

Evaluation of irreversibility in an ammonia-water absorption refrigeration system using three different mathematical models to calculate the thermodynamic properties

Evaluación de irreversibilidades en un sistema de refrigeración por absorción amoníaco-agua empleando tres modelos matemáticos diferentes para calcular las propiedades termodinámicas

Avaliação de irreversibilidades em um sistema de refrigeração por absorção amoníaco-água empregando três modelos matemáticos diferentes para calcular as propriedades termodinâmicas

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Iván Vera-Romero*
Christopher Lionel Heard-Wade**

Abstract

Second Law or Exergy Analyses of Absorption Refrigeration Systems (ARS) are very important for optimisations based on available work; these analyses are derived from the operating conditions and property calculations. There are several methods available for calculating the thermodynamic properties used in modelling these systems. A thermodynamic study on an ARS with the ammonia-water mixture (base case) was carried out with the objective of analysing the sensitivity of the overall and individual component irreversibility to the thermodynamic property. To this end, three existing methods were used: (M1), a model proposed by Ibrahim and Klein (1993) and used in the Engineering Equation Solver (EES) commercial software; (M2), a model proposed by Tillner-Roth and Friend (1998) and embodied in REFPROP v.8.0 developed by the National Institute of Standards and Technology (NIST); and (M3), a method proposed by Xu and Goswami (1999) that was programmed for this analysis. The obtained differences in the properties and the first law performance of the ARS are insignificant in the determination of the coefficient of performance (COP) (base case: 0.595, M1: 0.596, M2: 0.594, M3: 0.599). For the second law analysis, the overall irreversibility was the same (123.339kW) despite the irreversibilities per component had important differences: the solution heat exchanger (M1: 5.783kW, M2: 6.122kW, M3: 8.701kW), the desorber (generator) (M1: 51.302kW, M2: 45.713kW, M3: 49.098kW) and the rectifier (M1: 0.766kW, M2: 3.565kW, M3: 0.427kW). The components that destroy exergy the most are the desorber, the absorber and the condenser.

Keywords: ammonia-water properties; absorption refrigeration; coefficient of performance; irreversibility.

* M. Sc. Instituto Mexicano del Petróleo (San Bartolo Atepehuacan, México). ivera@ucienegam.edu.mx.

** Ph. D. Universidad Autónoma Metropolitana (Cuajimalpa, México). cheard@correo.cua.uam.mx.

Resumen

Los análisis por Segunda Ley, o de Exergía, en los Sistemas de Refrigeración por Absorción (SRA) son muy importantes, ya que permiten realizar análisis de optimización de acuerdo con el trabajo disponible, los cuales se establecen a partir de las condiciones de operación y del cálculo de sus propiedades. Para el modelado de estos sistemas existen diversas metodologías de cálculo para las propiedades termodinámicas. En este trabajo se realiza un estudio termodinámico sobre un SRA con mezcla amoníaco-agua propuesto (Caso Base), con la finalidad de evaluar la sensibilidad en las irreversibilidades globales y por equipo. Para tal efecto se emplearon tres metodologías existentes: (M1) el modelo de Ibrahim y Klein (1993), a través del software comercial Engineering Equation Solver (EES); (M2) el modelo propuesto por Tillner-Roth y Friend (1998), a través del software REFPROP v.8.0, desarrollado por el National Institute of Standards and Technology (NIST), y (M3) la metodología propuesta por Xu y Goswami (1999), programada para este análisis. Las diferencias entre las propiedades obtenidas y el funcionamiento del SRA por Primera Ley no son significativas en la evaluación del COP, obteniendo variaciones mínimas (Caso Base: 0.595, M1: 0.596, M2: 0.594, M3: 0.599). Para el análisis por Segunda Ley, la irreversibilidad total del sistema para los tres modelos resultó ser la misma (Irr Global: 123.339 kW), a pesar de que en la irreversibilidad por equipo sobresalen las diferencias entre el Intercambiador de la Solución (M1: 5.783kW, M2: 6.122kW, M3: 8.701kW), el Desorbedor (M1: 51.302kW, M2: 45.713kW, M3: 49.098kW) y el Rectificador (M1: 0.766kW, M2: 3.565kW, M3: 0.427kW). Los equipos que más destruyen exergía son el Desorbedor, el Absorbedor y el Condensador, respectivamente.

Palabras clave: coeficiente de desempeño; irreversibilidad; propiedades amoníaco-agua; sistema de refrigeración por absorción.

