Dossier

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Numerical Investigation of an Absorption-Diffusion Cooling Machine Using C_3H_8/C_9H_{20} as Binary Working Fluid

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Résumé — Étude numérique d'une machine frigorifique à absorption-diffusion utilisant le couple C_3H_8/C_9H_{20} — Ce papier est consacré à l'étude et l'analyse d'une machine frigorifique à absorption-diffusion. La machine est actionnée grâce à une source de chaleur de température modérée. La configuration et le principe de fonctionnement de l'appareil obéissent au modèle de Platen Munters [Platen B.C.V. and Munters C.G. (1928) Refrigerator, US Patent 1, 685-764]. Le fluide de travail utilisé est le binaire propane/*n*-nonane, le propane étant le réfrigérant et le *n*-nonane, l'absorbant. L'hydrogène est utilisé comme gaz inerte, égaliseur de pression. La machine est conçue pour une production frigorifique de 1 kW. La température maximale de la source de chaleur est fixée à 130 °C, une température qu'on pourrait atteindre aisément grâce à des capteurs solaires à tubes sous vide. Les simulations sont effectuées en utilisant un logiciel commercial de *flowsheeting*. L'équation d'état de Peng-Robinson est le modèle thermodynamique utilisé.
Nous analysons dans cet article les transferts thermiques et massiques dans les différents composants de l'appareil (absorbeur, condenseur, évaporateur, générateur et échangeurs de chaleur). Les résultats des simulations permettent de déterminer les valeurs des différentes grandeurs caractérisant le fonctionnement de la machine telles que les débits, les compositions et les températures. Une analyse paramétrique a été menée pour évaluer les performances de la machine pour un large éventail des conditions de fonctionnement.

Abstract — Numerical Investigation of an Absorption-Diffusion Cooling Machine Using C_3H_8/C_9H_{20} as Binary Working Fluid — *This paper is concerned with the analysis and the simulation of a heat-driven absorption-diffusion cooling machine which can operate with low-grade heat sources. The simplified configuration of the heat-powered absorption-diffusion refrigerating machine considered in this study is based on the Platen-Munters single pressure refrigerators principle [Platen B.C.V. and Munters C.G. (1928) Refrigerator, US Patent 1, 685-764]. Three working fluids are used, nonane as an absorbent, propane as a refrigerant and hydrogen as the inert auxiliary gas. The designed cooling capacity of the machine is 1 kW which is suitable for a domestic use*

for refrigeration purposes. We restricted the maximum temperature of the driving heat supplied to the generator to 130°C, a temperature achievable with evacuated-tube solar collectors.
The simulations are carried out using a commercially available flow sheeting software with the Peng-Robinson equation of state as property prediction method. In this paper, we analyze the heat and mass transfer characteristics in all relevant machine components (absorber, condenser, generator and solution heat exchangers). The simulations results allow determining the values of different parameters of the systems such as the refrigerant and the solvent temperatures in various points of the machine, the liquid and the vapor flow rates and compositions. The system performances were parametrically analyzed using the flow sheeting software. Performance characteristics were determined for a wide range of operating conditions allowing investigating and evaluating the effect of various design parameters.

INTRODUCTION

Researches dealing with the vapor absorption chillers and refrigerating systems have been since many decades yet attractive challenges to more save the energy and best protect the environment. The absorption-diffusion cooling system performance and its limiting operating conditions are closely related to the refrigerant/absorbent fluid system. The most used pair is NH_3/H_2O with either hydrogen or helium as inert auxiliary gaz. Absorption-diffusion cooling systems using this working fluid need high generator temperature. Thus, when only low-grade heat sources such as solar, geothermal or waste heat from industrial processes are available, the usage of NH_3/H_2O mixture as working fluid must be discarded. Regarding these limitations and others, the search for alternative working fluid systems is not ceasing.

