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# Modelling a solar absorption chiller using positive flash to estimate the physical state of streams and theoretical plate concept for the generator

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## A B S T R A C T

In this paper a general model for the steady state simulation of a solar absorption chiller is proposed. The novelty of this model is to calculate the physical state of all the streams rather than fix them (especially at the outlet of the condenser and evaporator). The thermodynamic properties of the mixture can be calculated by suitable predictive thermodynamic models, hence the working pair can be changed easily. Using this thermodynamic model, a general Positive Flash model is able to describe all the possible states (sub-cooled, super-heated, biphasic) of the various streams which are all considered as multicomponent mixtures. In the positive flash the same set of governing equations is valid for all phase regions. Another originality of the present study is that the generator is modelled as a distillation column, using the theoretical plate concept: MESH equations (Mass balance, Equilibrium, Summation, Heat balance) were written for each stage. Despite the modular structure of the software, a global solution strategy was implemented, using a Newton-Raphson method. This model is successfully compared to an example in the literature which deals with a GAX (Generator-Absorber heat eXchange) configuration absorption chiller using ammonia/water as the working pair.

## 1. Introduction

The use of compressor chillers to produce air conditioning has a major impact on environment. In a context of global warming, alternative solutions have to be proposed. Absorption chillers appear to be attractive solutions since they can be supplied by renewable energy (using solar collectors as in the present project) or waste heat (from biomass gasification such as the process presented by Narobe et al. [1], for example). In the present paper a general model for the steady state simulation of a solar absorption chiller is proposed.

Two types of model have been reported to describe absorption chillers: empirical or physical models. Empirical models consist of a set of non-physical equations that fit the relevant variables (temperature, power) to experimental data, when external source properties are known [2,3]. However, this kind of model cannot be

predictive. Physical models on the other hand, describe the phenomena according to equations based on physical laws; the relevant variables can then be computed. Two kinds of physical model can be distinguished: balance models and transfer models. Transfer models are more complete, where heat and mass transfer are solved at local level in the components [4–6]. These models can be very accurate but they require the devices to be meshed and require a long computation time. Balance models are less accurate but easier to handle and to solve. They calculate a set of variables expressing energy and mass balances between the inlet and outlet streams of the components. Since they are a good compromise between accuracy and computation time, we have focused our research on this kind of model.

Accuracy depends on assumptions. Isenthalpic expansions and negligible pressure drops are commonly used assumptions, which we will also apply. However, most of the models reported in the literature use other hypotheses which are restrictive and which cannot be used to simulate and accurately predict cycle behaviour.

The most common assumption is to consider that the refrigerant

fluid in the condenser and in the evaporator is pure. This may be an acceptable hypothesis when the working pair is  $\text{H}_2\text{O}/\text{LiBr}$  [7–9], because the separation into the generator produces nearly pure water steam. This hypothesis is sometimes proposed for the  $\text{NH}_3/\text{H}_2\text{O}$  working pair [10], but in this case, it is questionable since separation is more difficult. Thus, some authors propose to fix the concentration gap between a poor solution and rich solution [11] or the water concentration in the outlet from the top of the generator [12,13]. However, water concentration, even if very low, has a huge influence on the temperature in the evaporator and in the condenser. Therefore, it should be relevant to model the generator as a distillation column in order to properly estimate this concentration. To our knowledge, the only authors who have proposed such a model are Butz and Stephan [14] and it is also done in the model presented in the present paper.

Another common assumption made in the literature is to fix the physical state of the fluid at the component outlets: boiling liquid at the condenser outlet and saturated vapour at the evaporator outlet are very common assumptions [7–13]. However, depending on the flow rates and temperatures of the external sources, the phase change could be incomplete or overtaken. It is therefore more appropriate to estimate the physical state of the streams without making any assumptions.

Finally, in these studies, the thermodynamic properties of mixtures are often obtained from correlations specific to the working pair used in the cycle. The most commonly used correlations are those of Patek and Klomfar [15] who proposed empirical correlations involving more than forty parameters to estimate enthalpy and liquid-vapour equilibrium of a water-ammonia mixture. Using this kind of correlation precludes using the absorption chiller model with another working pair.

The key originalities of the proposed work are thus as follows:

- The software has been designed in a modular way allowing the simulation of various absorption chiller configurations (single or multi-stage). The modules and the resolution strategy are described in section 2.
- Thermodynamic properties of mixtures can be calculated by an Equation Of State (EOS) model or an excess free enthalpy model. The working pair can then be changed easily (changing the pure component properties and the binary interaction parameters). This kind of model is presented in section 3.
- All the streams are considered as multicomponent mixtures and a general Positive Flash model allows the use of the same set of equations irrespective of the physical state of the stream. This is described in section 4.
- The model is based on mass and energy balances applied to the various components of the machine, but the generator is

modelled using the theoretical plate concept. MESH equations (Mass balance, Equilibrium, Summation, Heat balance) were written for each stage. Consequently, neither the composition at the generator outlet nor the separation rate are fixed. They are both consequences of MESH equation solving. The model is described in section 5.

Finally, in section 6, the model is compared to the study by Butz and Stephan [14], which presented experimental and modelled results of a GAX (Generator-Absorber heat eXchange) configuration absorption chiller using ammonia-water as the working pair.

## 2. Definition of modules and resolution strategy

The basic components used to design the model of any absorption chiller configuration were defined. These modules are presented in Fig. 1.

It should be noted that no absorber module is proposed. An absorber is a heat exchanger in which the heat withdrawal enhances the absorption of the refrigerant fluid in the weak solution. Heat withdrawal occurs at the same time as the two inlet streams mix (refrigerant stream and weak solution stream). This study focuses on determining the physical state of each stream and the implementation of a theoretical plate-based model for the generator. As a first step, the absorber is represented by a mixer followed by one or two heat exchangers. This modelling is quite accurate. Further developments should be added to model the absorber in the same way as the generator with a theoretical plate-based model.

As has already been said, using the basic modules, any configuration can be designed. For example, Fig. 2-a shows a single stage, single effect configuration, while Fig. 2-b shows the same configuration with an additional sub-cooler and solution heat exchanger. Fig. 3 shows a GAX (Generator-Absorber heat eXchanger) configuration. The rich solution is preheated before it enters the generator by heat recovered from the partial condenser of the generator and from the absorber. In this configuration, the partial condenser of the generator is represented by an internal heat exchanger and the absorber is preceded by a pre-absorber, represented by a series association of a mixer and an internal exchanger.

Concerning the resolution strategy, there are three basic approaches [16]: the Sequential-Modular (SqM) approach, the Equation-Oriented (EO) approach and the Simultaneous-Modular (SiM) approach.

In the SqM approach, equations of each module are assembled in sub-systems, which we call units, and the computation takes place unit by unit following a calculation sequence. Each unit is solved using a suitable numerical method. This strategy can lead to

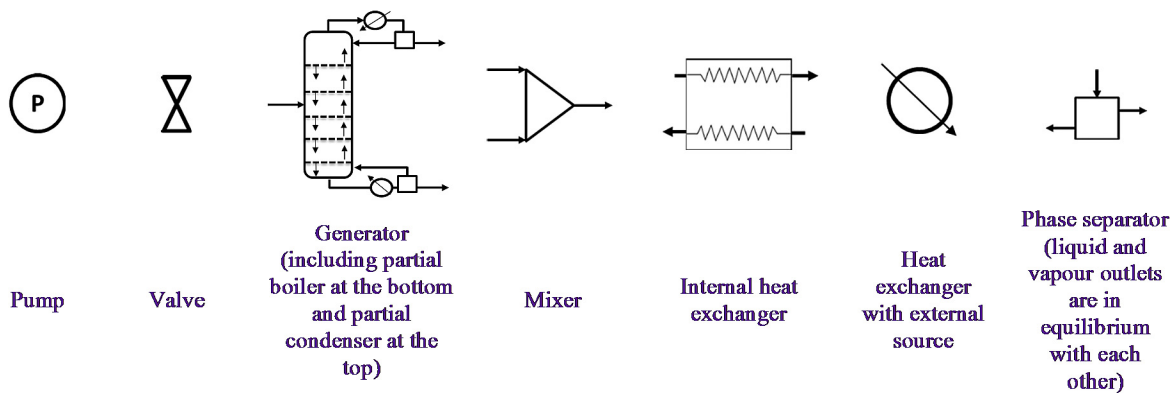
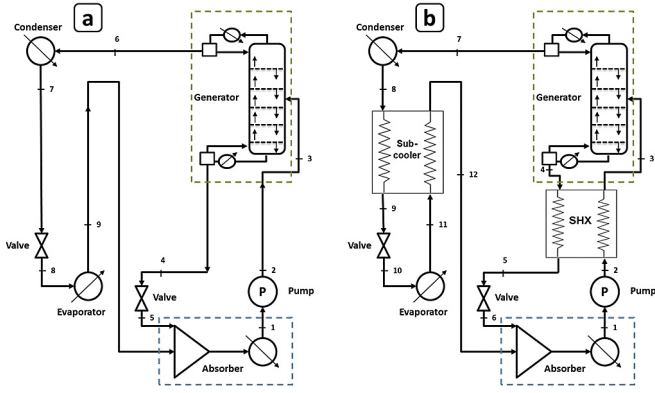


Fig. 1. Available modules.



