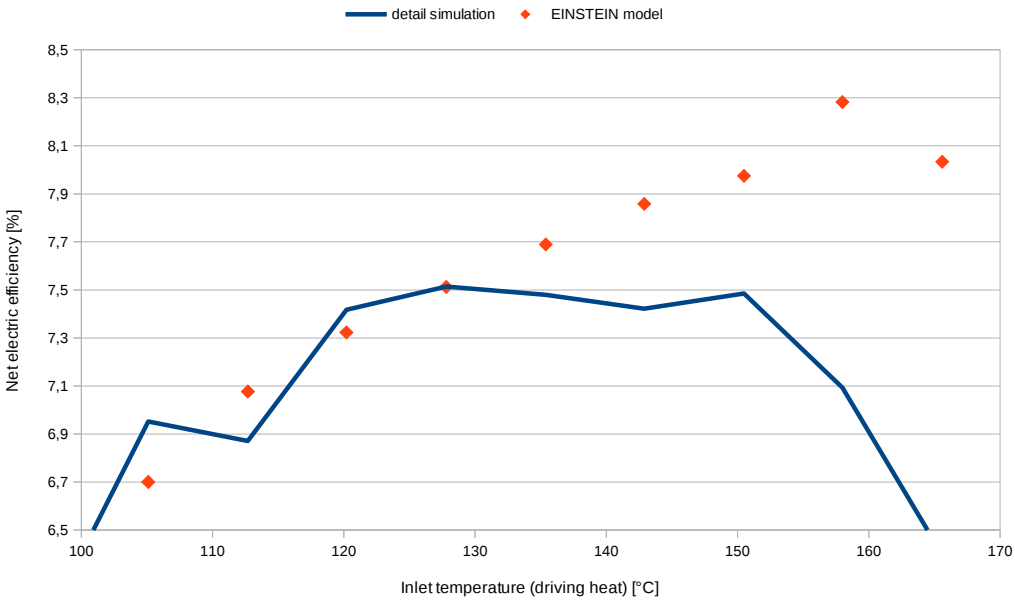


Figure 32 Net electric efficiency as a function of the inlet temperature for the driving heat. Base operation conditions for all other parameters.

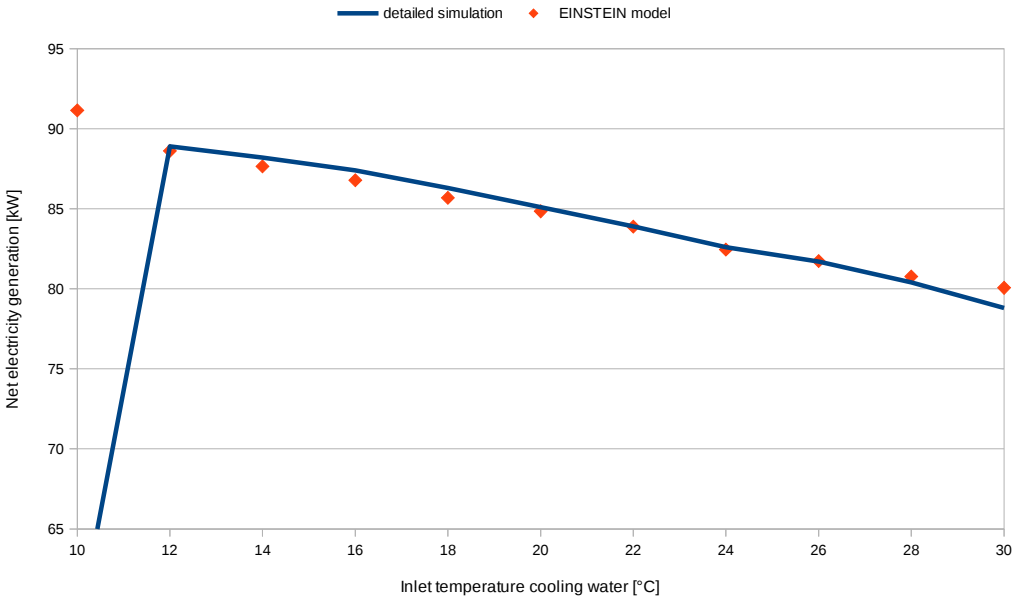


Figure 33 Net electric efficiency as a function of the inlet temperature for the heat rejection (cooling water). Base operation conditions for all other parameters.