Resumo

As análises por Segunda Lei, ou de Exergía, nos Sistemas de Refrigeração por Absorção (SRA) são muito importantes, já que permitem realizar análises de otimização de acordo com o trabalho disponível, os quais se estabelecem a partir das condições de operação e do cálculo de suas propriedades. Para a modelagem destes sistemas existem diversas metodologias de cálculo para as propriedades termodinâmicas. Neste trabalho realiza-se um estudo termodinâmico sobre um SRA com a mistura amoníaco-água proposta (Caso Base), com a finalidade de avaliar a sensibilidade nas irreversibilidades globais e por equipamento. Para tal propósito, empregaram-se três metodologias existentes: (M1) o modelo de Ibrahim e Klein (1993), através do software comercial Engineering Equation Solver (EES); (M2) o modelo proposto por Tillner-Roth e Friend (1998), através do software REFPROP v.8.0, desenvolvido pelo National Institute of Standards and Technology (NIST), e (M3) a metodologia proposta por Xu e Goswami (1999), programada para esta análise. As diferenças entre as propriedades obtidas e o funcionamento do SRA por Primeira Lei não são significativas na avaliação do COP, obtendo variações mínimas (Caso Base: 0.595, M1: 0.596, M2: 0.594, M3: 0.599). Para a análise por Segunda Lei, a irreversibilidade total do sistema para os três modelos resultou ser a mesma (Irr Global: 123.339 kW), apesar de que na irreversibilidade por equipamento sobressaem as diferenças entre o Intercambiador da Solução (M1: 5.783kW, M2: 6.122kW, M3: 8.701kW), o Dessorbedor (M1: 51.302kW, M2: 45.713kW, M3: 49.098kW) e o Retificador (M1: 0.766kW, M2: 3.565kW, M3: 0.427kW). Os equipamentos que mais destroem exergía são o Dessorbedor, o Absorvedor e o Condensador, respectivamente.

Palavras chave: coeficiente de desempenho; irreversibilidade; propriedades amoníaco-água; sistema de refrigeração por absorção.

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I. INTRODUCTION

The ammonia-water mixture (AWM) has been successfully used in many absorption refrigeration systems (ARS). AWM has played an important role in the use of heat pumps or as ARS applied or coupled to diverse external systems, such as distillation towers [1], Kalina cycles, which have higher pressures than a conventional system [2, 3], air conditioning systems, and combustion air cooling for gas turbines and streams in extractive industries such as coal and petroleum [4]. Most of the design and analysis of ARS until a little after the first half of the last century was based on graphical predictions. However, the range of pressures was small, and based only on few experimental data points and theoretical-empirical deductions [5, 6, 7].

The precise thermodynamic properties of the ammonia-water mixture are very important for the calculations in the design of ARS equipment and the prediction of their behaviour; this also applies to the operation of existing systems and their possible improvements. In the past few decades, the analysis of these systems has covered their performance based on both the first and the second law of thermodynamics; this analysis involves the use of the specific entropy value, which is fundamental to improve the prediction and optimization of cycle performance [1, 3, 8, 42]. The more than forty-five published methods for predicting the thermodynamic properties of AWMs have been classified into seven main groups according to Thorin *et al.* [9]. In these groups, there are combinations of cubic equations of state, excess Gibbs energy, corresponding states, perturbation theory, group contributions, and polynomial functions. Other developed methods are the Helmholtz free energy [14], the PC-SAFT equation [26], neural networks [19, 27], and others that mix two or more groups [10-13, 15-18, 20-25, 28-30].

Due to the above, in most cases, the precise estimation of the water concentration in the generator exit (desorber and rectifier) results in over or under design of these components [5, 31]. The disadvantage of some models is the restricted range over which they are valid, and in other cases is the lack of entropy

prediction [32]. Currently, due to the need of predicting exergy balances, the cubic equations of state, which are incorporated in commercial process simulators for such systems analyses, have been used [1, 8]. However, because the mixture in question is highly non-ideal, these equations of state lack the necessary adjustments to accurately predict its properties at ammonia concentrations close to unity. For this reason, many researchers have taken on the task of modifying or generating specialized equations. Nevertheless, there are few models with a wide range of applicability [9, 26, 33].

Here, an ARS has been evaluated according to both the first and the second law of thermodynamics, and the energy and irreversibility, with the aim of finding differences between three mathematical models for predicting thermodynamic properties [14, 18, 35]. A base case from the literature [34], in which the thermodynamic properties were calculated via a mathematical model based on Gibbs free energy, was employed to compare to the results obtained from the three methods herein considered.

II. METHODOLOGY

We used three different methods to obtain the thermodynamic properties of the operating conditions given in the proposed base case [34]. M1, a model developed by Ibrahim and Klein [35], is implemented in the commercial program Engineering Equation Solver (EES); M2, proposed by Tillner-Roth and Friend [14], is implemented in REFPROP v.8.0 developed by the National Institute of Standards and Technology (NIST); and M3, proposed by Xu and Goswami [18], was developed from work by Ibrahim and Klein, El-Sayed and Tribus, and Ziegler and Trepp [35-38, 40]. To carry out this analysis, the latter methodology [18] was programmed and validated [5, 12, 39, 43].

The analysed ARS [34] consisted of a simple single effect ammonia-water cycle with a solution heat exchanger and a pre-cooler (super heater), which had fourteen streams and ten components (Fig. 1).

