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Systematic Assessment of Model Robustness in Simulation of Absorption Refrigeration Processes

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A systematic sensitivity analysis approach is proposed to assess the robustness of thermodynamic model predictions employed in ABR processes. A sensitivity matrix is developed which incorporates the derivatives of multiple ABR performance indicators (e.g. coefficient of performance, generated cooling, mass flowrate of working fluid etc.) with respect to multiple thermodynamic property parameters propagated through different thermodynamic prediction models. The dominant eigenvector direction of the sensitivity matrix is identified and used to explore the ABR process behaviour as indicated by the change of ABR performance indicators under simultaneous, multiple and finite thermodynamic parameter variations. This enables the robust mapping of ABR performance toward the direction of maximum variability in the multiparametric space and hence the identification of a thermodynamic model which supports robust predictions regardless of variability. The approach is illustrated in a single effect ABR process system using the NH_3/H_2O mixture. Among various thermodynamic models we find that the Schwartzentruber-Renon with eNRTL are the most robust combination to parameter variability.

1. Introduction

Absorption Refrigeration (ABR) is a widely investigated process for transformation of renewable or waste heat into cooling (Kale et al., 2018). A detailed review of the absorption refrigeration technologies can be found in Papadopoulos et al. (2019). Performance evaluation of different ABR working fluids and process configurations is largely approached in published literature through process models (Wu et al., 2017). The latter are based on equations of state (EoS) and activity coefficient models to support the prediction of the equilibrium mixture properties necessary for process simulation. The thermodynamic models currently reported vary significantly from Peng-Robinson (Han et al., 2016) and soft-SAFT (Crespo et al., 2017) to NRTL and UNIFAC (Chaudhari et al., 2008). All these options result in significant prediction differences even for exactly the same ABR working fluid and process (Zehioua et al., 2010). As such, the validation of ABR models based on experimental data or available model-based results, and the assessment of ABR performance, include significant uncertainty. The latter reduces confidence in the obtained model predictions, as results may differ from the actual process operation.

In current literature, parameter estimation studies for the development of thermodynamic models used in ABR processes consider the difference of the predicted results from validated reference data (e.g. experimental) (Han et al., 2016), while ABR process model predictions are also compared with reference data (e.g. Adewusi and Zubair, 2004). However, this does not constitute a systematic treatment of uncertainty. Different sets of reference data used as input in a thermodynamic model affect the predictions provided for a desired property. Different thermodynamic models also result in divergent predictions for the same desired property. ABR process simulations require predictions of multiple properties over wide ranges of different temperatures, pressures and concentrations. Reference data are often only available for specific conditions and process parameters,

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prohibiting validation within wider ranges for all the desired parameters. The latter is very important because 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) which may result in unexpectedly detrimental process performance. It is therefore necessary to be able to quantify uncertainty and to select thermodynamic models which exhibit low sensitivity to multi-parametric variability, regardless of the availability of reference data.

2. Sensitivity analysis method

The above challenges are addressed through a systematic sensitivity analysis approach which accounts for the propagation of multi-parametric variability through multiple different thermodynamic models used in ABR processes. The purpose of the proposed approach is a) to identify the thermodynamic parameters that have the highest influence on the ABR performance and b) to select the thermodynamic models which exhibit the lowest sensitivity when such parameters are varied simultaneously toward a systematically identified direction of the highest variability. A model identified through such an approach would provide robust and reliable predictions even in cases of intense variability in the parameters used as input. The proposed method has been previously implemented in a single thermodynamic model to assess organic Rankine cycle working fluids (Papadopoulos et al., 2013). It is implemented here for the first time in ABR processes and considers for the first time multiple different thermodynamic models.

