Modelling and testing the performance of a commercial ammonia/water absorption chiller using Aspen-Plus platform

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Abstract

A steady-state simulation model of a commercial 3-ton ammonia/water absorption chiller is developed and validated using the flow-sheeting software Aspen-Plus. First an appropriate thermodynamic property model for the ammonia/water fluid mixture is selected. To this purpose nine methods from the software library are pre-selected and tested, but none of the methods predicts the vapour-liquid equilibrium (VLE) with sufficient accuracy. The interaction parameters of these models are then determined by fitting the equations of state (eos) to VLE data. It is finally found that the Boston-Mathias modified Peng-Robinson eos with fitted parameters predicts most accurately the VLE for the temperature and pressure ranges encountered in commercial chillers.

A simulation model of the machine is then developed. The simulation results are found to be in good agreement with data from literature at a cooling air temperature of 35 ºC. The heat transfer characteristics (*UA*) of the various heat exchangers of the machine are then determined and the model modified to make it accept these (*UA*) as input parameters. The

comparison of the simulation predictions at cooling air temperatures of 26.7 and 38 ºC with the bibliographical data showed good concordance. The proposed model could be very useful for the analysis and prediction of the performances of the commercial chiller.

Keywords: Absorption refrigeration, ammonia/water, thermodynamic property model, Aspen-Plus, Robur.

Highlights

- A commercial NH_3/H_2O absorption chiller is simulated using the software Aspen-Plus.
- Peng-Robinson-Boston-Mathias equation of state is used to predict VLE of NH_3/H_2O fluid mixture.
- A steady-state model describing the chiller operation is developed.
- The model predicts the internal operating conditions and *COP* of the chiller.

1. Introduction

Due to the rapid increase in global demand for energy and the need to reduce greenhouse gas emissions, the interest in finding new efficient ways of using energy is growing. Cooling technologies are of great economical, energetic and environmental importance. The conventional vapour compression refrigeration and air conditioning systems are driven by electrical energy which consumes worldwide huge amounts of this kind of energy and also contributes to the greenhouse effect in the atmosphere. Priority should be given to the investigation and use of alternative driving energy sources instead of electricity for cooling applications. The interest is focused on absorption cooling technology as it is an attractive alternative and sustainable solution to replace vapour compression units. Indeed, waste heat rejected in many industries is at higher temperatures than the heat source temperatures required for driving most of the absorption cooling systems [1-3]. The use of thermally driven cooling systems can help in reducing problems related to global warming, such as the green-house effect due to CO_2 emissions from the combustion of fossil fuels in thermal power plants. Also the common refrigerant/absorbent working fluids, namely water/lithium bromide and ammonia/water, used in absorption cooling systems are both environment-friendly. Nowadays, several studies are focused on finding new ways to directly use thermal or solar energy to drive cooling machines. Investigations are being carried out on the development of new and hybrid cycle configurations and finding new potential working fluids.

Lazzarin *et al*. [4] reported a detailed work on a gas-fired 5 tons ammonia/water absorption chiller for refrigeration applications. The authors studied the performance of the chiller by modifying its initial charge and proposed some modifications on the machine to produce cold at temperatures as low as -25°C. Chua *et al*. [5] presented a general framework for thermodynamic modelling of an irreversible absorption chiller focusing on the design and tested their theoretical approach on a single-stage ammonia/water unit. Component models of

71 the chiller have been assembled so as to quantify the internal entropy production and thermal
72 conductance (*UA*) in a thermodynamically rigorous formalism, which is in agreement with the
73 simultaneous heat and mass transfer processes occurring within the exchangers. Local
74 thermodynamic balances (energy, entropy and mass balances) and consistency within the
75 components are respected, in addition to the overall thermodynamic balance as determined by
76 the inlet and outlet states of the components. For the absorbers, Colburn-and-Drew mass
77 transfer equations are incorporated to describe the absorption process. Furthermore, the
78 impact of various irreversibilities on the performance of chiller is also evaluated through the
79 use of a general macroscopic equation. Horuz and Callander [6] carried out experimental
80 investigations on the 3 tons Robur gas-fired chiller and studied the response of the system to
81 variations of the chilled water flow rate, inlet temperature and level in the evaporator drum for
82 variable heat inputs by modifying the air-cooled components (a water-cooled absorber and a
83 water-cooled condenser units were incorporated into the system in order to test the
84 experimental system under wider range of condenser and absorber pressures). Darwish *et al*.
85 [7] analysed the Robur absorption refrigeration water/ammonia (ARWA) system using the
86 Aspen-Plus simulator. The results were compared with some manufacturer compiled data
87 reported in the open literature. The performance parameters employed for the analysis were:
88 coefficient of performance (*COP*), heat duties of the evaporator, absorber and condenser,
89 concentration in the ammonia poor and ammonia rich solutions, and flow rates of the
90 ammonia poor solution and refrigerant vapour leaving the evaporator. Agreement between the
91 simulation results and the experimental measurements was observed. Some innovative
92 modifications in the Robur cycle aimed at enhancing the generator operation showed a
93 significant improvement in the *COP*. In particular, introducing a throttling process directly
94 prior to the generator could alleviate the generator heat load and enhance the *COP* up to 20%.
95 Rossa and Bazzo [8] investigated theoretically the feasibility of a small-scale cogeneration

system for cold and electricity production. The system consisted of a 5-ton Robur absorption chiller and a 28 kWe natural gas micro-turbine whose exhaust gas was used to drive the absorption chiller. The authors reported a thermal efficiency of 41 % for the combined cooling and power system, which in turn represents an enhancement of 67% in the efficiency of a single natural-gas micro-turbine. El May *et al*. [9] developed a modular simulation program under Mathematica for absorption heat pumps, refrigerators and air conditioners. The modular approach is an easier way to simulate various complex configurations. As an application, the commercial Robur absorption machine was studied. The predicted results showed well agreement with experimental data from the open literature. El May *et al*. [10] presented and discussed the results of an energetic and exergetic analysis of a commercial air-cooled water/ammonia absorption machine with a cooling capacity of 10 kW. The comparison with a conventional single-effect absorption chiller operating under the same conditions showed that to achieve similar performances to those of the pre-absorber in the Robur chiller, an additional heat transfer area in the air-cooled absorber was required to ensure the complete absorption of the refrigerant. The second law analysis revealed that the highest exergy dissipation (75 %) is located in the driving compartment and that the irreversible absorption process was responsible for an important part (45%) of the *COP* degradation.

In the present work, a steady-state simulation model is developed using the Aspen-Plus platform to test and analyse the performance of a commercial 3-ton gas-fired absorption chiller (10 kW cooling capacity) at different operating conditions. This air-conditioner uses ammonia/water as a working fluid. This particular chiller has been chosen in this study for the following reasons:

i. Although absorption technique is used for cold production, its thermodynamic cycle presents some particularities and complex flow connections in comparison with

conventional absorption machines. In particular a solution cooled absorber, called pre-absorber, is incorporated in the Robur chiller to improve its performances;

ii. There is scarce information in the open literature on how to choose an appropriate thermodynamic property model for the ammonia/water mixture to simulate absorption chillers and heat pumps in Aspen-Plus [11];

iii. The absorption chiller is a commercial unit and operational experimental data is available in the open literature.

2. Chiller description and working principles

A schematic representation of the Robur absorption machine is shown in Figure 1. In the generator, the ammonia/water mixture is heated by thermal energy input provided from a gas burner to desorb the refrigerant. The refrigerant vapours (12) flow to the rectifier where they are cooled by the ammonia rich solution on its way to the generator and which is thus preheated. This causes partial condensation of the water vapours purifying further the ammonia vapours. These flow to the air-cooled condenser where they are liquefied. The liquid refrigerant (8) circulates then to the refrigerant heat-exchanger and further to the refrigerant expansion valve. After reduction of its pressure, the refrigerant is introduced in the evaporator (10) where it evaporates by absorbing heat from the chilled water. The refrigerant vapour flows to the absorber where it is absorbed by the ammonia poor solution returning from the generator in two steps: first, in the pre-absorber where the absorption heat released is used to preheat the ammonia rich solution on its way to the generator (4) and then in the air-cooled absorber to complete the absorption process. 3D-Sketches of the internal view of the machine and its components are presented in Appendix 1 (Figs 12 and 13).

3. Aspen-Plus modelling approach

3.1 Thermodynamic property models

Ammonia/water mixture has been used as a working fluid in absorption refrigeration systems for several decades. To simulate an absorption refrigeration cycle, the thermo-physical properties of the working fluid play a vital role [12]. Different equations are available in the literature [13-25] to calculate the thermodynamic properties of ammonia/water system: Virial equations of state, cubic equations of state, Polynomial functions, Helmholtz free energy, Perturbation theory and Gibbs excess energy.