For temperatures between the inlet temperature corresponding to the base operation conditions, the results of the EINSTEIN model and those of the detailed simulation are well in line (Figure 32). The same is valid also for the variation of the heat rejection temperature over the biggest part of the temperature range screened (Figure 33). This means, that in these temperature ranges the constant exergy efficiency model used by

EINSTEIN is appropriate to represent the real behaviour. The differences for higher driving heat temperatures are explained by the fact that due to the interaction of the single TFC system components there is a drop in system efficiency at very high heat input, so that the constant exergy efficiency model in this range is no longer valid. Also for very low heat rejection temperatures (10 °C in Figure 33) there appears a significant difference which has been explained by similar reasons, although in this case the difference appears abruptly and only for one (extreme) data point.

When operating the equipment at different input power (part load ratios; Figure 34), the EINSTEIN model and results from detailed simulations are well in line up to the input power corresponding to the base operating conditions (1.132 kW). Within the data from detailed simulations, for higher input power the electricity does not increase any more, but even decreases. Reasons for this deviation probably are similar to those mentioned above.

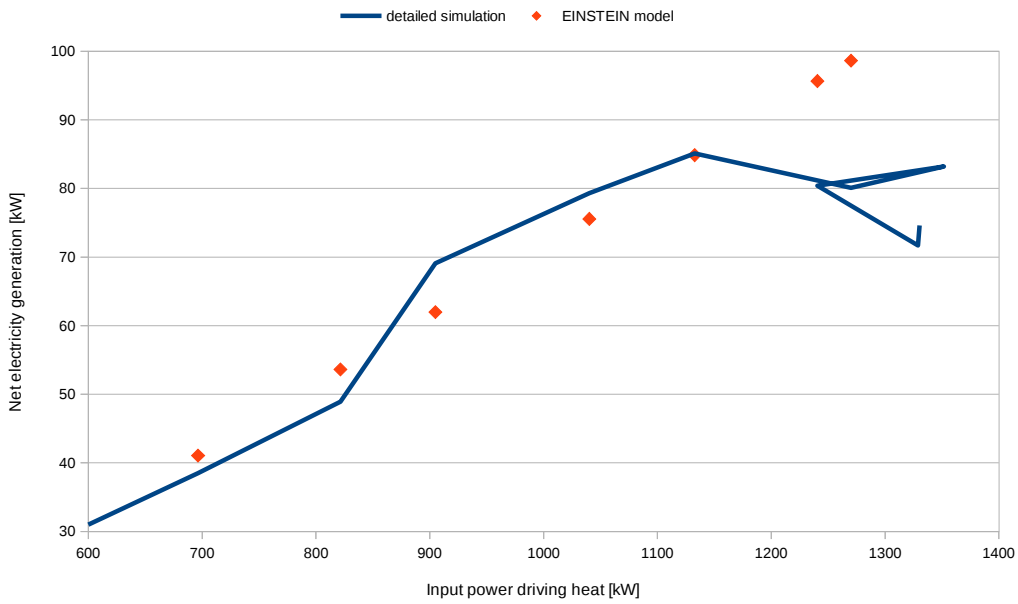


Figure 34 Net electricity generation as a function of the input power (driving heat). Base operation conditions for all other parameters.

5.1.3 Conclusions

The constant exergy efficiency model used within EINSTEIN gives a good approximation of results of detailed simulations. Differences appear if either the inlet temperature or the input power are higher than the values specified in the base operation conditions. Further research is necessary in order to (a) determine the reasons for these deviations and (b) to check whether an operation in these parameter ranges is of practical relevance. In the latter case the EINSTEIN model would have to be extended by some limiting mechanism getting active at extreme operation conditions. The analysis of the real system under real operation conditions will help to gain more insight on these open questions.