**Fig. 2.** a - Representation of a simple cycle with our modules; b - representation of a simple cycle with additional sub-cooler and SHX, with our modules.

numerous iterative levels especially when there are recycles, and all the more so for cycles.

In the EO approach, equations of all the modules are assembled in a large system of non-linear algebraic equations in steady-state simulation and differential algebraic equations in dynamic simulation.

The SiM approach is a combination of the other two but is not commonly used.

The most frequently used resolution strategy in steady-state simulation is the SqM approach, while the EO approach is very suitable for dynamic simulation. In order to simulate cycles using the SqM approach, a tear stream (a stream that “opens” the loop) must be initialized, the computation sequence of units defines a convergence loop and the steady state is obtained when the tear stream satisfies convergence criteria. In the present study, we deal with steady state, but we wanted to propose a strategy that could be easily adapted to dynamic simulation. Therefore the

Equation-Oriented resolution strategy is chosen: equations of all the modules (including material and energy balances) will be solved simultaneously. However, equations relating to thermodynamics will not be solved at this “flowsheet level”. Thermodynamic properties (enthalpies, fugacities, etc.) will be solved at a lower level.

### 3. Thermodynamic model

Thermodynamic models are used rather than correlations specific to the working pair so that the working pair can be easily changed.

Liquid-vapour equilibrium is reached when the fugacity of each component is identical in the two phases. Vapour phase fugacity is always expressed using the residual approach. Liquid phase fugacity can be computed using either the residual approach, leading to equilibrium equation (1) for component  $i$  (homogeneous method), or the excess approach, leading to equilibrium equation (2) (heterogeneous method) where the pure component liquid fugacity is approximated by the saturated pressure.

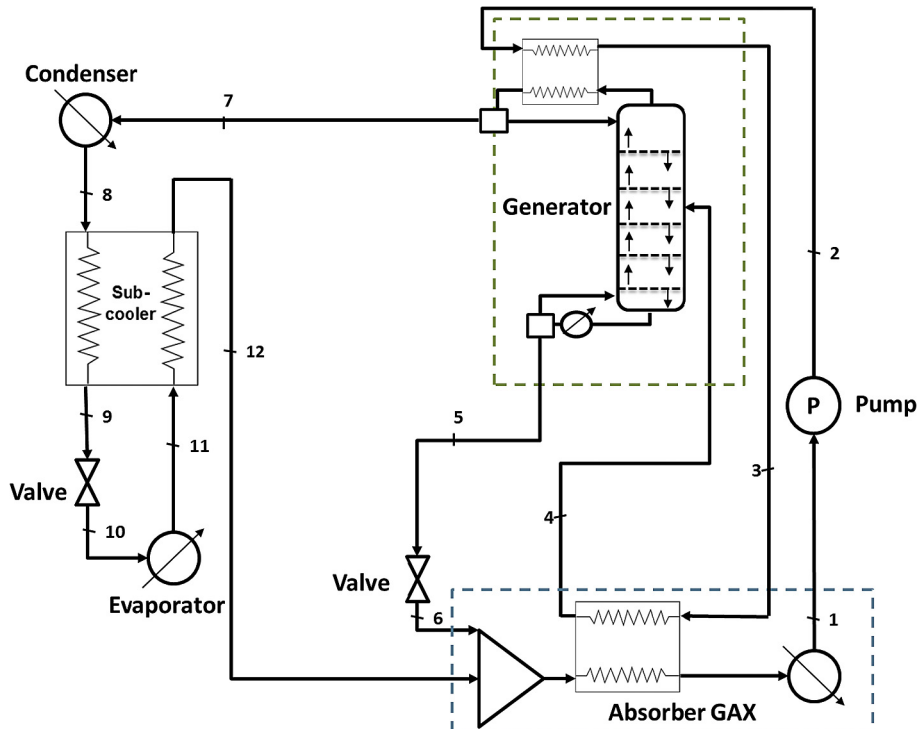
$$y_i \phi_i^v P = x_i \phi_i^l P \quad (1)$$

$$y_i \phi_i^v P = x_i \gamma_i^l P_i^{sat} \quad (2)$$

Fugacities ( $\phi_i^v$  and  $\phi_i^l$ ) can be expressed by the mean of an equation of state (EOS) for the mixture using appropriate mixing rules to obtain the parameters of the EOS. This is called the residual approach.

Activity coefficient ( $\gamma_i^l$ ) can be computed from a suitable equation depending on the chosen model (Margules, NRTL, UNIQUAC, etc.) of the excess molar free enthalpy  $g^E$ . This is called the excess approach.

In practice, vapour-liquid equilibria are often calculated using the so-called distribution coefficient or equilibrium coefficient  $k_i$



**Fig. 3.** Representation of a GAX cycle with our modules.

which describes, for each component  $i$ , the ratio of molar fraction in the vapour phase and in the liquid phase:

$$k_i = \frac{y_i}{x_i} \quad (3)$$

$k_i$  coefficient is calculated by the thermodynamic model:

$$mk_i = k_i(T, P, \mathbf{x}, \mathbf{y}) \quad (4)$$

where  $mk_i$  denotes the model deduced from equation (1) if a homogeneous approach is used or from equation (2) if a heterogeneous approach is used. It is a function of  $T, P, \mathbf{x}, \mathbf{y}$ .

Both the EOS model and the excess free enthalpy model give an accurate estimate of enthalpies.

In the case of a homogeneous method, molar enthalpy can be expressed as follows using a residual approach for both liquid and vapour phases:

$$mh^\alpha = h^\alpha(T, P, \mathbf{z}) = \sum_i \left( z_i h_i^{*GP}(T) \right) + \int_0^P \left( v^\alpha - T \left( \frac{\partial v^\alpha}{\partial T} \right)_{P, \mathbf{z}} \right) dP \quad (5)$$

$\mathbf{z}$  stands for  $\mathbf{y}$  (resp.  $\mathbf{x}$ ) and  $\alpha$  stands for V (resp. L) if the mixture is in vapour (resp. liquid) state.  $mh^L$  denotes the model of molar enthalpy for a liquid phase and  $mh^V$  denotes the model of molar enthalpy for a vapour phase. The first term on the right hand side represents the molar enthalpy of the mixture in a virtual perfect gas state. The second term is the molar residual enthalpy computed using the EOS to express the molar volume of the mixture  $v^\alpha$ .

In the case of a heterogeneous method, the molar enthalpy of a vapour mixture is still expressed by equation (5) using an EOS for the vapour phase and the molar enthalpy of a liquid mixture can be expressed as follows using the excess approach for the liquid phase:

$$mh^L = h^L(T, P, \mathbf{x}) = \sum_i \left( x_i h_i^{*L}(T, P) \right) - RT^2 \sum_i x_i \frac{\partial \ln \gamma_i}{\partial T} \quad (6)$$

The first term on the right hand side represents the molar enthalpy of the ideal mixture and the second term is the excess molar enthalpy computed using the chosen activity coefficient model (NRTL, Margules, etc).

The enthalpy of each stream is calculated as follows:

$$mh = h(T, P, \omega, \mathbf{x}, \mathbf{y}) = \omega h^V(T, P, \mathbf{y}) + (1 - \omega) h^L(T, P, \mathbf{x}) \\ = \omega mh^V + (1 - \omega) mh^L \quad (7)$$

where  $\omega$  is the vapour ratio and  $mh$  denotes the model for the molar enthalpy depending on  $T, P, \omega, \mathbf{x}, \mathbf{y}$ .

In the software, when  $\text{NH}_3/\text{H}_2\text{O}$  is used as the working pair, the homogeneous approach is used. As proposed by Figueira et al. [17], the Redlich-Kwong equation of state, with an asymmetric mixing rule and the SOF cohesion function, is used. These authors found this formulation to be very accurate for liquid-vapour equilibrium as well as for enthalpies for the  $\text{NH}_3/\text{H}_2\text{O}$  working pair over a wide range of temperatures (273 K–403 K) and pressures (0.5 bar–36 bar).