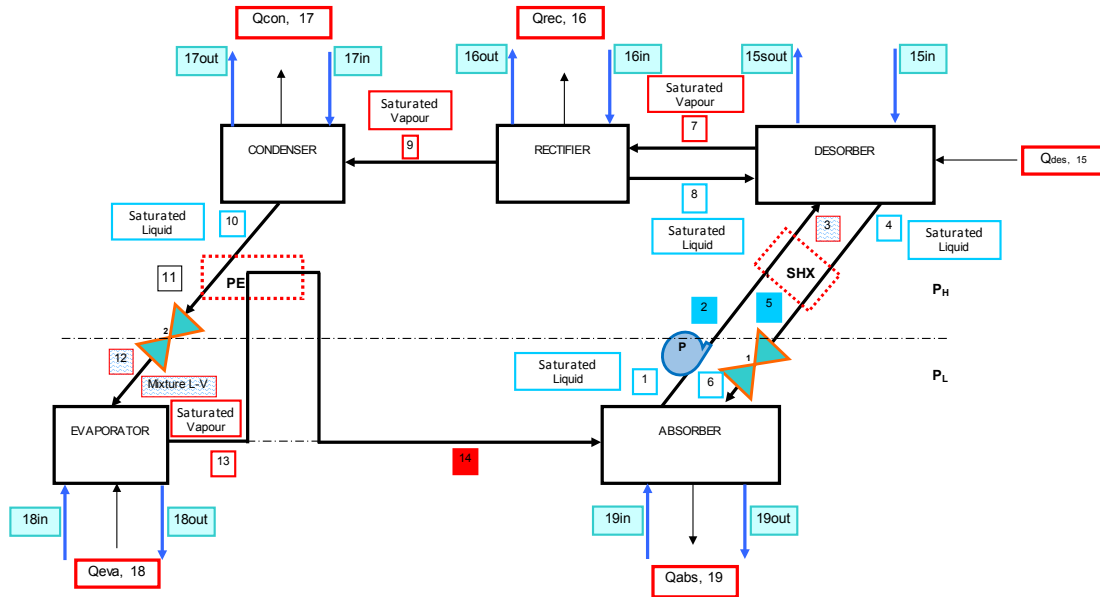


FIG. 1. Absorption Refrigeration System (ARS).

The initial conditions and mass and energy balance equations for the corresponding analyses under the

first and second laws of thermodynamics are given in tables 1 and 2.

TABLE 1

CONSIDERATIONS FOR THE ANALYSES WITH THE THREE MODELS EMPLOYED

Solution heat exchanger efficiency 95 (SHX)	95 %
Ammonia concentration in the mixture x_9 and z_9	0.999634
Solution pump isentropic efficiency	50 %
Ambient reference conditions	$T_0=303$ K $P_0=0.1013$ MPa
Constants*	$\alpha=100$ $\beta=350$
Conditions*	$p_{13}=p_{12}=p_1=p_6$ $p_2=p_3=p_4=p_5=p_7=p_8=p_9=p_{10}$ $p_1=p_6$ $x_9=x_{10}=x_{12}=x_{13}$ $x_1=x_2=x_3=x_8 > x_4=x_5=x_6$ $t_2=t_5$ $t_7=t_8$ $t_{10}=t_1$ $h_6 = h_5; h_{11} = h_{12}$

*Where α and β are random constants; x is the mass fraction of ammonia in the corresponding stream [41].

TABLE 2
EQUATIONS FOR THE MASS, ENERGY AND EXERGY BALANCES IN THE ARS UNDER ANALYSIS

Equation	No.	Equation	No.
Pump $W_p = (P_H - P_L) \frac{v_1 \dot{m}_1}{\eta_p}$ $\dot{m}_1 h_1 + \dot{W}_p = \dot{m}_2 h_2$	(1) (2)	Solution ratio $f = \frac{x_9 - x_4}{x_3 - x_4}$	(18)
Absorber $\dot{m}_{14} + \dot{m}_6 = \dot{m}_1$ $\dot{m}_{14} x_{14} + \dot{m}_6 x_6 = \dot{m}_1 x_1$ $\dot{m}_{14} h_{14} + \dot{m}_6 h_6 = \dot{m}_1 h_1 + \dot{Q}_{abs}$	(3) (4) (5)	Irreversibility $Irr = T_0 \left[\sum_{ent} \dot{m} s - \sum_{out} \dot{m} s \right]$	(19)
Desorber $\dot{m}_3 h_3 + \dot{Q}_{des} = \dot{m}_4 h_4 + \dot{m}_9 h_9 + \dot{Q}_{rec}$ $\dot{m}_7 h_7 + \dot{m}_4 h_4 = \dot{m}_8 h_8 + \dot{m}_3 h_3 + \dot{Q}_{des}$ $\dot{Q}_{des} = \dot{m}_7 [h_7 - h_4 + f(h_4 - h_3)] + \dot{Q}_{rec}$ $\dot{m}_7 + \dot{m}_4 = \dot{m}_8 + \dot{m}_3$ $\dot{m}_7 x_7 + \dot{m}_4 x_4 = \dot{m}_8 x_8 + \dot{m}_3 x_3$	(6) (7) (8) (9) (10)	Exergy $ex = (h - T_0 s) + \alpha + \beta x$ [41]	(20)
Condenser $\dot{Q}_{con} = \dot{m}_9 (h_9 - h_{10})$	(11)	Evaporator $\dot{Q}_{eva} = \dot{m}_{13} (h_{13} - h_{12})$	(21)
Heat Exchanger Solution (shx) $Q_{shx} = m_1 (h_3 - h_2)$ $\dot{m}_2 h_2 + \dot{m}_4 h_4 = \dot{m}_3 h_3 + \dot{m}_5 h_5$	(12) (13)	Coefficient of Performance (COP) $COP = \frac{\dot{Q}_{eva}}{\dot{W}_p + \dot{Q}_{des}}$	(22)
Rectifier $\dot{m}_7 = \dot{m}_9 + \dot{m}_8$ $\dot{m}_7 x_7 = \dot{m}_9 x_9 + \dot{m}_8 x_8$ $\dot{m}_7 h_7 = \dot{m}_9 h_9 + \dot{m}_8 h_8 + \dot{Q}_{rec}$ $\dot{Q}_{rec} = \dot{m}_7 [h_7 - h_8 + r(h_8 - h_9)]$	(14) (15) (16) (17)		

The matrix shown in Fig. 2 was used to solve the system mass, energy and exergy balances with vectors corresponding to the streams in the system.

