DTU Mechanical Engineering

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Documentation

Numerical models for the design and analysis of heat pumps with zeotropic mixtures

Main Features

- Numerical models for the design and analysis of heat pumps using zeotropic mixtures
- Standard cycle and internal heat exchanger cycle
- Access to all mixtures from Refprop 9.1
- Different approaches for heat exchanger design
- Numerical optimization of heat pump cycle w.r.t. thermodynamic and economic performance

Keywords: Design model, Heat pump, Process Integration, Refrigerant, Working fluid, Zeotropic mixture

Rev01:

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1 Introduction

The models were developed during different projects and were mainly utilized for the screening of working fluids among pure and mixed working fluids as described in [1]. The main purpose of the model is the heat pump design with the focus on the evaluation and comparison of working fluids and for the comparison of different cycle arrangements. The models are however capable of off-design simulations and may be coupled with more detailed heat exchanger models as described in [2].

1.1 Version control

Rev01:

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Changes:	- First version of models & documentation	

1.2 Applications of the models

This chapter gives an overview of studies that were conducted with the described models to demonstrate the capabilities of the models. Since some of the below mentioned articles used the current implementation of the models but previous preliminary unpublished versions of the models, representing the development of the current version Rev01. The mentioned studies could however be reproduced with the latest presented version of the model.

A first analysis [3] focused on the analysis of zeotropic working fluid mixtures in a heat pump application for recovering excess stream from a milk powder spray dryer for preheating the air stream. This study used a previous version of the models implemented in Modelica [4] The study included both a thermodynamic and economic evaluation of the investment and considered 6 pure fluids for the generation of mixtures.

A booster heat pump for the operation in a ultra-low-temperature district heating (ULTDH) network was analyzed in [5]. The booster heat pump is used to boost part of the forward stream of the ULTDH network from 40 °C to 60 °C for hot water supply, while the remaining part of the stream is utilized as a heat source being cooled down to the return temperature of 25 °C.

Another case study is given by [6], in which the possibilities to utilize excess heat from CO_2 supermarket refrigeration systems for supply of district heating was analyzed. In this study, the currently presented version of the numerical models was utilized to evaluate possible mixtures that were created from a list of 16 natural fluids and 4 HFOs.

The study [7] has analyzed the influence of the temperature glide matching in the heat exchangers on the performance. The models were used to evaluate four different boundary conditions for a list of 16 natural working fluids.

The publication [1] summarizes the different screening studies and presents a methodology to evaluate and compare pure and mixed working fluids.

2 Model description

The following chapter describes the thermodynamic model, the implemented possibilities for the estimation of the investment cost and the definition of different performance indicators. The presented study is limited to single stage cycles without devices for recovery of expansion work, but can be extended accordingly.

2.1 Thermodynamic cycles

Figure 1 and Figure 2 show the layout and a temperature-heat-diagram for the two implemented cycles. The first cycle is a standard vapor compression heat pump cycle, which consists of a compressor, heat sink heat exchangers including a desuperheater, a condenser and a subcooler, as well as a throttling valve and heat sink heat exchangers, including an evaporator and a superheater. The heat exchangers in the heat sink and source are modelled as separate units but might be realized as one component. The second cycle has an additional internal heat exchanger (IHX) that further cools the liquid before the throttling valve while superheating the working fluid at the compressor suction line.
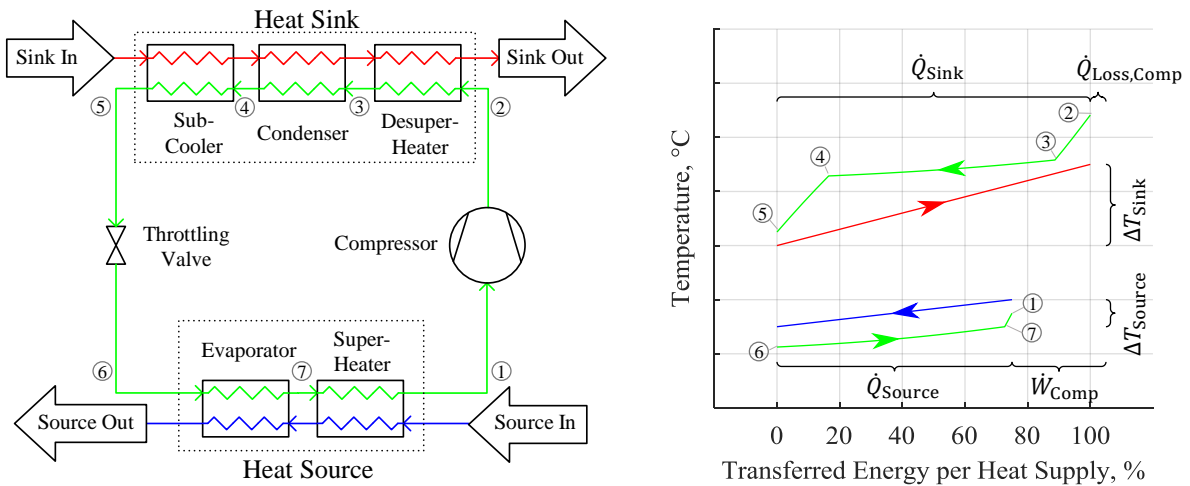

