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Systematic Modeling under Uncertainty of Single, Double and Triple Effect Absorption Refrigeration Processes

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ABSTRACT
A systematic approach is proposed to investigate the influence of different thermodynamic models and multi-parametric variations propagated through single, double and triple effect absorption refrigeration (ABR) processes and to identify the models with the least sensitivity to variability. The approach highlights the parameters which mainly affect the ABR process performance in all indicators simultaneously. A sensitivity index quantifies the variation range of the ABR performance indicators with respect to parameter variability. Cost functions are developed which combine both performance indicators and state process variables. These are used to identify thermodynamic models which simultaneously a) enable close match of simulation results and reference data, b) maintain low process variability and c) give rise to process state and performance profiles of low non-linearity, despite changes in model parameters. We employ up to 12 thermodynamic models for NH$_3$/H$_2$O, comprising different eNRTL models and equations of state such as Redlich-Kwong, Peng-Robinson, Schwartzentruber-Renon and Cubic-Plus-Association. We consider uncertainty in up to 6 component and process parameters and up to 7 ABR performance indicators. The e NRTL-Helgenson model is selected in all ABR process cases. Peng-Robinson for hydrocarbon water systems is selected in single-effect ABR, whereas Redlich-Kwong is selected for the double and triple-effect cases.

Keywords: Absorption refrigeration, working fluids, sensitivity analysis, thermodynamic models, modeling, Ammonia/water
1 Introduction

The absorption refrigeration (ABR) process is receiving attention in published literature as a means of cooling generation from renewable [1] or clean energy resources [2,3], while avoiding the energy intensive vapor compression process. The performance of the process largely relies on the characteristics of the employed working fluid mixture as well as on the flowsheet structure (e.g., single, double, triple-effect or other). Mixtures such as LiBr/H$_2$O and NH$_3$/H$_2$O represent the most investigated working fluid candidates, whereas other inorganic salts [4], organic [5], and ionic liquids [6] have also been investigated. In terms of process structures, single and double-effect systems have received significant attention in combination with various different working fluids. Triple-effect cycles as well as cycles with modifications in the equipment connectivity also receive attention as a means of improving operating process performance indicators [7]. While experimental investigations are widely used in cases of common working fluids and simpler process configurations such as single-effect systems, model-based approaches also represent a key technology in ABR systems development. They are very important in order to quickly identify fluid and process operating conditions which are worth of experimental investigation or to explore unconventional working fluids and process structures prior to investing on difficult and expensive, in terms of resources, experiments [5].

In the case of model-based approaches, the capabilities of the models employed for thermodynamic mixture property predictions are of utmost importance in order to obtain realistic working fluid and process performance insights. Published works often employ fluid-specific empirical models derived from direct fitting of experimental pressure-temperature-concentration data to predict important properties such as vapour pressure [8] or solubility [9], to name but a few. Generic activity coefficient models and equations of state (EoS) are also employed widely to model the liquid- and vapour-phase non-idealities and to provide mixture property predictions. Each one of such models maintains the same underlying structure regardless of the mixtures for which they are employed. Their use is adjusted to different mixture components by fitting component-specific parameters. Different types of activity coefficient models and EoS may be used for all types of mixtures employed in ABR processes, including inorganics, organics, and ionic liquids, but the majority of applications are for organic liquids. The non-random two liquid (NRTL) model [10] is the activity coefficient model used most frequently [11,12,21,13–20], [22], possibly because of the widely investigated NH$_3$/H$_2$O system, which has been modelled by the electrolyte-NRTL model [23]. The universal quasi-chemical functional-group activity coefficients (UNIFAC) model [24] has also been considered [25,26] as it enables the modelling of mixture components using functional groups, which makes the model very versatile. In terms of EoS, applications include Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), Patel-Teja (PT)
PR with various alpha functions and mixing rules [11,12,18,19,21], as well as soft-SAFT [28], to name but a few.

Whether mixture-specific correlations or general-purpose models, they both offer predictions that may vary significantly. Such variation is usually due to the underlying experimental data used for the fitting of model parameters [9,28] and the set of essential assumptions made for the derivation of the model. Such behavior is more pronounced in the case of activity coefficient models and EoS [11], which are developed to provide predictions for a wide range of molecular structures and conditions. Variability propagates through the employed parameters into the corresponding models and may result in different predictions for the same property through two different routes. The first route includes the case of exploiting different experimental datasets (e.g., from different sources) for the same parameter set introduced into a model of similar structure. The second route includes the use of the same parameter values (e.g. pure component properties) through different models used to predict the same desired mixture property. Uncertainty is therefore introduced in both cases in the ABR working fluid and process simulations. In this context, the main objective is to investigate the effect that the inherent uncertainty in the employed parameters and models has on the predicted process performance. Some models may be very sensitive to deviations in the model parameters within the defined uncertainty region, resulting in significant over- or under-estimation of the actual fluid and/or process performance. On the contrary, other models may be considerably less sensitive, enabling reliable predictions despite deviations due to uncertainty.

To this end, the consideration of uncertainty in model parameters or models used for predictions in working fluid and ABR simulations and its effect on process performance indicators has never been addressed systematically. On the other hand, thermodynamic models for working fluids used in ABR processes are often assessed compared to experimental or other, previously verified, model-based data. Although this is useful, this approach depends strongly on the quality of the experimental reference dataset, which may be unknown, or very hard to estimate due to limited availability of data for the operating conditions (e.g., temperature, pressure and/or concentration) encountered in the ABR process. In such cases, it may not be possible to assess the reliability of the employed model. It is also common in ABR processes that multi-parametric variations can occur on thermodynamic models causing the onset of nonlinear effects (e.g., non-smooth behaviour due to sharp changes in parameter profiles) that a simple, local sensitivity analysis will not be able to explore. In these cases, the lack of experimental-reference data should not prohibit validation and selection of models which are able to provide reliable predictions. Finally, thermodynamic models may be employed in ABR process optimization, where their convexity characteristics affect very significantly the ability of optimization algorithms to attain the optimum solution. Considering the multi-parametric nature of changes in the conditions observed in ABR processes, the effect of uncertainties may not be addressed either
through arbitrary approaches or through single-dimensional sensitivity analysis tools. In this context, the selection of reliable thermodynamic models for ABR processes includes challenges which have not been considered in published literature.

This work proposes a systematic approach to investigate the influence of different thermodynamic models and parameter variations on single, double and triple-effect ABR process performance and to identify the models which are least sensitive, in order to obtain robust predictions. The proposed approach analyzes the sensitivity of multiple ABR performance indicators on multi-parametric variations of thermodynamic model parameters as they are propagated through ABR process models. The underlying sensitivity analysis rationale was initially developed for post-optimality assessment in non-linear programming [29], and subsequently used for evaluation of process controllability under external disturbances in reactive separation [30] and separation systems [31], [32], as well as organic Rankine cycles (ORC) [33]. Papadopoulos et al. [34] further used the method to incorporate thermodynamic parameter uncertainties in the selection of ORC working fluid mixtures, without considering model selection or uncertainty in ORC optimization. In this work, the method considers uncertainty due to multiple different parameters and thermodynamic models, while it is expanded to account for both first- and second-order derivative information, the latter being important for process optimization purposes. In particular, we aim to identify thermodynamic models which simultaneously a) enable close match of simulation results and reference data, b) maintain low process variability and c) give rise to process state and performance profiles of low non-linearity despite wide changes in model parameters. The method itself and the corresponding upgrades are implemented for the first time on the identification of robust thermodynamic models for single, double and triple-effect ABR systems.

2 Nonlinear Sensitivity Analysis for Absorption Refrigeration Systems

2.1 Proposed approach

In this work, a nonlinear parametric sensitivity analysis method is used to identify the thermodynamic models and model parameters with high influence on the overall ABR process performance. The aim is to calculate the impact of multiple and simultaneous model parameter variations on a set of aggregate ABR process performance indicators for a set of considered thermodynamic models. The steps of the method are presented in detail, as follows:

**Step 1:** Let \( D \) be a set of thermodynamic models, \( e \in \mathbb{R}^{N_F} \), a vector incorporating the values of the parameters which will be subjected to variability as inputs in the thermodynamic models in \( D \), \( x \in \mathbb{R}^{N_x} \), a vector of state variables in the ABR process, \( F \in \mathbb{R}^{N_F} \), a vector of performance indicators, and \( h \in \mathbb{R}^{N_h}, \ g \in \mathbb{R}^{N_g} \), sets of vector of
which are the most sensitive with respect to the performance indicators imposed on model parameters. The logarithmic functions represent locally scaled transformations for the performance indicators and the model parameters, whereas matrix \( \mathbf{P} \) constitutes a measure of variation of the process model under the influence of infinitesimal changes imposed on model parameters.