5.2 Modelling of the sCO2 plant

5.2.1 Data set and EINSTEIN model

Table 7 shows the base operating conditions used for a parametric study of the plant. In the second column, the nominal parameters of the EINSTEIN model obtained by parameter fitting are shown.

Table 7. Base operating conditions and nominal conditions (result of parameter fit)

		Base operating conditions for parametric study	Nominal conditions EINSTEIN model
Driving heat	kW	326,0	370,1
inlet temperature	°C	353,7	353,7
inlet flow rate	kg/h	3.600	
Cooling water			
inlet temperature	°C	15	15
inlet flow rate	kg/h	5.832	
Net electricity generation	kW	67,90	81,81
Net electric efficiency	-	20,825%	22,105%
Part load correction (EINSTEIN model)			
Part Load ratio (at input)	-	0,8810	1
Part load correction (electric efficiency)	-	0,9421	1
Part load correction parameter	-	0,3000	

Real time simulations have been carried out with EINSTEIN, with the following parameters specified as input via the virtual monitoring data file:

- flow rates and inlet/outlet temperatures for driving heat and heat rejection
- part load ratio (master control) obtained as the ratio of actual driving heat (from input data) and nominal driving heat (as on the right column of Table 7)

In the following sections the net electricity generation and/or the corresponding net electric efficiency as obtained with the EINSTEIN simulations has been compared to the equivalent value from detailed simulations in the data

5.2.2 Results

a) Efficiency as a function of the inlet temperature

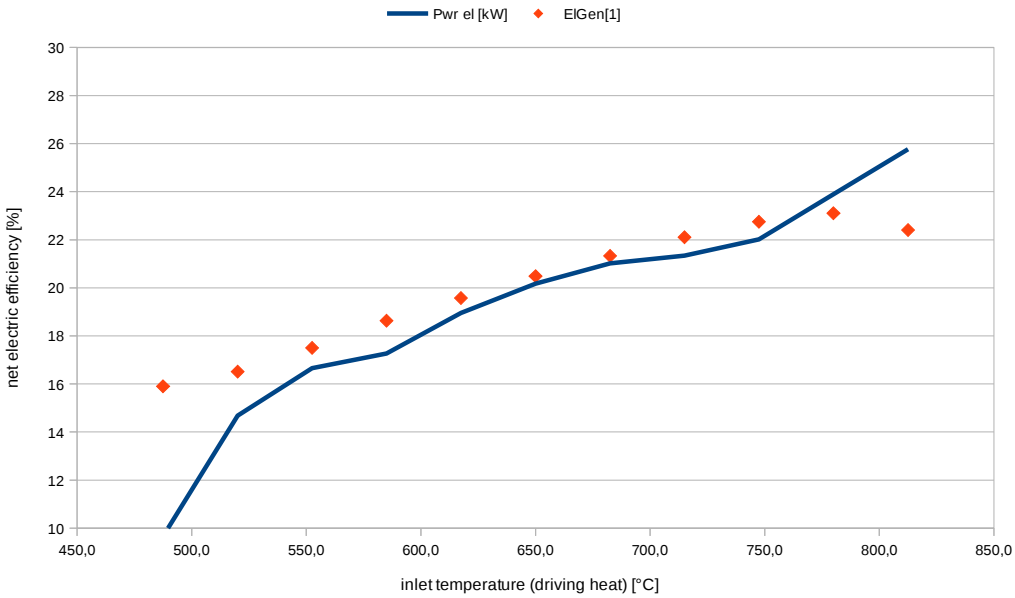


Figure 35 Net electric efficiency as a function of the inlet temperature for the driving heat. Base operation conditions for all other parameters.