Figure 1: Flow sheet (left) and Temperature-Heat-Diagram (right) of the standard cycle
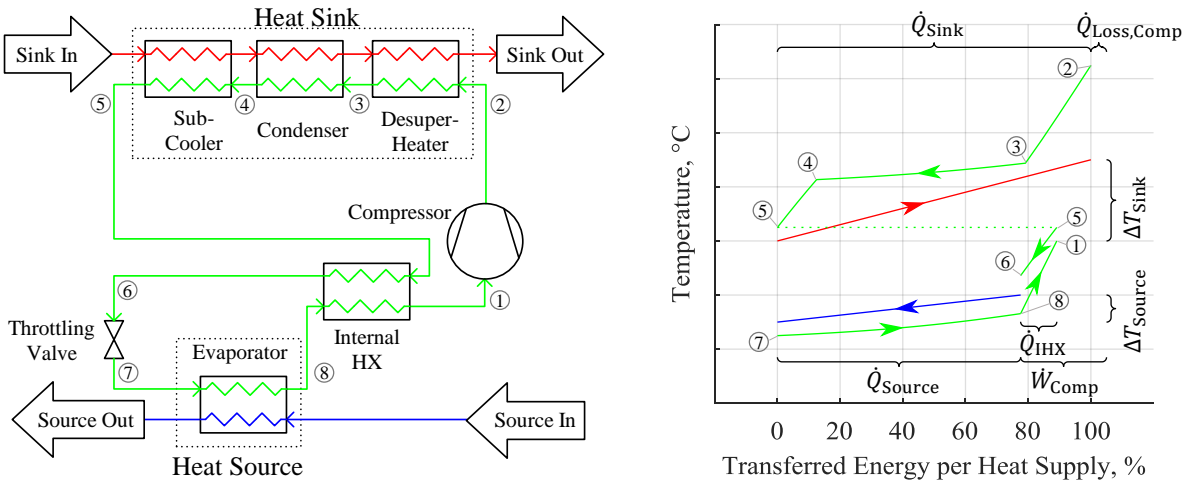
Figure 2: Flow sheet (left) and Temperature-Heat-Diagram (right) of the IHX-cycle

The thermodynamic models are based on steady state mass and energy balances for each component.

The compressor is modelled with an isentropic efficiency η_{is} to describe the compression process for an adiabatic compression $\left(h_{2,\text{adiabatic}} - h_1\right)$ in relation to an ideal isentropic compression process $\left(h_{2,\text{is}} - h_1\right)$.

$$\eta_{is} = \frac{h_{2,\text{is}} - h_1}{h_{2,\text{adiabatic}} - h_1} \tag{1}$$

Heat losses from the compressor can be considered as a fixed factor f_{hl}.

$$h_2 = h_{2,\text{adiabatic}} - f_{hl}\left(h_{2,\text{adiabatic}} - h_1\right) \tag{2}$$

For off-design analyses, the isentropic efficiency can be determined as described by [8] as a function of the pressure ratio $p_{\text{cond}}/p_{\text{evap}}$, the built-in pressure ratio π_i, the isentropic exponent κ and the isentropic efficiency at design operation $\eta_{\text{is,design}}$. The built-in pressure ratio is derived from the compressor specific built-in volume ratio $\pi_i = v_i^{\kappa}$.

$$\eta_{\text{is}} = \eta_{\text{is,design}} \frac{\left(p_{\text{cond}}/p_{\text{evap}}\right)^{(\kappa-1)/\kappa} - 1}{\pi_i^{(\kappa-1)/\kappa} - \frac{\kappa-1}{\kappa}\,\pi_i^{-\left(\frac{1}{\kappa}\right)}\left(\pi_i - \frac{p_{\text{cond}}}{p_{\text{evap}}}\right) - 1} \tag{3}$$

The throttling valve is modelled as an isenthalpic expansion process.