No. Equipment	Streams																									
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15ent	15out	16ent	16out	17ent	17out	18ent	18out	19ent	19out	20	
1 Absorber	-1	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	-1	0
2 Pump	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
3 Ed 1	0	0	0	0	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4 SHX	0	1	-1	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5 Desorber	0	0	1	-1	0	0	-1	1	0	0	0	0	0	0	1	-1	0	0	0	0	0	0	0	0	0	0
6 Rectifier	0	0	0	0	0	0	1	-1	-1	0	0	0	0	0	0	0	1	-1	0	0	0	0	0	0	0	0
7 Condenser	0	0	0	0	0	0	0	0	1	-1	0	0	0	0	0	0	0	0	1	-1	0	0	0	0	0	0
8 PE	0	0	0	0	0	0	0	0	0	1	-1	0	1	-1	0	0	0	0	0	0	0	0	0	0	0	0
9 Ed 2	0	0	0	0	0	0	0	0	0	0	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10 Evaporator	0	0	0	0	0	0	0	0	0	0	0	1	-1	0	0	0	0	0	0	0	1	-1	0	0	0	0
11 Environment	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	1	-1	1	-1	1	-1	1	-1	1	-1	-1
12 Balance	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

FIG. 2. Matrix used to solve mass, energy and exergy balances

III. RESULTS AND DISCUSSION

A. First law analysis

Tables 3 through 6 show the thermodynamic properties for each stream. Table 3 reports the data from the base case, which were compared to the other models: M1, M2 and M3. The data obtained from Model 1 (EES) showed differences with respect to the base case; however, no property (P, t, z) differed by more than 3 % (Table 4). Table 5 shows the data obtained using M2, implemented in the REFPROP NIST software. The differences in hm and sm compared to the base

case and M1 (Table 5) are mainly due to the fact that the reference properties from which the predictive model works are different [33]; nonetheless, when these properties (P, t, z) were compared, the percentage difference in pressure reached more than 10 %. For M3 (Table 6), the values were very similar to the base case and M1. Notwithstanding, there were differences in enthalpy and entropy in relation to M2 due to the reasons given above. The maximum percentage difference in P, t and z was in pressure, which was 6.036 %. The differences in temperature and concentration did not exceed 3 % in any of the models. M1, M2 and M3 have an extra column that corresponds to the entropy vector values (s_m).

TABLE 3
BASE CASE PROPERTIES [34]

Stream	h _m	m	Qvap	P	t	z (kg/kg)
1	-42.3	1.000	0.000	0.2402	40.0	0.368
2	-39.2	1.000	----	1.555	40.5	0.368
3	306.8	1.000	0.022	1.555	110.7	0.368
4	401.6	0.863	0.000	1.555	131.0	0.268
5	0.9	0.863	----	1.555	40.5	0.268
6	0.9	0.863	----	0.2402	40.7	0.268
7	1547	0.150	1.000	1.555	108.0	0.9444
8	264.1	0.013	0.000	1.555	108.0	0.368
9	1294	0.137	1.000	1.555	44.0	0.999634
10	190.1	0.137	0.004	1.555	40.0	0.999634
11	88.5	0.137	----	1.555	17.7	0.999634
12	88.5	0.137	0.119	0.2402	-14.5	0.999634
13	1264	0.137	0.998	0.2402	-10.0	0.999634
14	1372	0.137	----	0.2402	37.4	0.999634

TABLE 4
PROPERTIES CALCULATED BY M1 (EES) [35]

Stream	h _m	s _m	m	Qvap	P	t	z (kg/kg)	ADiff. (P)	ADiff. (t)	ADiff. (z)	PDiff. (P)	PDiff. (t)	PDiff. (z)
1	-43.258	0.472	1.000	0.000	0.2449	40.0	0.371	-0.0047	0.0000	0.0030	-1.957	0.000	0.815
2	-40.215	0.477	1.000	----	1.556	40.4	0.371	-0.001	0.1000	0.0030	-0.064	0.247	0.815
3	302.146	1.454	1.000	0.021	1.556	110.0	0.371	-0.001	0.7000	0.0030	-0.064	0.632	0.815
4	396.092	1.641	0.863	0.000	1.556	130.3	0.271	-0.001	0.7000	0.0030	-0.064	0.534	1.119
5	-0.724	0.531	0.863	----	1.556	40.4	0.271	-0.001	0.1000	0.0030	-0.064	0.247	1.119
6	-0.724	0.535	0.863	----	0.2449	40.7	0.271	-0.0047	0.0000	0.0030	-1.957	0.000	1.119
7	1544.008	4.882	0.150	1.000	1.556	107.3	0.9460	-0.001	0.7000	0.0016	-0.064	0.648	0.169
8	259.733	1.343	0.013	0.000	1.556	107.3	0.371	-0.001	0.7000	0.0030	-0.064	0.648	0.815
9	1308.905	4.218	0.137	1.000	1.556	44.7	0.999634	-0.001	-0.7000	0.00000	-0.064	-1.591	0.000
10	195.167	0.672	0.137	0.004	1.556	40.0	0.999634	-0.001	0.0000	0.00000	-0.064	0.000	0.000
11	82.958	0.301	0.137	----	1.556	17.8	0.999634	-0.001	-0.1000	0.00000	-0.064	-0.565	0.000
12	82.958	0.338	0.137	0.112	0.2449	-14.1	0.999634	-0.0047	-0.4000	0.00000	-1.957	2.759	0.000
13	1258.828	4.861	0.137	0.998	0.2449	-10.0	0.999634	-0.0047	0.0000	0.00000	-1.957	0.000	0.000
14	1371.036	5.249	0.137	----	0.2449	37.4	0.999634	-0.0047	0.0000	0.00000	-1.957	0.000	0.000