We start by considering a set D of thermodynamic models, an N_p-dimensional vector $\boldsymbol{\varepsilon}$ representing the parameters which will be subjected to variability as inputs in the thermodynamic models of D and an N_F-dimensional vector $\boldsymbol{F}$ of performance indicators. Let a vector $\boldsymbol{\varepsilon}^{nom}$ representing the nominal values for the model parameters of the ABR process. For every thermodynamic model $d \in D$, we identify the model parameters which are the most sensitive with respect to the performance indicators $\boldsymbol{F}$ by generating a local sensitivity matrix $\boldsymbol{P}$ around the nominal model parameter vector $\boldsymbol{\varepsilon}^{nom}$ as follows,

$$\boldsymbol{P} = \begin{bmatrix} \frac{\partial lnF_1}{\partial ln\varepsilon_1} & \cdots & \frac{\partial lnF_1}{\partial ln\varepsilon_{N_p}} \\ \vdots & \ddots & \vdots \\ \frac{\partial lnF_{N_F}}{\partial ln\varepsilon_1} & \cdots & \frac{\partial lnF_{N_F}}{\partial ln\varepsilon_{N_p}} \end{bmatrix}_{\boldsymbol{\varepsilon}^{nom}} . \tag{1}$$

The logarithmic functions represent locally scaled transformations for the performance indicators and the model parameters, whereas matrix $\boldsymbol{P}$ constitutes a measure of variation of the process model under the influence of infinitesimal changes imposed on model parameters.

The major directions of variability are identified by calculating the eigenvectors $\boldsymbol{\theta}^i$ $(i = 1, \dots, N_p)$ of the matrix $\boldsymbol{P}^T\boldsymbol{P}$ for every model D. The dominant direction of variability is represented as the combination of parameters $\boldsymbol{\varepsilon}$ which are causing the largest change in the performance indicators in a least square sense. The eigenvector $\boldsymbol{\theta}^1$, with the largest in magnitude eigenvalue of $\boldsymbol{P}^T\boldsymbol{P}$, is related to the largest change in the performance indices $\boldsymbol{F}$. The identification of major variability direction indicates that is not necessary to investigate other directions.

Following the determination of the sensitivity matrix, a sensitivity index Ω is defined, which accounts for the behavior of the performance indicators $\boldsymbol{F}$ within a wide variation range, explored through a magnitude parameter variation ζ 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

$$\begin{aligned} \underset{d \in D}{Calculate}\ \Omega(\zeta, d) &= 100 \cdot \sum_{i=1}^{N_F} \left| \frac{F_i(\boldsymbol{x}, d, \boldsymbol{\varepsilon}(\zeta)) - F_i(\boldsymbol{x}, d, \boldsymbol{\varepsilon}^{nom}))}{F_i(\boldsymbol{x}, d, \boldsymbol{\varepsilon}^{nom})} \right| \\ s.t. \quad h_i(\boldsymbol{x}, d, \boldsymbol{\varepsilon}) &= 0 \quad , \quad i = 1, \dots, N_h \\ g_i(\boldsymbol{x}, d, \boldsymbol{\varepsilon}) &\le 0 \quad , \quad i = 1, \dots, N_g \\ x_i^L \le x_i &\le x_i^U \quad , \quad i = 1, \dots, N_x \\ \frac{\varepsilon_i(\zeta) - \varepsilon_i^{nom}}{\varepsilon_i^{nom}} &= \zeta \cdot \theta_i^1 \quad , \quad i = 1, \dots, N_p \\ \zeta &\in [\zeta^L, \zeta^U] \end{aligned} \tag{2}$$

with N_x-dimensional vector $\boldsymbol{x}$ representing the state variables, with x^L and x^U being lower and upper bounds, N_h-dimensional vector $\boldsymbol{h}$ and N_g-dimensional vector $\boldsymbol{g}$ representing the equalities and inequalities of the ABR process. The Ω is calculated under the assumption that the eigenstructure of the local sensitivity matrix does not change considerably with the variation of parameters. The sensitivity index Ω represents the sum of the

relative change of performance indicators $\boldsymbol{F}$ from the nominal values, as a function of ζ, which is the parameter variation magnitude coordinate indicating the range of imposed change in the direction of $\boldsymbol{\theta}^1$. The maximum change along this direction is addressed through the lower and upper bound, ζ^L and ζ^U. Indices Ω 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.

3. Implementation

3.1 Absorption refrigeration process

Figure 1 illustrates the single stage, single effect ABR process. NH_3 is used as the refrigerant and H_2O as the absorbent. The latter has strong affinity for NH_3 and they are soluble with each other in a wide range of operating conditions. The main system components are the absorber, condenser, evaporator, and generator. Some other auxiliary components are solution (SHX) and condenser-evaporator (CEHX) heat exchangers, expansion valves, pump and rectifier. Low pressure conditions are indicated with blue color, whereas high pressure with red color.

