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# Modelling and Simulation of the Freezing Systems and Heat Pumps Using Unisim® Design

C. Patrascioiu

***Abstract*—**The paper describes the modeling and simulation of the heat pumps domain processes. The main objective of the study is the use of the heat pump in propene–propane distillation processes. The modeling and simulation instrument is the Unisim® Design simulator. The paper is structured in three parts: An overview of the compressing gases, the modeling and simulation of the freezing systems, and the modeling and simulation of the heat pumps. For each of these systems, there are presented the Unisim® Design simulation diagrams, the input–output system structure and the numerical results. Future studies will consider modeling and simulation of the propene–propane distillation process with heat pump.

***Keywords*—**Distillation, heat pump, simulation, Unisim Design.

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## I. Introduction

THE pipe transport of the vapours and gases represents an important operation of the chemical plants. This operation has a major influence to investment and operation costs. The vapours transport is made by using the centrifugal compressors.

The compressors are dynamic equipment used to increase the flow pressure. The compressors may be manipulated with steam turbines motor, gas turbines motor, gasoline or diesel engines or electric motors. The compressor engine is selected in relation to the compressor speed and inlet flow [1].

The gas compression applications are freezing systems [2] and heat pumps [3]. For the all gas compression applications, in order to realize a gut design and an optimal operation, it is necessary to model and simulate these processes. Many examples of the gas compressing systems modeling and simulation are presented in [4], [5]. The modern modeling and simulation instruments are usually chemical process simulators, respectively HYSYS or Unisim® Design, PROII [6]-[10].

The paper presents the research results of modeling and simulating freezing systems and heat pumps using Unisim® Design simulator. The target of this research is the integration of the distillation process model with the heat pump model.

## II. Overview of the Compressing Gas Systems

The gas compression systems in closed lump have four constitutive elements: vaporizer (V), compressor (C), condenser (K) and reducing pressure valve (D). A sample constructive scheme of this compressing system has a form presented in Fig. 1 (a) [2].

C. Patrascioiu, professor is with the Petroleum - Gas University of Ploiesti, Romania (e-mail: cpatrascioiu@upg-ploiesti.ro).

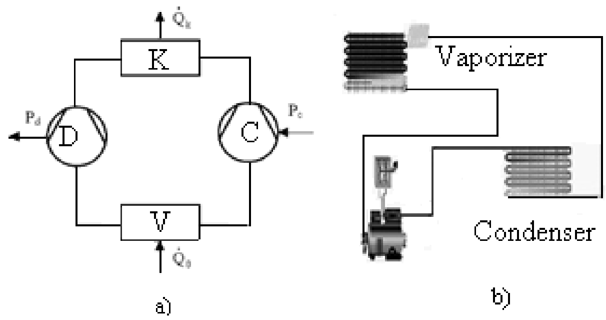


Fig. 1 Standard structure of the freezing systems and heat pumps: (a) block scheme; (b) freezing system example

The freezing systems have the structure presented in Fig. 1, that displays all the four components. An example of the freezing system is showed in Fig. 1 (b), which is a domestic freezing device.

The heat pumps are used to transfer the vapour heat to another flow, characterized by a high temperature, using pressure increasing. Among heat pump applications, there are the distillation processes. A standard structure of this distillation process type is presented in [3]. The use of a heat pump in a distillation process is possible just in the case when the temperature difference between the bottom and the top column is reduced. A basic structure of the propene – propane distillation column with heat pump is presented in Fig. 2 [5]. The vapours generated at the top column are compressed, so that the vapour temperature increases to a value greater than the bottom temperature. In this mode, the top column vapour will become the heat agent of the column reboiler. To restore the distillation mechanism, it is necessary that the vapour decompression should be combined with the temperature decreasing. The design of the heat pump must be realized using chemical simulators.

The control problems of the freezing systems and heat pumps are divided in two categories. The first category follows the chemical process objectives, and the second category is destined to centrifugal compressor control.

## III. Modeling of the Freezing System

### *A. Standard Freezing System Modelling*

A standard freezing system is presented in Fig. 3 [7], [12]. The freezing system contains propane, the flow characteristics being presented in Table I and the installation characteristics are shown in Table II.