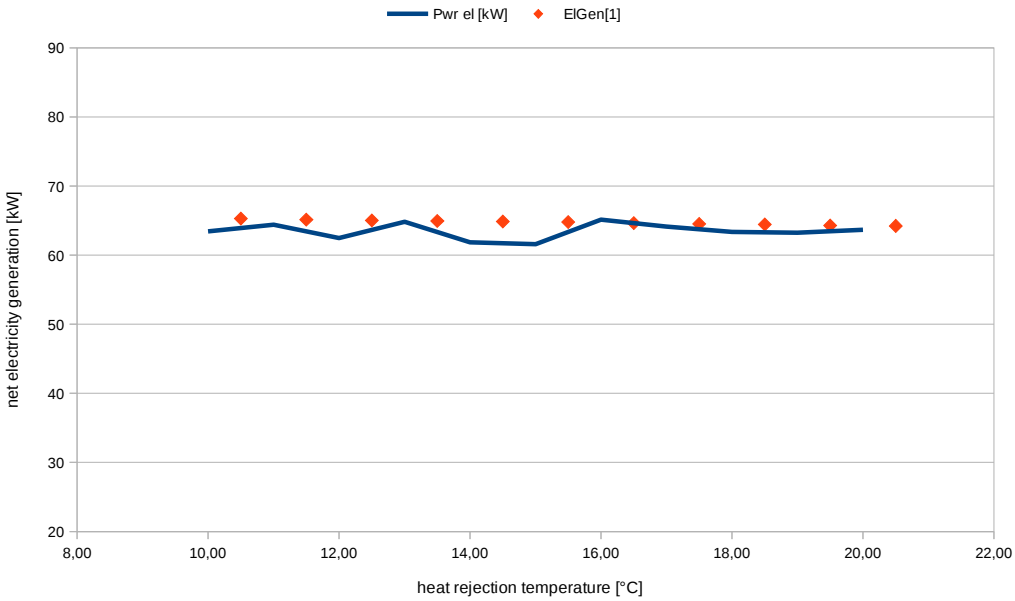


Figure 36 Net electric efficiency as a function of the inlet temperature for the heat rejection (cooling water). Base operation conditions for all other parameters.

The results of the EINSTEIN model and those of the detailed simulation are reasonably in line (Figure 35) for the most of the range of operating temperatures. Deviations are stronger at the extremes of the range of operating temperatures. Nevertheless it has to be noted, that the power input has not been kept constant when

varying the driving temperature, so that there may be an overlap of temperature effects and part load correction effects.

Electricity generation is not very sensitive to the heat rejection temperature over the the (small) temperature range screened (Figure 36). Detailed and EINSTEIN simulations are in good coincidence. This means, that in these temperature ranges the constant exergy efficiency model used by EINSTEIN is appropriate to represent the real behaviour.

When operating the equipment at different input power (part load ratios; Figure 37), the EINSTEIN model and results from detailed simulations are well in line for an input power above 250 kW (about 60% of nominal power). For lower part load ratios deviations are becoming higher.