#### 4. Positive flash

In the present model, each stream is considered as a multi-component mixture and is then described by its temperature  $T$ , its

pressure  $P$ , its molar flow  $D$  and the molar fractions of the stream  $z_i$  ( $i = 1, \dots, nc$ ) ( $nc$  being the number of components. This is 2 for an  $\text{NH}_3/\text{H}_2\text{O}$  working pair; it can be greater if the solvent or refrigerant is already a mixture.) When the stream is in the state of liquid-vapour equilibrium, the vapour ratio  $\omega$  and liquid molar fractions  $x_i$  ( $i = 1, \dots, nc$ ) and vapour molar fractions  $y_i$  ( $i = 1, \dots, nc$ ) have also to be determined and can be obtained by the following set of equations:

$$\omega y_i + (1 - \omega) x_i = z_i \quad (8)$$

$$y_i = x_i mk_i \quad (9)$$

$$\sum_{i=1}^{nc} x_i = 1 \quad (10)$$

$$\sum_{i=1}^{nc} y_i = 1 \quad (11)$$

It must be noted that one of the summation equations (10) and (11) is redundant because of the  $nc$  partial mass balances (8) and the fact that  $\sum_{i=1}^{nc} z_i = 1$ . However, it has been found that the combination of the two relationships ((10) and (11)) results in an equation with good numerical properties. Hence, solving the so-called Rachford-Rice equation (12) will ensure that equations (10) and (11) will be satisfied.

$$\sum_{i=1}^{nc} (y_i - x_i) = 0 \quad (12)$$

Since no assumption is made concerning the physical state of the streams, a classical approach would consist in two distinct and sequential steps: phase identification of each stream and selection, followed by solution of the proper governing equations. Phase identification of each stream could be based on calculation of the bubble and dew temperatures associated with pressure  $P$  and composition  $\mathbf{z}$  of the stream, and then, for each stream, when  $T$  is between these two temperatures,  $nc$  partial mass balance equation (8),  $nc$  equilibrium equation (9) and summation equation (12) could be solved together with the other equations in the absorption chiller model. This approach would demand a long computation time since two iterative subroutines are needed to calculate bubble and dew temperatures (which indeed consist in solving  $nc$  equation (8),  $nc$  equations (9) and (12) with  $\omega = 0$  for the bubble temperature and  $\omega = 1$  for the dew temperature). It is for this reason that we chose another approach: the positive flash. This is a set of equations used to describe a multi-component stream in the same way, irrespective of its physical state. Indeed, the set of equations is valid for all phase regions. As mentioned above, the present paper deals only with the steady state model, but it should be pointed out here that using the positive flash formulation for all the streams in a dynamic model leads to a global model which can handle the formation of a new phase or the disappearance of an existing one because of composition, pressure or temperature changes due to the dynamic state. Hence for the dynamic model, the positive flash approach will be of great interest. For the steady state model, this approach is also very interesting as far as computation time is concerned.

In 1989, Whitson and Michelsen [18] proposed an approach called the “negative flash” in which the vapour ratio is allowed to be outside the physical range 0–1. In their paper, the Rachford-Rice equation (10) is re-formulated as follows, combining equations (8), (9) and (12):

$$f(\omega) = \sum_{i=1}^{nc} \frac{(k_i - 1)z_i}{1 + (k_i - 1)\omega} = 0 \quad (13)$$

The solution to equation (13) gives the value of  $\omega$ , and compositions are then calculated as follows:

$$x_i = \frac{z_i}{\omega k_i + (1 - \omega)} \quad (14)$$

$$y_i = \frac{k_i z_i}{\omega k_i + (1 - \omega)} = k_i x_i \quad (15)$$

The authors showed that there is only one solution  $\omega$  to equation (13) which yields all non-negative phase compositions  $y_i$  and  $x_i$ . If this solution is between 0 and 1, liquid and vapour phases exist. Otherwise, if this solution is outside the physical range, the set of equations remains the same, but one of the phases does not exist (if  $\omega < 0$  (resp.  $\omega > 1$ ), only the liquid (resp. vapour) phase exists and the molar fractions  $y_i$  (resp.  $x_i$ ) are meaningless despite satisfying the equilibrium equation (9)). This “negative flash” approach is not convenient in our absorption chiller model since the value of  $\omega$  is useful for calculating stream enthalpy using equation (7). A non-physical value could be discarded and replaced by a physically acceptable value (0 if only the liquid phase exists and 1 if only the vapour phase exists), but this would lead to discontinuities which make this model unsuitable for use in dynamic modelling.

In 1998, Han and Rangaiah [19] proposed a method called the “ $\tau$  method” which keeps the physical meaning of  $\omega$ . They exploited the fact that the molar fraction summation of a non-existent phase is less than one (this can be demonstrated by analysing the defined function  $f(\omega)$  in equation (13)). They proposed to modify summation equations (10) and (11) as follows:

$$\sum_{i=1}^{nc} x_i + \tau^L = 1 \quad (16)$$

$$\sum_{i=1}^{nc} y_i + \tau^V = 1 \quad (17)$$

The resulting problem has more unknown variables than equations and is solved as the following minimization problem:

$$\begin{cases} \min(\tau^L + \tau^V) \\ \text{s.t. } \begin{cases} \text{equations (8)(9)(16)(17)} \\ 0 \leq \tau^L, \tau^V, x_i (i = 1, nc), y_i (i = 1, nc), \omega \leq 1 \end{cases} \end{cases} \quad (18)$$

The set of equations and the number of unknown variables are kept constant whatever the physical state. When the two phases exist,  $\tau^L$  and  $\tau^V$  are equal to zero. When the liquid phase does not exist,  $\tau^L$  is not equal to zero and  $\omega$  is equal to 1: it corresponds to a super-heated vapour state. When the vapour phase does not exist,  $\tau^V$  is not equal to zero and  $\omega$  is equal to 0: it corresponds to a sub-cooled liquid state.

In 2004, They et al. [20] extended this formulation to dynamic simulation and the minimization problem was transformed into a set of differential algebraic equations by adding equations to obtain the same number of unknown variables as the number of equations. They dealt with the liquid-liquid-vapour stage of a distillation column. Applying their method (which they called “positive flash”) to our liquid-vapour problem leads to a set of  $(2nc + 3)$  equations constituted by  $nc$  partial mass balance equation (8)  $nc$  equilibrium equation (9), the following new summation equation and two additional switch equations:

$$\sum_{i=1}^{nc} (y_i - x_i) + \tau^V - \tau^L = 0 \quad (19)$$

$$\tau^V \omega = 0 \quad (20)$$

$$\tau^L (1 - \omega) = 0 \quad (21)$$

This set of equations is associated to the  $(2nc + 3)$  variables:  $\tau^L, \tau^V, x_i, y_i (i = 1, nc), \omega$ . Equations (20) and (21) ensure that  $\tau^L$  and  $\tau^V$  are equal to zero in the case of a liquid-vapour state, since in this case the value of  $\omega$  is between 0 and 1. To take into account the fact that  $\omega$  is between 0 and 1, and then avoid converging to the solution of the negative flash, we have added the following substitution:

$$\omega = \frac{1}{1 + e^{-s\zeta}} \quad (22)$$

$\zeta$  is the new variable, which substitutes variable  $\omega$ , and  $s$  is a numerical parameter, which is chosen to ensure the accuracy of the solution.

Since  $\tau^L$  and  $\tau^V$  are also between 0 and 1, two other equations such as equation (22) have been added.

## 5. Steady state model

### 5.1. Variables and input parameters

The variables of the global model are:

- For each stream: temperature  $T$ , pressure  $P$ , molar flow rate  $D$ , vapour ratio  $\omega$ ,  $nc$  liquid molar fractions  $x_i (i = 1, \dots, nc)$ ,  $nc$  vapour molar fractions  $y_i (i = 1, \dots, nc)$ , and  $\tau^L$  and  $\tau^V$ , liquid and vapour gap variables. Thus there are  $6 + 2nc$  variables for each stream.
- Pump work  $W_{pump}$  for each pump.
- In each heat exchanger, exchanged power  $\dot{Q}$ , and for each heat exchanger with an external source there is another variable: molar flow of the external source,  $D_{source}$ , in the case of the generator boiler and outlet temperature,  $T_{source,out}$  in other cases (condenser, absorber, and perhaps rectifier).
- A set of variables for each theoretical stage of the generator (these are described in section 5.3)

Input parameters of the model are:

- Molar flow and composition of the pump outlet,
- Pump efficiency,  $\eta_{pump}$ , for each pump,
- Flow factors of the valves,  $K_v$ . It must be noted that the user of our tool can choose to fix a pressure instead of a flow factor. In this case, the flow factor is a variable of the system, and the pressure (upstream or downstream) is an input parameter,
- Number of theoretical plates  $N$  of the generator and feed stage number, “ $a$ ”,
- $UA$  product in each heat exchanger. In fact, the global coefficient  $U$  of each exchanger should be a function of the variables. In order to avoid a long computation time, these coefficients are kept constant and uniform. They are calculated beforehand using suitable correlations with estimated temperatures, flow rates and compositions. They are checked with the values obtained for these variables when solving the global system for the steady state of the cycle.
- Finally, for each heat exchanger with an external source, two variables: inlet and outlet temperature,  $T_{source,in}$  and  $T_{source,out}$  in

the case of the generator boiler. Inlet temperature,  $T_{source,in}$  and molar flow of the external source,  $D_{source}$ , in other cases.