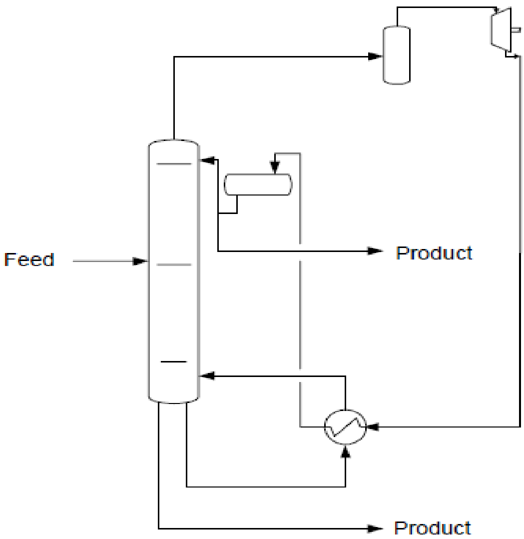


Fig. 2 The heat pump distillation column [5]

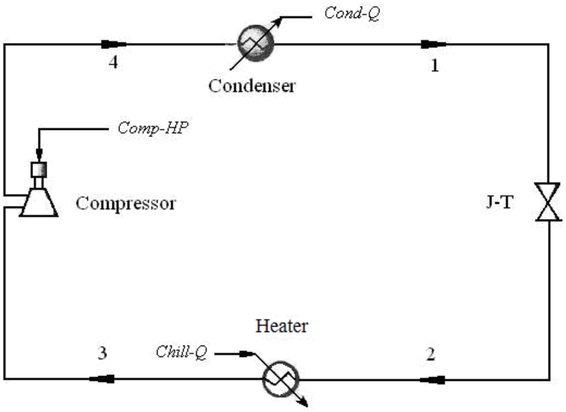


Fig. 3 The modeling of the standard freezing structure

TABLE I
MATERIAL FLOW CHARACTERISTICS

| Property | Flow 1 | Flow 3 |
|---|---|---|
| Vaporized fraction | 0 | 1 |
| Temperature | 50°C | -20°C |

The analysis of the input data indicates that the specifications of the flow 1 and flow 3 are not sufficient, because its flow rate or pressure are missing. This situation imposes that flow rate and pressure must be calculated using material and thermal balance.

Details of the programming are presented in [6]. The program modules are defined in the following order:

1) Flow 1 and flow 3;
2) Decompressing valve;
3) Heat exchanger named ***Heater***;
4) Compressor;
5) Condenser named ***Cooler***.

After uploading the last module, the mathematical model may be solved and the simulator determines the numerical solution. Thus, the flow rate of propane has the value 107.923 kmol/h and the pressure and temperature for each flow are presented in Table III.

By analyzing the simulation results, one may conclude that the freezer system is completely characterized. The imposed condition for the flows 1 and 3, as well as the condenser duty, determines the solution of the freezer system. Because the conditions for the flows 1 and 3 are very hard, the single input variable is the vaporizer duty. Table IV presents the variation of the condenser duty and the propane according to the vaporized duty.

TABLE II
CHEMICAL UNIT CHARACTERISTICS

| Chemical unit | Associated variable | | Unit parameter | | |
|---|---|---|---|---|---|
| | Signification | Name | Name | MU | Value |
| Heat exchanger | Thermal duty | *Chill Q* | Drop pressure | kPa | 7 |
| | | | Thermal duty | kJ/h | $10^6$ |
| Compressor | Power | *Comp HP* | Adiabatic efficiency | % | 75 |
| Condenser | Thermal duty | *Cond Q* | Drop pressure | kPa | 35 |

TABLE III
STANDARD REFRIGERATION SYSTEM SIMULATION RESULTS

| Flux | Temperature [ºC] | Pressure [bar] |
|---|---|---|
| 1 | 50.0 | 17.20 |
| 2 | -19.2 | 2.51 |
| 3 | -20.0 | 2.44 |
| 4 | 72.6 | 17.55 |

TABLE IV
OUTPUT VARIABLES CALCULATED VERSUS VAPORIZER DUTY

| Vaporizer duty [$10^6$ kJ/h] | Condenser duty [$10^6$ kJ/h] | Refrigerator flow rate [kmol/h] |
|---|---|---|
| 0.8 | 1.266 | 86.398 |
| 0.9 | 1.428 | 97.130 |
| 1.0 | 1.587 | 107.923 |
| 1.1 | 1.745 | 118.715 |
| 1.2 | 1.904 | 129.507 |
| 1.3 | 2.063 | 140.299 |

The analysis of the numerical results indicates that the condenser duty and propane flowrate are strongly correlated with the vaporizer duty. The variation of the propane flowrate and the compressor power are not desired and, consequently, the freezing structure does not function in variable duty.