Schulz [22] presented a fundamental equation of state for this binary mixture. Ziegler and Trepp [23] modified the Schulz equation of state and developed new correlations for predicting the equilibrium properties required in the analysis of absorption refrigeration cycles. The authors used the Gibbs excess energy equation to determine specific volume, specific entropy and specific enthalpy. Using the new correlation, the thermodynamic properties can be predicted up to a pressure of 50 bars and a temperature of 500 K. Renon *et al*. [13] derived an equation of state which can accurately estimate the properties of ammonia/water mixtures. An extended Redlich-Kwong equation of state with two adjustable parameters was used to predict VLE of the working fluid. Ruiter [24] presented a simplified thermodynamic model for the mixture. The equilibrium pressure and the excess enthalpy of the gas and liquid phases were described using 11 coefficients. Patek and Klomfar [15] presented five equations to predict VLE properties. The use of these equations avoids iterative procedures when calculating thermodynamic properties of ammonia/water mixture. The equations were developed by fitting critically assessed experimental data using simple functional forms. The results were presented in form of an enthalpy-concentration diagram. Barhoumi *et al*. [21] reported a detailed work on the reformulation of the thermodynamic

166 properties of the ammonia/water mixture using the Gibbs energy function. For the liquid
167 phase, a three constant Margules model of the excess free enthalpy was formulated. The
168 vapour phase was considered a perfect mixture of real gases, each pure gas being described by
169 a virial equation of state in pressure truncated after the third term. The model developed
170 predicts the thermodynamic properties of the mixture with great accuracy in the three states,
171 i.e. subcooled liquid, superheated vapour and liquid-vapour saturation in the temperature
172 range of 200 to 500 K and a pressure up to 100 bars.

173 Mejbri and Bellagi [25] modelled the thermodynamic properties of the ammonia/water
174 mixture using three different approaches: An empirical Gibbs free enthalpy model, the Patel-
175 Teja cubic equation of state and the PC-SAFT (Perturbed Chain Statistical Associating Fluid
176 Theory) equation of state. A comparison of these three methods proved the superiority of the
177 PC-SAFT equation of state to predict and extrapolate the thermodynamic properties of
178 ammonia/water system over a larger range of temperature ($273.16 \leq T \leq 613.15$ K) and
179 pressure ($0 < P \leq 210$ bar). Also, the authors recommended the use of the Gibbs free enthalpy
180 model for industrial applications that use ammonia/water as a working fluid at moderate
181 temperatures and pressures, such as absorption refrigeration.

182 The selection of a proper method for estimating the thermodynamic properties of the working
183 fluid is one of the most important steps that can affect the simulation of absorption
184 refrigeration cycles. Therefore, it is important to choose carefully an appropriate method to
185 estimate the different properties of the working fluid. Aspen-Plus includes a large databank of
186 thermodynamic property and transport models with the corresponding mixing rules for
187 estimating the mixture properties. Before performing a simulation in Aspen-Plus, it is
188 important to ensure that the selected property method is the best reliable thermodynamic
189 model. In this work, the choice of the ammonia/water mixture property model for use in the
190 simulation of the gas-fired chiller is investigated in detail. To this purpose the predictions of

191 the nine property models available in Aspen-Plus for this working fluid are evaluated and
192 compared with regressed experimental vapor-liquid equilibrium data reported by Mejbri and
193 Bellagi [25] in the pressure range from 2 to 25 bar and the temperature range from -19 to 220
194 ºC. In a second step, the Aspen-Plus Data Regression System facility is used to fit the
195 interaction parameters of the property models to the VLE data of reference [25]. The results
196 are presented in the form of *T-x-y* diagrams.

197 ## 3.2 Selection of the thermodynamic property model

198 The nine property models implemented in Aspen-Plus and considered for the calculation of
199 the properties of the ammonia/water mixture are listed in Table 1. This list includes cubic eos
200 methods (SRK, PR-WS and PR-MHV2, PENG-ROB, PR-BM, RKS-BM) as well as activity
201 coefficient methods (ENRTL-RK, NRTL-HOC, WILS-RK). The tests of these models are
202 performed in two steps. In the first one, *T-x-y* VLE prediction by each of the Aspen-Plus
203 property models are compared with the regressed data reported in [25] for 6 isobars, namely
204 2, 4, 10, 16, 20 and 25 bars. Figures 2, 3 and 4 illustrate this comparison for 2, 10 and 25 bar,
205 respectively. It is observed that the maximum equilibrium temperature deviation predicted by
206 the considered nine property models implemented in Aspen-Plus and the data reported by
207 Mejbri and Bellagi [25] is about 10 ºC. As regards the ammonia mass fraction in the liquid
208 phase, the values predicted by the property models SRK, PR-WS and PR-MHV2 are
209 inconsistent in the whole pressure range. This is the case also of the three activity coefficient
210 models (ENRTL-RK, NRTL-HOC, WILS-RK) for the pressures 10 and 25 bars, for which the
211 deviations increase with increasing pressure. It is concluded that none of these property
212 models reproduces the ammonia/water vapour-liquid equilibrium data with sufficient
213 accuracy.

In a second step, the data regression system of Aspen-Plus was used to fit the parameters of the property models by using the VLE data reported by Mejbri and Bellagi [25]. For the cubic equations of state it is the interaction parameter k_{ij} — or its coefficients $k_{ij}^{(1)}, k_{ij}^{(2)}, k_{ij}^{(3)}$ if it is supposed temperature dependent (see Appendix 2 for details) — that are fitted to the VLE data. Figures 5, 6 and 7 show the corresponding comparison for 2, 10 and 25 bars, respectively. As can be noted, all values of the ammonia mass fraction in the vapour phase predicted by the Aspen-Plus property models are now close to the data reported by Mejbri and Bellagi [25]. Regarding the ammonia mass fraction in the liquid phase, the PR-MHV2 model made the poorest predictions. These figures make also clear that the PR-BM model (Peng-Robinson eos with Boston-Mathias alpha function, see Appendix for details) is in better agreement with the considered vapour-liquid equilibrium data. The sum of squared errors for the nine Aspen-Plus property models tested and summarized in Table 2 confirms this conclusion. This table shows also that with the help of data regression eight of the nine property models have been successfully fitted to make them predict VLE close to the experimental data. Just one property model fails to accommodate well the data: PR-MHV2. It is concluded from these results that the Peng-Robinson-Boston-Mathias equation of state (PR-BM), with fitted parameters, is the most appropriate property method among those implemented in Aspen-Plus for the prediction of the ammonia/water vapour-liquid equilibrium in the investigated temperature and pressure ranges. Table 3 gives the default and regressed values of the parameters $k_{ij}^{(1)}, k_{ij}^{(2)}$ and $, k_{ij}^{(3)}$ for the considered cubic equation of state.

3.3 State points and assumptions

The steady-state simulation model developed in the present work using the flow-sheeting software Aspen-Plus is intended to analyse the performance of the air-cooled Robur

absorption chiller investigated experimentally by Klein [26]. This author carried out his experiments in an environmental chamber at three cooling air temperatures, namely 26.7°C, 35°C and 38°C, with 14 temperature measurement points in the chiller.

The analysis presented in the present paper is performed in two steps. Firstly, the heat transfer characteristics of the major heat exchanging devices of the machine: condenser, evaporator, absorber and refrigerant heat exchanger are deduced from operating data of the chiller at a cooling air temperature of 35 ºC. This heat exchanger characteristic, the heat conductance, sometimes referred to as the heat capacity of the heat exchanger, is generally defined by the equation

$$\dot{Q} = (UA)\Delta T_{ln}$$

Where $\dot{Q}$ is the heat duty and ΔT_{ln} the logarithmic mean temperature difference, LMTD, at the hot (subscript, *h*) and cold (subscript, *c*) ends of the exchanger,

$$\Delta T_{ln} = \frac{\left(T_{h,i} - T_{c,o}\right) - \left(T_{h,o} - T_{c,i}\right)}{\ln\left[\frac{\left(T_{h,i} - T_{c,o}\right)}{\left(T_{h,o} - T_{c,i}\right)}\right]}$$

With the subscripts *i* and *o* referring to inlet and outlet, respectively.

The simulations results are then compared with experimental data of Klein [26] and those obtained by simulation of El May *et al*. [10]. In a second step, the model is then modified to include the (*UA*) values of the heat exchangers determined in the previous step as input parameters. The results are compared with the two sets of data from the literature [10, 26] at cooling air temperatures of 26.7ºC and 38ºC.

Figure 8 shows the Robur model in Apen-Plus. The state points in the chiller are defined as follows. The absorber exit is state point 1A which also represents the inlet of the solution

pump at state point 1; the pump exit is state point 2. State point 5 represents the rectifier exit; the pre-absorber exit leading to the generator is state point 4; the solution exit of the generator leading to valve 2 is state point 6; the valve 2 exit leading to the pre-absorber is state point 3. The vapour exit of the generator is state point 7; the condenser exit is state point 8. The refrigerant heat exchanger exit leading to valve 1 is state point 13; the refrigerant valve exit is state point 9. The evaporator exit is state point 10; the refrigerant heat exchanger exit leading to the pre-absorber is state point 11, and the pre-absorber exit leading to the absorber is state point 14. The model assumptions and calculation sequence for the chiller simulation at a cooling air temperature of 35 ºC are summarized in Table 4.

