



Numerical Investigation of an Absorption-Diffusion Cooling Machine Using C₃H₈/C₉H₂₀ as Binary Working Fluid

H. Dardour, Pierre Cézac, Jean-Michel Reneaume, M. Bourouis, A. Bellagi

► To cite this version:

H. Dardour, Pierre Cézac, Jean-Michel Reneaume, M. Bourouis, A. Bellagi. Numerical Investigation of an Absorption-Diffusion Cooling Machine Using C₃H₈/C₉H₂₀ as Binary Working Fluid. Oil & Gas Science and Technology - Revue d'IFP Energies nouvelles, 2013, 68 (2), pp.249-254. 10.2516/ogst/2012086 . hal-01936088

HAL Id: hal-01936088

<https://hal.science/hal-01936088>

Submitted on 27 Nov 2018

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



This paper is a part of the hereunder thematic dossier published in OGST Journal, Vol. 68, No. 2, pp. 187-396 and available online [here](#)

Cet article fait partie du dossier thématique ci-dessous publié dans la revue OGST, Vol. 68, n°2, pp. 187-396 et téléchargeable [ici](#)

DOSSIER Edited by/Sous la direction de : Jean-Charles de Hemptinne

InMoTher 2012: Industrial Use of Molecular Thermodynamics InMoTher 2012 : Application industrielle de la thermodynamique moléculaire

Oil & Gas Science and Technology – Rev. IFP Energies nouvelles, Vol. 68 (2013), No. 2, pp. 187-396

Copyright © 2013, IFP Energies nouvelles

- 187 > Editorial
- 217 > *Improving the Modeling of Hydrogen Solubility in Heavy Oil Cuts Using an Augmented Grayson Streed (AGS) Approach*
Modélisation améliorée de la solubilité de l'hydrogène dans des coupes lourdes par l'approche de *Grayson Streed Augmenté* (GSA)
R. Torres, J.-C. de Hemptinne and I. Machin
- 235 > *Improving Group Contribution Methods by Distance Weighting*
Amélioration de la méthode de contribution du groupe en pondérant la distance du groupe
A. Zaitseva and V. Alopaeus
- 249 > *Numerical Investigation of an Absorption-Diffusion Cooling Machine Using C_3H_8/C_9H_{20} as Binary Working Fluid*
Étude numérique d'une machine frigorifique à absorption-diffusion utilisant le couple C_3H_8/C_9H_{20}
H. Dardour, P. Cézac, J.-M. Reneaume, M. Bourouis and A. Bellagi
- 255 > *Thermodynamic Properties of 1:1 Salt Aqueous Solutions with the Electrolyte Equation of State*
Propriétés thermophysiques des solutions aqueuses de sels 1:1 avec l'équation d'état de réseau pour électrolytes
A. Zuber, R.F. Checoni, R. Mathew, J.P.L. Santos, F.W. Tavares and M. Castier
- 271 > *Influence of the Periodic Boundary Conditions on the Fluid Structure and on the Thermodynamic Properties Computed from the Molecular Simulations*
Influence des conditions périodiques sur la structure et sur les propriétés thermodynamiques calculées à partir des simulations moléculaires
J. Janeček
- 281 > *Comparison of Predicted pKa Values for Some Amino-Acids, Dipeptides and Tripeptides, Using COSMO-RS, ChemAxon and ACD/Labs Methods*
Comparaison des valeurs de pKa de quelques acides aminés, dipeptides et tripeptides, prédites en utilisant les méthodes COSMO-RS, ChemAxon et ACD/Labs
O. Toure, C.-G. Dussap and A. Lebert
- 299 > *Isotherms of Fluids in Native and Defective Zeolite and Alumino-Phosphate Crystals: Monte-Carlo Simulations with "On-the-Fly" ab initio Electrostatic Potential*
Isothermes d'adsorption de fluides dans des zéolithes silicées et dans des cristaux alumino-phosphatés : simulations de Monte-Carlo utilisant un potentiel électrostatique *ab initio*
X. Rozanska, P. Ungerer, B. Leblanc and M. Yannourakou
- 309 > *Improving Molecular Simulation Models of Adsorption in Porous Materials: Interdependence between Domains*
Amélioration des modèles d'adsorption dans les milieux poreux par simulation moléculaire : interdépendance entre les domaines
J. Puibasset
- 319 > *Performance Analysis of Compositional and Modified Black-Oil Models For a Gas Lift Process*
Analyse des performances de modèles black-oil pour le procédé d'extraction par injection de gaz
M. Mahmudi and M. Taghi Sadeghi
- 331 > *Compositional Description of Three-Phase Flow Model in a Gas-Lifted Well with High Water-Cut*
Description de la composition des trois phases du modèle de flux dans un puits utilisant la poussée de gaz avec des proportions d'eau élevées
M. Mahmudi and M. Taghi Sadeghi
- 341 > *Energy Equation Derivation of the Oil-Gas Flow in Pipelines*
Dérivation de l'équation d'énergie de l'écoulement huile-gaz dans des pipelines
J.M. Duan, W. Wang, Y. Zhang, L.J. Zheng, H.S. Liu and J. Gong
- 355 > *The Effect of Hydrogen Sulfide Concentration on Gel as Water Shutoff Agent*
Effet de la concentration en sulfure d'hydrogène sur un gel utilisé en tant qu'agent de traitement des venues d'eaux
Q. You, L. Mu, Y. Wang and F. Zhao
- 363 > *Geology and Petroleum Systems of the Offshore Benin Basin (Benin)*
Géologie et système pétrolier du bassin offshore du Benin (Benin)
C. Kaki, G.A.F. d'Almeida, N. Yalo and S. Amelina
- 383 > *Geopressure and Trap Integrity Predictions from 3-D Seismic Data: Case Study of the Greater Ughelli Depobelt, Niger Delta*
Pressions de pores et prévisions de l'intégrité des couvertures à partir de données sismiques 3D : le cas du grand sous-bassin d'Ughelli, Delta du Niger
A.I. Opara, K.M. Onuoha, C. Anowai, N.N. Onu and R.O. Mbah