The heat exchangers are described by *n* state points and are accordingly discretized equidistantly in transferred heat rate into *n*-1 volumes. The general relation that describes the heat transfer for each volume relates the transferred heat $\dot{Q}$ to the UA-value and the logarithmic mean temperature difference ΔT_{lm}.

$$\dot{Q} = UA\,\Delta T_{\text{lm}} = \text{UA}\,\frac{\Delta T_{\text{in}} - \Delta T_{\text{out}}}{\ln(\Delta T_{\text{in}}/\Delta T_{\text{out}})} \tag{4}$$

The discretization of the heat exchanger is separated into single-phase and two-phase processes. As this distinction becomes indistinct above the critical point, the discretization is applied constantly throughout the entire heat rejection process. Separating the heat rejection process into single- and two-phase processes requires the determination of the saturation line. The saturation line is however difficult to determine in the region close to the critical point. Therefore, the transition between the discretization that is specific for single- and two-phase regions and the continuous discretization occurs at limit_sc*p_{crit}, whereas a value of limit_sc = 0.95 was found to yield relatively robust results.

The heat transfer relation allows fixation of e.g. the logarithmic mean temperature difference or the area, which allows comparison of different solutions for a comparable heat exchanger area. Alternatively, the minimum pinch point temperature differences can be defined. The model includes different options as described in section 3.5. and the fairness of the different approaches is extensively discussed in [1].

The discretized heat exchangers allow to consider any pressure drop between the state points. The pressure drops might be assumptions or results from detailed heat exchanger models. In [2], an approach for designing the heat exchangers was demonstrated and the study suggested a way for merging the cycle models with more detailed heat exchanger models.

2.2 Estimation of the investment cost

The investment cost for a heat pump can be estimated by different approaches. Bejan et al. [9] suggest to estimate the total capital investment cost TCI as a fixed multiple of the total purchased equipment cost PEC.

$$\text{TCI} = f_{\text{TCI}}\,\text{PEC} \tag{5}$$

The total purchased equipment cost PEC is the sum of the purchased equipment cost of the main components which are in this case the heat exchangers and the compressor. Examples of cost functions for these components are published in [5,10,11]. The factor f_{TCI} accounts for the cost for auxiliary equipment, assembly of the components, the company earnings and other aspects and varies between 4.16 for an extension of an existing plant to 6.32 for erection of a new system [9]. The value is however a case specific parameter and has to be validated for each specific application.

The cost functions for the equipment can e.g. use variables that give an indication of the size and thereby the investment cost. This variable can e.g. be the volume flow rate at inlet for the compressor or the area for the heat exchangers. While the volume flow rate at the compressor inlet is defined by the thermodynamic state point and the mass flow rate, the heat exchanger area requires estimating the heat transfer coefficients. The estimation of the heat transfer coefficients can be done by a detailed dimensioning of the heat exchangers [2,3] or by assuming feasible heat transfer coefficients [5].

2.3 Performance indicators

2.3.1 Thermodynamic performance

The thermodynamic performance can be described by the coefficient of performance COP, as the ratio of supplied heat $\dot{Q}_{Sink}$ and the consumed compressor power $\dot{W}_{Comp}$.

$$\text{COP} = \frac{\dot{Q}_{Sink}}{\dot{W}_{Comp}} \tag{6}$$

Although the COP is commonly used as a performance indicator, it can only serve for comparisons for constant boundary conditions in terms of source and sink inlet temperatures. For varying temperature levels, Second Law efficiencies might be a more appropriate basis for comparisons, as they consider the boundary conditions and relate the performance to the maximum achievable performances [12].

The Lorenz efficiency η_{Lor} is defined as the COP in relation to the maximum obtainable COP_{Lor} of a Lorenz cycle.

$$\eta_{Lor} = \frac{\text{COP}}{\text{COP}_{Lor}} \tag{7}$$

The COP_{Lor} is defined analogously as the Carnot COP_{Car} while accounting for the temperature glides, by using the thermodynamic average temperatures of the heat source $\bar{T}_{Source}$ and sink $\bar{T}_{Sink}$ [13]. The thermodynamic average temperatures are defined as the entropic mean temperature $\bar{T} = \Delta h/\Delta s$ and may be calculated as the logarithmic mean temperature $\bar{T}_{lm} = (T_1 - T_2)/\ln(T_1/T_2)$ for streams of constant heat capacity, [9].

$$\text{COP}_{Car} = \frac{T_{Sink,out}}{T_{Sink,out} - T_{Source,out}} \tag{8}$$

$$\text{COP}_{Lor} = \frac{\bar{T}_{Sink}}{\bar{T}_{Sink} - \bar{T}_{Source}} \tag{9}$$