3.4 Model components

Modelling a process in Aspen-Plus is based on the appropriate selection of the equivalent blocks for the main components to build a running model. Table 5 gives the Aspen blocks for the various machine elements as well as the input data for these elements for the 35 °C cooling air temperature case. The models for the pump and the two expansion valves are obvious. The default value of pump efficiency (100%) is used, as the effect of this parameter on the overall cycle performance is negligible. For the air-cooled condenser and absorber, the evaporator and the solution heat exchanger a two-flow heat exchanger model is used. For the separation of the refrigerant in the generator a multi-stage rectification column with condenser and boiler is needed. For the pre-absorber a simplified model combining a flash tank and a heater is adapted to account for the complex heat and mas transfer processes taking place in this machine element: On one side, hot ammonia poor solution from the generator is mixed with cold refrigerant vapours coming from the evaporator, resulting in a partial absorption and a liquid/vapour mixture leaving for the air-cooled absorber, and on other side, ammonia rich solution on its way to the generator preheated by the hot ammonia poor solution and by the heat released resulting from the partial absorption process.

Finally, the cooling medium air is modeled as gas mixture with 78 % Nitrogen by mole, 21 % Oxygen by mole and 1 % Argon by mole.

3.5 Simulation procedure

The simulation model developed in the present work uses in a first step a sequential modular approach in which each block is calculated separately. A “break point” is considered in the model for the cycle input conditions. This “break” point is inserted at state point 1, the solution pump inlet (Figure 8). The exit of the absorber (state point 1A) and the inlet of the solution pump (state point 1) represent the same state, and consequently state point 1A should have the same characteristics as those given as inputs at the solution pump inlet after the simulations are run. This constitutes the convergence criterion for the simulations.

As Equation Oriented Modelling is a more effective way of solving of complex problems, the simulations are run, in a second step, using the Equation-Oriented (EO) approach: the governing equations of the chiller model are solved simultaneously. To reach convergence in this approach, good initial estimates for all variables are necessary. A good practice is then to begin the simulation in sequential modular mode and to initialize (synchronize) the EO solution procedure using the results of the sequential simulation after complete convergence.

4. Results and discussion

4.1 Heat transfer characteristics of the main thermal components of the chiller

As mentioned previously the start input values are introduced into the chiller simulation considering a "break" point at state point 1. A well-formulated model will conserve mass and energy throughout the cycle, thus resulting in identical characteristics of the flows on either side of the break 1A. The cycle state points resulting from the Aspen-Plus model at a cooling air temperature of 35 ºC are given in Table 6. The experimental data reported by Klein [26]

and the simulation results obtained by El May *et al*. [10] are used to validate our Aspen-Plus model. The validation parameters employed are: driving heat input, coefficient of performance (*COP*) and temperature measured by Klein [26] at 14 locations in the chiller. Table 7 shows the thermal loads in the main components and the *COP* of the absorption chiller reported by Klein [26] and the values obtained in the present work. As regards the thermal loads, the maximum deviation is observed in the driving heat in the generator which is less than 7%. The deviation obtained in the *COP* is about 5%. In Figure 9, the temperature values measured experimentally by Klein [26] are compared with the corresponding values obtained in the present work and those obtained by El May *et al*. [10] in their simulation. This comparison shows excellent agreement between the Aspen-Plus model results and Klein's data, except for state point 11 (refrigerant vapour leaving the refrigerant heat exchanger) for which the deviation is more than 10 ºC. The results are also well in agreement with the simulation results obtained by El May *el al*. [10], except at 4 state points namely 4 (ammonia rich solution entering the generator), 13 (Refrigerant liquid leaving the refrigerant heat exchanger), 14 (ammonia poor solution entering the absorber) and 11 (refrigerant vapour leaving the refrigerant heat exchanger) for which the temperature deviation is higher than 5 ºC. The temperature values calculated in the present work and in El May *et al*. [10] for state point 11 are similar, which could mean that the experimental data from Klein [26] at this point is not of a good quality. The results commented above validate the model developed in Aspen-Plus for the Robur absorption chiller.

Next, the (*UA*) values were calculated for the condenser, evaporator, absorber and refrigerant heat exchanger (Table 8).

4.2 Model predictions with (*UA*) values as input parameters

In this second step, the Aspen-Plus model for this particular absorption chiller is then modified to include the heat transfer capacities (*UA*) of the condenser, evaporator, absorber and refrigerant heat exchanger – deduced from the simulation results at a cooling air temperature of 35 ºC – as input parameters for the simulations at cooling air temperatures of 26.7 °C and 38 °C. In Figure 10, the temperatures calculated using the Aspen-Plus model are compared with the experimental data from Klein [26] and simulated temperatures reported by El May *et al*. [10] at a cooling air temperature of 26.7 ºC. The results obtained in the present work are well in agreement with both sets of data. In the case of comparison with experimental data from Klein [26], the maximum deviations are observed in state points 4 (refrigerant vapour entering the generator) and 11 (refrigerant vapour leaving the refrigerant heat exchanger). Regarding the comparison with data obtained by El May *el al*. [10], the maximum deviation is observed in state point 14 (ammonia poor solution entering the absorber). Figure 11 shows the same comparison at a cooling air temperature of 38 ºC. In general terms, the results of the present work are well in agreement with data from Klein [26] and El May *et al*. [10]. The maximum deviations are obtained in state points 7 (Refrigerant vapour entering the condenser), 11 (refrigerant vapor leaving the refrigerant heat exchanger) and 13 (Refrigerant liquid leaving the refrigerant heat exchanger) for the comparison with experimental data from Klein [26] and in state points 11, 13, 14 and 3 (ammonia poor solution entering the pre-absorber) for the comparison with simulated data from El May *et al*. [10]. It is worth mentioning that the temperature values calculated in the present work and in El May *et al*. [10] for state points 11 and 13 are similar, which could mean that the Klein [26] experimental data at these points is not of such a good quality. Table 9 shows a comparison between experimental temperature data [26], the simulation results of [10] and the model calculated temperatures at a cooling air temperature of 38 ºC.

Based on these results, it is concluded that the version of the Aspen-Plus model that includes the (UA) values of the condenser, evaporator, absorber and refrigerant heat exchangers as input parameters could be very useful for predicting the internal operating conditions and the coefficient of performance of the Robur absorption chiller at different temperatures of the cooling air and taking in account the real size of the heat exchangers.

5. Conclusion

In this paper, a steady-state model of a commercial 3-ton ammonia/water absorption chiller was developed using the flow-sheeting software Aspen-Plus. For the selection of the appropriate property model for the working fluid mixture, nine different models implemented in Aspen-Plus were evaluated in two steps. Firstly, calculated VLE by each of the Aspen-Plus property models was compared with regressed VLE data reported by Mejbri and Bellagi [25] at different pressures. It was concluded that none of these property models predicts the ammonia/water vapor-liquid equilibrium with sufficient accuracy. Secondly, the aspen-Plus data regression system was used to calculate the parameters of the Aspen-Plus property models by fitting the vapour-liquid equilibrium data reported by Mejbri and Bellagi [25]. It was found that the Peng-Robinson-Boston-Mathias equation of state (PR-BM) with regressed interaction parameters is the most suitable property model for the system water/ammonia in the temperature and pressure ranges encountered in absorption air-conditioning units.

Once the appropriate property model for ammonia/water mixture selected, an Aspen-Plus model was developed to simulate the steady-state operation of the commercial gas-fired chiller. First, the heat transfer characteristics of the condenser, evaporator, absorber and refrigerant heat exchanger were deduced from data at a cooling air temperature of 35 ºC. Then, the results were compared with experimental data published by Klein [26] and those calculated by El May *et al*. [10]. The comparison showed good agreement between the

376 Aspen-Plus model results and the sets of data from the open literature. The model was then
377 modified to include the (*UA*) values of the heat exchangers calculated in the previous step as
378 input parameters. The results were compared with the experimental data from Klein [26] and
379 those reported by El May *et al*. [10] at cooling air temperatures of 26.7ºC and 38ºC. The
380 results showed agreement with the two sets of bibliographical data. Therefore, it is concluded
381 that the proposed Aspen-Plus model can be very useful tool for predicting the internal
382 operating conditions and the coefficient of performance of the commercial gas-fired
383 absorption chiller at different temperatures of the cooling air and taking in account the real
384 size of the heat exchangers.