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

H. Dardour^{1*}, P. Cézac², J.-M. Reneaume², M. Bourouis³ and A. Bellagi¹

¹ U.R. Thermique et Thermodynamique des Procédés Industriels, École Nationale d'Ingénieurs de Monastir, Université de Monastir, Avenue Ibn Jazzar, 5060 Monastir - Tunisia

² Laboratoire de Thermique, Énergétique et Procédés (EA 1932), ENSGTI, rue Jules Ferry, 64075 Pau - France

³ Center CREVER, Universitat Rovira i Virgili, 43006 Tarragona - Spain

e-mail: houda.dardour@gmail.com - pierre.cezac@univ-pau.fr - jean-michel.reneaume@univ-pau.fr - mahmoud.bourouis@urv.cat
a.bellagi@anim.rnu.tn

* Corresponding author

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 $\text{NH}_3/\text{H}_2\text{O}$ 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 $\text{NH}_3/\text{H}_2\text{O}$ 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 $\text{C}_3/n\text{-C}_9/\text{H}_2$ 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

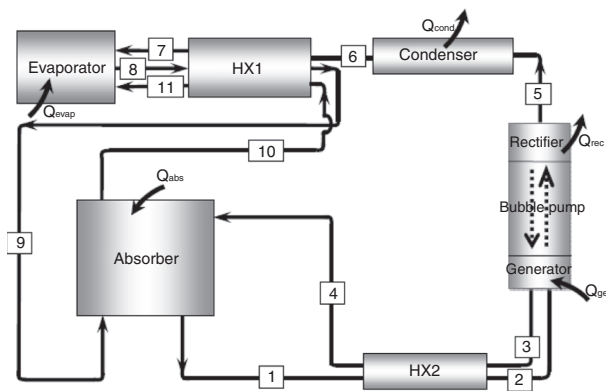


Figure 1

Schematic flow diagram of absorption – diffusion refrigeration system.