2.3.2 Economic performance

The economic performance is defined by one-time investments and operational costs. In order to compare one-time costs and annual cash flows, the capital recovery factor CRF might be used. The CRF converts annual cash flows that are constant over the plant life time n to one time investments or vice versa, for a defined effective interest rate i_{eff} [9].

$$\text{CRF} = \frac{(1 + i_{eff})^n - 1}{i_{eff}(1 + i_{eff})^n} \tag{10}$$

A measurement of the plant profitability is the net present value NPV. It describes the value of the investment over its entire lifetime at the time of the investment by accounting for both the investment cost and the accumulated cash flows.

$$\text{NPV} = -\text{TCI} + \frac{\text{CF}_{Supply} - \text{CF}_{el} + \text{CF}_{Source}}{\text{CRF}} \tag{11}$$

The annual cash flows consist of the expenses for the electricity consumption CF_{el}, the income from the supply of heat CF_{Supply} and a potential cash flow associated to the heat flow of the source CF_{Source}, which can either be an income when cooling is supplied or an expense, when the heat source is to be paid.

Furthermore, the simple payback time PBT can be used to evaluate the investment by calculating how many years are required to compensate the initial investment.

$$PBT = \frac{TCI}{CF_{Supply} - CF_{el} + CF_{Source}} \qquad (12)$$

An alternative for comparing the economic performance is the calculation of the specific levelized cost of heat c_h.

$$c_h = \frac{CF_{el} + CF_{Source} + TCI \cdot CRF}{\dot{Q}_{Sink} \cdot OH} \qquad (13)$$

3 Users guide

3.1 Requirements

All models are implemented and tested in Matlab 2018a [3] and were using medium properties from Refprop [4] for the working fluid of the cycle, as well as medium properties from Coolprop [5] for the medium properties of sink and source. The operating system was Windows 7.

For including the medium properties from Refprop, a slightly modified interface refpropm_v1.m is supplied. The modified interface enables to call medium properties for a fluid described by a medium string and a composition vector. The medium definition could describe a pure fluid or a mixture of two or more components and enables calling medium properties for pure or multi-component fluids without changing the function call. The original interface required adjustment of the function call dependent on the number of fluid components. Furthermore, a feature was implemented that calls the satspln function of Refprop, ensuring the interpolation of the saturation properties around the critical point. This requires that the user has writing permissions to its C-drive. The function call might alternatively be deactivated, which could potentially cause convergence problems, especially for fluids for which the heat sink is close to the critical temperature.

Coolprop should be installed as described in the documentation.

The interfaces must be placed on the active path and it is recommended to place them here `'C:\Program Files\REFPROP'` and here `'C:\Program Files\Coolprop'`. These paths are added to the active path during execution of the function calls.

In order to test the correct setup of the medium property interfaces, it is recommended to execute the script `'TestMediumProperties.m'`. If this script can be run without error messages, the medium property interfaces are installed correctly.

3.2 Structure of implementation

Figure 3 shows an overview of the folder structure in which the numerical models and the scripts for evaluating the functions are organized. The models are implemented as functions, meaning that they provide a certain set of output variables that were calculated for previously defined input variables. This ensures that only the most important variables are communicated, meaning a slim modelling code. For the communication among the scripts, so-called structures are used. Each of these contains a certain amount of information.

The cycle models itself are located under `'...\HPCycles\HP_std_cycle_Rev00\HP_std_cycle'` for the standard cycle and under `'...\HPCycles\HP_ihx_cycle_Rev00\HP_ihx_cycle'` for the internal heat exchanger cycle. The scripts for a potential exergy analysis are located in the same folder. The scripts for a potential economic analysis are located under `'...\HPEconomics\'`.

These models are not called directly but by a function that optimizes the cycle with respect to the defined objectives. The functions are located under '...\HPOptimizationCalls\'. Within these functions, the optimization call is adjusted according to the desired optimization boundary conditions.