385

Appendix 1

Commercial 3-ton ammonia/water absorption chiller

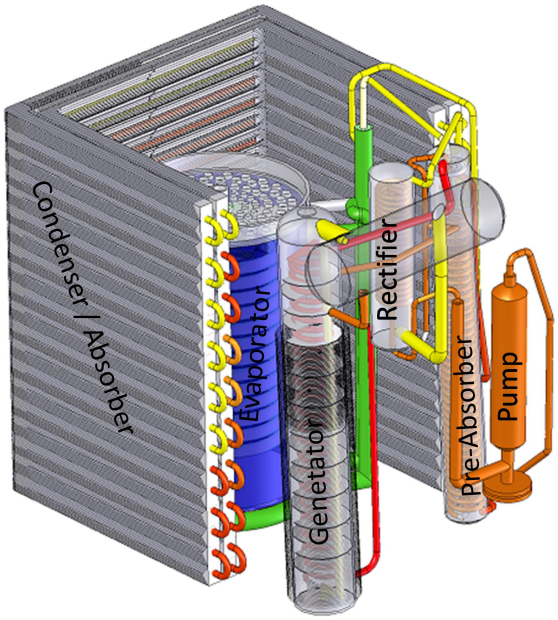
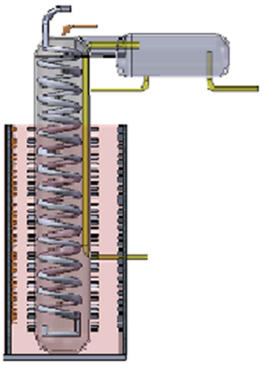
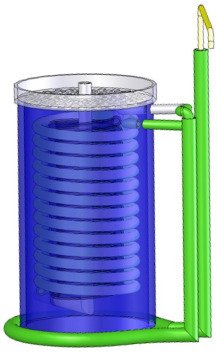


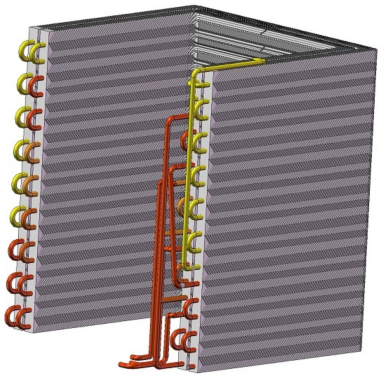
Figure12. Internal view of the commercial absorption chiller



(a) Generator

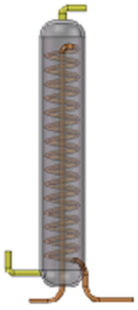


(b) Evaporator



(c) Absorber and Condenser

(d) Pre-absorber



(e) Rectifier

(f) Solution pump

393 Figure13. Schematic representation of the main components of the absorption chiller

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395

396

Appendix 2

Peng-Robinson Equation of State

This cubic eos writes for mixtures [11, 27]:

$$P = \frac{R\,T}{(\bar{V} - b)} - \frac{a}{\bar{V}(\bar{V} + b) + b(\bar{V} - b)}$$

Where P is the pressure, $\bar{V}$, the mixture molar volume, b, the mixture co-volume, a, the attraction term factor, and R the universal gas constant. The mixture a and b are deduced from the individual component constants a_i and b_i using the mixing rules:

$$b = \sum x_i\, b_i$$

$$a = \sum_{\boldsymbol{i}} \sum_{\boldsymbol{j}} x_i x_j \sqrt{a_i a_j}\left(1 - k_{ij}\right)$$

In these equations x_i is the mole fraction of component i in the mixture and $k_{ij}$the binary interaction parameter of components i and j. Usually it is supposed that:

$$k_{ij} = k_{ji}$$

It is this parameter that is deduced from VLE data by a regression procedure. To make the equation more flexible $k_{ij}$is often written as function of the temperature:

$$k_{ij} = k_{ij}^{(1)} + k_{ij}^{(2)}\,T + \frac{k_{ij}^{(3)}}{T}$$

So that three parameters are fitted to the VLE data: $k_{ij}^{(1)}, k_{ij}^{(2)}$ and $k_{ij}^{(3)}$.

The individual constants a_i and b_i are determined from the critical temperature and pressure of the compound, T_{ci} and P_{ci}, respectively:

$$a_i = \alpha_i(T)\left[0.45724\frac{R^2T_{ci}^2}{P_{ci}}\right]$$

$$b_i = 0.07780\frac{RT_{ci}}{P_{ci}}$$

410 In the $\alpha_i(T)$ function,

$$\alpha_i(T) = \left[1 + m_i\left(1 - \sqrt{T_r}\right)\right]^2$$

411 T_r is the reduced temperature, $\frac{T}{T_{ci}}$, and m_i, a component specific parameter depending on the

412 acentric factor ω_i,

$$m_i = 0.37464 + 1.54226\,\omega_i - 0.26992\,\omega_i^2$$

413 $\alpha_i(T) = 1$ at the critical temperature.

414 The Boston-Mathias modification of the Peng-Robinson equation of state is as follow:

$$\alpha_i(T) = \left[\exp\left[c_i\left(1 - T_{ri}^{d_i}\right)\right]\right]^2$$

415 with

$$d_i = 1 + \frac{m_i}{2} \;\; ; \;\; c_i = 1 - \frac{1}{d_i}$$

416 It's intended to extend the validity of the equation of state for temperatures larger than the
417 critical temperature. In fact, this is necessary for the water/ammonia mixture considered as a
418 working fluid in the absorption chiller because temperatures between 180 and 200°C are
419 needed in the generator to desorb the refrigerant. This temperature range is beyond the critical
420 temperature of ammonia (405.5 K corresponding to 132.4°C).

421

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Table captions

Table 1. Aspen-Plus thermodynamic property models tested

Table 2. Sum of squared errors for the regressed thermodynamic property models tested

Table 3. Interaction parameter k_{ij} for the considered cubic equations of state

Table 4. Calculation sequence of the chiller simulation

Table 5. Machine elements and their Aspen-Plus models with input data set

Table 6. Aspen-Plus model simulation results at a cooling air temperature of 35 ºC

Table 7. Comparison between experimental data [26] and simulation results in terms of component heat duties and chiller *COP* at a cooling air temperature of 35 ºC

Table 8. (*UA*) values of the heat exchangers calculated at a cooling air temperature of 35 ºC

Table 9. Comparison between experimental temperature data [26], the simulation results of [10] and the model calculated temperatures at a cooling air temperature of 38 ºC.

504 Table 1. Aspen-Plus thermodynamic property models tested

505

506

Aspen-Plus property model	Model name
ENRTL-RK	Electrolyte NRTL/Redlich-Kwong
RKS-BM	Redlich-Kwong-Soave-Boston-Mathias
PENG-ROB	Standard Peng-Robinson
PR-MHV2	Modified Peng-Robinson-Huron-Vidal
PR-WS	Peng-Robinson-Wong-Sandler
NRTL-HOC	Non-Random-Two-Liquid/Hayden-O'Connell
SRK	Soave-Redlich-Kwong
WILS-RK	Wilson/Redlich-Kwong
PR-BM	Peng-Robinson-Boston-Mathias

517

518 Table 2. Sum of squared errors for the regressed thermodynamic property models tested.

519

Aspen-Plus property model	Sum of squared errors
PR-BM	36.55
PENG-ROB	38.36
WILS-RK	41.92
RKS-BM	44.86
SRK	45.07
ENRTL-RK	48.31
NRTL-HOC	53.00
PR-WS	80.42
PR-MHV2	226.62

520

Table 3. Interaction parameter k_{ij} for the considered cubic equations of state

Aspen-Plus property model	$\boldsymbol{k^{(1)}_{NH_3\ H_2O}}$ **Default**	$\boldsymbol{k^{(2)}_{NH_3\ H_2O}}$ **Default**	$\boldsymbol{k^{(3)}_{NH_3\ H_2O}}$ **Default**	$\boldsymbol{k^{(1)}_{NH_3\ H_2O}}$ **Regressed**	$\boldsymbol{k^{(2)}_{NH_3\ H_2O}}$ **Regressed**	$\boldsymbol{k^{(3)}_{NH_3\ H_2O}}$ **Regressed**
PR-BM	-0.3147	$1.4\ 10^{-4}$	0	-1.0017	$1.1\ 10^{-3}$	119.82
PENG-ROB	-0.2589	0	0	-1.0610	$1.2\ 10^{-3}$	130.30
RKS-BM	-0.280	-0.280	0	-1.2146	$1.3\ 10^{-3}$	162.214
SRK	0	$1.77\ 10^{-5}$	0	-0.4246	$1.95\ 10^{-4}$	26.492

Table 4. Calculation sequence of the chiller simulation

State point	**Calculation step**
1	Saturated liquid, composition, total mass flow and pressure
1A	Determined by the absorber model
2	Determined by the high pressure solution pump model
3	Determined by the solution valve 2 model
4	Determined by the pre-absorber model
5	Determined by the rectifier model
6	Determined by the generator model
7	Determined by the generator model
8	Determined by the condenser model
9	Determined by the refrigerant valve 1 model
10	Determined by the evaporator model
11	Determined by the vapor-liquid heat exchanger model
13	Determined by the vapor-liquid heat exchanger model
14	Determined by the pre-absorber model