Hydrocarbons and alkane mixtures as refrigerants in vapor-compression-based refrigerating machines and heat pumps were widely considered in the literature (Granryd, 2001; Palm, 2008) but researches concerning their use in absorption and absorption-diffusion machines are unfortunately rare, more extensive investigations are still needed. Chekir *et al.* (2006) presented Fortran-based simulation results of an absorption refrigeration model based on mass and energy conservation equations. Ten alkane mixtures were considered with both air and water cooling. Semanani-Rahbar and Le Goff (2002) analyzed cooling and heating performances in absorption systems using hydrocarbon pairs. In the present study, we analyze relying on Aspen (2001) simulations, the global behavior and performance of an absorption-diffusion system using the $C_3/n\text{-}C_9/H_2$ as working fluids.

1 CYCLE DESCRIPTION

A schematic diagram of an absorption-diffusion refrigeration machine based on Platen-Munters's principle is given in Figure 1. In this study, we consider a cycle using propane-nonane-hydrogen as the working fluid. Propane is the refrigerant, nonane is the absorbent and hydrogen is the inert auxiliary gaz. The cycle is driven by the heat supplied to the generator which drives some propane out of the rich solution (rich in propane) coming into the generator after having left the water-cooled absorber and been pre-heated while passing through the solution heat exchanger. The heat supplied to the generator forms bubbles which push up liquid up in the bubble pump assuring thus the liquid circulation in the cycle. The refrigerant vapor enters the rectifier with a negligible content of nonane and leaves it in a purified state. It flows then to the condenser where it condenses by rejecting heat to the water used as cooling medium. The refrigerant liquid passes through the vapor-liquid heat exchanger HX1 where it is sub-cooled and enters then the evaporator where it meets the hydrogen-propane residual mixture coming from the absorber. Before entering the evaporator, the hydrogen-propane residual mixture has passed and been cooled through the vapor-liquid heat exchanger HX1. Evaporation takes place at low temperature and low propane partial

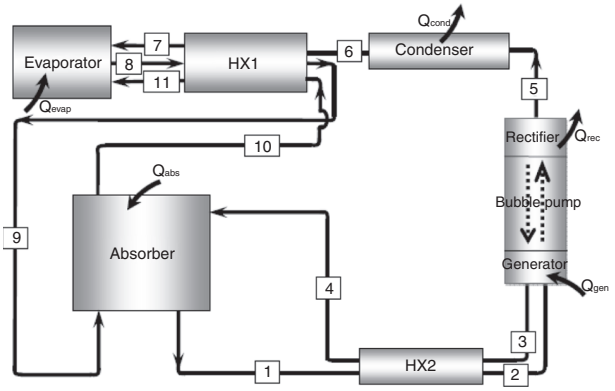

Figure 1

Schematic flow diagram of absorption – diffusion refrigeration system.

pressure. Propane-hydrogen mixture leaves the evaporator, passes through the vapor-liquid heat exchanger and moves onto the absorber where it comes into contact with the weak solution (weak in propane) coming from the generator after having passed through the solution heat exchanger HX2. The absorption of propane takes place and the hydrogen leaves the absorber with however some amount of propane which were not absorbed. Propane rich solution leaves the absorber, passes through the solution heat exchanger (HX2) and moves on towards the generator. The cycle begins again.

2 MODELING AND SIMULATION

2.1 Machine Model

Processes are defined on Aspen Plus *via* a graphical interface. The absorption-diffusion refrigeration system studied in this work is modeled by series of unit operations, blocks (*Fig. 2*). Simulations are made using the sequential modular mode of the flow sheeting program, thus each block is simulated in sequence. While the condenser is modeled using a Heater block, the evaporator is modeled using two blocks a Mixer and a Heater. A Mheatx block is used to model the vapor-liquid heat exchanger and a RadFrac block is used to model the section composed of the three elements (generator, bubble pump and rectifier). The absorber is also modeled using a RadFrac block. The solution heat exchanger is modeled using two Heater blocks connected with a heat stream. After specifying the components, choosing the thermodynamic model and indicating the parameters of each unit operation, simulation could be run. However, design specification convergence blocks must be added. It allows to iteratively adjust the values of some variables, first indicated as manipulated, to meet the problem design specifications.