## 5.2. Module equations

The generator equations are presented in section 5.3. For all the other modules, the following equations can be written: total mass balance,  $nc$  partial mass balances, energy balance, and, for each outlet stream, the summation equation (19), the vapour gap equation (20) and the liquid gap equation (21).

Depending on the module, the following rules are applied:

- Since the expansion in the valves is considered isenthalpic,  $\dot{Q}$  is zero in the energy balance of the valves.
- As far as the energy balance is concerned, for the pump module,  $\dot{Q}$  must be replaced by the product  $W_{pump} \cdot \eta_{pump}$  which can be estimated with the help of the pump equation:

$$W_{pump} = D_{out} \frac{(P_{out} - P_{in})}{\eta_{pump} \rho(T_{in}, P_{in}, \mathbf{x}_{in})} \quad (23)$$

where  $\rho(T_{in}, P_{in}, \mathbf{x}_{in})$  is the density of the inlet fluid which can be evaluated using the COSTALD method [21].

- For the internal heat exchanger module, since the two streams are separate in the device, the set of equations has to be written for each stream.
- For every heat exchanger with an external source, in addition to the energy balance for the fluid, the energy balance for the source has to be written too.
- The logarithmic mean temperature difference equation is used in each heat exchanger (heat losses are neglected).

$$\dot{Q} = UA \frac{\Delta T_1 - \Delta T_2}{\ln \frac{\Delta T_1}{\Delta T_2}} \quad (24)$$

where  $\Delta T_1$  is the difference between hot inlet temperature and cold outlet temperature in the exchanger (at end "1" of the exchanger), and  $\Delta T_2$  is the difference between the hot outlet temperature and cold inlet temperature in the exchanger (at end "2" of the exchanger).  $U$  is the global heat transfer coefficient. It depends on temperatures, flow rates and geometry of the exchanger. In order to avoid a too long computation time, this is fixed (using suitable correlations to estimate temperatures and flow rates beforehand). It is also assumed to be constant along the exchanger although this may not be the case if phase change occurs. In this case another model using different zones can be used [22]. In the example of the present paper  $U$  is assumed to be constant.

Pressure drops in the pipes have been neglected. They have also been neglected in the components, apart from in the valves and pumps. An equation stating that the outlet pressure is equal to the inlet pressure must therefore be added, except in the valves and pumps.

The valve equation can be written as follows:

$$D_{out} = K_V \sqrt{\frac{(P_{in} - P_{out})}{\rho(T_{in}, P_{in}, \mathbf{x}_{in}) / \rho_{water, 20^\circ C}}} \quad (25)$$

## 5.3. Generator model. MESH equations

The generator is the device where the rich solution is separated in order to recover the ammonia vapour. The generator therefore

has to be modelled as a distillation column. As already mentioned, most authors make assumptions about the composition of generator outputs in papers dealing with absorption chillers. Nevertheless, in chemical engineering science, two ways of modelling the distillation unit operation are reported in order to estimate these compositions. The first relies on partial mass transfer balances at the liquid-vapour interface, and the second uses the concept of stackable theoretical plates. From a theoretical point of view, the former produces more representative models which are closest to reality. However, these models are difficult to use since they require a lot of parameters, which are often difficult to assess. Moreover, they require more computation time. Therefore models based on the theoretical plate concept are a good compromise: compositions of the output streams are calculable without assumptions while keeping a reasonable computation time.

A theoretical plate is a hypothetical zone in which the liquid and vapour phases of the mixture establish equilibrium with each other. The liquid and vapour flows that leave a theoretical plate are therefore in equilibrium. A schematic representation of the generator is given in Fig. 4. It can be seen that the first stage is the partial condenser of the distillation column (sometimes called the rectifier). It extracts  $\dot{Q}_C$ , the power needed to generate the reflux which ensures the required purity at the top of the distillation column. Stage  $N$  is the distillation column boiler. In this stage the solar heated water provides the necessary power,  $\dot{Q}_B$ . The generator has one feed (rich solution) which enters the column at stage number "a" ("a" is an input parameter). It can be seen that the generator is a diabatic distillation: heat is transferred on the trays below the feed tray inside the column as opposed to classical adiabatic columns where heat is only supplied to the boiler and extracted from the condenser. Thus in Fig. 4, the heat at each stage below the feed stage is supplied by the bottom fluid circulating in series from the bottom stage to the feed stage. The rate of subcooling of the poor solution leaving the generator is a given parameter.

MESH equations (Mass balance, Equilibrium, Summation, Heat Balance equations) are written for each theoretical stage.

For the  $j$ th theoretical stage ( $j = 1, N$  and  $j \neq a$ ):

$$V_{j+1} + L_{j-1} = L_j + V_j \quad (26)$$

$$V_{j+1} y_{i,j+1} + L_{j-1} x_{i,j-1} = L_j x_{i,j} + V_j y_{i,j} \quad (27)$$

$$y_{i,j} = x_{i,j} m k_{i,j} \quad (28)$$

$$\sum_{i=1}^{nc} (y_{i,j} - x_{i,j}) = 0 \quad (29)$$

$$\dot{Q}_j + V_{j+1} m h_{j+1}^V + L_{j-1} m h_{j-1}^L = L_j m h_j^L + V_j m h_j^V \quad (30)$$

$$\text{with : } L_0 = 0, V_{N+1} = 0$$

$$\text{and : } \dot{Q}_1 = -\dot{Q}_C, \quad \dot{Q}_j = 0 \text{ if } 1 < j < a, \quad \dot{Q}_j = \dot{Q}_{SC} \text{ if } a < j < N-1, \quad \dot{Q}_N = \dot{Q}_B$$

For the  $a$ th theoretical stage, the MESH equations are written as follows:

$$D_{in} + V_{a+1} + L_{a-1} = L_a + V_a \quad (31)$$

Partial condenser:  
internal heat exchanger  
or exchanger with  
external source

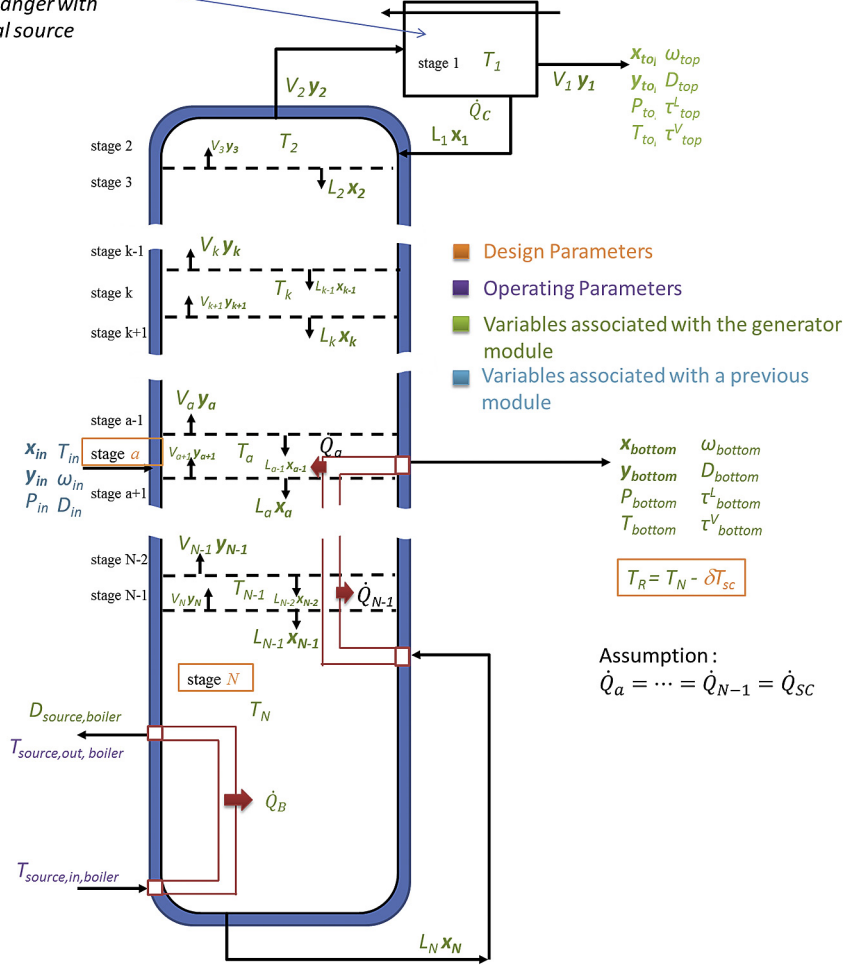


Fig. 4. Diagram of generator.

$$D_{in} [\omega_{in} y_{i,in} + (1 - \omega_{in}) x_{i,in}] + V_{a+1} y_{i,a+1} + L_{a-1} x_{i,a-1} = L_a x_{i,a} + V_a y_{i,a} \quad (32)$$

$$y_{i,a} = x_{i,a} m k_{i,a} \quad (33)$$

$$\sum_{i=1}^{nc} (y_{i,a} - x_{i,a}) = 0 \quad (34)$$

$$\dot{Q}_{SC} + D_{in} m h_{in} + V_{a+1} m h_{a+1}^V + L_{a-1} m h_{a-1}^L = L_a m h_a^L + V_a m h_a^V \quad (35)$$

Thus, for each stage, there are  $3 + 2nc$  variables ( $L_j, V_j, T_j, x_j, y_j$ ) associated with  $3 + 2nc$  MESH equations.