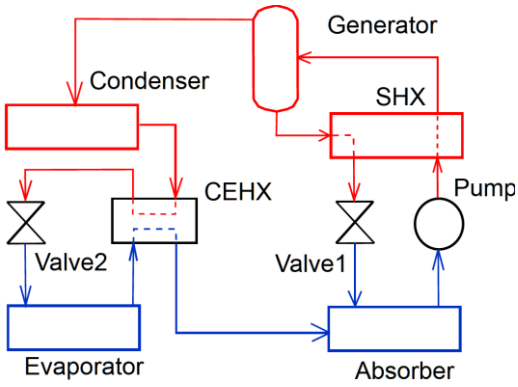


Figure 1:Single-stage, single-effect NH_3/H_2O ABR configuration.

3.2 Investigated thermodynamic models and reference data

The proposed sensitivity analysis method is addressed through the consideration of different EoS, based on the available options in AspenPlus Version 9 Software (www.aspentech.com). The Redlich-Kwong, the Schwartzentruber-Renon, the Cubic-Plus-Association and the Peng-Robinson (with Boston-Mathias modification) EoS are selected in order to describe the vapor-phase properties of NH_3/H_2O mixture. The liquid-phase non-ideality of NH_3/H_2O mixture is modelled using the Electrolyte NRTL (ELECNRTL) model. The package used for the calculation of thermodynamic properties was mainly ASPENPCD, followed by AQUEOUS, ELECPURE, PURE20, ENRTL-RK and EOS-LIT databanks. Our results are validated against data obtained from simulations performed by Adewusi and Zubair (2004). This source is selected mainly for two reasons. Firstly, it includes detailed stream data for a single effect cycle hence facilitating both the modeling and comparison of results obtained from the simulation of the cycle. Secondly, it employs correlations developed directly from NH_3/H_2O experimental mixture data by Ibrahim and Klein (1993). These correlations have been validated by Thorin et al. (1998), showing that for temperature and pressure conditions similar to those in our work the predicted mixture properties match experimental data closely.

3.3 Process operating assumptions

AspenPlus Version 9 Software has been used for ABR process design and simulation. The majority of the components has been considered as “Heater Blocks”, pump and valves as adiabatic “Pump Block” and “Valve Blocks”, respectively and the generator-rectifier system as distillation column. The simulation assumptions have been selected to be similar with the operating conditions in Adewusi and Zubair (2004). Low and high pressure are considered as the vapour pressures of NH_3/H_2O mixture and NH_3 at 40 ^oC, respectively. Their values are equal to 244.85 kPa and 1,555.76 kPa. The strong-solution mixture mass flow is 1 kg/sec with 0.3709 NH_3 mass fraction. The SHX and CEHX effectiveness are 1 and 0.95, respectively, while on evaporator’s exit, the requirement is 0.998 vapor fraction. The generator’s heat flow input is equal to 267.9 kW. However, for the

generator-rectifier's distillate-to-feed ratio and number of stages, there is no information in Adewusi and Zubair (2004). Therefore, the distillate-to-feed value was determined equal to 0.13224 kg/kg so that the temperature in the rectifier refrigerant vapour stream matches the corresponding steam in the literature source. The number of stages was determined equal to 5 so that the purity of NH_3 in the rectifier refrigerant vapour stream matches that of the literature source.

3.4 Technical details and constraints

Table 1 summarizes the parameters varied during the sensitivity analysis (vector $\boldsymbol{\varepsilon}$) and the performance indicators of vector $\boldsymbol{F}$. Uncertainty is introduced in selected critical parameters and NH_3 vapor pressure (corresponding to the high pressure of the cycle), using experimentally obtained values as nominal points. These parameters are selected as they affect both the operational conditions of the ABR process, and the employed EoS. Note that coefficient of performance is defined as the ratio of evaporator heat flow to generator's heat flow input.