2.2 Thermodynamic Property

Aspen Plus has an extensive library of built-in thermodynamic models. The choice of the suitable one is of crucial importance to get results with a high degree of accuracy. According to the Aspen Plus documentation (2001) the Pen-Robinson equation of state is the most efficient and reliable method to accurately predict the thermodynamic behavior and the phase equilibrium of light hydrocarbon mixtures. Investigations done by Jaubert *et al.* (2010) by comparing calculated and experimental data allow concluding the same. On the other hand, Luyben (2006) recommend the Chao-Seader model as the most appropriate method within the Aspen Plus built-in property methods.

The Aspen Plus Peng-Robinson-based predictions as well as the Chao-Seader-based-ones are compared with the experimental vapor-liquid equilibrium data for the C_3H_8/C_9H_{20} binary mixture. Figure 3, displaying this comparison, shows that the Peng-Robinson equation of state is in better agreement with the experimental values. Simulations on Aspen Plus are thus done specifying the Peng-Robinson equation of state as the property method.

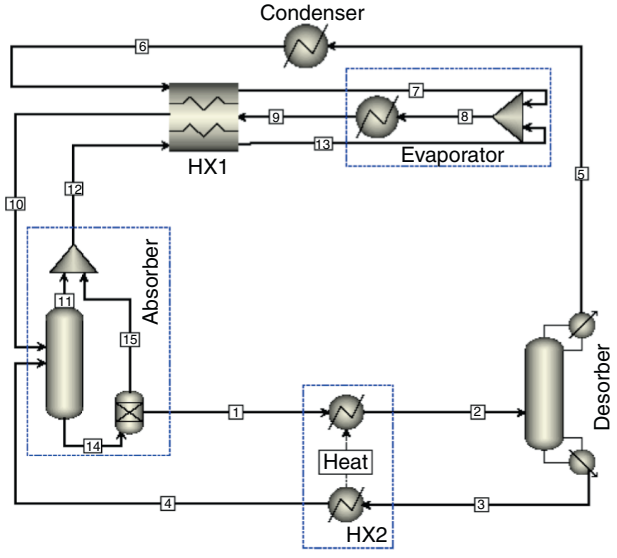

Figure 2

Schematic representation of the absorption chiller-diffusion in Aspen Plus.

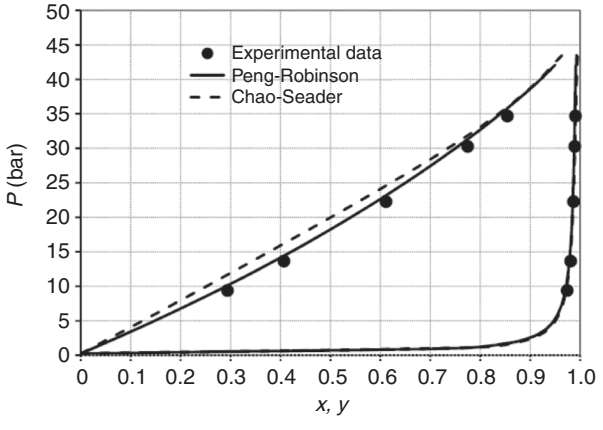

Figure 3

P-x-y diagram of $C_3/n\text{-}C_9$ (T = 376.15 K). Experimental data reported by Jennings and Schucker (1996).

3 RESULTS

The diffusion absorption refrigerator cycle is modeled taking into account the assumptions and operating conditions given in Table 1. Water at 25°C is utilized for cooling the absorber and the condenser. The condensation temperature is assumed to be 13°C higher than the temperature of the cooling water and is thus equal to 38°C. This yields to a total pressure of about 13.1 bar. Pressure drops and heat losses along and through the pipes are neglected. Numerical steady state simulations are conducted using the Aspen plus program in sequential modular mode. The thermodynamic properties of C_3H_8 and C_9H_{20} pure substances and their binary solution properties are retrieved from the software databank using the Peng-Robinson equation of state. Simulations are performed with a molar flow of the rich solution equal to 0.4 mol/s. This value corresponds, according to the considered assumptions and operating conditions, to a refrigeration capacity of about 1 kW. Detailed simulation results are presented in Table 2 and Table 3. The reference state for enthalpy and entropy is the component's constituent elements in an ideal gas state at 25°C and 1 atm. The Cooling Coefficient of Performance (COP) is defined as the ratio of the evaporator heat duty to the generator power input and is expressed as follows:

$$COP = \frac{\dot{Q}_{ev}}{\dot{Q}_{gen}} \quad (1)$$

To determine its Carnot (reversible) cooling coefficient of performance, the heat driven cooling system can be considered as a combined cycle of Carnot engine operating between T_a and T_h, and a Carnot refrigeration system producing cold at T_c and rejecting heat at T_a. T_c, T_a and T_h are respectively the evaporator, the cooling medium and the heat driving temperatures. Applying the first and second laws of thermodynamics, the cooling coefficient of performance can thus be expressed as follows:

TABLE 1
Assumptions and operating conditions

	State point
Saturated solution at the desorber exit	3
Saturated vapor at the desorber exit	5
Vapor purity at the desorber exit: 99.99%	5
Sub-cooled liquid at the condenser exit: 3 K	6
Saturated solution at the absorber exit	1
Evaporator exit temperature: 0°C	9
HX2 et HX1 pinch approach temperature: 2 and 5 K	-
Generator temperature: 130°C	3

TABLE 2
Point characteristics at a strong solution flow of 0.4 mol/s

State point	Temperature T (°C)	C_3 molar fraction x, y	Molar flow rate $\dot{n}$ (kmol/h)	Molar enthalpy h (kcal/mol)	Molar entropy s (cal/mol.K)
1	35	$x_{C_3} = 0.44$	1.5	−48.9	−161.6
2	110	$x_{C_3} = 0.44$	1.5	−44.5	−149
3	130	$x_{C_3} = 0.28$	1.18	−48.9	−168.9
4	37	$x_{C_3} = 0.28$	1.18	−54.5	−184.8
5	39	$y_{C_3} \approx 1$	0.34	−25.1	−69.4
6	35	$x_{C_3} \approx 1$	0.34	−28.6	−80.4
7	5	$x_{C_3} \approx 1$	0.34	−29.4	−83.3
8	−9	$y_{C_3} = 0.42$	1.5	−11.7	−35
9	0	$y_{C_3} = 0.42$	1.5	−11.1	−31
10	23	$y_{C_3} = 0.42$	1.5	−10.6	−31.1
11-12	37	$y_{C_3} = 0.26$	1.19	−6.3	−20.2
13	5	$y_{C_3} = 0.26$	1.19	−6.7	−21.3

TABLE 3
Component thermal performances at a strong solution flow of 0.4 mol/s

Generator (kW)	5.5
Rectifier (kW)	−4
Condenser (kW)	−1.3
Evaporator (kW)	1.1
Absorber (kW)	−1.3
Coefficient of performance	0.2

$$COP_{Carnot} = \frac{T_c}{T_a - T_c}\frac{T_h - T_a}{T_g} \quad (2)$$

For the considered temperature levels the COP_{Carnot} of the system is about 2.85. The real COP obtained is only about 0.2. This difference is partially due to losses from the rectifier and various irreversibilities. The COP of Carnot is too rough to predict the COP of practical absorption-diffusion cooling machines (Yan and Chen, 1989). However, it remains highly important in theory.

Figure 4 illustrates the effect of the generator temperature on the system cooling coefficient of performance and the generator heat input power at a fixed strong solution flow of 0.4 mol/s. Results are shown for generator temperatures ranging between 105°C and 130°C. 105°C is the minimum value of the system driving heat temperature allowing the C_3/n-C_9 separation under the considered operating conditions and assumptions. We fix the maximum generator temperature to 130°C. 130°C as maximum value of generator temperatures corresponds to driving heat sources of low potential. Figure 4 shows that the optimal generator temperature is about 120°C and corresponds to a COP of about 0.21. As expected the COP sharply decreases near the limiting values the generator temperature. In our case, it is especially seen near the minimum value since simulations stop at 130°C which is a value strongly inferior to the maximum generator temperature. The effect of the generator temperature on the generator heat input power is also shown in Figure 4. Increasing generator temperature leads to an almost linear increase of the generator heat input power. This result is in good agreement with simulated and experimental results of (Chen, 1995; Chen *et al.*, 1996) for the absorption diffusion cooling machine using NH_3-H_2O-H_2 as working fluid.