527

528 Table 5. Machine elements and their Aspen-Plus models with input data set

Machine Element	**Aspen Block**	**Input values**
Condenser (COND)	Two-flow heat exchanger HEATX	Pinch temperature: Hot outlet-Cold inlet = 13.5 °C
Evaporator (EVAP)	Two-flow heat exchanger HEATX	Pinch temperature: Hot outlet-Cold inlet = 3 °C
Absorber (ABS)	Two-flow heat exchanger HEATX	Pinch temperature: Hot outlet-Cold inlet = 10.2 °C
Solution heat exchanger (SHX)	Two-flow heat exchanger HEATX	Pinch temperature: Hot outlet-Cold inlet = 16 °C
Expansion valve1 (DET1)	VALVE	Outlet pressure = 4.936 bar
Pre-absorber (PREAB)	FLASH block and HEATER block	Pressure = 4.936 bar Exit temperature = 76 °C
	MIXER	Pressure drop = 0 bar
Expansion valve2 (DET2)	VALVE	Outlet pressure = 4.936 bar
Generator (GEN)	RADFRAC	Reflux mass ratio = 0.09 Mass flow rate at the bottom = 55.06 kg/h
	HEATER	Pressure drop = 0 bar Exit temperature = 115°C
PUMP	PUMP	High pressure = 22.380 bar Isentropic efficiency = 1 **State point 1** - Pressure = 4.936 bar - Temperature = 45.2°C - Total mass flow = 90.718 kg/h - Vapour fraction = 0 - NH_3 Mass fraction = 0.437 - H_2O Mass fraction = 0.563

529

530

531 Table 6. Aspen-Plus model simulation results at a cooling air temperature of 35 ºC

State point	From	To	Pressure (bar)	Temperature (°C)	Vapour fraction	Mass flow rate (kg/h)	NH_3 Mass fraction (%)
1A	Absorber	Pump	4.936	45.2	0	90.718	43.7
2	Pump	Rectifier	22.380	46.6	0	90.718	43.7
3	DET2	PREAB12	4.936	115.3	0	55.060	9.0
4	PREAB2-2	Generator	22.380	108.1	0.006	90.718	43.7
5	Rectifier	PREAB2-2	22.380	64.3	0	90.718	43.7
6	EXCH	DET2	22.380	115.0	0	55.060	9.0
7	Generator	Condenser	22.380	105.6	1	35.658	97.0
8	Condenser	H-EXCH1	22.380	48.5	0	35.658	97.0
9	DET1	Evaporator	4.936	4.9	0.073	35.658	97.0
10	Evaporator	H-EXCH1	4.936	9.5	0.819	35.658	97.0
11	H-EXCH1	PREAB1-2	4.936	16.7	0.901	35.658	97.0
12	PREAB1-2	Mixer	4.936	76.0	1	22.425	94.8
13	H-EXCH1	DET1	22.380	24.0	0	35.658	97.0
14	Mixer	Absorber	4.936	76.0	0.254	90.718	43.7
15	PREAB1-2	Mixer	4.936	76.0	0	68.293	26.9
20	Generator	EXCH	22.380	192.6	0	55.060	9.0

532

533

534 Table7. Comparison between experimental data [26] and simulation results in terms of
535 component heat duties and chiller *COP* at a cooling air temperature of 35 ºC

Parameter	**Experimental value**	**Calculated value**
Q generator (kW)	17	15.91
Q evaporator (kW)	9.59	9.51
Q condenser (kW)	-	12.84
Q absorber (kW)	-	12.85
COP	0.56	0.59

536
537
538 Table 8. (*UA*) values of the heat exchangers calculated at a cooling air temperature of 35 ºC

Heat exchanger	**[*UA*] (W/K)**
Condenser	390.0
Evaporator	3304.9
Absorber	630.0
H-EXCH1	55.9

539
540 Table 9. Comparison between experimental temperature data [26], the simulation results of
541 [10] and the model calculated temperatures at a cooling air temperature of 38 ºC.

542

543

State points	Experimental data [26]	El May et al. [10]	Aspen-Plus simulation
	Temperature (°C)	Temperature (°C)	Temperature (°C)
1	52.6	50.9	47.4
2	51.6	51.2	47.3
3	119.7	128.3	120.2
4	111.9	109.6	107.6
5	70.4	68.8	65.1
7	113.9	119.4	104.7
8	53.1	49.9	55.2
9	7.1	5.2	5.5
10	11.3	8.5	8.2
11	24.3	13.3	13.1
13	16.4	29.6	28.2
14	76.9	86.0	77.0

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547 **Figure captions**

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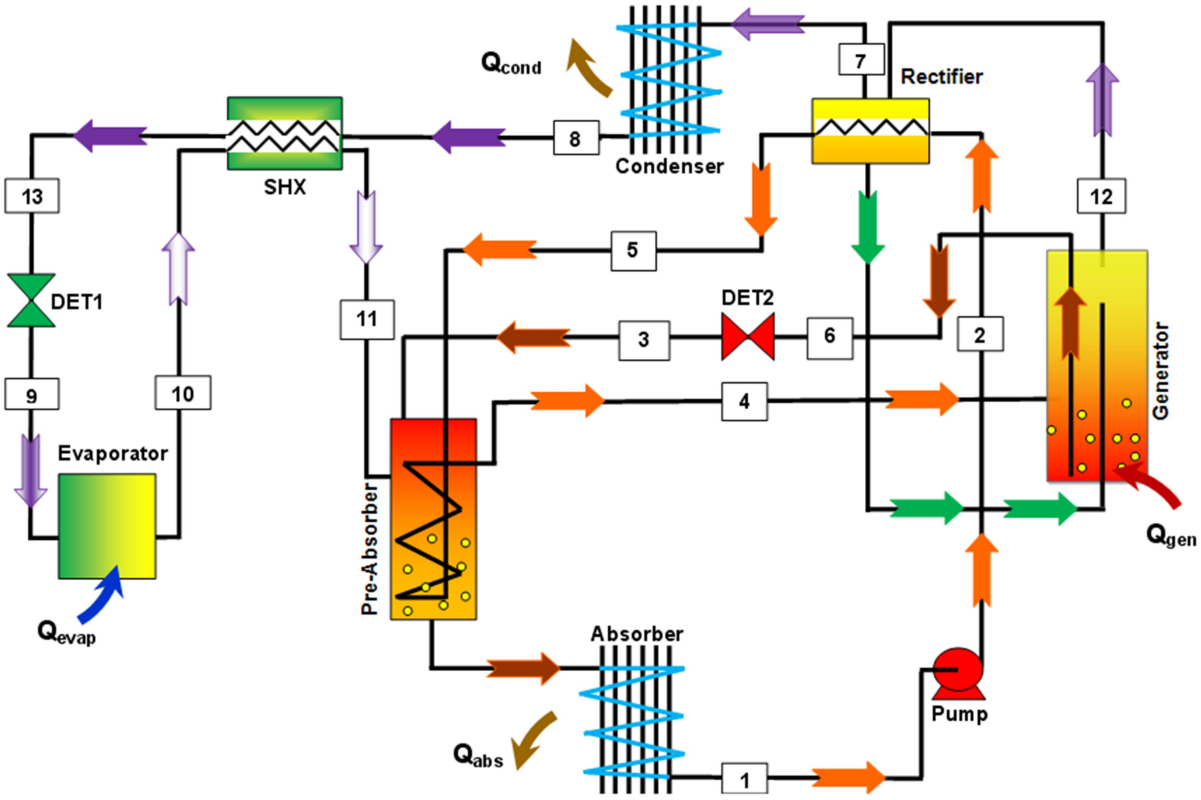

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574 Figure1. Schematic representation of the absorption chiller