TABLE 5
PROPERTIES CALCULATED BY M2 (REFPROP-NIST) [14]

Stream	h _m	s _m	m	Q _{vap}	P	t	z (kg/kg)	ADiff. (P)	ADiff. (t)	ADiff. (z)	PDiff. (P)	PDiff. (t)	PDiff. (z)
1	68.736	0.940	1.000	0.000	0.2411	40.000	0.372	-0.0009	0.0000	0.0040	-0.375	0.000	1.087
2	70.264	0.940	1.000	----	1.555	40.102	0.372	0.0000	0.3980	0.0040	0.000	0.983	1.087
3	427.057	1.959	1.000	0.023	1.555	110.852	0.372	0.0000	-0.1520	0.0040	0.000	-0.137	1.087
4	488.011	2.002	0.862	0.000	1.555	131.000	0.271	0.0000	0.0000	0.0030	0.000	0.000	1.119
5	73.972	0.844	0.862	----	1.555	40.102	0.271	0.0000	0.3980	0.0030	0.000	0.983	1.119
6	73.972	0.848	0.862	----	0.2411	40.355	0.271	-0.0009	0.3450	0.0030	-0.375	0.848	1.119
7	1871.768	3.825	0.151	1.000	1.555	108.268	0.9449	0.0000	-0.2680	0.0005	0.000	-0.248	0.053
8	386.909	1.854	0.013	0.000	1.555	108.268	0.372	0.0000	-0.2680	0.0040	0.000	-0.248	1.087
9	1650.128	5.681	0.138	1.000	1.555	44.910	0.999634	0.0000	-0.9100	0.00000	0.000	-2.068	0.000
10	533.336	2.116	0.138	0.000	1.555	40.000	0.999634	0.0000	0.0000	0.00000	0.000	0.000	0.000
11	417.087	1.730	0.138	----	1.555	15.823	0.999634	0.0000	1.8770	0.00000	0.000	10.605	0.000
12	417.087	1.753	0.138	0.000	0.2411	-14.500	0.999634	-0.0009	0.0000	0.00000	-0.375	0.000	0.000
13	1593.431	6.314	0.138	0.997	0.2411	-10.845	0.999634	-0.0009	0.8450	0.00000	-0.375	-8.450	0.000
14	1709.679	6.722	0.138	----	0.2411	37.500	0.999634	-0.0009	-0.1000	0.00000	-0.375	-0.267	0.000

TABLE 6
PROPERTIES CALCULATED BY M3 [18]

Stream	h _m	s _m	m	Q _{vap}	P	t	z (kg/kg)	ADiff. (P)	ADiff. (t)	ADiff. (z)	PDiff. (P)	PDiff. (t)	PDiff. (z)
1	-41.207	0.475	1.000	0.000	0.2414	40.000	0.364	-0.0012	0.0000	-0.0040	-0.500	0.000	-1.087
2	-39.689	0.476	1.000	----	1.553	40.089	0.364	0.0020	0.4110	-0.0040	0.129	1.015	-1.087
3	297.947	1.468	1.000	0.022	1.553	108.592	0.364	0.0020	2.1080	-0.0040	0.129	1.904	-1.087
4	394.207	1.654	0.862	0.000	1.553	129.131	0.262	0.0020	1.8690	-0.0060	0.129	1.427	-2.239
5	2.332	0.536	0.862	----	1.553	40.089	0.262	0.0020	0.4110	-0.0060	0.129	1.015	-2.239
6	2.332	0.540	0.862	----	0.2414	40.360	0.262	-0.0012	0.3400	-0.0060	-0.500	0.835	-2.239
7	1532.892	4.868	0.151	1.000	1.553	105.870	0.94802	0.0020	2.1300	-0.0036	0.129	1.972	0.383
8	254.474	1.327	0.012	0.000	1.553	105.870	0.364	0.0020	2.1300	-0.0040	0.129	1.972	-1.087
9	1295.915	4.187	0.138	1.000	1.553	41.344	0.999634	0.0020	2.6560	0.00000	0.129	6.036	0.000
10	190.727	0.658	0.138	0.000	1.553	40.000	0.999634	0.0020	0.0000	0.00000	0.129	0.000	0.000
11	81.465	0.287	0.138	----	1.553	17.434	0.999634	0.0020	0.2660	0.00000	0.129	1.503	0.000
12	81.465	0.326	0.138	0.113	0.2414	-14.501	0.999634	-0.0012	0.0010	0.00000	-0.500	-0.007	0.000
13	1256.171	4.865	0.138	0.999	0.2414	-10.000	0.999634	-0.0012	0.0000	0.00000	-0.500	0.000	0.000
14	1365.434	5.257	0.138	----	0.2414	37.500	0.999634	-0.0012	-0.1000	0.00000	-0.500	-0.267	0.000

The results from the first law analysis of the system showed slight variations compared to the base case (Table 7). The overall differences were of little significance, even though the solution heat exchanger and the solution pump showed greater variations. In the case of the solution pump, the simulations using REFPROP and M3 had the least difference between each other, compared with their differences from the base case. For the solution heat exchanger, the differences with respect to the base case were the lowest for the EES method and M3, compared to the results with REFPROP. Despite the differences among the various models, the coefficient of performance was substantially the same for all models; hence, any of the models is adequate for first law analysis of the system.