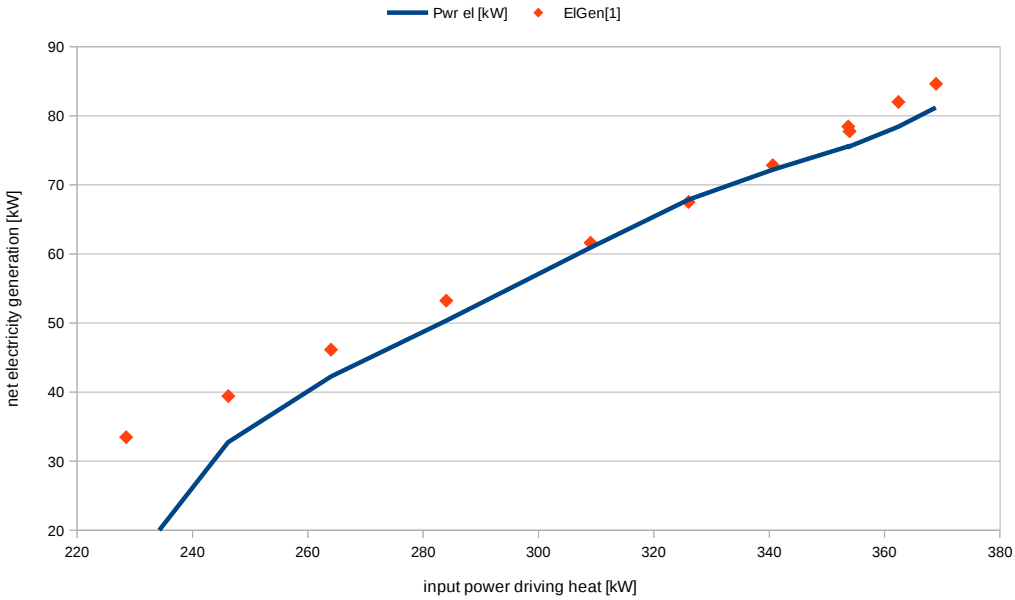


Figure 37 Net electricity generation as a function of the input power (driving heat). Base operation conditions for all other parameters.

5.2.3 Conclusions

The constant exergy efficiency model used within EINSTEIN gives a good approximation of results of detailed simulations. Differences appear at extreme values for the inlet temperature or at low input powers. Further research is necessary in order to (a) determine the reasons for these deviations and (b) to check whether an operation in these parameter ranges is of practical relevance. The analysis of the real system under real operation conditions will help to gain more insight on these open questions.

References

[1] *EINSTEIN Guide for Thermal Energy Audits*. Available for download at http://www.einstein-energy.net/index.php/tool-kit

[2] *EINSTEIN Technical Manual*, available for download at http://einstein.sourceforge.net/technical/manual.html

[3] *EINSTEIN User Manual*, available online at http://einstein.sourceforge.net/

[4] I-Therm report D3.2: *"Extension of EINSTEIN: Calculation and design algorithm for heat pipes (Prototype)"*.

[5] I-Therm report D3.3: "*Extension of EINSTEIN: Calculation and design algorithm for (waste) heat to power (Prototype)*".

[6] I-Therm report D3.4: "*Extension of EINSTEIN: Automatic processing of historical monitoring data and system optimisation (Prototype)*".

[7] scipy.optimize: Library of functions for optimisation and root finding within the Package SciPy: "*Scientific Computing Tools for Python*". Documentation available online at https://docs.scipy.org/doc/scipy/reference/optimize.html.

Annexes

1 Protocol for the data base interface between system control and EINSTEIN

2 Comparison of relative (energy, cost, environmental) savings for heat to power vs. alternative technologies

3 Annotations on the Review Report from January 2018

Annex 1: Protocol for the data base interface between system control and EINSTEIN

Data transfer between the system control and data acquisition unit (SCADA, as e.g. the systems developed by SYNESIS in WP8) and EINSTEIN can be done via an SQL (MySQL) data base.

The data set is formed by the following tables:

data / ctrl

These tables ontain pairs (time stamp: value) associated to a -> sensor (table data, used for reading plant data by EINSTEIN) and to a -> controller (table ctrl, for feed-back from EINSTEIN to the plant control).

Parameter	**type**	**description**
id	integer	unique identifier of the data point
sensorId / controllerId	integer	link (id) to the associated sensor
dateTime	datetime	date and time of measurement
value	float	value of measurement

sensor / controller

Table sensor contains a list of sensors (measurement points) and the analogous table controller contains a list of controller parameters.

Parameter	**type**	**description**
id	integer	unique identifier of the sensor / controller
label	text	short name of the sensor / controller (e.g. T_in, T_out, ...)
plantId	integer	link (id) to the associated plant
unit	text	unit for value (e.g. °C, kg/h, ...)
frecuency	float	frequency of measurements / controller updates in minutes
description	text	optional: description of the sensor / controller

plant

This additional table in the data base allows to monitor several plants within a single data base (e.g. all demo plants of the i-Therm project.

Parameter	**type**	**description**
id	integer	unique identifier of the plant
description	text	optional: description of the plant
lastUpdate	datetime	time of last update of plant data

Annex 2: Calculation of Relative Savings for Heat to Power vs. Alternative Technologies

In this annex the mathematics behind the graphs in Figure 3 is given.