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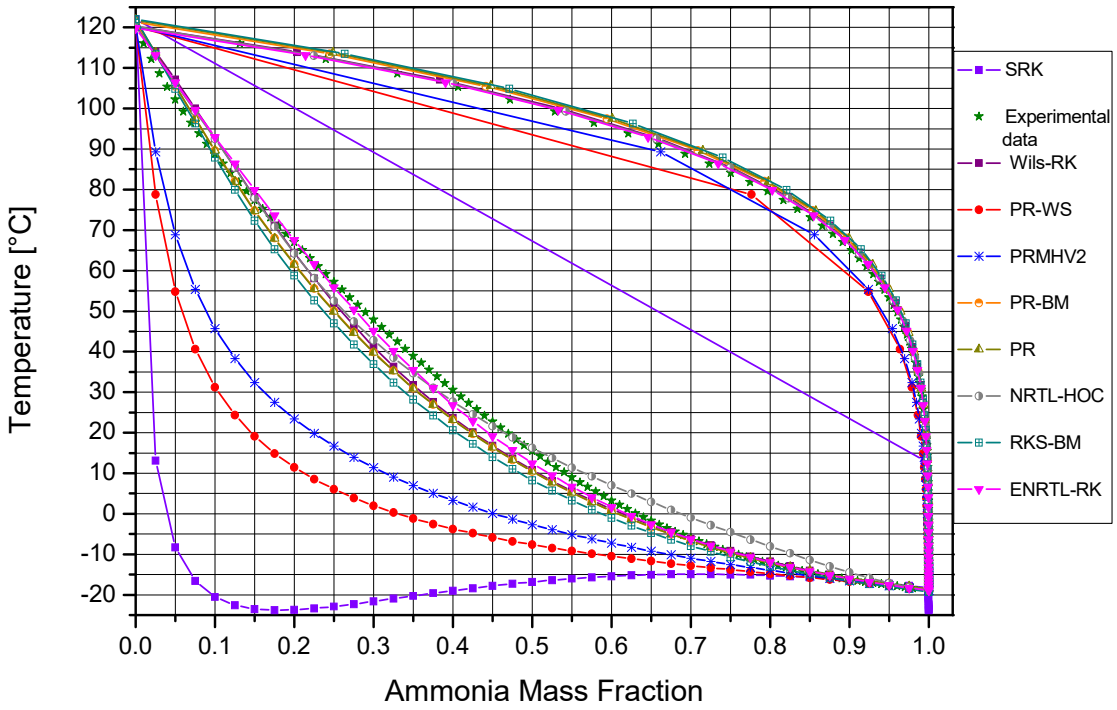

Figure 2. *T-x-y* VLE diagram at $P = 2$ bar for ammonia/water mixture (predicted by models with default interaction parameters)

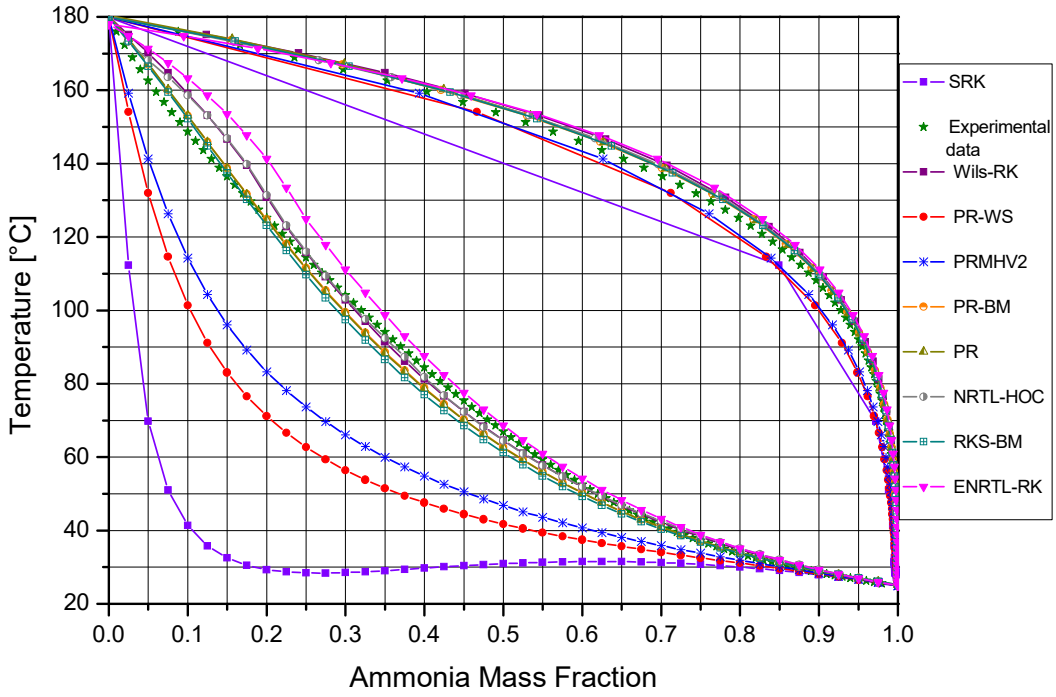

Figure 3. *T-x-y* VLE diagram at P = 10 bar for ammonia/water mixture (predicted by models with default interaction parameters)

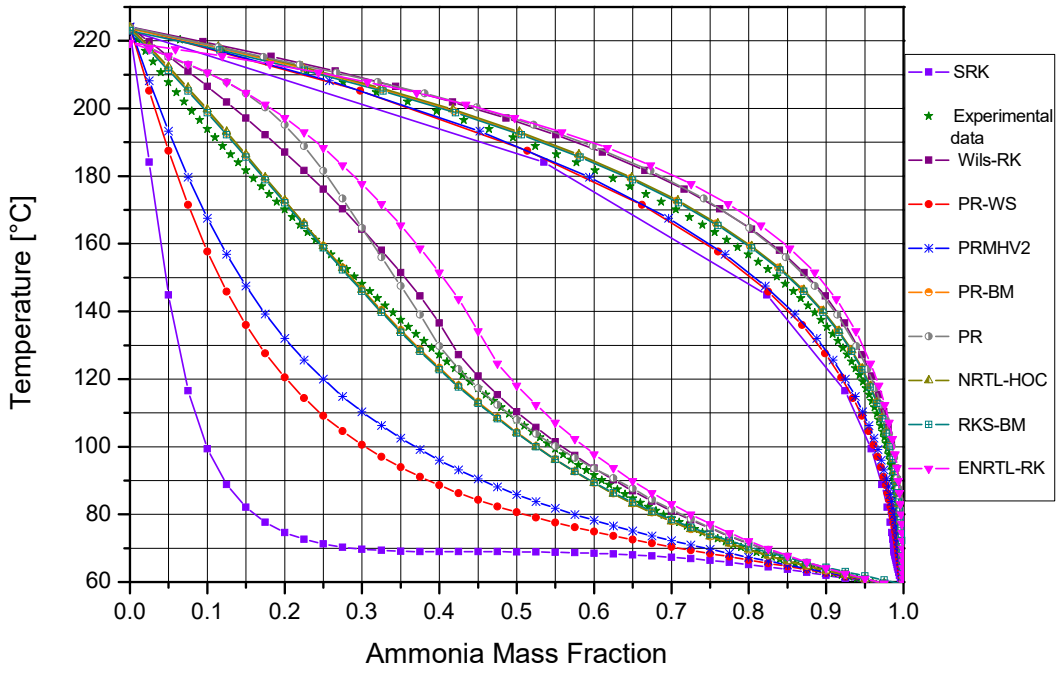

Figure 4. *T-x-y* VLE diagram at P = 25 bar for ammonia/water mixture (predicted by models with default interaction parameters)

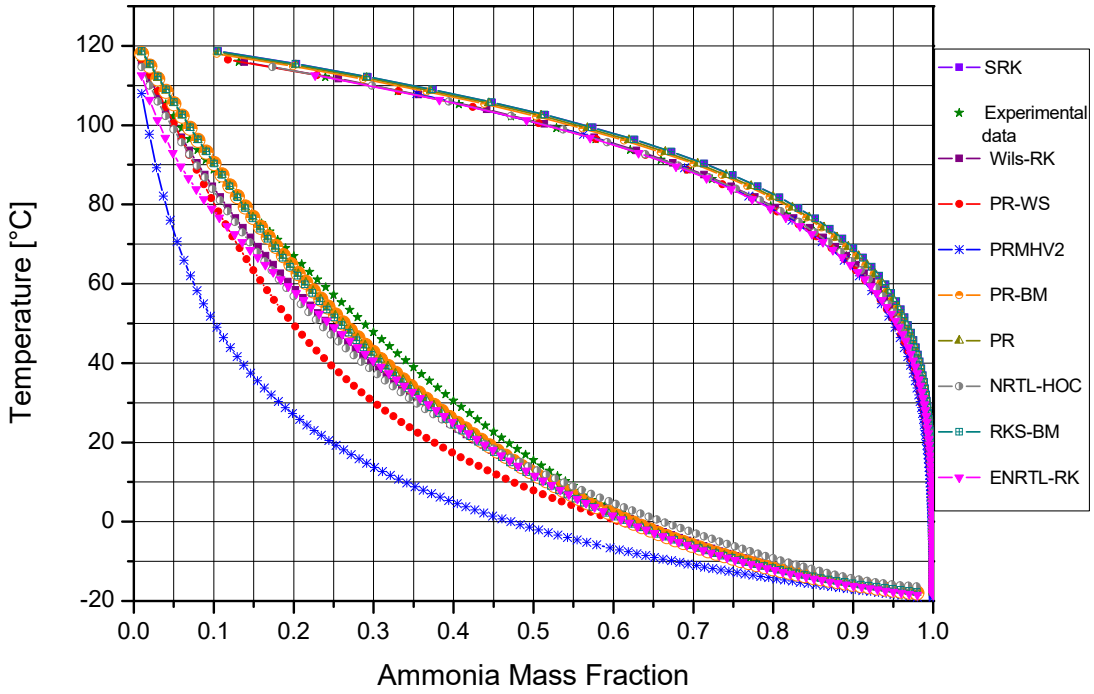

Figure 5. *T-x-y* VLE diagram at $P = 2$ bar for ammonia/water mixture (predicted by models with regressed interaction parameters)