A partial condenser can be modelled as a heat exchanger with an external source (this is the case in Fig. 2) or as an internal heat

exchanger if an internal stream is used to condense the vapour (this is the case in Fig. 3).

Finally, both generator outlets have to be modelled by positive flash model variables. We add  $2 \times (6 + 2nc)$  equations described in Table 1, associated to  $2 \times (6 + 2nc)$  outlet stream variables. However, since the partial condenser (stage 1) and the boiler (stage N) are assumed to be equilibrium stages, outlet flows are assumed to be in equilibrium (saturated vapour at the top and boiling liquid at the bottom) and this leads to the equations in Table 1.  $\dot{Q}_C$  in the partial condenser (resp.  $\dot{Q}_B$  in the boiler) is estimated using equation (24) with a constant temperature of the solution,  $T_1$  (resp.  $T_N$ ). Inlet and outlet temperatures of the other fluid are not the same.

#### 5.4. Resolution

Although the model equations have been written in a modular way, a global resolution using Newton-Raphson's method has been implemented to solve the model. The programme has been written

Table 1  
Positive flash equations for the generator outlets.

Top outlet	$D_{top} = V_1$	$T_{top} = T_1$	$\omega_{top} = 1$	$x_{top} = x_1$	$y_{top} = y_1$	$\tau_{top}^L = 0$	$\tau_{top}^V = 0$
Bottom outlet	$D_{bottom} = L_N$	$T_{bottom} = T_N$	$\omega_{bottom} = 0$	$x_{bottom} = x_N$	$y_{bottom} = y_N$	$\tau_{bottom}^L = 0$	$\tau_{bottom}^V = 0$

Bold variables are array variables.

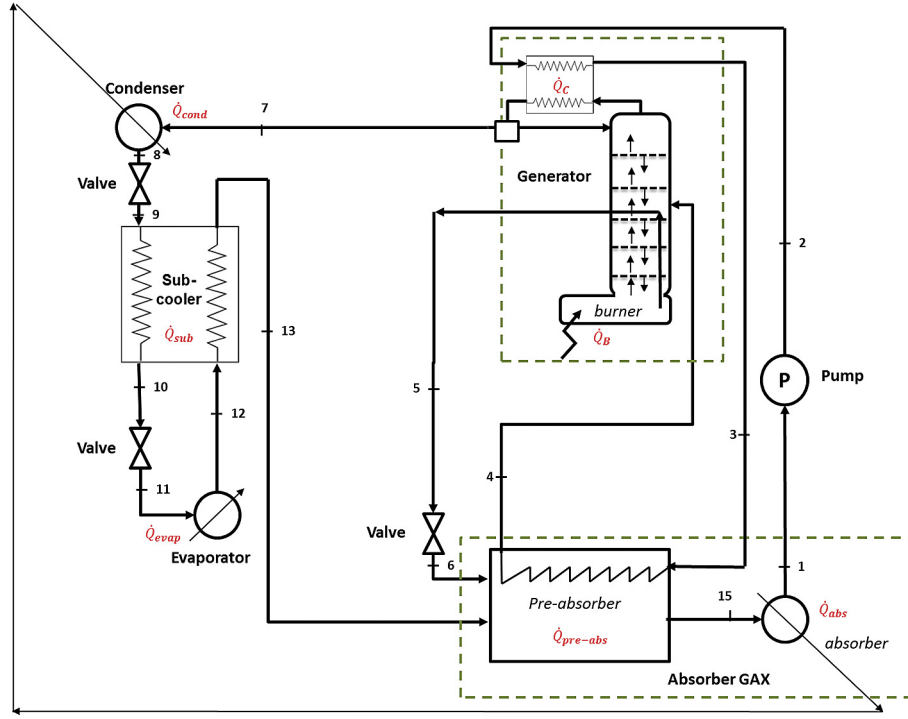


Fig. 5. Diagram of Butz and Stephan's experimental test rig.

in FORTRAN. The biggest challenge to solving the system of equations was the choice of the initial point.

## 6. Results and discussion

The model has been tested with the example presented by Butz

and Stephan in 1989 [14]. These authors presented experimental and modelled results for an existing commercial machine, of which the components and their interconnections are shown in Fig. 5. It is a GAX configuration, which significantly improves COP (Coefficient Of Performance) by recovering the heat produced by absorption and using it as extra heat to supplement the solar source [23]. Fig. 6

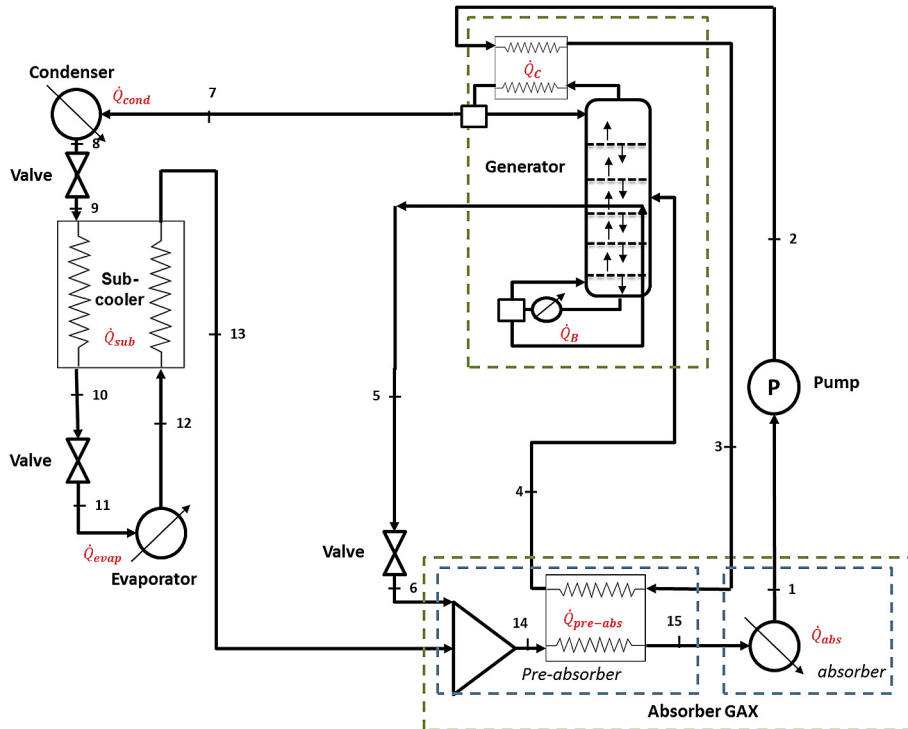


Fig. 6. Diagram of Butz and Stephan's test rig with our modules.

**Table 2**  
Input parameters.

Parameter	Value	Parameter	Value	Parameter	Value
$T_{source,in,abs}$ (°C)	36.19	$\eta_{pump}$	0.8	$UA_{pre-abs}$ (W/K)	316.87
$D_{source,abs}$ (kg/s)	0.61	$T_{source,in,boil}$ (°C)	196.85	$UA_{abs}$ (W/K)	615.2
$T_{source,in,cond}$ (°C)	43.47	$T_{source,out,boil}$ (°C)	186.85	$UA_{cond}$ (W/K)	893.99
$D_{source,cond}$ (kg/s)	0.61	$N$	4	$UA_{evap}$ (W/K)	2825.19
$T_{source,in,evap}$ (°C)	10.07	$a$	2	$UA_c$ (W/K)	70.7
$D_{source,evap}$ (kg/s)	0.44			$UA_B$ (W/K)	1503.7
$D_2$ (kg/s)	0.0216			$\delta T_{sc}$ (°C)	62
$x_{NH_3,2}$	0.4297			Sub-cooling at the bottom outlet of the generator	
$P_{low} = P_1$ (bar)	4.6				
$P_{high} = P_2$ (bar)	21.6				
$P_{intermediate} = P_9$ (bar)	12.0				

is the representation of this machine with our modular tool. It differs slightly from Fig. 3: there is a second valve between the condenser and the sub-cooler and the generator is not adiabatic as specified in section 5.3. The working pair is ammonia/water.