These optimization calls can be called by different scripts with different boundary conditions. Each call corresponds to one model evaluation for the boundary conditions for the specific case. Examples of these calls are presented for two cases, which correspond to the two cases presented in [1]. The examples are located under '...\CaseStudyI\' and '...\CaseStudyII\', respectively.
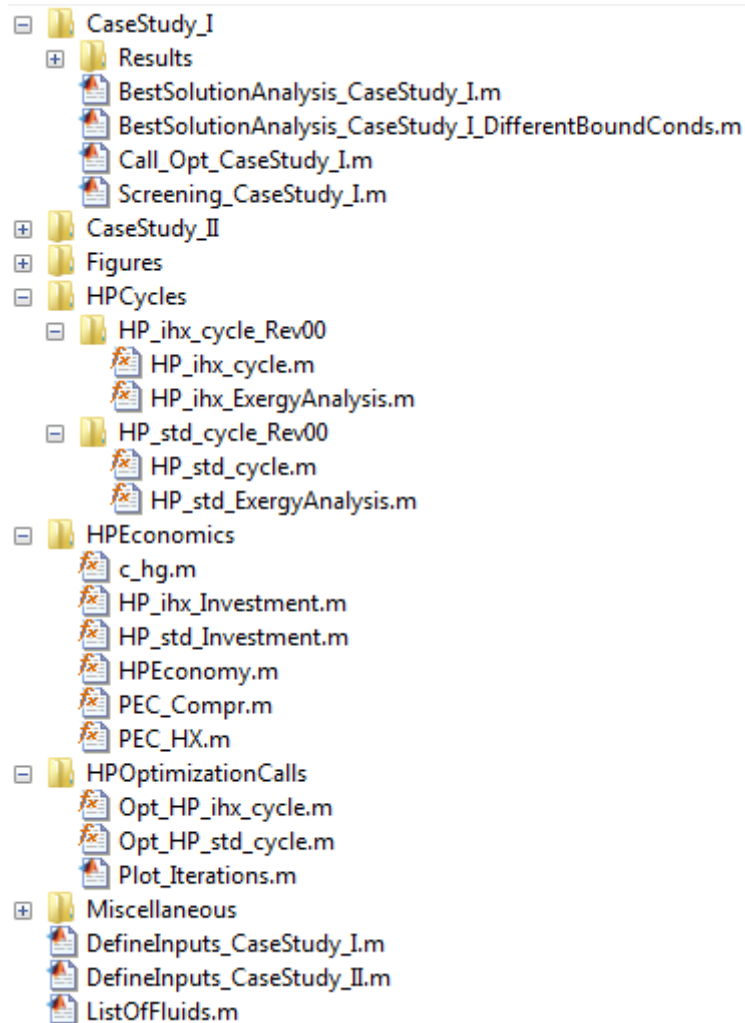

Figure 3: Folder structure of numerical model

The most intuitive script is a simple evaluation of a cycle for given boundary conditions, as implemented in '...\CaseStudyI\Call_Opt_CaseStudy_I.m'. The functions calls can however also be called to e.g. evaluate a list of promising fluids for a set of defined boundary conditions, as e.g. in '...\CaseStudyI\BestSolutionAnalysis_CaseStudy_I', or for varying boundary conditions for comparison purposes, as '...\BestSolutionAnalysis_CaseStudy_I_DifferentBoundaryConds.m'. The script '...\ScreeningCaseStudy_I.m' executes the screening procedure as described in [1].

The inputs for the model evaluations are defined by the file `'...\DefineInputs_CaseStudy_I.m'`. The script defines the most important parameter, as described in the following section, and saves them into the folder of the current case study. The script adds all required folders to the current Matlab-path.

If the user wants to analyze a new case study, it is recommended to either duplicate the folder structure and the files as they are available for CaseStudy_I and CaseStudy_II before adjusting the values or to reuse the existing file and folder structure of the available case studies.

3.3 Inputs

The evaluation of the model requires the following set of inputs:

- `boundaryCond:` Includes all boundary conditions, such as medium, temperatures and pressures of sink and source
- `cycleInput:` Includes all inputs with respect to the cycle, such as the required minimum superheating, pinch point temperature differences
- `componentInput:` Includes all component specific inputs, such as number of states in the heat exchangers or efficiencies of the compressor
- `solverInput:` Includes information for the solver, such as maximum solving time, tolerances
- `economyInput:` Includes all inputs related to economic calculations, such as interest rate, plant lifetime, annual operating hours

The full set of required inputs, including examples and units, is given by the provided examples.

3.4 Outputs

The optimization calls evaluate the model and yield the following outputs:

- `COP:` The COP is the main results and is directly given as a variable
- `summary:` The remaining important variables are summarized in the summary structure. The structure has among others the following substructures, which each include the according information: `medium`, `composition`, `Performance`, `EB` (Energy Balance), `TQ` (Temperatures and Heat rates in the HX), `Component`, `Exergy`, `Investment`, `Economy`, `exitflag`
- `cycle:` The cycle structure includes all information that describe the state points of the cycle, e.g. enthalpy, entropy, pressures, Temperatures, mass flow rate, … for the main state points of the cycle as well as vectors including the discretized states of the heat exchangers.

3.5 Options for model evaluations

The model implementations include some features for evaluating the functions. These different options are explained in the following.