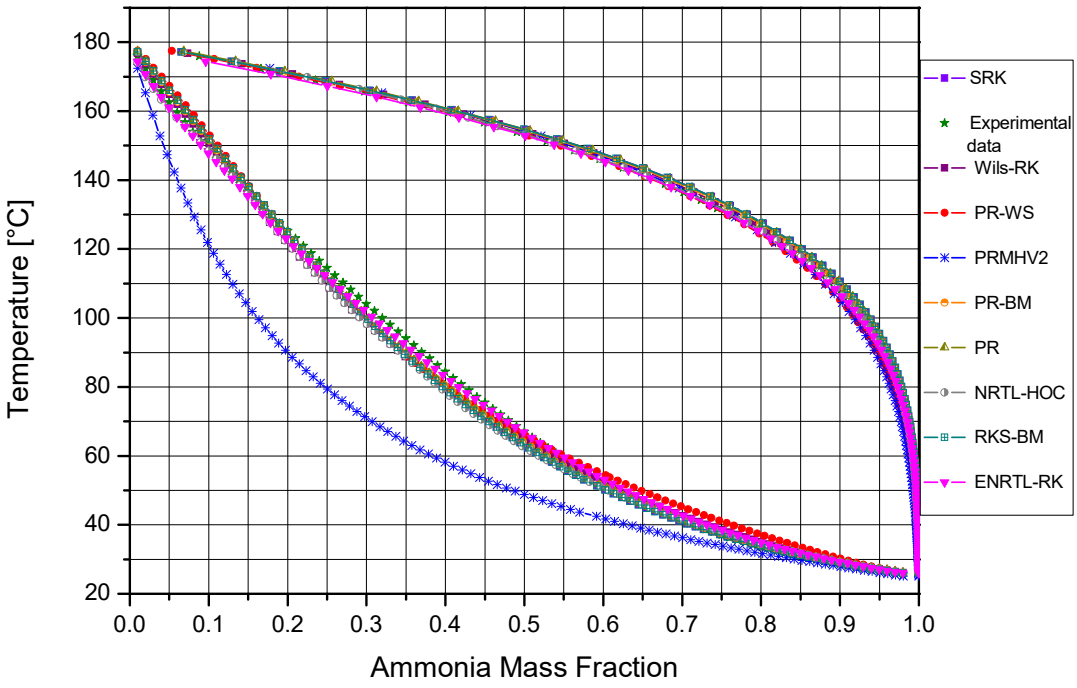

Figure 6. *T-x-y* VLE diagram at P = 10 bar for ammonia/water mixture (predicted by models with regressed interaction parameters)

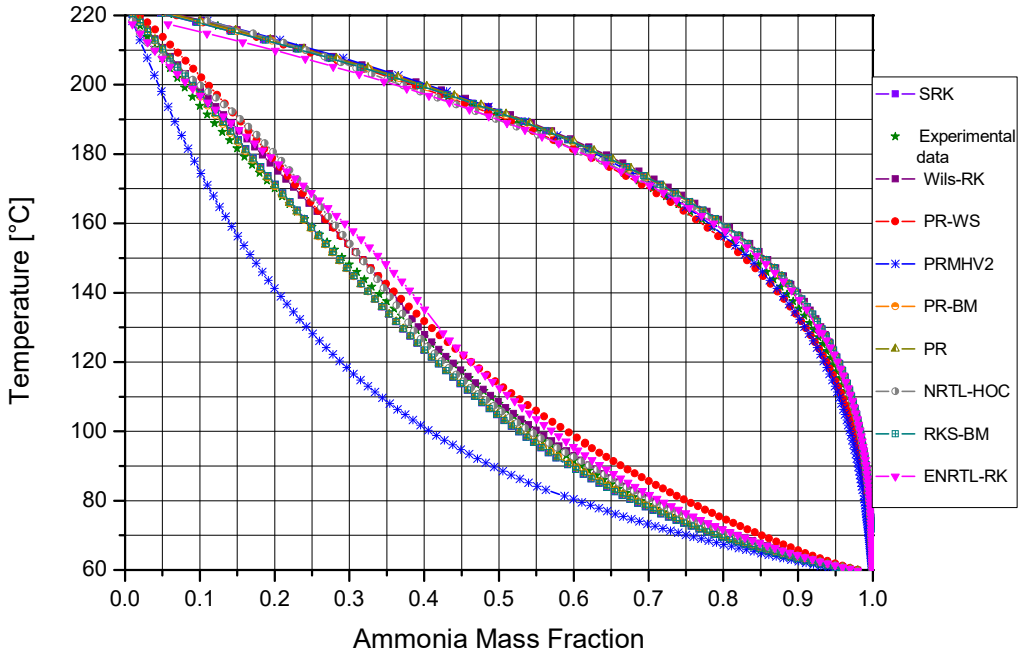

Figure 7. *T-x-y* VLE diagram at P = 25 bar for ammonia/water mixture (predicted by models with regressed interaction parameters)

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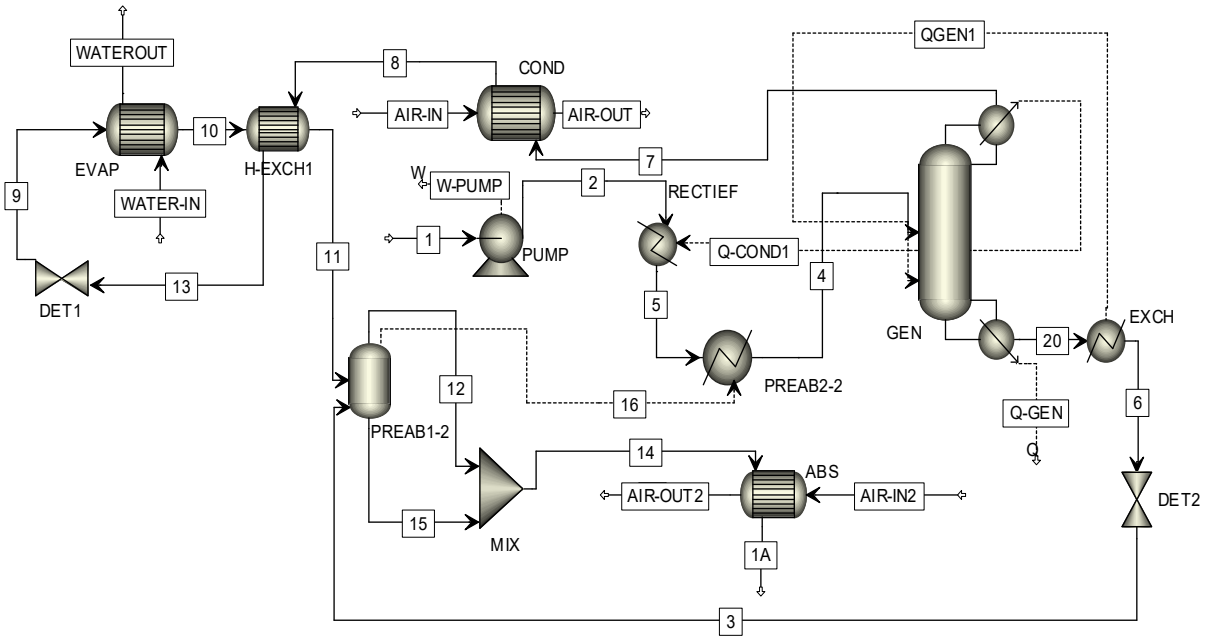

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605 Figure 8. The absorption machine model in Aspen-Plus