Butz and Stephan also used the concept of theoretical stages to model the generator and they also assumed constant heat transfer coefficient even if a phase change occurred. They used a Ziegler and Trepp model [24] to estimate thermodynamic properties. Thus the present model is very similar but it uses a more recent thermodynamic model and above all, it uses the positive flash formulation to estimate the physical state of each stream.

The parameters of the model are shown in Table 2.

- Some parameters are taken from Butz and Stephan's paper (Column1, Table 2).
- Others were chosen (Column 2). Hence, the pump efficiency is fixed at 0.8, which is a standard value [25,4]. We also fixed the

inlet and outlet temperatures of the solar heated water, which is the source of the boiler. In the commercial absorption machine described by Butz and Stephan, heat is supplied by a gas burner. So we chose to fix the outlet temperature 5 °C higher than the boiler temperature reported by Butz and Stephan, and the inlet temperature 10 °C higher than the outlet temperature. Several simulations were carried out to choose suitable values for the number of theoretical plates  $N$  of the generator and the feed stage number, "a".

- Lastly, some parameters ( $UA$  products and outlet temperature of the poor solution) are deduced from reported values of temperatures and exchanged heats from Butz and Stephan's paper and are reported in Column 3, Table 2.

It should be pointed out that since we have estimated the inlet and outlet temperatures of hot utility at the generator boiler, the estimate of  $UA$  product at the boiler is probably not very

**Table 3**  
Comparison of obtained results with modelled and experimental results of Butz and Stephan.

Variable	Present model A	Butz & Stephan model B	Experience Exp	% Error A-B	% Error A-Exp	% Error B-Exp
$T_{source,out,abs}$ (°C)	41.69	41.26	43.47	1.04%	-4.09%	-5.08%
$T_{source,out,cond}$ (°C)	47.07	45.09	45.14	4.39%	4.28%	-0.11%
$T_{source,out,evap}$ (°C)	5.60	5.54	5.46	1.08%	2.56%	1.47%
$D_5$ (kg/s)	0.0142	0.0136	Nd	0.01357		
$x_{NH_3,5}$	0.1220	0.1138	Nd	7.2%		
$D_7$ (kg/s)	0.0074	0.0080	Nd	0.00802		
$x_{NH_3,7}$	0.9907	0.9912	Nd	-0.05%		
$T_1$ (°C)	46.08	45.40	44.10	1.50%	4.49%	2.95%
$\varpi_1$	0	0	Nd	0%		
$T_2$ (°C)	46.17	45.93	45.30	0.52%	1.92%	1.39%
$T_3$ (°C)	66.83	64.23	63.10	4.05%	5.91%	1.79%
$T_4$ (°C)	90.76	104.21	105.20	-12.91%	-13.73%	-0.94%
$\varpi_4$	0	0	Nd	0%		
$T_N$ (boiler) (°C)	181.16	181.83	Nd	-0.37%		
$T_5$ (°C)	119.16	119.38	115.30	-0.18%	3.35%	3.54%
$T_6$ (°C)	114.16	114.68	113.10	-0.45%	0.94%	1.40%
$\Pi_6$	0.0057	0.0167	Nd	-65.87%		
$T_7$ (°C)	86.54	81.75	86.90	5.86%	-0.42%	-5.93%
$T_8$ (°C)	44.41	42.64	49.10	4.15%	-9.55%	-13.16%
$\Pi_8$	0	0	Nd	0%		
$T_9$ (°C)	31.93	31.26	31.50	2.13%	1.35%	-0.76%
$\Pi_9$	0.0531	0.0516	Nd	2.91%		
$T_{10}$ (°C)	20.37	10.81	22.00	88.46%	-7.40%	-50.86%
$\Omega_{10}$	0	0	Nd	0%		
$T_{11}$ (°C)	2.58	2.10	2.50	22.90%	3.24%	-16.00%
$\Pi_{11}$	0.0647	0.0306	Nd	111.54%		
$T_{12}$ (°C)	7.21	7.41	7.50	-2.66%	-3.83%	-1.20%
$\Pi_{12}$	0.9350	0.8790	Nd	6.37%		
$T_{13}$ (°C)	30.23	15.89	25.60	90.25%	18.09%	-37.93%
$\Pi_{13}$	0.9830	0.9760	Nd	0.72%		
$T_{15}$ (°C)	85.90	80.52	74.70	6.69%	15.00%	7.79%
$\Pi_{15}$	0.2942	0.2766	Nd	6.36%		

**Table 4**  
Calculated powers.

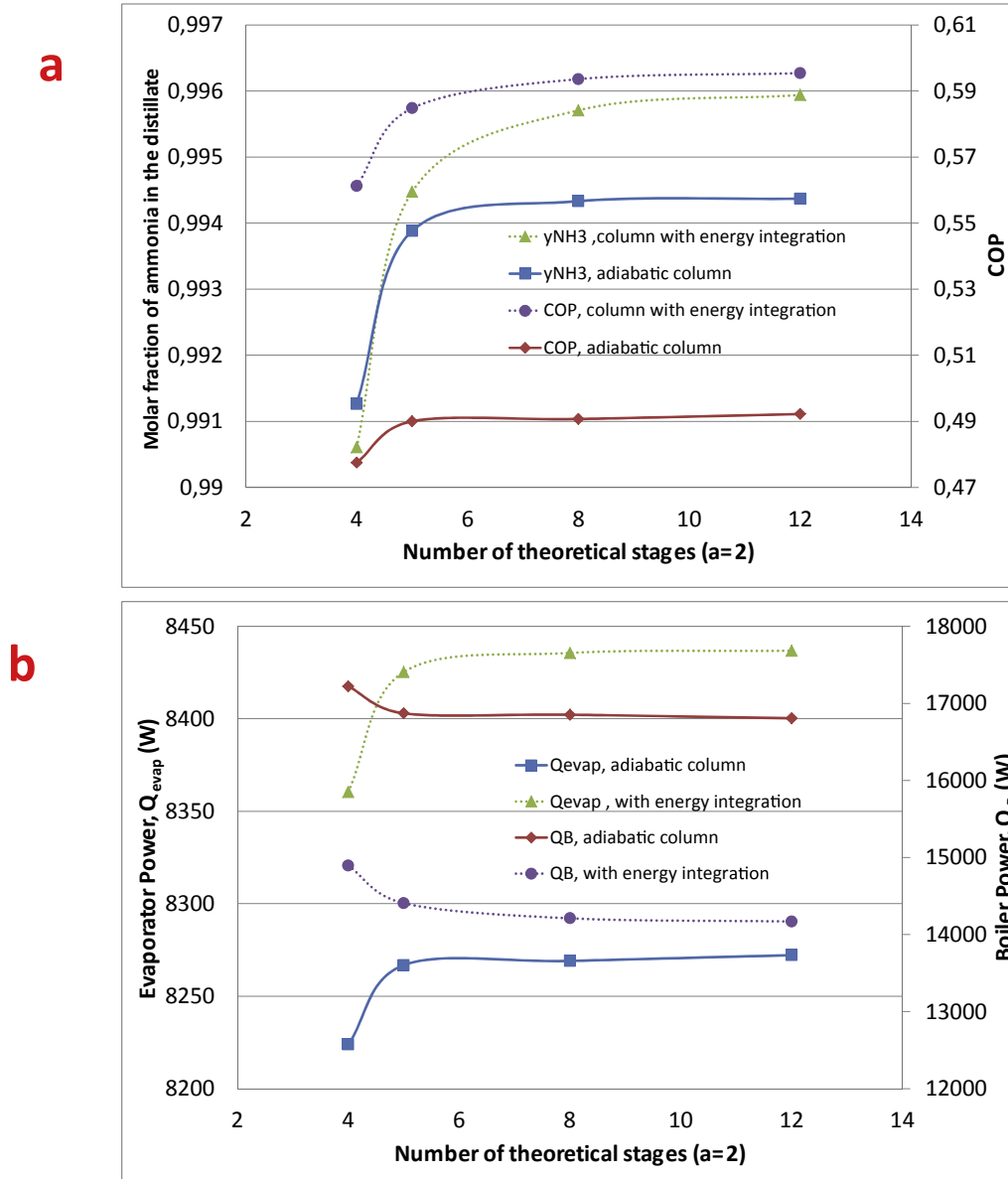
Variable	Model	Butz Model	% Error Mod. – Butz Mod.
$\dot{Q}_B$ (kW)	14.85	13.72	8.26%
$\dot{Q}_C$ (kW)	2.04	1.81	12.60%
$\dot{Q}_{pre-abs}$ (kW)	2.39	4.05	-40.94%
$\dot{Q}_{abs}$ (kW)	14.08	12.76	10.39%
$\dot{Q}_{cond}$ (kW)	9.16	9.62	-4.71%
$\dot{Q}_{evap}$ (kW)	8.35	8.57	-2.59%
$\dot{Q}_{sub}$ (kW)	0.88	1.24	-29.49%
COP	0.5620	0.6246	-10.02%

representative of Butz and Stephan's experimental device. Modeling the GAX pre-absorber is also a problem insofar as we describe this pre-absorber as an adiabatic mixture and an internal exchanger in series. Since the outlet flow of the mixer (inlet flow of the

exchanger) has no physical reality, its temperature is not given by Butz. A first attempt consisted of a preliminary calculation of the mixer (using our model and thermodynamics). This attempt was unsuccessful: the hot temperature of the outlet flow of the mixer was less than the cold temperature of the outlet flow of the exchanger (value of Butz).  $UA$  product was therefore approached by setting a temperature difference of 10 °C at the hot end of the exchanger. As for the boiler, the estimated  $UA$  product is probably not very representative of Butz and Stephan's experimental device.