TABLE 7
ARS FIRST LAW PERFORMANCE EVALUATION

	Base Case	M1	M2	M3
		[35]	[14]	[18]
f	7.32	7.29	7.23	7.23
Q _{SHX}	346	342	357	338
Q _{abs}	230	231	231	232
r	----	----	0.913	0.919
Q _{rect}	51	49	50	48
Q _{des}	268	268	272	270
Q _{con}	151	153	154	153
Q _{eva}	161	161	163	163
W _p	3.05	3.00	2.295	2.28
COP	0.595	0.596	0.594	0.599

B. Second law analysis

The irreversibility analysis did not include the base case since no entropy values were reported (Table 8).

TABLE 8
SPECIFIC EXERGY VECTORS FOR EACH MODEL
(KJ/KG)

Stream	M1 [35]	M2 [14]	M3 [18]
1	299.2	269.9	296.9
2	300.8	271.4	298.1
3	347.1	319.5	335.1
4	334.4	316.9	324.0
5	273.9	253.7	270.9
6	272.7	252.5	269.7
7	837.8	1485.2	831.9
8	338.3	311.1	334.4
9	830.7	728.6	827.1
10	791.4	692.0	791.2
11	791.6	692.7	794.3
12	780.4	685.7	782.5
13	585.8	480.1	581.9
14	580.4	472.7	572.4

Table 9 shows the size of the irreversibilities (Irr) for each component (kW), while Table 10 gives the representativity of these irreversibilities as a percentage for each component. All the models gave the same total irreversibility (Overall Irr = 123.339 kW). However, the solution heat exchanger, the desorber, the rectifier and to a lesser degree the absorber were remarkable, since for them there were significant differences among the models and the resulting values of exergy loss. This is due to the differences in the specific entropy calculated by each model in the vapor phase when the ammonia concentration was close to unity. For the other components, the results were very similar and, therefore, they can be considered generally acceptable for a second law analysis and design decisions. The components with the greatest exergy destruction were the desorber, followed by the absorber and the condenser.

TABLE 9
IRREVERSIBILITIES FOR EACH COMPONENT OF
THE ARS

Equipment	M1 [35]	M2 [14]	M3 [18]
	Irr		
Absorber	36.485	37.955	35.186
Pump	0.758	0.759	1.070
Ed 1	1.043	1.223	1.043
SHX	5.783	6.122	8.701
Desorber	51.302	45.713	49.098
Rectifier	0.766	3.565	0.427
Condenser	19.109	18.661	18.640
PE	0.711	0.917	0.878
Ed 2	1.547	0.977	1.631
Evaporator	5.835	7.448	6.665
Global Irr	123.339	123.339	123.339

TABLE 10
IMPORTANCE OF THE IRREVERSIBILITY FOR EACH
COMPONENT OF THE ARS

Equipment	M1 [35]	M2 [14]	M3 [18]
	Irr (%)		
Absorber	29.581	30.773	28.528
Pump	0.614	0.615	0.868
Ed 1	0.845	0.991	0.845
SHX	4.688	4.964	7.054
Desorber	41.594	37.063	39.808
Rectifier	0.621	2.890	0.346
Condenser	15.493	15.129	15.113
PE	0.576	0.743	0.712
Ed 2	1.254	0.792	1.322
Evaporator	4.731	6.038	5.404

IV. CONCLUSIONS

The values of the properties calculated by the three methods (M1, M2 and M3) compared to the base case showed significant differences for only some of the streams, and particularly for the pressure prediction in the case of nearly pure ammonia in the vapour phase. However, when the overall system heat and mass balances were analysed, the differences were small, and in particular, the coefficient of performance was reasonably consistent. When the second law analysis was considered, differences were found in the exergy values for the process streams calculated by the models used in this study. The orders of magnitude of the percentage contributions to the overall irreversibility of the system were consistent among models; that is, desorber, absorber, and condenser were the components with the greatest irreversibilities. Notwithstanding, the observed differences in the overall irreversibility were the same in all cases.

Nomenclature

SHX	Solution heat exchanger
COP	Coefficient of performance
W	Power (kW)
PE	Pre-cooler (or super heater)
Ed	Expansion device
f	Flow ratio
h	Specific enthalpy (kJ kg ⁻¹)
s	Specific entropy (kJ kg ⁻¹ K ⁻¹)
m	Mass flow rate (kg s ⁻¹)
P	Pressure (MPa)
Q	Heat (kW)
Q _{vap}	Vapour fraction
t	Temperature (°C)
T	Absolute temperature (K)
x, z respectively	Fraction mass and mol ammonia respectively
I _{rr}	Irreversibility (kW)
ex	Exergy (kJ kg ⁻¹)
AD _{iif}	Absolute difference
PD _{iff}	Percentage difference

Subindex

rec	rectifier
abs	absorber
con	condenser
des	desorber
eva	evaporator
m	mixture
p	pump
H	high pressure
L	low pressure
0	reference state