*B. Freezing System Analysis*

We consider the same freezer structure, Fig. 3. From an industrial point of view, it is necessary to correctly define the input variables. The safety compressor operation imposes that the flows 3 and 4 have to be in vapour steady. In these conditions, the input variables are the following: the output compressor pressure, the condenser thermal duty, the propane flowrate and the open valve percentage. Based on the previous example, the input variable for the second case have the values presented in Table V. In this case, the Unisim simulation diagram has been realized using the specification presented as:

1. Flow 4;
2. Heat exchanger;
3. Valve;
4. Condenser;

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5. Flow 3;
6. Compressor.

TABLE V
INPUT VARIABLE SPECIFICATIONS

| Variable | Associated to | MU | Specification |
|---|---|---|---|
| Output compressor pressure | Flow 4 | kPa | 1755 |
| Condenser duty | Condenser | kJ/h | $1.587x10^6$ |
| Freezer flow rate | Flow 4 | kmol/h | 107.923 |
| Open valve | VLV | % | 69.51 |

From a systemic point of view, the freezer system, defined in the second case, can be considered as a multivariable system, Fig. 4. The freezing system has been simulated using the Unisim Design simulator. The numerical results are presented in Table VI.

TABLE VI
NUMERICAL SIMULATION RESULTS

| Variable | Associated to | UM | Value |
|---|---|---|---|
| Temperature | Flow 4 | °C | 50.9 |
| Temperature | Flow 1 | °C | 34.7 |
| Drop pressure | Valve | kPa | 1500 |
| Temperature | Flow 2 | °C | -22.8 |
| Vapour/Phase fraction | Flow 2 | % | 37.0 |
| Thermal duty | Heat exchanger | kJ/h | $1.207x10^6$ |
| Temperature | Flow 3 | °C | -23.7 |
| Compressor power | Compressor | kW | 105.5 |

The analysis of the results confirms that the variable selection determines the numerical simulation results. So, there have been registered significant differences for the temperature of the stream "Flow 1" (34.7°C/50°C). This difference is generated by the input data specification and, consequently, by the mathematical model imposed by the input data.

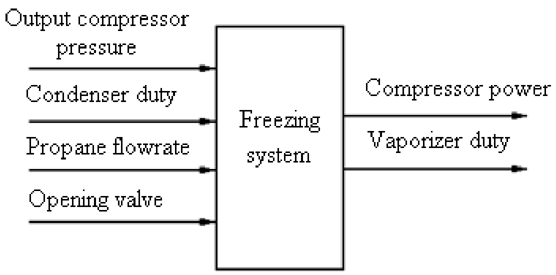


Fig. 4 Input/output freezer system structure

The analysis of the Unisim simulation diagram and the analysis of the mathematical models of the physical processes generate the following conclusions:

– The output compressor pressure, the algorithm of the valve drop pressure and the propane flowrate generate the pressure profile for the freezing system.
– The vaporizer duty is calculated using the condition that the flow aspired by the compressor has to be in a vapour phase.

Thereby, this approach of the freezing mathematical model is better for modeling in case 1. The obtained results when only the propane flow rate has been modified are presented in Table VII. An increasing flow rate generates the increasing of the compressor power, the decreasing of the vaporizer duty and, most important, the increasing of the Vapor/Phase fraction of flow 2. As a consequence of the last observation, the vaporizer duty decreases and the function of the vaporizer is possible to be replaced (for example, with a direct blending of the flow 2 with another heat flow).