Table 1: Varying parameters and performance indicators

Varied parameters of vector ε	Symbol	Performance indicators of vector F	Symbol
Critical temperature of H_2O	$T_c^{H_2O}$	Absorber heat flow	Q_{abs}
Critical temperature of NH_3	$T_c^{NH_3}$	Condenser heat flow	Q_{cond}
Critical pressure of H_2O	$P_c^{H_2O}$	Evaporator heat flow	Q_{evap}
Critical pressure of NH_3	$P_c^{NH_3}$	Coefficient of performance	COP
High pressure of cycle	P_{High}		

The process operability is ensured by avoiding cavitation in the pump's entrance. Consequently, a saturated (or subcooled) liquid mixture is required, as parameter variability may lead to vapor-liquid phase conditions, by altering the mixture's vapor pressure in pump inlet. For this reason, AspenPlus Software introduces the constraint that the vapor fraction in the pump entrance should be less than 0.1 %.

4. Results and discussion

4.1 Influence of model parameters on absorption refrigeration process under variability

Table 2 summarizes the contribution of varied parameters to the dominant direction of variability for every thermodynamic model. Parameters on the left side of the table have a higher impact on the eigenvector $\boldsymbol{\theta}^1$ and, subsequently, on the performance indices compared to the right-aligned table parameters. For every thermodynamic model, the parameter with the highest influence is $T_c^{NH_3}$, as it is a major input parameter on the applied EoS. For the same reason, $P_c^{NH_3}$ contributes significantly to the process variability. It is obvious that variability introduced to the critical properties of NH_3 influences significantly performance indexes due to use of NH_3 on every stream of the working cycle either as vapour-refrigerant or as liquid-component of binary mixture. Moreover, P_{High} has a high variability contribution as it affects all the high pressure streams and components of the system. $T_c^{H_2O}$ and $P_c^{H_2O}$ have the lowest impact on the ABR working cycle, with $P_c^{H_2O}$ having zero contribution to Schwartzentruber-Renon EoS. Note that this is reasonable considering that H_2O participates mainly only to the liquid binary mixture.

Table 2: Ordering of most influential parameters from left to right for each model on ABR process. Most dominant parameter is marked with bold. Sign in brackets indicate negative values and opposite directions of change compared to positive values; zero in brackets indicate no influence of the parameter on the process.

Model	Parameters ordered based on contribution to eigenvalue direction
ELECNRTL – Redlich-Kwong	$\boldsymbol{T_c^{NH_3}}$, $P_c^{NH_3}(-)$, P_{High} , $T_c^{H_2O}$, $P_c^{H_2O}(-)$
ELECNRTL – Schwartzentruber-Renon	$\boldsymbol{T_c^{NH_3}}$, $P_{High}(-)$, $T_c^{H_2O}$, $P_c^{NH_3}(-)$, $P_c^{H_2O}(0)$
ELECNRTL – Peng-Robinson	$\boldsymbol{T_c^{NH_3}}$, $P_c^{NH_3}(-)$, P_{High} , $T_c^{H_2O}$, $P_c^{H_2O}(-)$
ELECNRTL – CPA	$\boldsymbol{T_c^{NH_3}}$, $P_{High}(-)$, $P_c^{NH_3}(-)$, $T_c^{H_2O}$, $P_c^{H_2O}(-)$

4.2 Evaluation of sensitivity index Ω and performance indicators

This section presents the proposed sensitivity analysis method implementation. Figure 2 illustrates the sensitivity index Ω with respect to the magnitude parameter ζ. Thermodynamic models with steep profile close

to region $\zeta = 0$ exhibit significantly different performance compared to their nominal point, implying that they are very sensitive to variability. A small change in the model parameters will lead to a large variation on the performance indicators. On the other hand, thermodynamic models with a flat profile close to region $\zeta = 0$ absorb efficiently model disturbances. As a result, their performance is more robust to model variations and does not vary significantly compared to the nominal operation. Models with Redlich-Kwong and Peng-Robinson Eos exhibit a steeper profile, whereas models with Schwartzentruber-Renon and CPA EoS exhibit a profile with a lower slope. Furthermore, nonlinear thermodynamic model behaviour is observed in regions with small ζ positive values. After a critical ζ positive value, the model's behaviour could be approached as linear. In addition, note that upper bound $\zeta^U \approx 0.05$ corresponds to 5 % increment of the most influential parameter of Table 2 from its AspenPlus Software nominal value. Negative ζ values are bounded by the cavitation phenomenon on pump's inlet.