**Step 2:** Let \( \mathbf{\varepsilon}^{\text{nom}} \in \mathbb{R}^{N_p} \), be a vector representing the nominal values for the model parameters of the ABR process. The nominal values are the parameter estimates provided in published literature. For every thermodynamic model \( d \in D \), identify the model parameters which are the most sensitive with respect to the performance indicators \( \mathbf{F} \) by generating a local sensitivity matrix \( \mathbf{P} \) around the nominal model parameter vector \( \mathbf{\varepsilon}^{\text{nom}} \) as follows,

\[
\mathbf{P} = \left( \frac{\partial \ln \mathbf{F}}{\partial \ln \mathbf{\varepsilon}} \right)^{\text{nom}} = \begin{bmatrix}
\frac{\partial \ln F_1}{\partial \ln \varepsilon_1} & \cdots & \frac{\partial \ln F_1}{\partial \ln \varepsilon_{N_p}} \\
\vdots & \ddots & \vdots \\
\frac{\partial \ln F_{N_F}}{\partial \ln \varepsilon_1} & \cdots & \frac{\partial \ln F_{N_F}}{\partial \ln \varepsilon_{N_p}}
\end{bmatrix}_{\mathbf{\varepsilon}^{\text{nom}}}.
\]

Sensitivity matrix \( \mathbf{P} \) can be calculated numerically, by applying a vector of infinitesimal variations \( \Delta \mathbf{\varepsilon} \) so that the nominal vector \( \mathbf{\varepsilon}^{\text{nom}} \) is transformed to the perturbed vector \( \mathbf{\varepsilon}^{\text{pert}} = \mathbf{\varepsilon}^{\text{nom}} + \Delta \mathbf{\varepsilon} \). The logarithmic functions represent locally scaled transformations for the performance indicators and the model parameters, whereas matrix \( \mathbf{P} \) constitutes a measure of variation of the process model under the influence of infinitesimal changes imposed on model parameters.

**Step 3:** For every thermodynamic model \( d \in D \), derive the major directions of variability by calculating the eigenvectors \( \mathbf{\Theta}^i (i = 1, \ldots, N_p) \) of the matrix \( \mathbf{P}^T \mathbf{P} \). Identify the dominant direction of variability for the system, represented as the combination of parameters \( \mathbf{\varepsilon} \) which are causing the largest change in the performance indicators in a least square sense. It can be proven that the eigenvector \( \mathbf{\Theta}^1 \), which corresponds to the largest in magnitude eigenvalue of \( \mathbf{P}^T \mathbf{P} \) (or singular value of \( \mathbf{P} \)), is related to the largest change in the performance indices \( \mathbf{F} \) [30]. The dominant direction of variability is representative of the worst-case scenario for the system and judging the robustness of the model along this direction is sufficient. As a result, the dimensionality of the sensitivity analysis is significantly reduced.

**Step 4:** The identification of the dominant direction of variability enables the calculation of the perturbed parameter model vector \( \mathbf{\varepsilon}(\zeta) \), by the following relation:

\[
\frac{\varepsilon_i(\zeta) - \varepsilon_i^{\text{nom}}}{\varepsilon_i^{\text{nom}}} = \zeta \cdot \Theta_i^1 , \quad i = 1, \ldots, N_p.
\]
of $\mathbf{\Theta}$. The maximum change along this direction is addressed through the introduction of lower and upper bounds, $\zeta^L$ and $\zeta^U$, with $\zeta \in [\zeta^L, \zeta^U]$. These limits may change in case a physical or a process constraint is violated, leading to an update of the bounds on $\zeta$ coordinate.

**Step 5:** It is essential to define a sensitivity index $\Omega$, which accounts for the behavior of the performance indicators $\mathbf{F}$ within a wide variation range, explored through a magnitude variation $\mathbf{x}$ along the dominant direction of variability. As a result, for every thermodynamic model $d \in D$, the sensitivity metric is obtained for finite parameter variations, as follows:

$$
\Omega(\zeta, d) = 100 \sum_{i=1}^{N_F} \left| \frac{F_i(\mathbf{x}, d, \mathbf{e}(\zeta)) - F_i(\mathbf{x}, d, \mathbf{e}^{\text{nom}})}{F_i(\mathbf{x}, d, \mathbf{e}^{\text{nom}})} \right|
$$

subject to:

$$
h_i(\mathbf{x}, d, \mathbf{e}) = 0, \quad i = 1, \ldots, N_h$$

$$
g_i(\mathbf{x}, d, \mathbf{e}) \leq 0, \quad i = 1, \ldots, N_g$$

$$
x_i^L \leq x_i \leq x_i^U, \quad i = 1, \ldots, N_x$$

$$
\frac{e_i(\zeta) - e_i^{\text{nom}}}{e_i^{\text{nom}}} = \zeta \cdot \theta^1, \quad i = 1, \ldots, N_p
$$

$$
\zeta \in [\zeta^L, \zeta^U].
$$

(4)

Index $\Omega$ is calculated under the assumption that the eigenstructure of the local sensitivity matrix does not change considerably within the parameter variation space. The sensitivity index $\Omega$ represents the sum of the relative change of performance indicators $\mathbf{F}$ from the nominal values, as a function of $\zeta$, which is the parameter variation magnitude coordinate indicating the range of imposed change in the direction of $\mathbf{\Theta}^1$.

**Step 6.** Indices $\Omega$ resulting from different models are rank-ordered identifying the model with the lowest sensitivity to model parameter changes. The emphasis is therefore concentrated on the sensitivity of the process performance rather than on the actual value of the performance indicators. In this way, the model that ensures a predicted performance near the nominal design point can be determined.

### 2.2 Cost function criteria

The evaluation of sensitivity index $\Omega$ indicates the impact of parameters of vector $\mathbf{e}$ on the performance indicators of the system, while the former are varied from their nominal values. However, information related to the state variables $x_i$, to the deviation of system values from reference (ref) values or to the profile characteristics of state variables and performance indicators under parameter variability, is not included. For this reason, several cost functions are introduced that contain additional information about the state variables and the performance indicators of the process. Therefore, for every thermodynamic model $d \in D$ the following cost functions are defined:

$$
J_1(d) = \sum_{k=-N_{\zeta}}^{N_{\zeta}} \sum_{i=1}^{N_x} \left( \frac{x_i(d, \zeta_k) - x_i^{\text{ref}}}{x_i^{\text{ref}}} \right)^2
$$

(5)
\[ J_2(d) = \sum_{k=-N_\zeta}^{N_\zeta} \sum_{i=1}^{N_P} \left( \frac{F_i(x(\zeta_k), d, e(\zeta_k)) - F_i^{\text{ref}}}{F_i^{\text{ref}}} \right)^2 \]  

\[ J_3(d) = \sum_{k=-N_\zeta}^{N_\zeta} \sum_{j=1}^{N_P} \sum_{i=1}^{N_x} \left( \frac{x_i(d, \zeta_k) - x_i(d, \zeta_0)}{e_j(\zeta_k) - e_j(\zeta_0)} \right)^2 \left( \frac{e_j(\zeta_0)}{x_i(d, \zeta_0)} \right)^2 \]

\[ J_4(d) = \sum_{k=-N_\zeta}^{N_\zeta} \sum_{j=1}^{N_P} \sum_{i=1}^{N_x} \left( \frac{F_i(x(\zeta_k), d, e(\zeta_k)) - F_i(x(\zeta_0), d, e(\zeta_0))}{e_j(\zeta_k) - e_j(\zeta_0)} \right)^2 \]

\[ J_5(d) = \left( \sum_{k=-N_\zeta}^{N_\zeta} \sum_{j=1}^{N_P} \sum_{i=1}^{N_x} \left( \frac{x_i(d, \zeta_{k+1}) - x_i(d, \zeta_0)}{e_j(\zeta_{k+1}) - e_j(\zeta_0)} \right)^2 \right) \]

\[ J_6(d) = \left( \sum_{k=-N_\zeta}^{N_\zeta} \sum_{j=1}^{N_P} \sum_{i=1}^{N_x} \left( \frac{F_i(x(\zeta_{k+1}), d, e(\zeta_{k+1})) - F_i(x(\zeta_0), d, e(\zeta_0))}{e_j(\zeta_{k+1}) - e_j(\zeta_0)} \right)^2 \right) \]

Cost functions \( J_1 \) and \( J_2 \) pertain to the deviations of state variables and performance indicators, respectively, from their reference values for every value of the coordinate \( \zeta \). In other words, they indicate the proximity of the simulation results to the reference data when parameter variability and propagation through different thermodynamic models is considered. Cost functions \( J_3 \) and \( J_4 \) explore how steep or flat are the profiles of the state variables and the performance indicators, respectively, while the model parameters are varied. They
illustrate the magnitude of variability for every thermodynamic model, by investigating the first derivative of state variables and performance indicators with respect to the change of parameters of vector $\epsilon$. Finally, cost functions $J_5$ and $J_6$ include information about the underlying nonlinear characteristics of every thermodynamic model by accounting for the convexity of the profiles under varying parameters. This is addressed through the estimation of the second derivatives of state variables and performance indicators with respect to the change of model parameters. Having defined the cost functions and analyzed their physical meaning, a systematic approach is proposed to assess them. The steps of the assessment procedure are presented as follows:

**Step 1:** For every thermodynamic model $d \in D$, apply the proposed sensitivity analysis method in order to identify the dominant direction of variability, corresponding to the eigenvector $\theta^1$, and the varying parameters of vector $\epsilon$. Then, evaluate the values of the state variable vector $x$ and the performance indicators of vector $F$ for every coordinate $\zeta$. Having evaluated the necessary elements, for every thermodynamic model $d \in D$, calculate the cost functions $J_i$ ($i = 1, \ldots, 6$).