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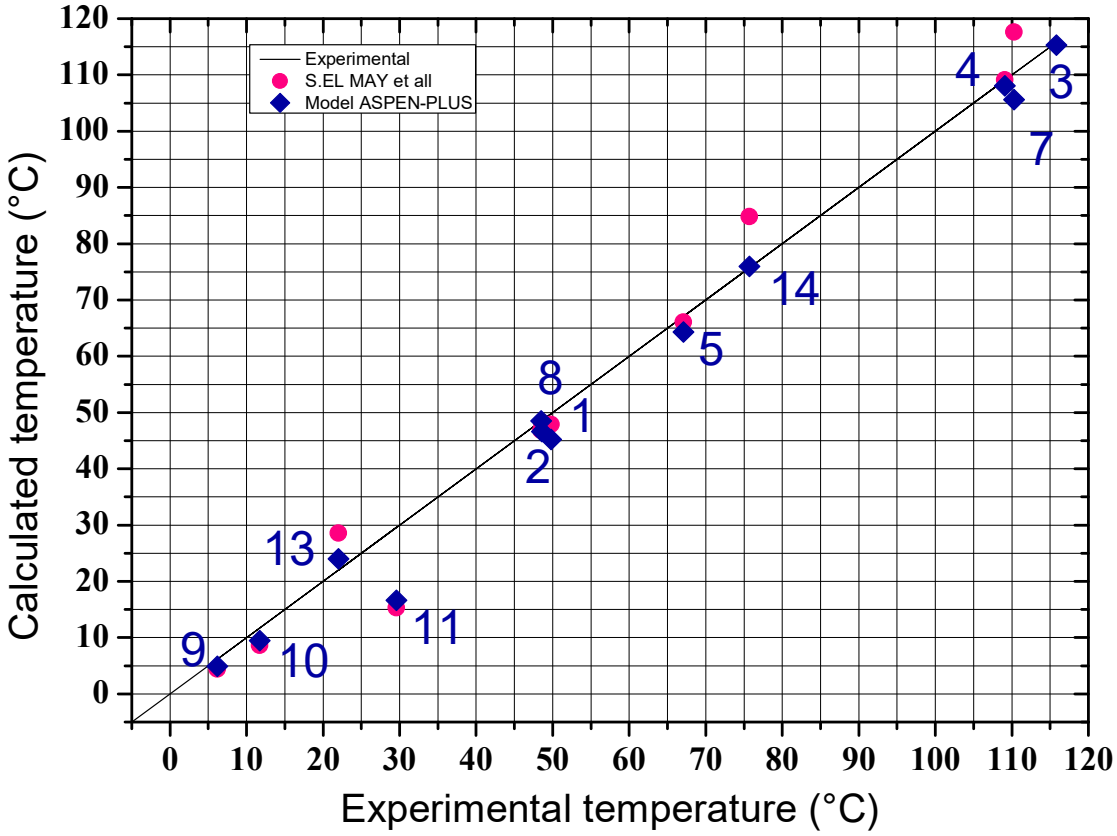

Figure 9. Temperature comparison at different locations in the chiller at a cooling air temperature of 35 ºC (*UA* values as output parameters of the model)

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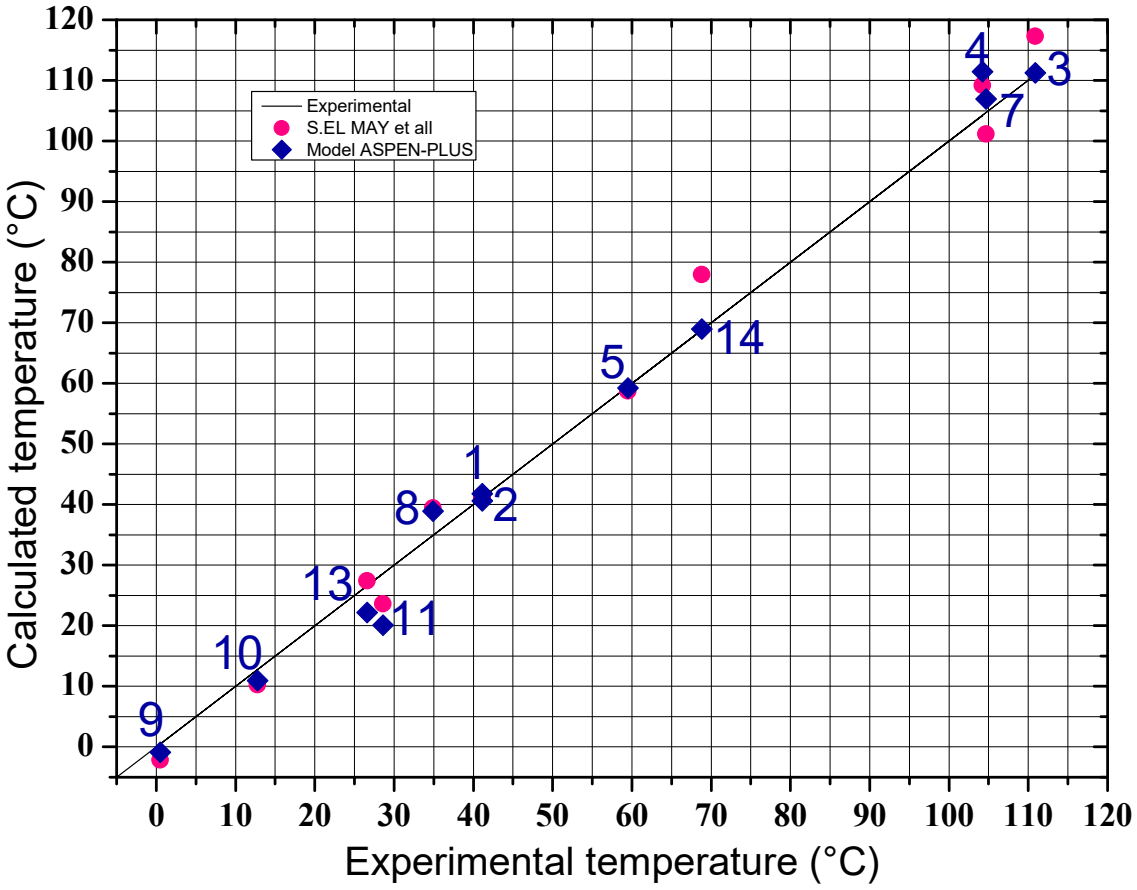

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614 Figure 10. Temperature comparison at different locations in the chiller at a cooling air

615 temperature of 26.7 ºC (*UA* values as input parameters in the model)

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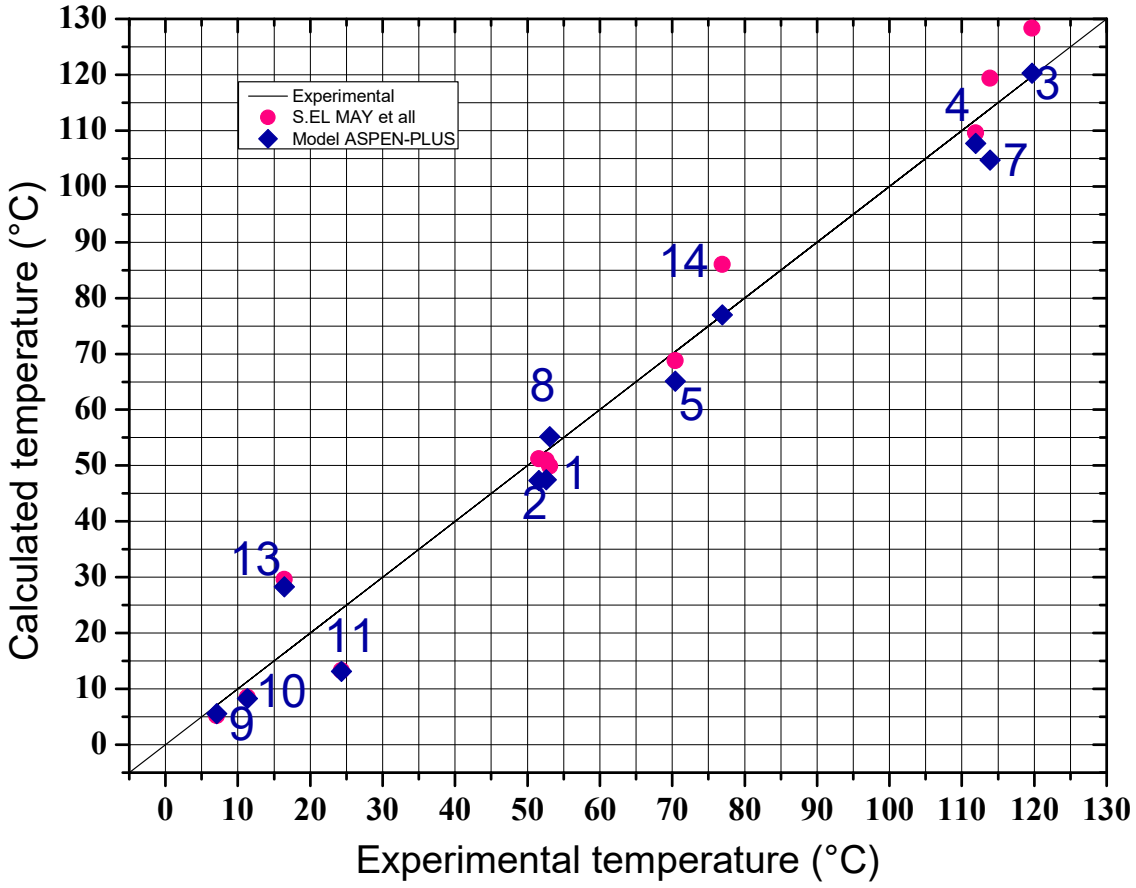

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619 Figure 11. Temperature comparison at different locations in the chiller at a cooling air

620 temperature of 38 ºC (*UA* values as input parameters in the model)