The following three options for using a certain amount of waste heat Q are compared:

- direct heat recovery
- heat to power conversion with a net electric efficiency of hel
- heat pump with a certain COP of heating COP_h

A conversion efficiency from LCV of fuel to useful heat of $\eta_{ref} = 0,9$ is supposed.

Relative savings are then calculated by

- assigning an index (e.g. tariff, relative primary energy consumption, generation of CO_2) for both electricity and fuel savings:

$$S = i_{el} S_{el} + i_{fuel} S_{fuel} \tag{A2.1}$$

a) direct heat recovery

The saving in this case is given by

$$S = i_{fuel} S_{fuel} = i_{fuel} \frac{Q}{\eta_{ref}} \tag{A2.2}$$

b) heat to power conversion

Electricity saved in this case is given by the net average conversion efficiency during operation

$$S = i_{el} S_{el} = i_{el} \eta_{el} Q \tag{A2.3}$$

c) heat pump

With the simplifying assumption of zero energy losses the energy balance over the heat pump gives

$$Q_h = E + Q_c \tag{A2.4}$$

where Q_h and Q_c are the heat delivered / absorbed at the hot and cold side respectively and E is the electric power input.

Then, with $Q_c = Q$ and $Q_h = COP_h E$ this results in:

$$E = \frac{Q}{COP_h - 1} \tag{A2.5}$$

$$Q_h = \frac{COP_h}{COP_h - 1} Q \tag{A2.6}$$

$$S = \frac{i_{fuel}}{\eta_{ref}} * Q_h - i_{el} E = \frac{\frac{i_{fuel}}{\eta_{ref}} COP_h - i_{el}}{COP_h - 1} Q \quad \text{(A2.7)}$$

If the savings in the first case (direct heat recovery) are defined as a reference, then relative savings s can be calculated, simplifying by using the relative index $r = i_{el} / i_{fuel}$:

- for direct heat recovery:

s = 1 (by definition)

- for heat to power

$$s = r\ \eta_{ref}\ \eta_{el} \quad \text{(A2.8)}$$

- for heat pumps

$$s = \frac{COP_h - r\ \eta_{ref}}{COP_h - 1} \quad \text{(A2.9)}$$

Annex 3: Annotations on the Review Report from January 2018

The current Deliverable D3.6 has been proposed – among other reasons – on request of the project review carried out between November 2017 and January 2018.

As far as possible, within the present document the requested information is provided. Nevertheless, it was not possible to respond to all of the reviewers' requests, as in some cases comments were very generic and/or not very explicit and it was not clear what was exactly the point; and in other cases we do not agree with the critique as expressed by the reviewers.

Therefore, in the following we want to make some remarks to each of the comments referring to the EINSTEIN tool / work on WP3 as mentioned in the review report (Ref.: Ares(2018)202161 – 12/01/2018).

Comments to Deliverable D3.2 (Review Report pp. 14/15)

Reviewers' comment: „*the figures (on the evaluation of energy, environmental and economic savings), however, are not realistic and misleading*".

It is not possible for us to answer to this critique unless we get more information about (a) which of the figures is considered as "not realistic" or "misleading". In any case we would like to highlight, that the scope of D3.2 is not the feasibility analysis of technologies, but to describe the features of the software. Given examples are only illustrative, and in this context the discussion whether some (economic ?) figures are realistic or not seems to be secondary. The figures (e.g. estimated system costs, etc.) and system configuration – at the stage when this report was written - were very preliminary and do not necessarily have to represent the real systems in a 1:1 manner.

Comments to Deliverable D3.3

Reviewers' comment: „*the proposed control strategy* [in the second use case TC-ITHERM-05] *is not correct and should be revised*".