**Step 2:** For every thermodynamic model $d \in D$, every cost function is required to be scaled. Assuming $N_d$ the number of investigated models, $\mu$ a desired mean value and $\sigma$ a standard deviation, the standard score magnitude for every cost function $()$ can be defined as follows:

$$
\bar{J}_i(d) = \frac{J_i(d) - \mu_i}{\sigma_i}
$$

(11)

with

$$
\sigma_i = \sqrt{\frac{\sum_{m=1}^{N_d} (J_i(d_m) - \mu_i)^2}{N_d - 1}}
$$

(12)

Regardless of the thermodynamic model or the cost function, the desired mean value is set to zero ($\mu = 0$). Assuming this condition, the scaled cost functions express the deviation between the absolute value of a cost function and a desired set point cost function. An ideal thermodynamic model would have zero-valued cost functions, corresponding to exactly similar behavior to the reference data and nonexistent sensitivity to variations of parameters.

**Step 3:** Cost functions containing information of same type should be combined. By defining a new amount of cost functions, including both the effect of state variables and performance indicators, the investigation of the behavior of a thermodynamic model under parameter variability would become more informative and comprehensive. Therefore, for every thermodynamic model $d \in D$ calculate the new cost functions $J_{REF}$, $J_{MV}$ and $J_{NL}$ as follows,

$$
\text{Calculate } J_{REF}(d), J_{MV}(d), J_{NL}(d)
$$

with

$$
J_{REF}(d) = \bar{J}_1(d) + \bar{J}_2(d)
$$

$$
J_{MV}(d) = \bar{J}_3(d) + \bar{J}_4(d)
$$
\[ J_{NL}(d) = \bar{f}_5(d) + \bar{f}_6(d) \]

s.t.
\[ h_i(x, d, \varepsilon) = 0 \quad , \quad i = 1, \ldots, N_h \]
\[ g_i(x, d, \varepsilon) \leq 0 \quad , \quad i = 1, \ldots, N_g \]
\[ x_i^L \leq x_i \leq x_i^U \quad , \quad i = 1, \ldots, N_x \]
\[ \frac{\varepsilon_i(\zeta) - \varepsilon_i^{\text{nom}}}{\varepsilon_i^{\text{nom}}} = \varepsilon \cdot \theta_i^T \quad , \quad i = 1, \ldots, N_p \]
\[ \zeta \in [\zeta^L, \zeta^U] . \] (1)

Cost functions \( J_{REF}, J_{MV} \) and \( J_{NL} \) include the impact of the variation of parameters to the state variables, as well as to the performance indicators. Cost function \( J_{REF} \) represents the deviation between the reference data and the investigated thermodynamic models of set \( D \), whereas cost function \( J_{MV} \) explores the magnitude of variability of each thermodynamic model, while the parameters of vector \( \varepsilon \) change towards the dominant direction of variability based on the elements of the eigenvector \( \Theta^T \). Furthermore, cost function \( J_{NL} \) is a measure of the underlying nonlinear characteristic, which are included internally to each thermodynamic model. The estimation of these cost functions allows the identification of the impacts to process performance and operation of uncertainties introduced to the model parameters. The calculation of \( J_{REF}, J_{MV} \) and \( J_{NL} \) enables the selection of the most robust in uncertainty among a set of available thermodynamic models.

3 Implementation

3.1 Description of absorption refrigeration ammonia/water system

In this study, three types of absorption refrigeration systems are investigated; namely the single-stage, single-effect cycle, the two-stage, double-effect cycle and the two-stage, triple-effect cycle. The single and double-effect configurations are both explained in detail in [35] and [36], whereas the triple-effect is mainly analyzed in [36]. Briefly, the ABR processes convert an amount of heat input energy into a cooling load in order to provide refrigeration. The process utilizes a mixture of two working fluids, also known as the refrigerant and the absorbent. In these systems, \( \text{NH}_3 \) is used as a refrigerant fluid and \( \text{H}_2\text{O} \) is used as the absorbent. The latter has strong affinity for \( \text{NH}_3 \) as they are soluble with each other in a wide range of operating conditions. Heat input supplied to the system drives to the separation of refrigerant vapor from a refrigerant/absorbent liquid mixture. Then, the refrigerant is liquified by a condenser and flows through an evaporator providing a cooling load during a liquid-to-vapor phase change procedure. Finally, the refrigerant vapor is mixed again with the remaining binary mixture of the separation process in order to repeat the ABR cycle.

Regarding the process topology, the single-stage, single-effect system is the simplest configuration of vapor absorption technology with respect to the number of involved equipment components. Reduced complexity and minor computational effort of this cycle establish a more convenient way to apply the current sensitivity analysis approach and extract
results. The two-stage processes may be considered as a natural extension of the single-stage system, based on the fact that they consist of two discrete individual single-stage circuits. Generally, the multi-stage, multi-effect cycles provide increased efficiency compared to single-stage systems. In current work, we investigate two of the most common two-stage cycles, that have been already investigated in detail by [35] and [36] in order to assure the reliability of the validation models. A detailed analysis review related to the variety of different types and configurations of ABR cycles is reported by Papadopoulos et al. [5].

3.1.1 Single-Stage, Single-Effect Process

The single-stage, single-effect absorption refrigeration system consists of four main components, namely the condenser, evaporator, absorber and generator, as shown in Figure 1. Other auxiliary components include the expansion valves, pump, rectifier and heat exchangers. Table 1 illustrates qualitatively the phases and compositions in every stream. In atmospheric pressure, the evaporation temperature of NH$_3$ is -33.73 °C, meaning that the evaporator may operate in very low temperatures. However, this is not possible as the absorption fluid H$_2$O will crystallize. As a result, the NH$_3$/H$_2$O working cycle operates at higher pressures on the evaporator, so that the evaporation temperature of NH$_3$ may be increased. In real applications, the NH$_3$ evaporation temperature is between -15 °C and 5 °C. Typical values of the absorber and condenser temperature are around 40 °C. The high pressure of the cycle, in which the generator and the condenser operate, is around 15 bar.
Figure 1. Flowsheet Diagram of single-stage, single-effect NH$_3$/H$_2$O cycle.

Table 1. Thermodynamic conditions of single-effect NH$_3$/H$_2$O cycle, streams 2,3,4,5,9,10 operate at high pressure level, the rest at low pressure level.

<table>
<thead>
<tr>
<th>Stream</th>
<th>Phase</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Saturated liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>2</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>3</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>4</td>
<td>Saturated liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>5</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>6</td>
<td>Vapor-liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>9</td>
<td>Superheated vapor</td>
<td>NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>10</td>
<td>Saturated liquid</td>
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</tr>
<tr>
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<td>Subcooled liquid</td>
<td>NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>12</td>
<td>Vapor-liquid</td>
<td>NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>13</td>
<td>Saturated vapor with small amount of liquid</td>
<td>NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>14</td>
<td>Superheated vapor</td>
<td>NH$_3$ with a small amount of H$_2$O</td>
</tr>
</tbody>
</table>
3.1.2 Two-Stage, Double-Effect Process

Figure 2 shows a two-stage, double-effect NH$_3$/H$_2$O cycle. The first inner stage of the cycle (components with index 1) is similar to the single-effect structure consisting of the absorber 1, generator-rectifier 1, solution heat exchanger (SHX 1) and the pump 1. Moreover, it includes the condenser, the condenser-evaporator heat exchanger (CEHX) and the evaporator. The circuit of the second outer stage (components with index 2) connects to the first stage through intrastate heat exchange. The heat, required for the operation of generator 1, is obtained from the rectifier and the absorber of the second stage. Both of the absorbers operate with the vapor produced by the evaporator, whereas the condenser obtains high NH$_3$ quality vapor produced by the generators-rectifiers of both stages. Therefore, the evaporator, as well the condenser, participate on the operation of two stages. The operation conditions per stream are shown on Table 2.

Table 2. Thermodynamic conditions of two-stage, double-effect NH$_3$/H$_2$O cycle, streams 2,3,4,5,9,10,11,17,18,19,20,25,27 operate at high pressure level, the rest at low pressure level.