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REFERENCES

- [1] A. Rivera, J. Cerezo, R. Rivero, *et al.*, "Single Stage and Double Absorption heat transformers used to recover energy in a distillation column of butane and pentane," *Int J of Energy Research*, vol. 27 (14), pp. 1279-1292, Nov. 2003. DOI: <http://doi.org/10.1002/er.943>.
- [2] A. I. Kalina, "Combined Cycle and waste-heat recovery power systems based on a novel thermodynamic energy cycle utilizing low-temperature heat for power generation," *ASME paper No. 83-JPGC-GT-3*, 1983.
- [3] S. Stecco, and U. Desideri, "A thermodynamic analysis of the kalina cycles: comparisons, problems and perspectives," *Gas Turbine and Aeroengine Congress and Exposition: ASME*, 1989.
- [4] S. H. Rizvi, and R. A. Heidemann, "Vapor-Liquid equilibria in the ammonia-water system," *J Chem Eng Data*, vol. 32 (2), pp. 183-191, Apr. 1987. DOI: <http://doi.org/10.1021/je00048a017>.
- [5] R. A. Macris, B. E. Eakin, R. T. Ellington, *et al.*, "Physical and thermodynamic properties of ammonia-water mixtures," *Research Bulletin No. 14*. Inst. of Gas Technology, 1964.
- [6] R. T. Ellington, G. Kinst, R. E. Peck, *et al.*, "The absorption cooling process," *Research Bulletin*, Institute of Gas Technology, 1957.
- [7] R. Tillner-Roth, and G. Friend, "Survey and Assessment of available measurements on thermodynamic properties of the mixture

- {Water+Ammonia},” *J Phys Chem Ref Data*, vol. 27(1), pp. 45-61, Jan. 1998. DOI: <http://doi.org/10.1063/1.556014>.
- [8] A. Vidal, R. Best, R. Rivero, *et al.*, “Analysis of a combined power and refrigeration cycle by the exergy method,” *Energy*, vol. 31 (15), pp. 3401-3414, Dec. 2006. DOI: <http://doi.org/10.1016/j.energy.2006.03.001>.
- [9] E. Thorin, C. Dejfors, and G. Svedberg, “Thermodynamic properties of ammonia-water mixtures for power cycles,” *Int J Thermophys*, vol. 19(2), pp. 501-510, 1998. DOI: <http://doi.org/10.1023/A:1022525813769>.
- [10] A. A. Zatorskii, “Algorithm for calculation of the parameters of the junction points of the cycles of absorption-type water-ammonia refrigeration machines in a digital computer,” *Plenum Publishing Corporation*, pp. 716-719, 1979.
- [11] K. E. Herold, K. Hain, and M. J. Moran, “AMMWT: A computer program for calculating the thermodynamic properties of ammonia and water mixtures using a Gibbs Free Energy formulation,” *ASME* 4, pp. 65-75, 1988.
- [12] Y. M. Park, and R. E. Sonntag, “Thermodynamic properties of ammonia-water mixtures: a generalized equation-of-state approach,” *ASME Trans*, vol. 97, pp. 150-159, 1991.
- [13] S. N. Mumah, S.S. Adefila, and E.A. Arinze, “Properties generation procedures for first and second law analyses of ammonia-water heat pump system,” *Energy Convers Mgmt*, vol. 35 (8), pp. 727-736, Aug. 1994. DOI: [http://doi.org/10.1016/0196-8904\(94\)90058-2](http://doi.org/10.1016/0196-8904(94)90058-2).
- [14] R. Tillner-Roth, and G. Friend, “A Helmholtz free energy formulation of the thermodynamic properties of the mixture {Water+Ammonia},” *J Phys Chem Ref Data*, vol. 27(1), pp. 63-96, Jan. 1998. DOI: <http://doi.org/10.1063/1.556015>.
- [15] A. Nowarski, and D. G. Friend, “Application of the Extended Corresponding States Method to the Calculation of the Ammonia-Water Mixture Thermodynamic Surface,” *International Journal of Thermophysics*, vol. 19 (4), pp. 1133-1142, 1998. DOI: <http://doi.org/10.1023/A:1022641709904>.
- [16] R. M. Enick, G. P. Donahy, and M. Holsinger, “Modeling the High-Pressure Ammonia-Water System with WATAM and the Peng-Robinson Equation of State for Kalina Cycle Studies,” *Ind Eng Chem Res*, vol. 37 (5), pp. 1644-1650, May. 1998. DOI: <http://doi.org/10.1021/ie970638s>.
- [17] L. A. Weber, “Estimating the virial coefficients of the ammonia + water mixture,” *Fluid Phase Equilibria*, vol. 162 (1-2), pp. 31-49, Aug. 1999. DOI: [http://doi.org/10.1016/S0378-3812\(99\)00181-8](http://doi.org/10.1016/S0378-3812(99)00181-8).
- [18] F. Xu, and D. Y. Goswami, “Thermodynamic properties of ammonia-water mixtures for power-cycle applications,” *Energy*, vol. 24 (6), pp. 525-536, Jun. 1999. DOI: [http://doi.org/10.1016/S0360-5442\(99\)00007-9](http://doi.org/10.1016/S0360-5442(99)00007-9).
- [19] R. Sharma, D. Singhal, R. Ghosh, and A. Dwivedi, “Potential applications of artificial neural networks to thermodynamics: vapor-Liquid equilibrium predictions,” *Computers and Chemical Engineering*, vol. 23 (3), pp. 385-390, Feb. 1999. DOI: [http://doi.org/10.1016/S0098-1354\(98\)00281-6](http://doi.org/10.1016/S0098-1354(98)00281-6).
- [20] R. Lugo, J. Guilpart, and L. Fournaison, “Calculation method of thermophysical properties of ammonia-water mixtures,” *Presentacion Second Workshop on Ice Slurries, Paris France: International Institute of Refrigeration*, 2000.
- [21] A.A. Vasserman, A. G. Slyenko, S. V. Bodyul, *et al.*, “A Thermophysical Property Databank for Technically Important Gases and Liquids,” *International Journal of Thermodynamics*, vol. 22 (2), pp. 477-485, 2001. DOI: <http://doi.org/10.1023/A:1010774831521>.
- [22] R. Lugo, L. Fournaison, J. M. Chourot, *et al.*, “An excess function method to model the thermophysical properties of one-phase secondary refrigerants,” *International Journal of Refrigeration*, vol. 25 (7), pp. 916-923, Nov. 2002. DOI: [http://doi.org/10.1016/S0140-7007\(01\)00105-0](http://doi.org/10.1016/S0140-7007(01)00105-0).
- [23] R. Span, and W. Wagner, “Equations of State for Technical Applications. I. Simultaneously Optimized Functional Forms for Nonpolar and Polar Fluids,” *Int J of Thermophysics*, vol. 24 (1), pp. 1-39, 2003. DOI: <http://doi.org/10.1023/A:1022390430888>.
- [24] R. Span, and W. Wagner, “Equations of State for Technical Applications. III. Results for Polar Fluids,” *Int J of Thermophysics*, vol. 24 (1), pp. 111-162, 2003. DOI: <http://doi.org/10.1023/A:1022362231796>.
- [25] M. Barhoumi, A. Snoussi, E. N. Ben, *et al.*, “Modélisation des données thermodynamiques du mélange ammoniac/eau,” *Int J Refrig*, vol. 27 (3), pp. 271-283, May. 2004. DOI: <http://doi.org/10.1016/j.ijrefrig.2003.09.005>.
- [26] Kh. Mejbri, and A. Bellagi, “Modelling of the thermodynamic properties of the water-ammonia mixture by three different approaches,” *Int J Refrig*, vol. 29 (2), pp. 211-218, Mar. 2006. DOI: <http://doi.org/10.1016/j.ijrefrig.2005.06.002>.
- [27] A. Sencan, “Artificial intelligent methods for thermodynamic evaluation of ammonia-water refrigeration system,” *Energy Conv & Man*, vol. 47, pp. 3319-3332, 2006. DOI: <http://doi.org/10.1016/j.enconman.2006.01.002>.
- [28] A. H. Farokh-Niae, H. Moddarress, and M. Mohsen-Nia, “A three-parameter cubic equation of state for prediction of thermodynamic properties of fluids,” *J Chem Thermodynamics*, vol. 40 (1), pp. 84-95, Jan. 2008. DOI: <http://doi.org/10.1016/j.jct.2007.05.012>.
- [29] N. S. Ganesh, and T. Srinivas, “Evaluation of thermodynamic properties of ammonia-water mixture up to 100 bar for power application systems,”