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

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.

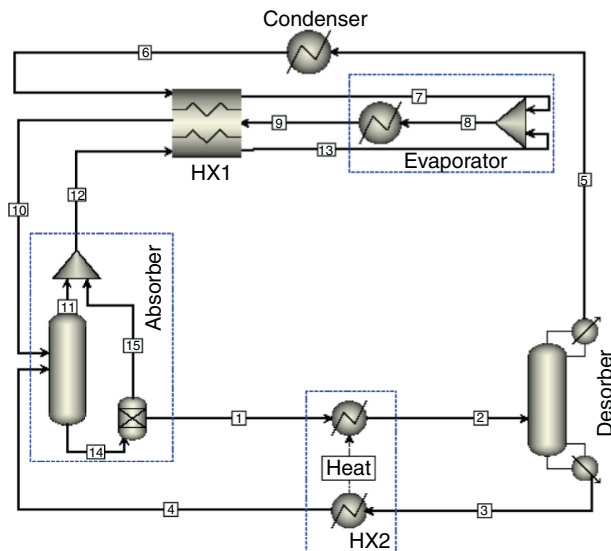


Figure 2

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

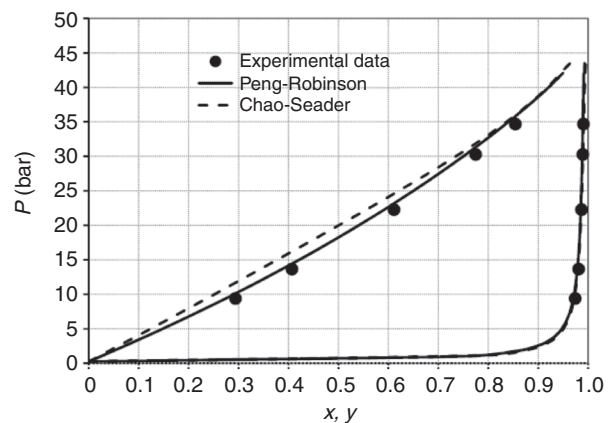


Figure 3

P - x - y diagram of $C_3/n-C_9$ ($T = 376.15$ 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

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

are conducted using the Aspen plus program in sequential modular mode. The thermodynamic properties of C₃H₈ and C₉H₂₀ 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 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).