<table>
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<td>Mixture</td>
</tr>
<tr>
<td>3</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>4</td>
<td>Saturated liquid</td>
<td>Mixture</td>
</tr>
</tbody>
</table>
3.1.3 Two-Stage, Triple-Effect Process

As a consequence of the wide operating range of NH$_3$/H$_2$O, an unusual cycle with high COP can be accommodated. In Figure 3, a two-stage, triple-effect, absorption refrigeration configuration is illustrated. In this process, two single-stage absorption cycles can be identified, one inside a second, larger one. The inner stage (smaller cycle) operates at the conditions of a conventional single-stage cycle. The heat transfer input of this stage is supplied by the condenser 2 and absorber 2 of the larger single-stage cycle. Both stages utilize the same evaporator. The outer stage operates at sufficiently high temperatures so that the heat rejection, from absorber 2 and condenser 2, can be utilized entirely to drive generator 1 of the first cycle. As a result, one thermal energy unit supplied to the outer stage (components with indices 2) drives a specific amount of refrigerant that provides a cooling load in the evaporator. Furthermore, the rejected absorption and condensation heats of condensation and absorption of this refrigerant are used to produce additional refrigerant and capacity, by feeding thermally the inner stage. Therefore, a unit of input energy is utilized three times to provide refrigeration capacity, that is the definition of a triple-effect system. In contrast to the double-effect cycle, each stage of the triple one includes a separate condenser.

With respect to the cycle temperatures, similar to the double-effect conditions are applied for the evaporator and inner stage condenser 1. Moreover, the triple-effect cycle operates at three pressure stages. The inner stage pressures are similar to those of the double-effect cycle, whereas the outer stage pressure is the vapor pressure of refrigeration fluid at 70 °C (typical temperature value). The thermodynamic conditions on every stream of the triple-effect cycle are shown in Table 3.

<table>
<thead>
<tr>
<th>Stream Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>Subcooled liquid Mixture</td>
</tr>
<tr>
<td>6</td>
<td>Vapor-liquid Mixture</td>
</tr>
<tr>
<td>9</td>
<td>Superheated vapor NH$_3$</td>
</tr>
<tr>
<td>10</td>
<td>Saturated liquid NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>11</td>
<td>Subcooled liquid NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>12</td>
<td>Vapor-liquid NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>13</td>
<td>Saturated vapor with small amount of liquid NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>14</td>
<td>Superheated vapor with small amount of liquid NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>15</td>
<td>Superheated vapor with small amount of liquid NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>16</td>
<td>Saturated liquid Mixture</td>
</tr>
<tr>
<td>17</td>
<td>Subcooled liquid Mixture</td>
</tr>
<tr>
<td>18</td>
<td>Subcooled liquid Mixture</td>
</tr>
<tr>
<td>19</td>
<td>Saturated liquid Mixture</td>
</tr>
<tr>
<td>20</td>
<td>Subcooled liquid Mixture</td>
</tr>
<tr>
<td>21</td>
<td>Vapor-liquid Mixture</td>
</tr>
<tr>
<td>25</td>
<td>Superheated vapor NH$_3$</td>
</tr>
<tr>
<td>26</td>
<td>Superheated vapor with small amount of liquid NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>27</td>
<td>Superheated vapor NH$_3$</td>
</tr>
</tbody>
</table>
Figure 3. Flowsheet Diagram of two-stage, triple-effect NH$_3$/H$_2$O cycle.

Table 3. Thermodynamic conditions of two-stage, triple-effect NH$_3$/H$_2$O, streams 13,14,15,16,19,20 operate at outer stage high pressure, streams 3,4,5,6,9,10,11 operate at inner stage high pressure level, the rest at low pressure level.

<table>
<thead>
<tr>
<th>Stream</th>
<th>Phase</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Saturated vapor with small amount of liquid</td>
<td>NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>2</td>
<td>Saturated liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>3</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>4</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>5</td>
<td>Saturated liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>6</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>7</td>
<td>Vapor-liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>9</td>
<td>Superheated vapor</td>
<td>NH$_3$</td>
</tr>
<tr>
<td>10</td>
<td>Saturated liquid</td>
<td>NH$_3$ with a small amount of H$_2$O</td>
</tr>
<tr>
<td>11</td>
<td>Superheated vapor</td>
<td>NH$_3$</td>
</tr>
<tr>
<td>12</td>
<td>Saturated liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>13</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>14</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>15</td>
<td>Saturated liquid</td>
<td>Mixture</td>
</tr>
<tr>
<td>16</td>
<td>Subcooled liquid</td>
<td>Mixture</td>
</tr>
</tbody>
</table>
3.2 Investigated Thermodynamic Models

To illustrate the proposed sensitivity analysis method, twelve combinations of activity coefficient models and EoS are investigated, as shown in Table 4. The models are selected from the options available in ASPEN Plus [37]. The liquid-phase non-ideality of NH$_3$/H$_2$O mixture is modelled using either the Electrolyte NRTL (ELECNRTL) model or the ENRTL-HG [38–40] which uses the Helgeson model for mixture property estimation. Electrolyte-NRTL model types are appropriate for the calculation of properties of electrolyte-based binary mixtures, especially in case vapor-liquid equilibrium is present. The vapor-phase non-ideality is modelled using EoS. The Redlich-Kwong [41] EoS is applicable to systems at low to moderate pressures and is the default option when the ELECNRTL option is selected in ASPEN Plus. The Schwartzentruber-Renon [42] EoS is recommended for polar mixtures and highly non-ideal systems at high temperatures and pressures, while Cubic-Plus-Association [43] model’s applicability covers the vapor-liquid equilibrium of mixtures containing polar/associating chemicals. Finally, the Peng-Robinson equation of state and its modifications (with Boston-Mathias alpha functions and for hydrocarbon-water systems) [44,45] are mainly recommended for hydrocarbon processing, covering, however, a broad variety of mixtures and applications.

Table 4. Investigated Thermodynamic Models of set $D$.

<table>
<thead>
<tr>
<th>Thermodynamic Model ID</th>
<th>Base Method</th>
<th>Equation of State</th>
</tr>
</thead>
<tbody>
<tr>
<td>d$_1$</td>
<td>ELECNRTL</td>
<td>Redlich-Kwong</td>
</tr>
<tr>
<td>d$_2$</td>
<td>ELECNRTL</td>
<td>Schwartzentruber-Renon</td>
</tr>
<tr>
<td>d$_3$</td>
<td>ELECNRTL</td>
<td>Peng-Robinson with Boston-Mathias alpha function</td>
</tr>
<tr>
<td>d$_4$</td>
<td>ELECNRTL</td>
<td>Peng-Robinson for hydrocarbon-water systems</td>
</tr>
<tr>
<td>d$_5$</td>
<td>ELECNRTL</td>
<td>Peng-Robinson</td>
</tr>
<tr>
<td>d$_6$</td>
<td>ELECNRTL</td>
<td>Cubic-Plus-Association</td>
</tr>
<tr>
<td>d$_7$</td>
<td>ENRTL-HG</td>
<td>Redlich-Kwong</td>
</tr>
<tr>
<td>d$_8$</td>
<td>ENRTL-HG</td>
<td>Schwartzentruber-Renon</td>
</tr>
<tr>
<td>d$_9$</td>
<td>ENRTL-HG</td>
<td>Peng-Robinson with Boston-Mathias alpha function</td>
</tr>
<tr>
<td>d$_{10}$</td>
<td>ENRTL-HG</td>
<td>Peng-Robinson for hydrocarbon-water systems</td>
</tr>
<tr>
<td>d$_{11}$</td>
<td>ENRTL-HG</td>
<td>Peng-Robinson</td>
</tr>
<tr>
<td>d$_{12}$</td>
<td>ENRTL-HG</td>
<td>Cubic-Plus-Association</td>
</tr>
</tbody>
</table>
Our results are validated against data obtained from simulations performed by Adewusi and Zubair [35] and Herold et al. [36]. These sources are selected mainly for two reasons. Firstly, they include detailed stream data for single, double and triple-effect cycles hence facilitating both the modeling and comparison of results obtained from the three cycles. Secondly, they employ correlations developed directly from NH$_3$/H$_2$O mixture data by Ibrahim and Klein [46]. These correlations have been validated by Thorin et al. [47], showing that for temperature and pressure conditions similar to those in our work the predicted mixture properties match experimental data closely. In this respect, the simulation results in [35] and [36] are used as reference data.

3.3 Operating conditions and simulation assumptions

The flowsheet diagrams of the single, double and triple-effect cycles have been designed using ASPEN Plus. Every component of the process is considered as “Heater Block”, except from the generator and the rectifier. The generator-rectifier systems are represented as distillation columns for the separation of liquid and vapor phase. The pumps and the valves are simulated as “Pump Blocks” and “Valve Blocks”, respectively, assuming adiabatic models.