Figure 5 illustrates the COP as a function of the generator temperature at various evaporator exit temperature. It is shown that the higher the evaporator exit temperatures, the higher the COP. This result is also in good agreement with previous studies on the absorption-diffusion cooling machine using NH_3-H_2O-H_2 as working fluid especially those done by (Zohar *et al.*, 2005).

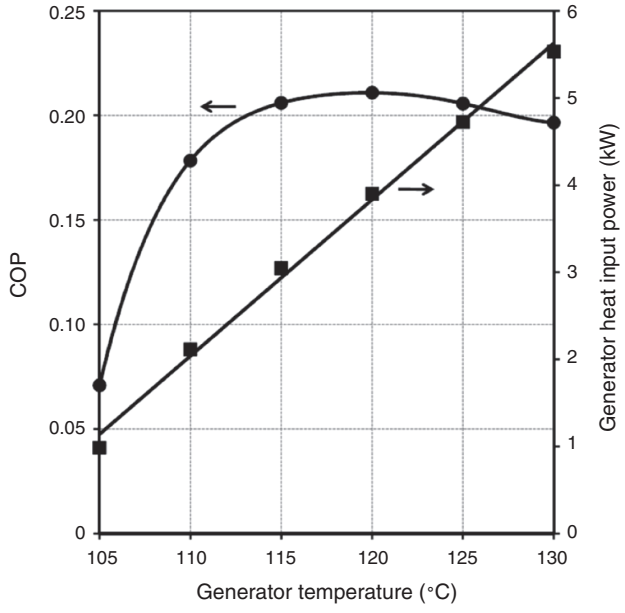

Figure 4

COP and generator heat input power *vs* generator at a strong solution flow of 0.4 mol/s.

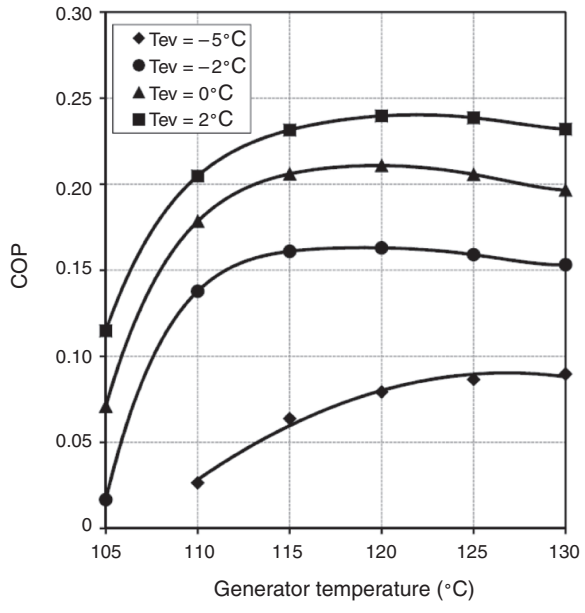

Figure 5

COP *vs* generator temperature and evaporator exit temperature at a strong solution flow of 0.4 mol/s.

CONCLUSION

Modeling and simulation of a $C_3/n\text{-}C_9/H_2$ absorption-diffusion cooling system using Aspen Plus flow-sheeting program are done. Until now, there is no published study that had been carried out to investigate the possible use of the $C_3/n\text{-}C_9/H_2$ working fluid in absorption-diffusion cooling machines. It is also the first time that Aspen Plus flow-sheeting program is used to model and simulate such systems. This program allows us in next works to conduct easy and highly professional sizing of the considered cooling machine. The results of this study showed that our system reaches good cooling performances with low generator temperatures which could be assured by low-grade driving heat sources. This makes the $C_3/n\text{-}C_9/H_2$ preferable to the $NH_3/H_2O/H_2$, the absolutely most used working fluid in commercialized cooling units.

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