- Mass flow rate and load:
  The mass flow rate of the cycle and respectively the cooling and heating load can be defined by different inputs. One variable defines which option is selected for the specification (`cycleInput.DefineLoad = …`) and accordingly a second variable has to be defined as an input. Examples are listed in the following:
  - o Supplied heat sink (heating):
    ```
    cycleInput.DefineLoad   = 'Q_dot_sink';   % Fixed supplied heat
    load
    cycleInput.Q_dot_sink   = 13900;          % [W]
    ```
  - o Supplied heat source (cooling):

```
cycleInput.DefineLoad   = 'Q_dot_source';  % Fixed supplied heat
source
cycleInput.Q_dot_sink   = 12331;           % [W]
```
o Volume flow rate at compressor inlet:
```
cycleInput.DefineLoad   = 'V_dot_comp_in'; % Fixed volume flow
cycleInput.Q_dot_sink   = 300/3600;        % [m3/s]
```

- Minimum required superheating:

The minimum required superheating is respected at both the compressor inlet and outlet. It is defined as the following:

    o Standard cycle:
```
cycleInput.delta_T_minSH= 5;               % [K]
```
    o IHX-Cycle
The IHX-cycle has the additional degree of freedom of varying the evaporator outlet quality.
```
cycleInput.Q_evap_out = 1;
```

- Pressure drops:

The pressure drops in the heat exchangers can be given as a vector including the pressure drop in each control volume for each heat exchanger:

    o Example for the condenser (using `n_vol_cond = n_states_cond-1`):
```
cycleInput.dp_cond  = dp_cond_tot/(n_vol_cond)*ones(n_vol_cond,1);
```
The definition of the other heat exchangers is analogue.

- Compressor efficiency:

The compressor efficiency can be either set to a constant value or it can, e.g. for off-design analysis, estimated with correlation depending on the operating conditions.

    o Constant isentropic efficiency:
```
cycleInput.Define_Efficiency = 'constant';
componentInput.Comp.eta_is_comp_design = 0.75;  % [-] Isentropic
Eff.
```
    o Accounting for the pressure ratio and the built-in-volume-ratio:
```
cycleInput.Define_Efficiency = 'BuiltInPressureRatio';
componentInput.Comp.eta_is_comp_design = 0.75;  % [-] Isentropic
Eff.
componentInput.Comp.pi_comp = 3;                % Built in volume
ratio
```

- Heat exchanger area/temperature differences:

The heat exchanger area can be defined in various ways. Considering that the cycle load is fixed, the minimum temperature differences, the average temperature differences, the UA-values and the heat exchanger area are linked. Dependent on how the cycle is solved or optimized, the degree of freedom might be more or less constraint by the heat exchanger inputs. The different implemented options are:

    o Fixed Minimum pinch point temperature differences:
```
cycleInput.DefineHX     = 'Pinch';
componentInput.HX.delta_T_pinch_source_min = 3; % [K]
componentInput.HX.delta_T_pinch_sink_min   = 3; % [K]
componentInput.HX.delta_T_pinch_sub_min    = 3; % [K]
```
    o Minimum pinch point temperature differences (as inequality constraint for optimization -> actual minimum pinch point temperature differences might be larger, if beneficial for objective, e.g. COP):
```
cycleInput.DefineHX     = 'minPinch';
componentInput.HX.delta_T_pinch_source_min = 3; % [K]
```

```
componentInput.HX.delta_T_pinch_sink_min   = 3; % [K]
componentInput.HX.delta_T_pinch_sub_min    = 3; % [K]
```
     o Fixed UA-values:
```
cycleInput.DefineHX    = 'UA';
componentInput.HX.UA_source_total = 4.4699e+04; % [W/K]
componentInput.HX.UA_sink_total = 6.0396e+04;   % [W/K]
% Temperature differences are only used for defining the guess
values!
componentInput.HX.delta_T_pinch_sub_min = 5;    % [K]
componentInput.HX.delta_T_pinch_source_min = 5; % [K]
componentInput.HX.delta_T_pinch_sink_min = 5;   % [K]
```
     o Fixed total Heat Exchanger Investment:
```
cycleInput.DefineHX     = 'Invest';
economyInput.HX.PEC_HX_total = 10000;        % [€] Summed PEC for all
HXs
% Temperature differences are only used for defining the guess
values!
componentInput.HX.delta_T_pinch_sub_min = 5;    % [K]
componentInput.HX.delta_T_pinch_source_min = 5; % [K]
componentInput.HX.delta_T_pinch_sink_min = 5;   % [K]
```
- Objective:
  Dependent on the degree of freedom that is given by the other inputs, it makes sense to either solve to e.g. the maximum COP or the maximum net present value NPV:
       o Maximum COP:
```
cycleInput.Objective    = 'COP';
```
       o Maximum Net present value:
```
cycleInput.Objective    = 'NPV';
```
- Calculation options:
  Dependent on the defined boundary conditions and the required results, it can make sense to accelerate the calculations by not always executing all possible calculations. The following scripts can be activated or not:
       o Calculation of Investment cost:
```
economyInput.calcInv    = 'on';
```
       o Calculation of Economy:
```
economyInput.calcEco    = 'on';
```
       o Calculation of Exergy Analysis:
```
cycleInput.calcExergy   = 'on';
```