Table 5, Table 6 and Table 7 illustrate the simulation assumptions of the single, double and triple-effect system, respectively. The single and double-effect assumptions have been selected to be similar with the operating conditions in reference [35], whereas the triple-effect assumptions with the conditions in reference [36]. Note that data from references [35] and [36] are used as provided for all parameters of Table 5, Table 6 and Table 7, except for distillate-to-feed ratio and number of stages in rectifier(s). For these parameters there is no information in the literature sources regarding the used values. The distillate-to-feed values were determined so that the temperature in the rectifier refrigerant vapour stream matches the corresponding steam in the literature sources. The number of stages were determined so that the purity of NH$_3$ in the rectifier refrigerant vapour stream matches that of the literature sources. Low and high pressures of the cycle represent the vapor pressures of binary mixture and cooling fluid NH$_3$, respectively, at slightly different evaporation temperatures (0.3 °C to 4 °C deviations) compared to the [35], [36]. These are slight deviations which occur due to the use of different thermodynamic models compared to those of the literature sources. For double-effect process, the heat input of the inner stage generator is calculated by the rejected heat flows of outer stage absorber and outer stage rectifier, as follows,

$$Q_{gen1} = |Q_{abs2}| + |Q_{rec2}|.$$  (14)
whereas, for triple-effect process, it is obtained by the sum of the rejected heat flows of the outer stage absorber and the outer stage condenser as follows,

\[ Q_{gen1} = |Q_{abs2}| + |Q_{cond2}|. \quad (15) \]

The coefficient of performance (COP) of the process is equal to the ratio of useful cooling provided to heat and work required. The cooling energy is given by the heat flow of the evaporator \( Q_{evap} \), whereas the input energy is given by the sum of the reboiler duty \( Q_{gen} \) (of outer stage on double and triple-effect cycles) and the work pumps \( W_{pumps} \). The value of work pumps is negligible compared to the reboiler duty and is not included on the calculation of the coefficient of performance. Therefore, the COP is defined as

\[ COP = \frac{Q_{evap}}{Q_{gen} + W_{pumps}} \approx \frac{Q_{evap}}{Q_{gen}}. \quad (16) \]

### Table 5. Simulation Assumptions of the single-stage, single-effect NH\textsubscript{3}/H\textsubscript{2}O cycle based on [35].

<table>
<thead>
<tr>
<th>Operating Parameter</th>
<th>Assumption</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong-Solution Mixture Mass Flow</td>
<td>( m = 1 \text{ kg/sec} )</td>
</tr>
<tr>
<td>Low and High Pressure Cycle</td>
<td>( P_{low} = 244.85 \text{ kPa and } P_{high} = 1555.76 \text{ kPa} )</td>
</tr>
<tr>
<td>Strong-Solution Mixture Mass Fraction</td>
<td>( x^{NH3} = 0.3709 \text{ kg NH}_3/\text{kg mixture} )</td>
</tr>
<tr>
<td>Generator Heat Input (Reboiler Duty)</td>
<td>( Q_{gen} = 267.9 \text{ kW} )</td>
</tr>
<tr>
<td>Distillate to Feed Ratio (Generator)</td>
<td>( 0.13224 \text{ kg/kg} )</td>
</tr>
<tr>
<td>Heat Exchangers Effectiveness</td>
<td>( \varepsilon_{SHX} = 1 \text{ and } \varepsilon_{CEHX} = 0.95 )</td>
</tr>
<tr>
<td>Vapor Fraction on Evaporator Exit</td>
<td>( x^{vapor} = 0.998 )</td>
</tr>
<tr>
<td>Number of stages in Rectifier (Distillation column)</td>
<td>5</td>
</tr>
<tr>
<td>Purity of NH\textsubscript{3} in rectifier refrigerant vapour stream</td>
<td>0.9996 with relative error ±0.2% from nominal</td>
</tr>
</tbody>
</table>

### Table 6. Simulation Assumptions of the two-stage, double-effect NH\textsubscript{3}/H\textsubscript{2}O cycle based on [35].

<table>
<thead>
<tr>
<th>Operating Parameter</th>
<th>Assumption</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong-Solution Mixture Inner Stage Mass Flow</td>
<td>( m_{inner} = 1 \text{ kg/sec} )</td>
</tr>
<tr>
<td>Strong-Solution Mixture Outer Stage Mass Flow</td>
<td>( m_{outer} = 0.27 \text{ kg/sec} )</td>
</tr>
<tr>
<td>Low and High Pressure Cycle</td>
<td>( P_{low} = 277.97 \text{ kPa and } P_{high} = 1548.03 \text{ kPa} )</td>
</tr>
<tr>
<td>Strong-Solution Mixture Inner Stage Mass Fraction</td>
<td>( x_{inner}^{NH3} = 0.3913 \text{ kg NH}_3/\text{kg mixture} )</td>
</tr>
<tr>
<td>Strong-Solution Mixture Outer Stage Mass Fraction</td>
<td>( x_{outer}^{NH3} = 0.0671 \text{ kg NH}_3/\text{kg mixture} )</td>
</tr>
<tr>
<td>Outer Stage Generator Heat Input (Reboiler Duty)</td>
<td>( Q_{gen2} = 120 \text{ kW} )</td>
</tr>
<tr>
<td>Inner Stage Distillate to Feed Ratio (Generator 1)</td>
<td>0.0645 \text{ kg/kg}</td>
</tr>
<tr>
<td>Outer Stage Distillate to Feed Ratio (Generator 2)</td>
<td>0.058148 \text{ kg/kg}</td>
</tr>
<tr>
<td>Heat Exchangers Effectiveness</td>
<td>( \varepsilon_{SHX1} = 1, \varepsilon_{SHX2} = 1 \text{ and } \varepsilon_{CEHX} = 0.746 )</td>
</tr>
<tr>
<td>Vapor Fraction on Evaporator Exit</td>
<td>( x^{vapor} = 0.9 )</td>
</tr>
<tr>
<td>Number of stages in Rectifiers (Distillation columns)</td>
<td>5</td>
</tr>
<tr>
<td>Purity of NH\textsubscript{3} in rectifier refrigerant vapour stream</td>
<td>0.995 with relative error ±0.3% from nominal</td>
</tr>
</tbody>
</table>
Table 7. Simulation Assumptions of the two-stage, triple-effect NH$_3$/H$_2$O cycle, based on [36].

<table>
<thead>
<tr>
<th>Operating Parameter</th>
<th>Assumption</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong-Solution Mixture Inner Stage Mass Flow</td>
<td>$m_{\text{inner}} = 1$ kg/sec</td>
</tr>
<tr>
<td>Strong-Solution Mixture Outer Stage Mass Flow</td>
<td>$m_{\text{outer}} = 0.622$ kg/sec</td>
</tr>
<tr>
<td>Low, Medium and High Pressure Cycle</td>
<td>$P_{\text{Low}} = 494.8$ kPa, $P_{\text{Medium}} = 1344.1$ kPa and $P_{\text{High}} = 3365.4$ kPa</td>
</tr>
<tr>
<td>Strong-Solution Mixture Inner Stage Mass Fraction</td>
<td>$x_{\text{NH}_3}^\text{inner} = 0.5295$ kg NH$_3$/kg mixture</td>
</tr>
<tr>
<td>Strong-Solution Mixture Outer Stage Mass Fraction</td>
<td>$x_{\text{NH}_3}^\text{outer} = 0.3273$ kg NH$_3$/kg mixture</td>
</tr>
<tr>
<td>Outer Stage Generator Heat Input (Reboiler Duty)</td>
<td>$Q_{\text{gen}2} = 156.7$ kW</td>
</tr>
<tr>
<td>Inner Stage Distillate to Feed Ratio (Generator 1)</td>
<td>0.10415 kg/kg</td>
</tr>
<tr>
<td>Outer Stage Distillate to Feed Ratio (Generator 2)</td>
<td>0.08796 kg/kg</td>
</tr>
<tr>
<td>Heat Exchangers Effectiveness</td>
<td>$\epsilon_{\text{SHX}1} = 0.8$ and $\epsilon_{\text{SHX}2} = 0.8$</td>
</tr>
<tr>
<td>Vapor Fraction on Evaporator Exit</td>
<td>$x_{\text{vapor}} = 0.98$</td>
</tr>
<tr>
<td>Number of stages in Rectifiers (Distillation columns)</td>
<td>5</td>
</tr>
<tr>
<td>Purity of NH$_3$ in rectifier refrigerant vapour stream</td>
<td>0.995 with relative error ±0.45% from nominal</td>
</tr>
</tbody>
</table>

3.4 Implementation and technical details

3.4.1 Performance indicators and varied parameters

Table 8 summarizes the parameters varied during the sensitivity analysis (vector $\mathbf{e}$) and the performance indicators of vector $\mathbf{F}$ for the single, double and triple-effect systems. Uncertainty is introduced in selected critical parameters and vapor pressure of the refrigerant (corresponding to the high pressure of the cycle) as their values are usually obtained either experimentally or through empirical modeling. In current work, the nominal values of critical temperatures and pressures are obtained through the ASPEN Plus ASPENPCD databank, while the nominal vapor pressures are calculated by a modified version of the extended Antoine equation [48], as recommended by ASPEN Plus. These parameters are selected as they affect the operational conditions of the ABR process, the employed EoS, described in Table 4, and a plethora of pure compound or mixture properties. As a result, the impact of these parameters to the system’s performance is significant, considering that the thermodynamic properties of every stream are affected.