It should be also noted that the inlet temperature of the source in the condenser,  $T_{source,in,cond}$ , was fixed, whereas Butz and Stephan's model calculated this value. Indeed in the present formulation condenser and absorber sources are independent, whereas in their model the outlet source flow of the absorber is the inlet source flow of the condenser.

Despite all these differences and uncertainties, results from the present model compared quite well with those of Butz and Stephan, as can be seen in Table 3.

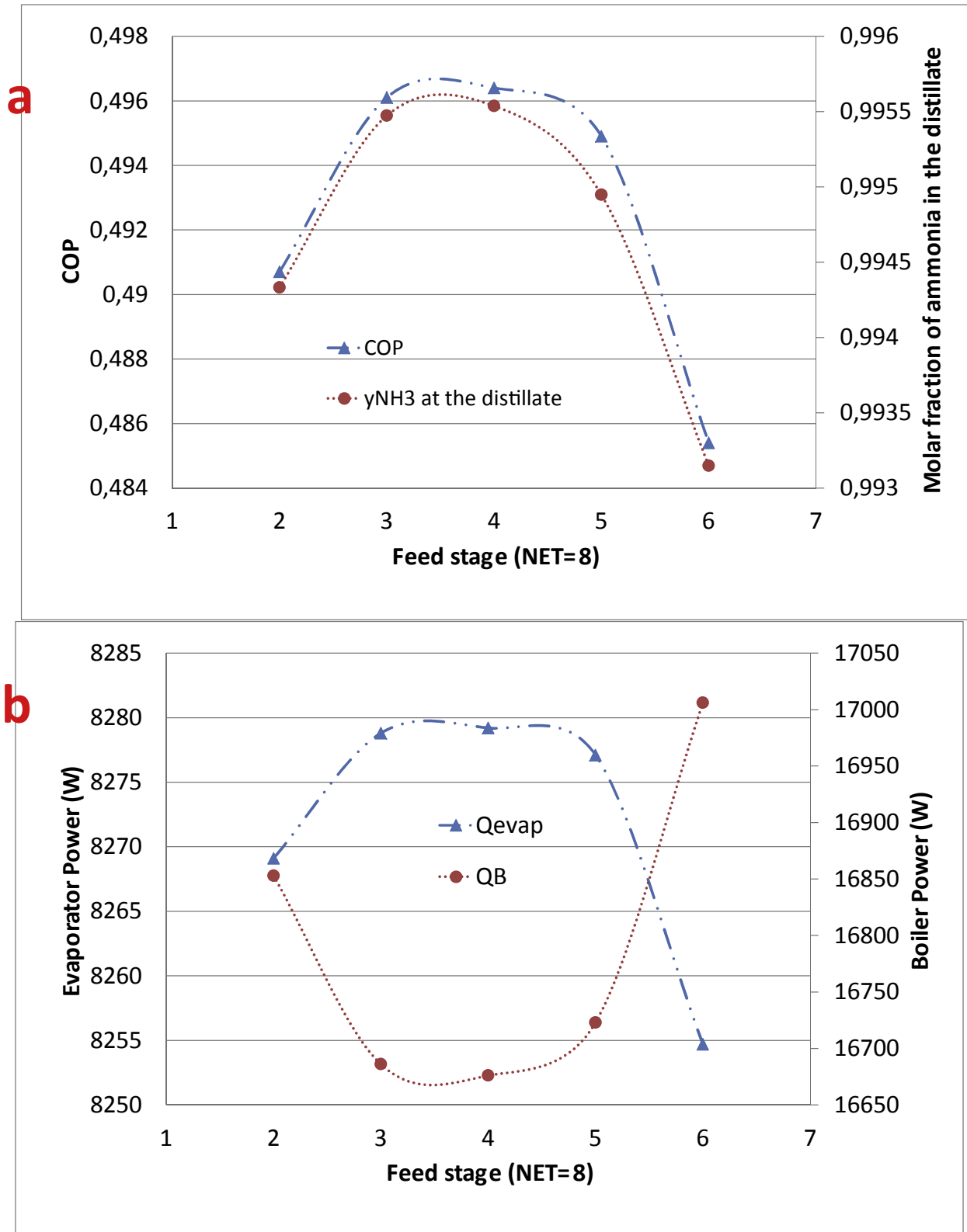


**Fig. 7.** Influence of the number of theoretical stages on the COP and the molar fraction of ammonia in the distillate (a) and on the evaporator power and the boiler power (b). The feed is located at stage number 2. This influence is shown in cases of adiabatic and diabatic columns.

Deviations from the experiment are less than 10%, except for points 4, 13 and 15 (these flows are involved in the pre-absorber or in the sub-cooler). We will discuss these points later. In Table 4, the calculated powers are compared to those of Butz and Stephan. Once

again, results are quite good except for the pre-absorber and the sub-cooler.

As far as the pre-absorber is concerned, remember that  $UA$  product had to be approached very approximately. This explains (at



**Fig. 8.** Influence of the position of the feed on the COP and the molar fraction of ammonia in the distillate (a) and on the evaporator power and the boiler power (b). The number of theoretical stages is 8. This influence is shown in case of an adiabatic column.

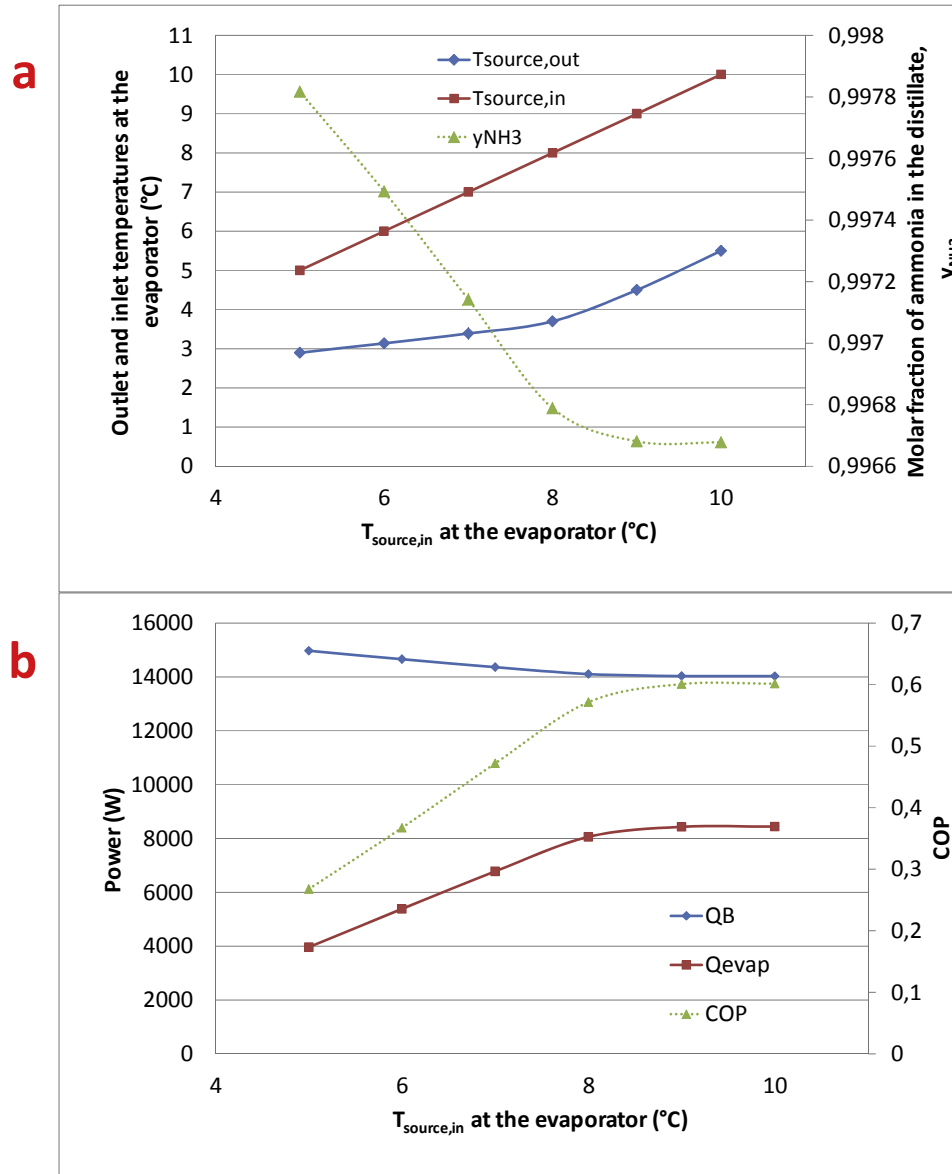
least partially) the gap between our result and that of Butz and Stephan. In an attempt to validate this hypothesis, a sensitivity analysis on the  $UA$  product of the heat exchanger of the pre-absorber was performed. It was noted that by increasing  $UA$  product, the exchanged power also increases, but only up to a maximum of 2.56 kW. The gap is therefore reduced but only slightly. The limit is linked to the modelling of the pre-absorber. By introducing a counter-current heat exchanger, the temperature of the cold outlet flow ( $T_4$ ) is limited, for an infinite  $UA$ , by the temperature of the hot inlet flow ( $T_{14}$ ). We can conclude that this gap is thus intrinsic to the modelling of the pre-absorber.