3.6 Examples for model evaluations

Examples of possible combinations of the inputs and evaluations with different purposes are given by the Matlab examples. In the following, some of the most important examples are explained.

3.6.1 Implemented procedures

- Single model evaluation:
  The file `call_Opt_CaseStudy_I.m` demonstrates single model evaluation of the standard cycle for one specific fluid.
- Screening procedure:
  The script `ScreeningCaseStudy_I.m` executes the full screening for the standard cycle. The cycle is evaluated for fixed minimum pinch point temperature differences and a fixed supplied cooling load. The summary file is saved for each successfully solved model evaluation and can be analyzed during post processing. The results are saved to a folder as specified in the screening script. It is recommended

to generate a new folder for each screening. The screening script checks for each results, if the fluid was evaluated before. If that condition is true, it jumps to the next fluid to avoid multiple evaluations of the same fluid. This does however require to save new screenings into empty folders.

- Analysis of a list of promising fluids:
  The script `BestSolutionAnalysis_CaseStudy_I.m` evaluates the standard model for the list of mixtures that is defined in the beginning of the file.

- Analysis of a list of promising fluids for different boundary conditions:
  The script `BestSolutionAnalysis_CaseStudy_I_DifferentBoundaryConds.m` evaluates the standard model for the list of mixtures that is defined in the beginning of the file for different boundary conditions. During the first run, the cycle is evaluated by fixed pinch point temperature differences, in another evaluation, all fluids are solved for a fixed heat exchanger investment that was set to the value of Ammonia and in the last run, the pinch point temperatures are released and optimized with respect to COP.

3.6.2 How to call the procedures

1. The file `DefineInputs_CaseStudy_....m` is the first script that has to be run. It defines the main input parameters of the case study and adds all required paths to the active Matlab path. The list of fluids is evaluated in this execution by calling the script `ListOfFluids.m` and if the list should be adjusted, it has to be done in this file before the definition of the inputs.

2. Call of the above described procedures:
   a. Single model evaluation:
      The single evaluation of a model requires the definition of some further inputs as described in the available scripts before the actual function is called, e.g. the definition of cycle parameters. If required, inputs that are specific for any function evaluation may be given and the default values in the defined inputs may be overwritten. Further inputs are e.g. the medium, the composition, the required superheating and other inputs.
      Afterwards the model is evaluated accordingly.
      Lastly, the most important performance parameters are displayed and a temperature-heat diagram and a $\log(p)$-h-diagram is plotted.

   b. Screening procedure:
      Analogously to a single model evaluation, some cycle inputs and screening specific inputs have to be defined. The script is then running through all possible combinations of the mixtures for composition steps of 10 % and evaluates the cycle model accordingly. The result file is saved for each mixture and before each model evaluation, it is checked if the fluid was evaluated before. It is recommended to define a new folder in which the screening results are saved and to change the path in the screening script accordingly. The result folder into which the screening results are saved should be empty before every screening procedure.
      After the screening procedure was conducted, the results should be summarized by running the script `SummarizeResults.m` after having adjusted the path pointing to the results that were generated by the screening procedure. The algorithm yields a table containing all results in both Matlab and excel format, as well as a structure containing all results.
      The generated excel file may be used for further analyses by employing the available functions for filters.
      The results may be visualized by using the scripts `plot_c_HG_over_x2.m` and `plot_COP_over_x2.m`, which however requires that the Result structure was generated before.

c. The evaluation of the best cases is conducted analogously to the single model evaluation. In this case, a list of fluids has to be defined for further evaluation. The script runs through this list of fluids and evaluates the model for each fluid and saves the results to a table. For the script comparing the different boundary conditions, this procedure is repeated 3 times for different boundary conditions.