TABLE VII
RESULTS OF THE FREEZING SYSTEM SIMULATION

| Propane flowrate [kmol/h] | Vaporizer duty [kJ/h] $x10^{-6}$ | Compressor power [kW] | Vapor/Phase flow 2 [%] |
|---|---|---|---|
| 107.9 | 1.207 | 105.5 | 35 |
| 120.0 | 1.165 | 117.3 | 47 |
| 140.0 | 1.094 | 136.9 | 55 |
| 180.0 | 0.953 | 176.0 | 70 |
| 250.0 | 0.707 | 244.0 | 83 |

## IV. MODELING AND SIMULATION OF THE THERMAL PUMP

### *A. Distillation Column with Thermal Pump*

The distillation heat recuperation is not possible because the heat extracted in the condenser is not used by the column reboiler, due to the low temperature of the hot flow. The solution of this problem is to compress the column vapours to a high pressure, in order to ensure a high temperature of this flow [11]. This column type uses a centrifugal compressor that will introduce new elements in the distillation process: aspiration vessel, antidumping control system, protection systems, auxiliary device. The compressor is an important energy user and, in consequence, the consumed power will depend on the difference between bottom and top column temperature. The most important applications of this system are used in ethylene – ethane distillation and propylene – propane distillation. An example is the industrial distillation column presented in Fig. 4.

### *B. Modelling and Simulation*

In present, the simulation of the distillation column with a heat pump is very difficult. The heat pump study may be realized using the next simplifying hypothesis:

a) The vapours flow of the top column is compressed and divided into two circuits: a circuit is used to column reboiler because the flow has a high temperature, and the second circuit is cooled and condensed in a heat exchanger.
b) After the heat exchanger, each circuit has a decompressing valve used to cool and condense the flow.
c) The liquid obtained from the two circuits is collected into a reflux vessel associated to the distillation column. After separation of the two phases, the reflux flow is used in the distillation column, the distillate flow represents the product and the vapour flow will be returned in the compressor feed.

The process input variables are the following: the output compressor pressure, the column vapours flow rate and the flow rate of the reboiler circuit (circuit number 2). The heat

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pump Unisim diagram simulation is presented in Fig. 5 and the input data are presented in Table VIII.

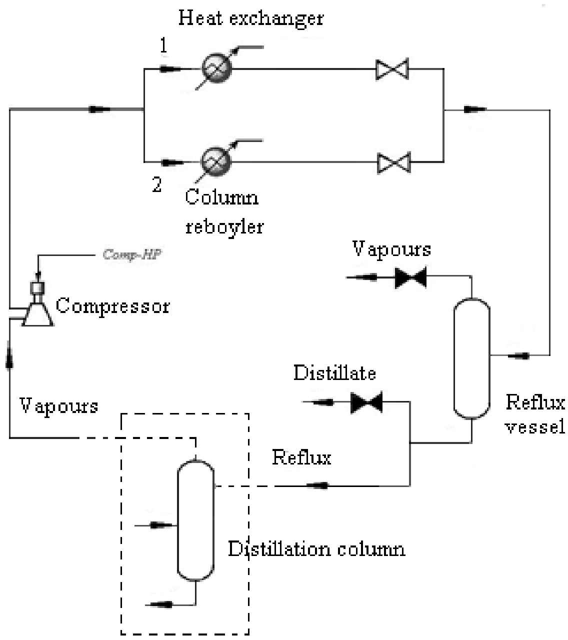


Fig. 5 The thermal pump structure

The Unisim simulation diagram is presented in Fig. 6 and the numerical results are presented in Table IX.

TABLE VIII
HEAT PUMP SIMULATION INPUT DATA

| Variable | UM | Value |
|---|---|---|
| Distillation column vapors flowrate | kg/h | $3.037x10^5$ |
| Distillation column pressure | kPa | 900 |
| Output compressor pressure | kPa | 1700 |
| Circuit 2 flow rate (column reboiler) | % | 80 |
| Column reboiler thermal duty | kJ/h | $7x10^7$ |
| Heat exchanger heat duty | kJ/h | $1x10^7$ |
| Valve 1 / valve 2 drop pressure | kPa | 50 |
| Reflux vessel distillate flowrate | % | 6.9 |

