# Modelling and Simulation of the Freezing Systems and Heat Pumps Using Unisim<sup>®</sup> 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.

### I. INTRODUCTION

 $T^{\rm HE}$  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).

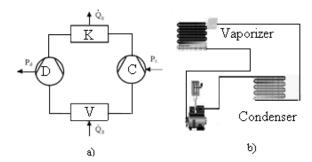


Fig. 1 Standard structure of the freezing systems and heat pumps: (a) block scheme; (b) freezing system example

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.

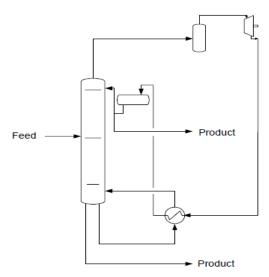


Fig. 2 The heat pump distillation column [5]

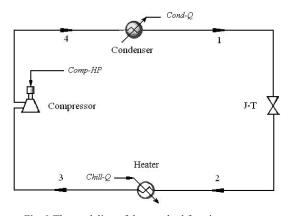


Fig. 3 The modeling of the standard freezing structure

TABLE I Material Flow Characteristics

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

CHEWICAL ONLY CHARACTERISTICS					
Chemical	Associated variable Unit		parameter		
unit	Signification	Name	Name	MU	Value
Heat	Thermal duty	Chill O	Drop pressure	kPa	7
exchanger	Thermai duty	Chili Q	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 [°C]	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	Condenser duty	Refrigerator flow rate			
[10 <sup>6</sup> kJ/h]	$[10^6  kJ/h]$	[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;

- 5. Flow 3;
- 6. Compressor.

TABLE V
INPUT VARIABLE SPECIFICATIONS

INFOT VARIABLE SECURICATIONS				
Variable	Associated to	MU	Specification	
Output compressor pressure	Flow 4	kPa	1755	
Condenser duty	Condenser	kJ/h	$1.587 \times 10^6$	
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	$1.207 x 10^6$		
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.

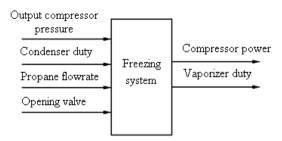


Fig. 4 Input/output freezer system structure

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 <sup>-6</sup>	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

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

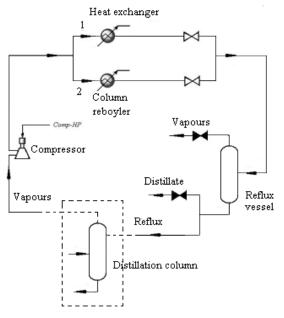


Fig. 5 The thermal pump structure

TABLE VIII HEAT PUMP SIMULATION INPUT DATA

Variable	UM	Value
Distillation column vapors flowrate	kg/h	3.037x10 <sup>5</sup>
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	$7.859 \times 10^4$
Reflux flow	Mass flow	kg/h	$2.096 x 10^5$
Distillate flow	Mass flow	kg/h	$1.553 \times 10^4$

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

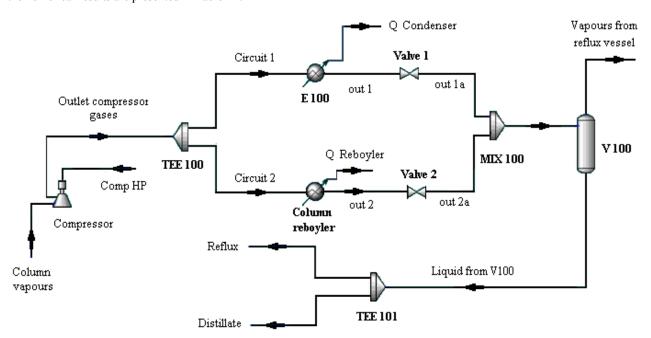


Fig.6 Heat pump simulation Unisim diagram

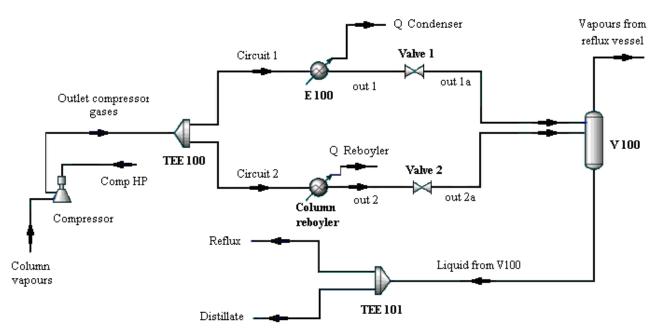


Fig. 7 Heat pump simulation Unisim diagram without MIX module

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.

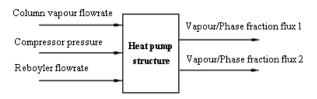


Fig. 8 Heat pump input/output structure

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.

### REFERENCES

- W. F. Stoecker, *Industrial Refrigeration Handbook*, McGraw-Hill: New York, 1998.
- M. Bălan, Instalații frigorifice teorie și programe pentru instruire, www.termo.utcluj.ro/if (Accessed date 08.15.2015)
- [3] United States Patent, 4,753,667, Jun. 28, 1988.
- [4] N. Uddin, J. T. Gravdahl, A compressor surge control system: combination active surge control system and surge avoidance system, ISUAAAT Scientific Committee with JSASS Publication, 2012.
- [5] R. Taboada, C. I. Ferreira, Compression Resorption Cycles in Distillation Columns, International Refrigeration and Air Conditioning Conference, 2008, http://docs.lib.purdue.edu/iracc. (Accessed date 08.15.2015)
- [6] N. Paraschiv, A. Băieşu, G. Stamatescu, Using an Advanced Control Technique for Controlling a Distillation Column, IEEE International Conference on Control and Automation, 2009.
- [7] C. Patrascioiu, M Popescu, Sisteme de conducere a proceselor chimice -Aplicatii, MatrixRom, Bucuresti, 2013.
- [8] C. Patrascioiu, M. Popescu, and N. Paraschiv, Specific Problems of Using Unisim Design® in the Dynamic Simulation of the Propylene-Propane Distillation Column, Revista de Chimie, Vol. 65, No. 9, pp. 1086-1091, 2014.
- [9] G. Bucur, A. Moise, C. Popescu, Simulation of gas dehydratation plants safe operation in chemical industry, Revista de chimie, vol. 66, no. 11, 2015.

# International Journal of Chemical, Materials and Biomolecular Sciences

ISSN: 2415-6620 Vol:10, No:5, 2016

- [10] C. Patrascioiu, Cao M. Anh, M. Popescu, Control of Propylene Propane Distillation Process using Unisim® Design, Proc. of 19th International Conference on System Theory, Control and Computing, October 14-16, Cheile Gradistei, Romania, p 747-752.
  [11] D. F. Sneider, Heat Integration Complications Heat Pump Troubleshoting, Don Sneider, 2001.
  [12] Honeywell, Process Modelling Using Unisim Design Training, Student Course 4576, 2009
- Course 4526, 2009.