3.7   Scripts for post-processing

The screening procedure is comprehensive and produces a large amount of output data. The summary structures are saved for each model evaluation and can be summarized and processed in different formats. In order to support during the post-processing of the simulation results, the following scripts are supplied:

- Summarize results and export as tables:

  The file `SummarizeResults.m` summarizes the results and saves it as a structure in Matlab-format and a table in Matlab-format as well as in Excel. The excel file is an effective tool for the analysis of the results as it allows to filter and sort the results by different criteria. Note that no filter may be active while the results are exported to the excel file, since this causes errors. During the collection of the results, the results are checked for validity and only feasible results are saved to the summary files.

- The exported structure serves as a basis for the generation of the plots of the COP and e.g. the c_{hg} over the composition of component 2, which can be generated with the scripts `plot_COP_over_x2.m` and `plot_c_hg_over_x2.m`.

3.8   Further comments

The folder `Miscellaneous` contains supporting functions from other authors that are e.g. used for plotting purposes. References to the authors of these functions are given within the functions itself.

Author contributions

Benjamin Zühlsdorf was responsible for the development, implementation, testing and documentation of the numerical models. Jonas Kjær Jensen and Brian Elmegaard contributed by discussions throughout the process. All authors have given approval to the final version of the numerical models.

Acknowledgements

Nomenclature

Abbreviations:

GWP	Global warming potential	IHX	Internal heat exchanger
HFC	Hydrofluorocarbon	ODP	Ozone depletion potential
HFO	Hyrdofluoroolefin		

Latin Symbols:

A	Heat exchange area, m^2	$\bar{T}_{Cond,pure}$	Thermodynamic average temperature of condenser for ideal pure fluid, °C or K
c_{HG}	Levelized specific cost of heat generation, €/MWh		
COP	Coefficient of performance, -	$\bar{T}_{Cond,mix}$	Thermodynamic average temperature of condenser for ideal mixture, °C or K
COP_{Car}	Carnot COP, -		
COP_{Lor}	Lorenz COP, -	$\bar{T}_{Evap}$	Thermodynamic average temperature of evaporator, °C or K
$COP_{Int,max}$	Maximum Lorenz COP of internal cycle, -		
		$\bar{T}_{Evap,pure}$	Thermodynamic average temperature of evaporator for ideal pure fluid, °C or K
CF_{el}	Annual cash flow associated to electricity consumption, €/year		
CF_{Source}	Annual cash flow associated to heat consumption, €/year	$\bar{T}_{Evap,mix}$	Thermodynamic average temperature of evaporator for ideal mixture, °C or K
CF_{Supply}	Annual cash flow associated to heat supply, €/year		
CRF	Capital recovery factor, 1/year	$\bar{T}_{Sink}$	Thermodynamic average temperature of sink, °C or K
f_{TCI}	Factor for estimation of TCI, -	$T_{Sink,in}$	Sink inlet temperature, °C or K
h_i	Specific enthalpy at state point i, kJ/kg	$T_{Sink,out}$	Sink outlet temperature, °C or K
i_{eff}	Effective interest rate, -	$\bar{T}_{Source}$	Thermodynamic average temperature of source, °C or K
n	Life time of plant, years		
NPV	Net present value, €	$T_{Source,in}$	Source inlet temperature, °C or K
OH	Annual operating hours, h/year	$T_{Source,out}$	Source outlet temperature, °C or K
PBT	Payback time, years		
PEC	Purchased equipment cost, €	U	Heat transmission coefficient, $kW/(m^2K)$
$\dot{Q}_{IHX}$	Heat transferred in IHX, kW		
$\dot{Q}_{Loss.Comp}$	Heat loss from compressor, kW	UA	Heat conductance, kW/K
$\dot{Q}_{Sink}$	Heat load transferred to sink, kW	UA_{Sink}	Overall heat conductance of condenser, kW/K
$\dot{Q}_{Source}$	Heat load transferred from source, kW	UA_{Source}	Overall heat conductance of evaporator, kW/K
TCI	Total capital investment cost, €	VHC	Volumetric heating capacity, kJ/m^3
$\bar{T}_{Cond}$	Thermodynamic average temperature of condenser, °C or K	v_i	Specific volume at state point i, m^3/kg

$\dot{W}_{\text{Comp}}$ Compressor work, kW

Greek Symbols:

ε	Exergetic efficiency, -	$\Delta T_{\text{Pinch,Sink}}$	Pinch point temperature difference in condenser, K
η_{Lor}	Lorenz efficiency, -	$\Delta T_{\text{Pinch,Source}}$	Pinch point temperature difference in evaporator, K
ΔT_{in}	Temperature difference at heat exchanger inlet, K	ΔT_{Sink}	Sink temperature glide, K
ΔT_{out}	Temperature difference at heat exchanger outlet, K	ΔT_{Source}	Source temperature glide, K
ΔT_{Pinch}	Pinch point temperature difference, K		

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