TABLE IX
HEAT PUMP SIMULATION OUTPUT DATA

| Unit/stream | Variable | UM | Value |
|---|---|---|---|
| Output compressor | Temperature | °C | 56 |
| Out 1 | Temperature | °C | 48 |
| Out 1A | Temperature | °C | 46.8 |
| | Vapour/phase fraction | - | 1 |
| Out 2 | Temperature | °C | 48 |
| Out 2A | Temperature | °C | 46.7 |
| | Vapour/phase fraction | - | 0.07 |
| To reflux vessel | Temperature | °C | 46.7 |
| | Vapour/phase fraction | - | 0.258 |
| Reflux vessel vapor | Mass flow | kg/h | $7.859x10^4$ |
| Reflux flow | Mass flow | kg/h | $2.096x10^5$ |
| Distillate flow | Mass flow | kg/h | $1.553x10^4$ |

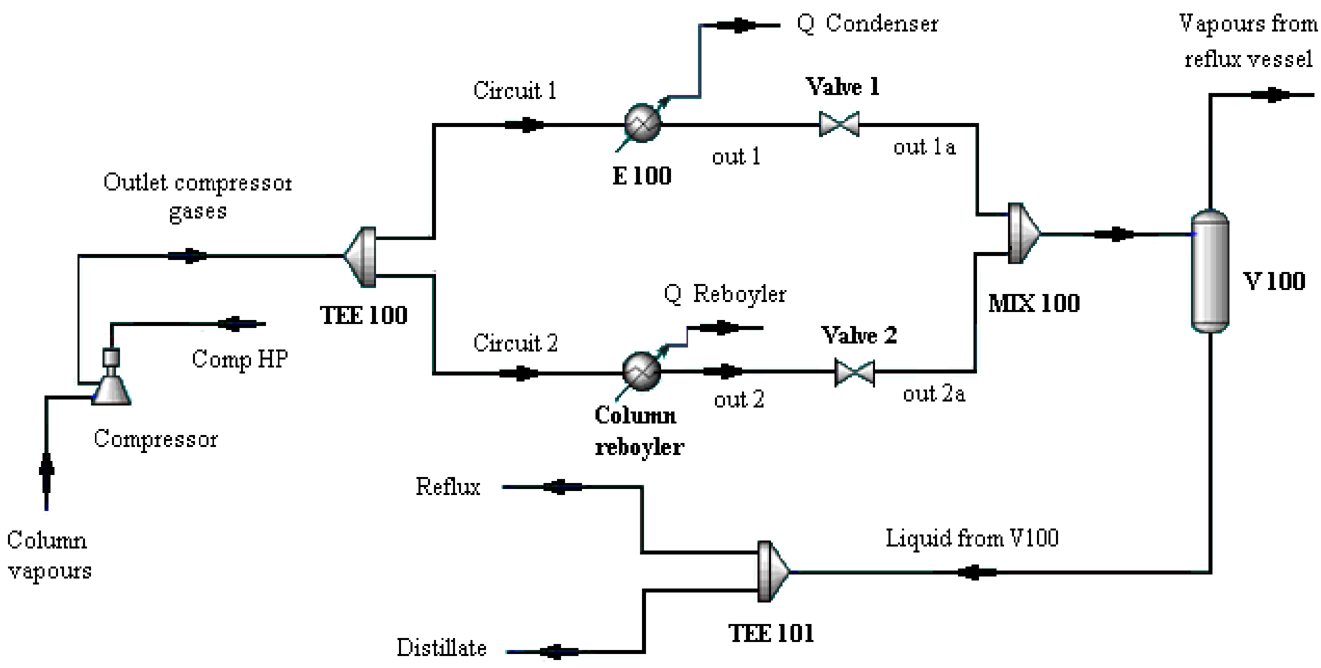


Fig.6 Heat pump simulation Unisim diagram

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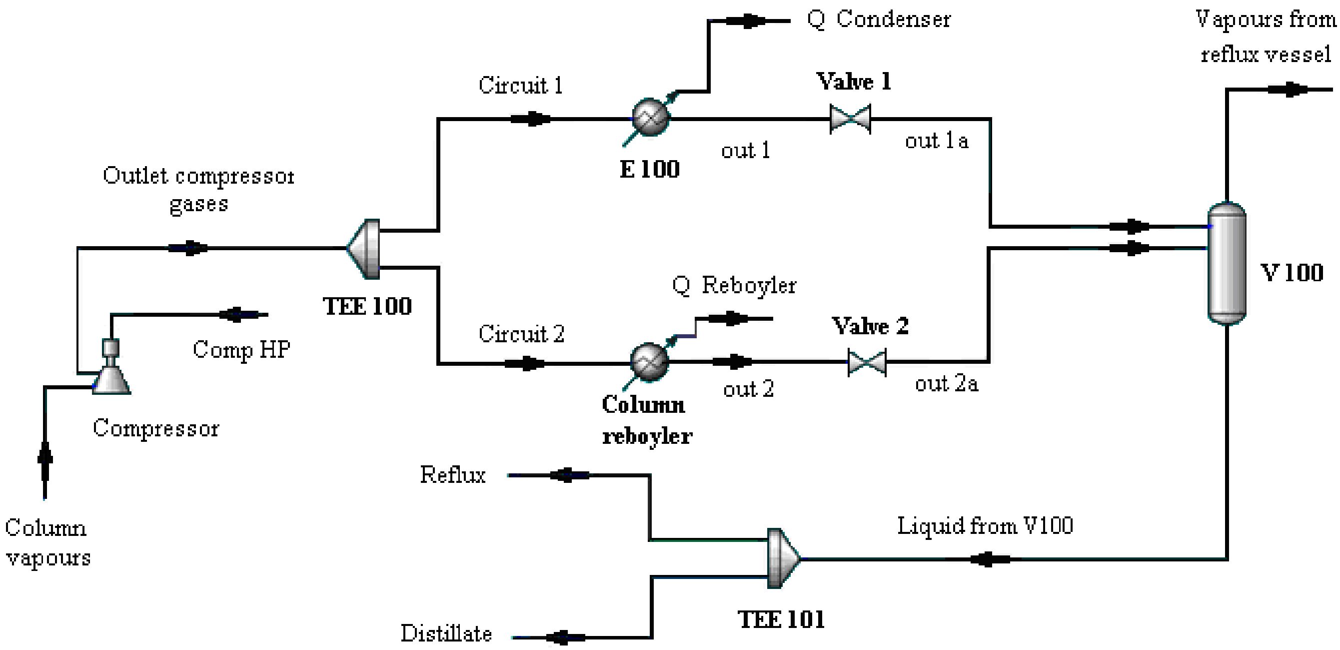


Fig. 7 Heat pump simulation Unisim diagram without MIX module

One of the process modeling is represented by the stream mixing. The Unisim simulator has the MIX module that allows the representation of the mathematical mixing model. In the configuration of the MIX module, it is necessary to select one of two variants of the Automatic Pressure Assignment function: Equalizer all or Set outlet to lowest inlet. The author has studied another variant of the industrial process presented in Fig. 5, respectively the elimination of the MIX module and the configuration of the reflux vessel module with two input streams, Fig. 7. In this mode, the mixing of the out1A and out2A will be realized in the reflux vessel and the pressure and temperature will be calculated using the separator module.