The double-effect configuration contains two additional main components, the absorber 2 and the generator 2. Consequently, the heat flows of the absorber 2 and generator 1 are added on the performance indicator vector $\mathbf{F}$. The investigated parameters are similar to those of the single-stage, single-effect system.
With respect to the triple-effect system, the heat flow of the condenser 2 is added on the vector $F$. Furthermore, the triple-effect configuration operates on three pressure stages. Assuming that uncertainty is introduced on high inner stage pressure $P_{Medium}$ and high outer stage pressure $P_{High}$, these parameters are added on the model parameter vector $\epsilon$.

### Table 8. Varying parameters and performance indicators for single, double and triple-effect systems.

<table>
<thead>
<tr>
<th>System type</th>
<th>Varying parameters of vector $\epsilon$</th>
<th>Performance indicators of vector $F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-effect</td>
<td>$T_{c}^{H_{2}O}$, $T_{c}^{NH_{3}}$, $P_{c}^{H_{2}O}$, $P_{c}^{NH_{3}}$, $P_{High}$</td>
<td>$Q_{abs}$, $Q_{cond}$, $Q_{evap}$, COP</td>
</tr>
<tr>
<td>Double-effect</td>
<td>$T_{c}^{H_{2}O}$, $T_{c}^{NH_{3}}$, $P_{c}^{H_{2}O}$, $P_{c}^{NH_{3}}$, $P_{High}$</td>
<td>$Q_{abs1}$, $Q_{abs2}$, $Q_{cond}$, $Q_{evap}$, $Q_{gen1}$, COP</td>
</tr>
<tr>
<td>Triple-effect</td>
<td>$T_{c}^{H_{2}O}$, $T_{c}^{NH_{3}}$, $P_{c}^{H_{2}O}$, $P_{c}^{NH_{3}}$, $P_{Medium}$, $P_{High}$</td>
<td>$Q_{abs1}$, $Q_{abs2}$, $Q_{cond1}$, $Q_{cond2}$, $Q_{evap}$, $Q_{gen1}$, COP</td>
</tr>
</tbody>
</table>

### 3.4.2 State variables of cost functions

The purpose of the cost function evaluation method, described in (13), is to identify the contribution of the performance indicators and the state variables to the model’s behavior. The performance indicators of vector $F$ have been previously mentioned in Table 8. The state variables of vector $x$ have been selected such that the deviations from reference values, the model variabilities and the nonlinearities may be investigated. Table 9 illustrates the state variables of the single, double and triple-effect process. Temperatures $T_i$, mass flow rates $m_i$ and ammonia mass fractions $x_{i}^{NH_{3}}$ of selected streams have been considered.

### Table 9. State variables of cost functions.

<table>
<thead>
<tr>
<th>System Type</th>
<th>State Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-effect</td>
<td>$T_{2}, T_{3}, T_{4}, T_{5}, T_{6}, T_{9}, T_{10}, T_{11}, T_{12}, T_{13}, T_{14}, m_{4}, x_{4}^{NH_{3}}, x_{9}^{NH_{3}}$</td>
</tr>
<tr>
<td>Double-effect</td>
<td>$T_{1}, T_{2}, T_{3}, T_{4}, T_{5}, T_{6}, T_{9}, T_{10}, T_{11}, T_{12}, T_{13}, T_{14}, T_{15}, T_{16}, T_{17}, T_{18}, T_{19}, T_{20}, T_{21}, T_{22}, T_{23}, T_{24}, T_{25}, T_{26}, T_{27}, m_{4}, m_{19}, x_{9}, x_{9}^{NH_{3}}, x_{9}^{NH_{3}}, x_{9}^{NH_{3}}, x_{9}^{NH_{3}}$</td>
</tr>
<tr>
<td>Triple-effect</td>
<td>$T_{1}, T_{2}, T_{3}, T_{4}, T_{5}, T_{6}, T_{7}, T_{9}, T_{10}, T_{11}, T_{12}, T_{13}, T_{14}, T_{15}, T_{16}, T_{17}, T_{18}, T_{19}, T_{20}, T_{21}, T_{22}, T_{23}, T_{24}, T_{25}, T_{26}, T_{27}, m_{5}, m_{15}, x_{5}, x_{9}, x_{15}, x_{19}$</td>
</tr>
</tbody>
</table>

### 3.4.2 System operation constraint

One of the factors that ensure the safe operation of the process is the requirement that the binary liquid mixture at the entrance of the pump is saturated (or subcooled) to avoid cavitation. The change of model parameters of vector $\epsilon$ through the dominant direction of variability may lead to a vapor-liquid binary mixture, by increasing the vapor pressure of the mixture. For that reason, a physical constraint, including the vapor fraction in the pump inlet, must be defined. The default value of ASPEN Plus for the upper bound of vapor fraction is 0.1%. The following inequality for single, double (inner and outer stage pump) and triple
(inner and outer stage pump) effect systems represent the highest value of vapor fraction preventing from pump cavitation,

\[ x_{pump-entrance}^{vapor} < 0.1 \% \]  \hspace{1cm} (17)

### 3.5 Goals of investigations

Prior to presenting an overview of the obtained results, note that for completeness we provide detailed, stream-by-stream simulation results as Supporting Information without considering any variability. The default ASPEN Plus thermodynamic model for electrolyte binary mixtures is used, comprising the ELECNRTL activity coefficient model, combined with the Redlich-Kwong EoS.

The following section presents the results of the investigated methods to the ABR system. Initially, the impact of parameters on ABR process is identified by applying the sensitivity analysis approach in (4) in order to identify the dominant direction of variability and calculate the sensitivity index \( \Omega \) along the major eigenvector direction for every thermodynamic model \( d \). The decomposition of the \( \Omega \) index into its component performance indicators is then performed to provide useful insights regarding the nature of variability impacts. Finally, the combined contribution of state variables and performance indicators on ABR process is illustrated by studying the cost functions defined on (13) in order to identify the model with the most favorable sensitivity behavior.

### 4. Results and Discussion

#### 4.1 Influence of model parameters on absorption refrigeration process under variability

The results of the identification of the dominant direction of variability are illustrated in Table 10, Table 11 and Table 12 for single, double and triple-effect process, respectively. Based on the sensitivity analysis procedure, the local sensitivity matrix is decomposed into a set of eigenvectors. Instead of exploring, the behavior of the ABR process under multiple arbitrary parameter variations, the eigenvectors incorporate the directions in which the system will be more susceptible to variability. Dominant eigenvector \( \Theta^1 \), with the largest eigenvalue, is then selected and the parameters in vector \( e \) are ordered based on the highest absolute value of the elements in \( \Theta^1 \). The combined consideration of model parameter changes along this eigenvector direction causes the largest change in the performance indicators of vector \( F \) compared to other eigenvector directions. For each thermodynamic model, the parameters appearing towards the left of the tables, have a higher impact on the eigenvector direction and subsequently on the performance indices compared to the parameters appearing towards the right of the tables. The most dominant parameters are marked in bold based on the corresponding entry (in absolute value) in the eigenvector.

Table 10 illustrates the influence of parameters on single-stage, single-effect process. The most influential parameter in the dominant direction of variability is the \( T_c^{NH3} \) of NH3 for
every thermodynamic model. This is reasonable, because it directly affects the EoS as a major input parameter. For the same reason, the $p_{NH_3}^c$ of NH$_3$ has a significant impact on the process variability, contributing, however, less than $T_{NH_3}^c$. It is important to mention that the investigated ranges of variability for NH$_3$ have a dominant influence on the process, as this compound participates with high concentration, either in vapor phase or in liquid phase, to each stream of the cycle. The $P_{High}$ of the cycle (or the vapor pressure of the refrigerant at a specific temperature) is an operational characteristic of the process, meaning that it influences all the high-pressure stages of the system. The group of parameters with the lowest impact on the operating cycle, are $T_{H_2O}^c$ and $P_{H_2O}^c$. In some thermodynamic models, the influence of $P_{H_2O}^c$ is completely insignificant. Considering that H$_2$O is mainly present in the liquid binary mixture, without participating in the vapor phase, the minor contribution of these parameters is reasonable.

The influence of parameters on two-stage, double-effect system is displayed in **Table 11**. Thermodynamic models ds, ds, d9 and d11 are not included in the analysis, as they violate the cavitation constraint (17) at nominal operating conditions. Similarly, to the case of the single-effect cycle, the major influential parameters are the critical properties of NH$_3$. The main difference between the single and the double-effect cycle is observed in $P_{High}$, which has the lowest influence on the cycle performance.

**Table 12** presents the impact of parameters on two-stage, triple-effect cycle. The only valid thermodynamic models are d1 and d7, both of them using the Redlich-Kwong EoS. The rest of the models violate constraint (17) at nominal operating conditions. However, for the purpose of the extension of the analysis, all the thermodynamic models previously considered in the double-effect cycle are investigated. With the exception of model d4, the most influential parameter is $T_{NH_3}^c$, whereas the second major parameter is $P_{High}$ except from model d1. For the remaining parameters, a certain pattern cannot be identified.