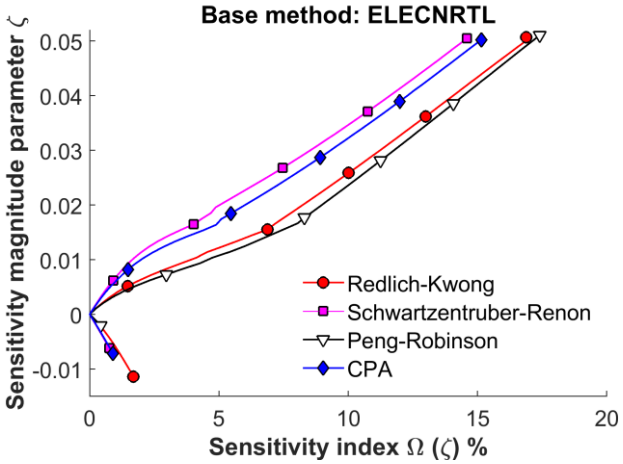
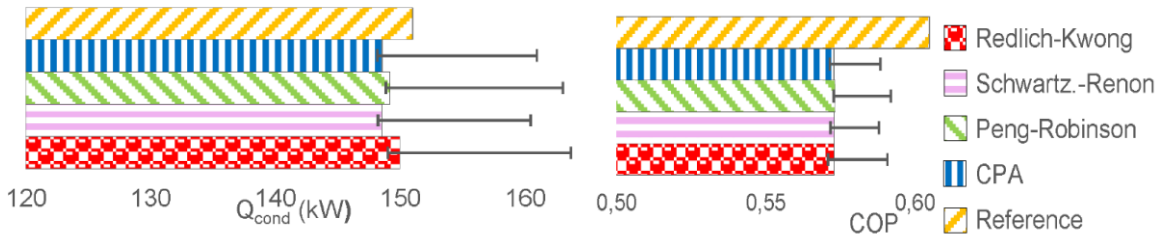


Figure 2: Index Ω with respect to variation of coordinate magnitude ζ

Figures 3a and 3b illustrate the nominal values of condenser heat flow Q_{cond} and process coefficient of performance COP for every thermodynamic model compared to reference values from Adewusi and Zubair (2004). Variability on these elements is introduced through black errorbars with right-direction corresponding to increase of positive ζ values. Nominal and reference values of Q_{cond} are very close to each other. However, the sensitivity of this performance indicator to parameter variation is high, hence moving towards the positive ζ-direction increases Q_{cond} values so that it deviates significantly from nominal and reference point. For every thermodynamic model COP nominal value deviates slightly from the reference value, while exhibits, simultaneously, a low range of variability. As a result, the process performance remains unaffected to model uncertainties introduced in the parameter vector $\boldsymbol{\varepsilon}$.



(a) (b)

Figure 3: (a) nominal Q_{cond} and (b) COP values under variability (black errorbars) compared to reference values (Adewusi and Zubair, 2004) on ABR single-effect process.

5. Conclusions

Current work presents a nonlinear sensitivity analysis of the NH_3/H_2O single-effect absorption refrigeration process under model parameter variability using different thermodynamic models. Firstly, the most influential parameters on ABR process performance are identified, by calculating the dominant direction of variability. Then, sensitivity index Ω is introduced, representing the sum of the relative change of performance indicators from their nominal values. Thermodynamic models with different EoS have been considered, while literature studies are introduced for validation and comparison purposes. In terms of variability, a few parameters contribute to the ABR process variation with $T_c^{NH_3}$ being the most crucial. Observing the sensitivity index Ω curves towards the dominant direction of variability, the deviations among the models are considered small. The Schwartzentruber-Renon EoS appears as the least sensitive to the parameter uncertainty. The decomposition of sensitivity index to its performance indicators reveals that variability is more intense to the condenser, whereas system's efficiency is not significantly affected as COP still remains close to the reference values.

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