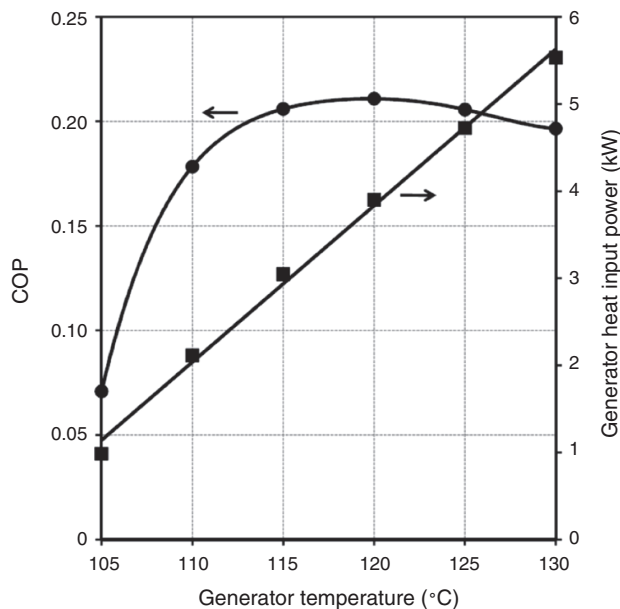


Figure 4

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

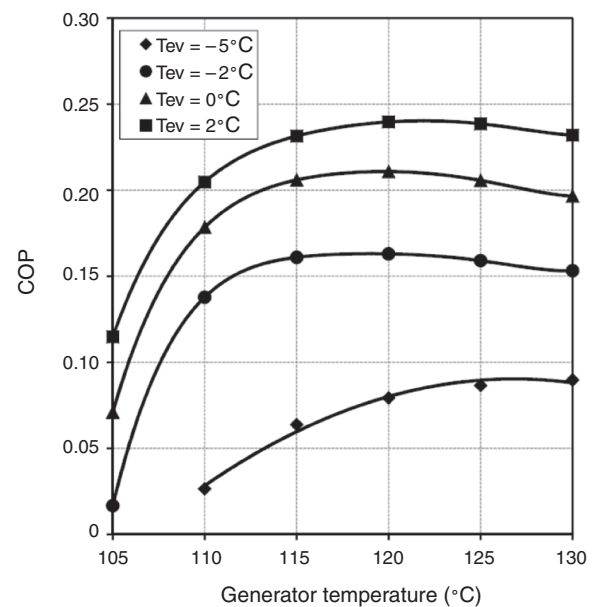


Figure 5

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

CONCLUSION

Modeling and simulation of a $C_3/n-C_9/H_2$ 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 $C_3/n-C_9/H_2$ 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 $C_3/n-C_9/H_2$ preferable to the $NH_3/H_2O/H_2$, the absolutely most used working fluid in commercialized cooling units.

REFERENCES

- Aspen Plus. Version 11.1 (2001) Aspen Technology, Inc., Ten Canal Park, Cambridge, MA, USA. www.aspentech.com.
- Aspen Plus Documentation, user guide (2001) Aspen Technology Inc.
- Chekir N., Mejbri Kh., Bellagi A. (2006) Simulation d'une machine frigorifique à absorption fonctionnant avec des mélanges d'alcane, *Int. J. Refrig.* **29**, 3, 469-475.
- Chen J. (1995) Investigation of the diffusion absorption refrigeration, *PhD Dissertation*, University of Maryland at College Park.
- Chen J., Kim K.J., Herold K.E. (1996) Performance enhancement of a diffusion absorption refrigerator, *Int. J. Refrig.* **19**, 3, 208-218.
- Granryd E. (2001) Hydrocarbons as refrigerants-an overview, *Int. J. Refrig.* **24**, 1, 15-24.
- Jaubert J.N., Privat R., Mutelet F. (2010) Predicting the Phase Equilibria of Synthetic Petroleum Fluids with the PPR78 Approach, *AIChE J.* **56**, 12, 3225-3235.
- Jennings D.W., Schucker R.C. (1996) Comparison of High-Pressure Vapor-Liquid Equilibria of Mixtures of CO_2 or Propane with Nonane and C_9 Alkylbenzenes, *J. Chem. Eng. Data* **41**, 4, 831-838.
- Luyben W.L. (2006) *Distillation Design and Control using Aspen Simulation*, Wiley, New York.
- Palm B. (2008) Hydrocarbons as refrigerants in small heat pump and refrigeration systems – A review, *Int. J. Refrig.* **31**, 4, 552-563.
- Platen B.C.V. and Munters C.G. (1928) Refrigerator, US Patent 1, 685-764.
- Semanani-Rahbar M., Le Goff P. (2002) Utilisation de couples d'hydrocarbures dans les frigopompes et les thermofrigopompes à absorption, *Int. J. Refrig.* **25**, 1, 75-88.
- Yan Z., Chen J. (1989) An optimal endoreversible three-heat-source refrigerator, *J. Appl. Phys.* **65**, 1, 1-4.
- Zohar A., Jelinek M., Levy A., Borde I. (2005) Numerical investigation of a diffusion absorption refrigeration cycle, *Int. J. Refrig.* **28**, 4, 515-525.

Final manuscript received in November 2012

Published online in May 2013

Copyright © 2013 IFP Energies nouvelles

Permission to make digital or hard copies of part or all of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than IFP Energies nouvelles must be honored. Abstracting with credit is permitted. To copy otherwise, to republish, to post on servers, or to redistribute to lists, requires prior specific permission and/or a fee: Request permission from Information Mission, IFP Energies nouvelles, fax. +33 1 47 52 70 96, or revueogst@ifpen.fr.