As already stated above on D3.2, and equally valid for D3.3, given examples are only illustrative. The numbers and system configuration are very preliminary and do not pretend to represent the real systems in a 1:1 manner. The case of a waste heat to power equipment following the availability of waste heat is already demonstrated in the first test case TC-ITHERM-02 (section 3.1 of the report). The objective of the second test case described in section 3.2 was on the one hand to represent the laboratory situation foreseen at the time of elaboration of the report for the corresponding i-Therm demonstration plant (in which indeed the heat supply would have followed the requirement of driving heat), and on the other hand to demonstrate the capability of the software to simulate also such a situation: an external control of the waste heat to power generation equipment driven by an active heat supply.

Reviewers' comment: "*the parameters used for obtaining the data in Table 2 (footnote 3), however, are not realistic and too optimistic*".

First of all, following our experience we consider the parameters given as quite realistic and, therefore, disagree with this comment, but as energy costs vary widely depending on the size of the companies and from country to country it is possible that there are different opinions and points of view. But in any case, as already stated above on the comments to D3.2., the scope of the example (and the deliverable D3.3.) is to illustrate the software features and not to carry out a feasibility analysis of the technology.

Reviewers' comment: "*The program, however, cannot be installed properly. The installation procedure needs to be revised*".

We checked this as soon as we got aware and detected a minor bug in the installer of the free version 2.4 of the software which, however, affected only new users, and which has been immediately repaired.

Comments to Deliverable D3.4 (Review Report p. 15)

Reviewers' comment: „*Reference is made to Guides and Manuals of the EINSTEIN software package. The information in these documents is insufficient to use the software. Several items in the Technical Manual are unclear or show shortcomings (e,g Pinch analysis in the EINSTEIN software is neither following standard procedures nor conventional presentation and listing as in typical pinch analysis; the description of the EINSTEIN – CHP module is unclear and confusing).*"

In order to be able to improve the documentation of the software, we would appreciate some more details in order to work on specific issues if necessary. Generic comments such as "is insufficient / unclear / confusing / shows shortcomings" are not very helpful in this sense, if they are not supported by some more specific critique.

With respect to pinch analysis, in our opinion the EINSTEIN module follows closely the standard pinch procedure and representation. Maybe the reviewers' comment was motivated by a difference to the classical representation used in many textbooks which is that we use energy and not power for the quantity scale. This, nevertheless, is well motivated by the fact that the modelling and optimisation in EINSTEIN is done in a dynamic and not a stationary context. Whenever dynamic behaviour of both source and sink streams and the possibility of storage is included in the analysis, then using energy (or, what would be equivalent, *average* power) gives a better approximation of the real heat recovery potential than using (however defined) *instantaneous* power.

Reviewers' comment: „*The package has not demonstrated to provide a trade-off between energy and capital.*"

The EINSTEIN software tool disposes of a module for economic and financial analysis where both investment cost (capital) and energy saving / energy cost saving are calculated. The trade-off between energy saving and capital is central in the economic analysis in EINSTEIN (as in any economic analysis tool) and is – among others - reflected in the EINSTEIN concept of "*total energy system cost*" which includes both capital cost and current costs for energy and O&M (see the EINSTEIN Audit Guide Chapter 2 for further details of the economic analysis). The EINSTEIN economic analysis module is rather standard and has not been subject to further development in work package 3, and, therefore, has not been described within D3.4.

We included a demonstration of economic analysis in the show case included in this deliverable in section 2.3.

Reviewers' comment: „*Therefore, D3.4 needs revision in order to provide the examples discussed during the review meeting which should demonstrate the functionality of the Einstein software.*“

The scope of Deliverable D3.4 is to summarise the features of „*Automatic processing of historical monitoring data and system optimisation*“, mainly the work of Tasks 3.3a and 3.3b.

During the review process we received two example cases from one of the reviewers, Mr. Declercq, which refer to pinch analysis (and some economic parameters) and, therefore, do not fit into the scope of D3.4. Nervertheless, we already elaborated some EINSTEIN projects on these examples, but did not receive a feed-back on this. A description of these examples can be included as an additional annex within this report if needed.

Examples demonstrating the functionality of the EINSTEIN software in general and the capability to model specific i-ThERM pilot projects are included within this Deliverable D3.6.

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