As far as the sub-cooler is concerned, the gap probably comes from the thermodynamic model. Butz and Stephan used the Ziegler and Trepp model [24]. However, this model has been upgraded [26] and in it the vapour phase is assumed to be a perfect gas. In the present model, the Redlich-Kwong equation of state was used for both phases with a mixing rule and a cohesion parameter proposed by Figueira et al. [17]. In order to check this point, we simulated

only the sub-cooler setting inlet temperature, flow rate, pressure, composition of the inlet flows (9 and 12) using those of Butz and Stephan. The first observation was that the physical state of inlet flow 9 was not the same. A sub-cooled liquid was calculated whereas Butz and Stephan reported liquid-vapour equilibrium. This strongly suggests that the gap results from the thermodynamic model. In addition, in our case, only sensible heat was exchanged whereas in their case latent heat was also exchanged. Finally, it can be noted (Table 2) that temperatures  $T_7$  to  $T_{13}$  predicted by the present model are a better fit for experimental values than those predicted by their model. This emphasizes the importance of the thermodynamic model for estimating the thermodynamic properties of a refrigerant-absorbent mixture.

Now, since the model is validated, a sensibility analysis is presented. The following parameters were studied:

- The number of theoretical stages of the generator,
- The energetic integration in the generator,



**Fig. 9.** Influence of the temperature of the cold source at the inlet of the evaporator. This influence is shown for a diabatic column (with energetic integration) of 8 theoretical stages fed at stage number 4.

- The feed position in the generator,
- The inlet temperature of the source at the evaporator.

The influence of the first two parameters is shown in Fig. 7. For the adiabatic column, as the number of theoretical stages increases, the purity of the distillate, the provided frigories at the evaporator, and the COP increase too, while the boiler power decreases, until all these variables reach a plateau. Since the investment cost of a distillation column is linked to its stage number, the optimal stage number, from an economic point of view, stands at the beginning of this plateau. For the diabatic column (with energetic integration described in section 5.3), the same conclusions can be drawn. It can be also pointed out that the COP of the diabatic column is always higher than the one of the adiabatic column not only because of a lower boiler power (about 2500 W), but also because of a slightly higher provided cold power at the evaporator (about 160 W).

The influence of the feed position in the generator is shown in Fig. 8. It clearly appears that there is an optimal stage to feed the column, which maximizes the purity, the COP and the provided frigories while minimizing the boiler power.

At last, the influence of the inlet temperature of the cold water at the evaporator is shown in Fig. 9. The inlet temperature of the cold source was decreased from 10 °C to 5 °C in a diabatic column of 8 theoretical stages fed at the stage number 4. It can be seen that from 8 °C, the decrease of the outlet temperature is slowed, while the increase of the boiler power and the decrease of the provided cold power and the COP are sped up. These observations are congruent with the fact that the COP of a three-heat-source cycle decreases when the temperature of the cold source decreases. It can be also noted that the purity at the top of the generator is higher when the cold source temperature is lower.

## 7. Conclusions and perspectives

Within the framework of a project which aims to develop a reversible solar cooling system which responds to thermal requirements in the industrial and tertiary building sectors, we have focused on modelling absorption chillers. Our final aim is to propose a formulation for a model which will be suitable for implementing a dynamic model, easily able to handle the formation of a new phase or the disappearance of an existing one because of changes in composition, pressure or temperature due to the dynamic state. To achieve this, the positive flash proposes the same set of governing equations for all phase regions. Thus, all streams are multicomponent mixtures and their physical states are not previously fixed but are calculated using positive flash equations. In the present work, the generator is modelled using the theoretical plate concept. This type of model, which is well-known in chemical engineering modelling, has only been used once, several years ago, by Butz and Stephan in the context of absorption chillers. However, the theoretical plate model is a useful model which ensures good compromise: compositions of the output streams can be calculable without assumptions while keeping a reasonable computation time. However, in such a model an accurate thermodynamic model has to be used to estimate liquid-vapour equilibrium coefficients. Generally speaking, the thermodynamic model is an important tool to accurately estimate the thermodynamic properties (liquid-vapour equilibrium as well as enthalpies) of a refrigerant-absorbent mixture. In the case of water/ammonia it is suggested that the Redlich-Kwong equation be used (for both phases) with the mixing rule and cohesion parameter proposed by Figueira et al. [17].

The present formulation has been tested in steady state and compared, in the case of the GAX configuration using water/ammonia as a working pair, to Butz and Stephan's results [14]. It gives satisfactory results, given that some parameters are missing.

Although the present model has been designed in order to be general, some adaptations are required to use it with different working fluids: the binary parameters have to be changed if the EOS is still valid. If components such as alcohol are used, excess enthalpy model has to be implemented. Finally, in future this work will be used to test the present formulation in the context of a dynamic model. The absorber could also be modelled using the theoretical plate concept, just like the generator.

At last the model developed in this contribution could be solved together with the model of the heat supply process in order to perform the global optimization of the whole system.

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## Nomenclature

$A$	heat exchanger surface, m <sup>2</sup>
$D$	molar flow rate, kmol/s
$c_p$	molar specific heat, J/(K.mol)
$h$	molar enthalpy, J/kmol
$k_i$	liquid-vapour equilibrium coefficient for component $i$
$K_v$	Flow factor, m <sup>3</sup> /s
$L$	liquid flow rate, kmol/s
$M$	Molar weight
$N$	number of theoretical plates in the generator
$nc$	number of components
$mh$	model for molar enthalpy
$mk$	model for equilibrium coefficient
$P$	pressure, Pa
$P_i^{sat}$	saturated vapour pressure of component $i$ , Pa
$\dot{Q}$	exchanged power, W
$R$	gas ideal coefficient, J/(K.mol)
$T$	temperature, K
$U$	global heat transfer coefficient, W/(K.m <sup>2</sup> )
$V$	vapour flow rate, kmol/s
$v$	molar volume, m <sup>3</sup> .mol <sup>-1</sup>
$W_{pump}$	pump work supplied, W
$\mathbf{x}$	molar liquid fraction vector
$\mathbf{y}$	molar vapour fraction vector
$x_i$	molar liquid fraction of component $i$
$y_i$	molar vapour fraction of component $i$

## Greek symbols

$\gamma$	activity coefficient
$\eta_{pump}$	pump efficiency
$\varpi$	massic vaporization rate
$\rho$	density, kg/m <sup>3</sup>
$\tau^L$	liquid gap variable
$\tau^V$	vapour gap variable
$\varphi$	fugacity coefficient
$\omega$	molar vaporization rate

## Subscripts

<i>a</i>	feed stage
<i>abs</i>	absorber
<i>B</i>	generator boiler
<i>C</i>	generator partial condenser
<i>cond</i>	condenser
<i>evap</i>	evaporator
<i>i</i>	component <i>i</i>
<i>in</i>	inlet
<i>j</i>	theoretical plate number
<i>out</i>	outlet
<i>pre-abs</i>	pre-absorber
<i>source</i>	external source
<i>sub</i>	sub-cooler

## Superscripts

*	pure component
V	vapour phase
L	liquid phase
GP	Perfect gas

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