**Table 10. Ordering of most influential parameters from left to right for each model on single-stage, single-effect process.**

<table>
<thead>
<tr>
<th>Model ID</th>
<th>Parameters ordered based on contribution to eigenvalue direction*</th>
</tr>
</thead>
<tbody>
<tr>
<td>d1</td>
<td>$T_{NH_3}^c, P_{NH_3}^c (-), P_{High}, T_{H_2O}^c, P_{H_2O}^c (-)$</td>
</tr>
<tr>
<td>d2</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
<tr>
<td>d3</td>
<td>$T_{NH_3}^c, P_{NH_3}^c (-), P_{High}, T_{H_2O}^c, P_{H_2O}^c (-)$</td>
</tr>
<tr>
<td>d4</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
<tr>
<td>d5</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
<tr>
<td>d6</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
<tr>
<td>d7</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
<tr>
<td>d8</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
<tr>
<td>d9</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
<tr>
<td>d10</td>
<td>$T_{NH_3}^c, P_{High} (-), T_{H_2O}^c, P_{NH_3}^c (-), P_{H_2O}^c (0)$</td>
</tr>
</tbody>
</table>
4.2 Evaluation of sensitivity index $\Omega$

This section illustrates the implementation of the proposed sensitivity analysis method. The dominant direction of variability identified in Table 10 provides an initial indication regarding the variability impacts on the ABR performance. The purpose of calculating the sensitivity index $\Omega$ is to investigate the behavior of the system under variability of finite magnitude along the dominant eigenvector direction, in order to unveil nonlinear effects and identify process interactions due to simultaneous parameter variations.

Figure 4 illustrates the single-stage, single-effect sensitivity index $\Omega$, which represents the combined effect of all model parameters on the change of the performance indicators of
vector $\mathbf{F}$ for magnitudes defined by the sensitivity magnitude parameter $\zeta$. Thermodynamic models with steep profile close to region $\zeta = 0$ exhibit significantly different performance compared to their performance at the nominal point. As a result, they are very sensitive to variability and they will have a detrimental effect on ABR performance, as a small change in the model parameters will have a large effect on the performance indicators. Thermodynamic models with a flat profile close to region $\zeta = 0$ can absorb efficiently model deviations, meaning that their performance is not altered significantly compared to the nominal operation. Among all the thermodynamic models, the $d_1$, $d_3$, $d_5$, $d_7$, $d_9$ and $d_{11}$ exhibit a steeper profile, whereas the $d_2$, $d_4$, $d_6$, $d_8$, $d_{10}$ and $d_{12}$ exhibit a profile with a lower slope. In addition, it is worth mentioning that the underlying nonlinear behavior of the thermodynamic models is mainly present in regions of the sensitivity magnitude parameter $\zeta$ with small positive values. After a critical value of $\zeta$ in the positive value region, the behavior of the thermodynamic model could be considered as linear. Another significant observation is that thermodynamic models with different activity coefficient model but with the same EoS exhibit similar behavior. For example, thermodynamic models $d_6$ and $d_{12}$, both using the Cubic-Plus-Association EoS, exhibit very small deviations. Consequently, the EoS of a thermodynamic model could be considered as a major impact element on the performance of the process compared to the employed activity coefficient model. However, since the activity coefficient models are very similar this conclusion may not be generalized. The upper bound $\zeta^U \approx 0.05$ corresponds to 5% increment of the most influential parameter of vector $\mathbf{e}$, as indicated by Table 10, from its ASPEN Plus based nominal value. In the negative direction region of the sensitivity magnitude parameter, the values of $\zeta$ are bounded by the pump cavitation constraint (17). Thermodynamic models including Peng-Robinson based EoS, appear to be more sensitive to the violation of this constraint, allowing the investigation of only a few values of the coordinate $\zeta$ in the negative direction.

Figure 5 illustrates the sensitivity index $\Omega$ of the two-stage, double-effect cycle. It appears that the profiles are very similar to each other, indicating that the variability of the performance indicators is not affected significantly by the selection of the thermodynamic model. Models $d_1$ and $d_7$, containing the Redlich-Kwong equation of state, exhibit the highest variability, while models $d_2$ and $d_6$ exhibit the lowest. For values close to the region $\zeta = 0$, the deviations between the indexes $\Omega$ are negligible. Moreover, the upper bound $\zeta^U$ corresponds to 5% increase from its nominal value of the parameter with the highest impact to the performance indicators, whereas in the negative direction region of the sensitivity magnitude parameter, the $\zeta$-values are bounded due to the vapor contained in the binary liquid mixture, damaging the pumps (constraint (17)). Models $d_1$, $d_7$ and $d_8$ enable the highest flexibility related to the cavitation constraint, allowing higher variability in the parameters of vector $\mathbf{e}$. 
Figure 6 investigates the two-stage, triple-effect sensitivity index $\Omega$. It has already been mentioned that the only models not violating constraint (17) at the nominal operation point are $d_1$ and $d_7$.. However, Figure 6 illustrates that there is a feasible region (in which the constraint (17) is not violated) for models $d_2$, $d_4$, $d_6$, $d_8$, $d_{10}$ and $d_{12}$ at points of $\zeta > 0.005$. Excluding $d_4$ and $d_{10}$, the remaining models exhibit similar profile characteristics. Models $d_2$, $d_6$, $d_8$ and $d_{12}$ exhibit the highest values of sensitivity index $\Omega$ under parameter variability, whereas models $d_4$ and $d_{10}$ require the highest increase of sensitivity magnitude coordinate $\zeta$ in order to avoid violation of constraint (17). The valid models $d_1$ and $d_7$, including the Redlich-Kwong EoS, present similar $\Omega$ index values. Also, they extend slightly to the negative direction of the sensitivity magnitude $\zeta$ before constraint (17) is violated. The upper bound of $\zeta$ corresponds to 2.65% increase of the most influential parameter from its nominal value.

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**Figure 4.** Sensitivity index $\Omega$ with respect to variation of sensitivity parameter magnitude $\zeta$ on single-stage, single-effect system.
Figure 5. Sensitivity index $\Omega$ with respect to variation of sensitivity parameter magnitude $\zeta$ on two-stage, double-effect system.

Figure 6. Sensitivity index $\Omega$ with respect to variation of sensitivity parameter magnitude $\zeta$ on two-stage, triple-effect system.

4.3 Decomposition of sensitivity index $\Omega$ to performance indicators

The evaluation of sensitivity index $\Omega$ illustrates the effect of the model parameter variability of vector $\mathbf{e}$ in the overall performance process. This section presents a decomposition of sensitivity index $\Omega$, investigating separately the absolute values of each performance index. The study of performance indicators indicates how each one of them is affected under changing parameters towards to the major direction of variability. Figure 7, Figure 8 and Figure 9 for single, double and triple-effect cycle illustrate error bars between the absolute minimum and maximum value of every performance indicator for every
thermodynamic model. Moreover, values of the literature studies [35] and [36] have also been introduced, for comparison purposes.

**Figure 7** illustrates the absolute values of the four performance indicators of single-stage, single-effect process under parameter variability. For every thermodynamic model, the nominal values of the heat flow $Q_{abs}$ of the absorber are very close to the literature values, while the variability introduced by the change of model parameters, is relatively low. Despite the fact that the nominal and literature values of $Q_{cond}$ are similar, the sensitivity of this performance indicator to parameter variation is more significant. The nominal point of $Q_{evap}$ performance index deviates slightly from the literature data point used as reference, exhibiting simultaneously a low variability range. The $COP$ presents the same profile characteristics with the $Q_{evap}$ as they are directly related.

**Figure 8** illustrates the two-stage, double-effect performance indicators of vector $F$. The nominal point values are close to the literature, regardless of the selected thermodynamic model. In contrast to the single-effect configuration, the increase of the sensitivity magnitude parameter $\zeta$ in the two-stage, double-effect system causes a decrease in the performance indicators values, except for the $Q_{cond}$. Generally, the variability level of performance indices under parameter variation is relatively low. The performance indicator with the lowest variability is $Q_{abs2}$, whereas the highest change occurs on the heat flow $Q_{cond}$.

**Figure 9** illustrates the decomposition of the two-stage, triple-effect sensitivity index $\Omega$ into its performance indicators. The triple-effect process behaves similarly to the single-effect cycle. In other words, the increase of coordinate $\zeta$ leads the increase of the heat flows and $COP$. The nominal performance indicator values deviate from the literature, except from the $Q_{evap}$ and the $COP$. This could be explained by the mismatches observed in temperatures of outer-stage high pressure streams, as it is presented in Table A.5 and Table A.9 of the Supporting information section. Especially, temperatures $T_{14}$ and $T_{19}$ of Table A.9 exhibit the highest mean average percentage error values among the investigated magnitudes. This implies that the investigated thermodynamic models may be challenged by the high pressure conditions observed in this case. Note that the literature results used as a reference point in our study have been obtained using empirical correlations to predict thermodynamic properties, hence there may be some scattering there too. Our main observation here is merely that, compared to the single and double-effect cycle, the level of variability of the triple-effect process is more intense. In any case, the proposed approach enable the quantification of the uncertainty that induces the observed variability irrespectively of the employed reference points.