The simulation of the Unisim diagram presented in Fig. 7 has generated similar results to the numerical results presented in Table IX. The analysis of the process structure may generate a simplified input/output structure, Fig. 8.

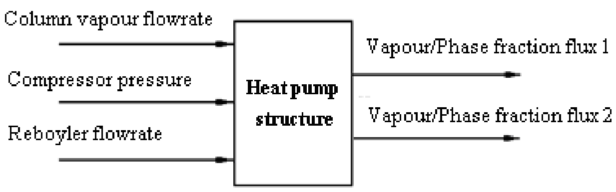


Fig. 8 Heat pump input/output structure

The input variables of the heat pump are the column vapours flowrate, the compressor pressure and the reboiler duty. From an industrial point of view, the reboiler duty is dependent to out2 flow rate, but the Unisim simulator uses two variables: the flowrate of out2 stream and the duty exchanger (column reboiler). The output variables are vapour/phase fraction of the streams out1 and out2. Finally, the industrial output variables are the reflux vessel vapours flow rate and the reflux flow rate.

## V. Conclusions

The paper presents the modeling and simulation of the freezing systems and heat pump systems using the Unisim Design simulator. For each system type there have been defined the input and output variables. The numerical simulation has highlighted the steady state process characteristics and the best Unisim simulation diagram of the two processes. In future, the numerical results will enable performing the distillation process on the basis of the heat pump simulation.

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