As a general result and regardless of the type of the process, the component affected most by the varying parameters of vector $e$ is the heat flow in the condenser. In addition, the heat flow of the evaporator and, consequently, the coefficient of performance $COP$, are not only close to the literature values but they, also, present a low level of variability.
*Upward direction positive $\zeta$ values, downward direction negative $\zeta$ values.

Figure 7. Performance indicators $F$ of single-stage, single-effect cycle with respect to variations of sensitivity magnitude parameter $\zeta$ and literature [44].
Figure 8. Performance indicators $F$ of two-stage, double-effect cycle with respect to variations of sensitivity magnitude parameter $\zeta$ and literature [44].

*Upward direction negative $\xi$ values, downward direction positive $\xi$ values.*
*Upward direction positive $\zeta$ values, downward direction negative $\zeta$ values.

Figure 9. Performance indicators $F$ of two-stage, triple-effect cycle with respect to variations of sensitivity magnitude parameter $\zeta$ and literature [45].
4.4 Calculation of cost functions

This section elaborates on the calculation of cost functions, described in equations (13). The main purpose of the cost functions is to support the identification of the thermodynamic model which a) provides simulation results as close as possible to the reference data under variability and b) exhibits the lowest possible sensitivity in case of parametric variability when used either in simulations or in optimization. For every thermodynamic model, the cost function $J_{REF}$ investigates the deviation of the process, under varying parameters, from the literature values. The cost function $J_{MV}$ indicates how steep or flat is the change of state variables and performance indicators, while the elements of the vector $\mathbf{e}$ change to the dominant direction of variability, identified by the eigenvector $\mathbf{\Theta}^1$. The cost function $J_{NL}$ refers to the convexity and the nonlinear characteristics of every thermodynamic model, by calculating the second derivatives of performance indicators and state variables with respect to the model parameter variation. The combination of these cost functions illustrates the complete behavior of each thermodynamic model, exploring how they would react to the uncertainty introduced in the parameter vector. Note that a detailed presentation of the numerical values of the cost functions is given in section A.3 of Supporting Information.

Figure 10 illustrates a diagram for the single-stage, single-effect cycle, investigating simultaneously all the cost functions for every thermodynamic model. With respect to deviations from reference data, models $d_1$, $d_3$, $d_5$, $d_7$, $d_9$, and $d_{11}$ exhibit the largest deviations, as their cost function $J_{REF}$ is higher compared to the same cost function of models $d_4$, $d_6$, $d_{10}$, and $d_{12}$. In addition, models $d_3$, $d_4$, and $d_{10}$ seem to have both the smallest grade of sensitivity to model parameter variations and minor nonlinear characteristics. The cost functions $J_{MV}$ and $J_{NL}$ of these models obtain very low values, meaning that the process performance indicators and state variables may absorb parameter variation effects and retain curvature characteristics around the nominal operating point, while the parameters vary along the dominant direction of variability. Moreover, model $d_{10}$ has the lowest cost function values, hence, it is considered as the most appropriate.

Figure 11 illustrates the diagram of the two-stage, double-effect process. All models present similar deviation characteristics compared to the literature. The lowest magnitude of variability and nonlinearity is observed for models $d_1$, $d_4$, $d_7$ and $d_{10}$. Model $d_7$ seems to combine the lowest values on all three cost functions, hence, it is considered as the best one. A triple-effect cycle diagram is not illustrated due to the low number of models that provide valid results under variability (i.e. only $d_1$ and $d_7$). Both models contain a $J_{REF}$ value equal to 1.414. Model $d_7$ contains $J_{MV}$ and $J_{NL}$ values equal to 0.0154 and 0.0001, respectively, whereas model $d_1$ equal to 1.99 and 2, respectively. Therefore, it is obvious that model $d_7$ is the most appropriate.
Models $d_2$ and $d_8$ are not included in the diagrams, as they contain significantly higher $J_{MV}$ and $J_{NL}$ values than the rest of the models.

Figure 10. Cost functions for single-stage, single-effect cycle
5 Conclusions

The present work deals with the nonlinear sensitivity analysis of the absorption refrigeration NH₃/H₂O system under different thermodynamic methods and model parameter variability. A systematic methodology has been introduced so that the impact of varying parameters to the system’s performance to be investigated. Two criteria are introduced, the first one called sensitivity index $\Omega$, representing the sum of the relative change of performance indicators from their nominal values and the second one consisting of cost functions $J$, investigating the combined effect of performance indicators and state variables to the system’s behavior. The proposed methodology is implemented on three absorption refrigeration process types, the single-stage, single-effect cycle, the two-stage, double-effect cycle and the two-stage, triple-effect cycle. A variety of parameters, performance indicators and thermodynamic models have been considered.

The results of this work are compared to similar literature studies. It has been shown that the nominal point values are very close to the literature for every thermodynamic model of the single-effect and the double-effect system, whereas slight deviations have been observed for the triple-effect system. Furthermore, there are only a few parameters that affect
significantly the absorption refrigeration process in terms of variability, with $T_c^{NH_3}$ being mainly the most influential. Exploring the curves of the sensitivity index $\Omega$ towards the dominant direction of variability, the deviations between the models could be considered small, whereas the effect of equation of state is more significant than the activity coefficient method. The decomposition of the sensitivity index to its performance indicators reveals that variability is more intense in the condenser component, whereas the cooling load of the evaporator and, subsequently, the coefficient of performance still remain close to the literature values. Finally, the evaluation of the cost functions for every model elaborates the combined contribution of the performance indicators and the state variables to the system’s deviation from literature, variability and nonlinearity. With respect to the single-effect cycle, models $d_4$ and $d_{10}$ with Peng-Robinson for hydrocarbon-water systems EoS are the most appropriate, as they contain the lowest cost function values. In terms of the double-effect cycle, the value of $J_{LT}$ is similar for the most of the models, while models $d_1$ and $d_7$ with Redlich-Kwong EoS, $d_4$ and $d_{10}$ with Peng-Robinson for hydrocarbon-water systems EoS present the lowest values of the model variability and nonlinearity cost functions. For the triple-effect system, the only valid models were $d_1$ and $d_7$ with Redlich Kwong EoS. The $d_7$ with ENRTL-HG contained the lowest cost function values between the two valid models.

**Nomenclature**

- **COP**: coefficient of performance
- **$D$**: set of thermodynamic models
- **$d$**: candidate thermodynamic model
- **$F$**: vector of performance indicators of dimension $N_F$
- **$g$**: vector of inequality constraints of dimension $N_g$
- **$h$**: vector of equality constraints of dimension $N_h$
- **$J$**: cost function
- **$m$**: mass flow rate (kg/sec)
- **$N_d$**: total number of investigated thermodynamic models
- **$N_F$**: total number of performance indicators
- **$N_g$**: total number of inequality constraints
- **$N_h$**: total number of equality constraints
- **$N_p$**: total number of model parameters
- **$P$**: pressure (kPa)
- **$P$**: sensitivity matrix of dimensions $N_F \times N_p$
\( Q \)  
heat flow rate (kW)

\( \mathbb{R} \)  
set of real numbers

\( T \)  
temperature (K) (or °C if noted so)

\( \mathbf{x} \)  
vector of state variables of dimension \( N_x \)

\( x^{NH_3} \)  
ammonia quality mass fraction (kg NH\(_3\)/kg mixture)

\( x^{vapor} \)  
vapor fraction (dimensionless)

**Greek Symbols**

\( \Delta \varepsilon \)  
infinitesimal model parameter variations

\( \varepsilon_{CEHX} \)  
effectiveness of condenser-evaporator heat exchanger

\( \varepsilon_{SHX} \)  
effectiveness of solution heat exchanger

\( \varepsilon \)  
vector of model parameters of dimension \( N_p \)

\( \zeta \)  
sensitivity magnitude parameter

\( \Theta \)  
eigenvector of dimension \( N_p \) of matrix \( P^T P \)

\( \mu \)  
mean value

\( \sigma \)  
standard deviation

\( \Omega \)  
sensitivity index (dimensionless)

**Superscript/Subscript Indices**

\( abs \)  
absorber

\( c \)  
critical magnitude

\( CEHX \)  
condenser-evaporator heat exchanger

\( cond \)  
condenser

\( evapor \)  
evaporator

\( gen \)  
generator

\( L \)  
lower bound

\( LIT \)  
literature

\( MV \)  
model variability

\( NL \)  
nonlinear

\( nom \)  
nominal

\( per \)  
perturbated

\( rect \)  
rectifier
6. Acknowledgements

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7. References


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Highlights

- Consideration of multiple thermodynamic models in absorption refrigeration
- Systematic identification of appropriate model using sensitivity analysis
- Application to single, double and triple effect systems
- Model selected based on proximity to reference data, parameter variability and non-linearity