- Journal of Mechanical Engineering Research*, vol. 3(1), pp. 25-39, 2011.
- [30] K. Sadhukhan, A. K. Chowdhury, and B. K. Mandal, "Computer Based Thermodynamic Properties of Ammonia-Water Mixture for the Analysis of Power and Refrigeration Cycles," *Int J of Thermodynamics*, vol. 12(3), pp. 133-139, 2012. DOI: <http://doi.org/10.5541/ijot.375>.
- [31] E. Thorin, "Thermophysical properties of ammonia-water mixtures for prediction of heat transfer areas in power cycles," *Int J Thermophys*, vol. 22(1), pp. 201-214, 2001. DOI: <http://doi.org/10.1023/A:1006745100278>.
- [32] J. Pátek, and J. Klomfar, "Simple functions for fast calculations of selected thermodynamic properties of the ammonia-water system," *Int J Refrig*, vol. 18(4), pp. 228-234, May. 1995. DOI: [http://doi.org/10.1016/0140-7007\(95\)00006-W](http://doi.org/10.1016/0140-7007(95)00006-W).
- [33] E. Thorin, "Comparison of correlations for predicting thermodynamic properties of ammonia-water mixtures," *Int J Thermophys*, vol. 21(4), pp. 853-870, 2000. DOI: <http://doi.org/10.1023/A:1006658107014>.
- [34] K. E. Herold, R. Radermacher, and S. A. Klein, "Absorption chillers and heat pump," CRC Press Inc, USA, 1996.
- [35] O. M. Ibrahim, and S. A. Klein, "Thermodynamic properties of ammonia-water mixtures," *ASHRAE Trans*, pp. 1495-1502, 1993.
- [36] F. Xu, and D. Y. Goswami, "Erratum to: Thermodynamic properties of ammonia-water mixture for power-cycle applications," *Energy*, vol. 24 (1999), pp. 525-536, *Energy*, vol. 27 (6), p. 203, Jun. 2002. DOI: [http://doi.org/10.1016/S0360-5442\(99\)00007-9](http://doi.org/10.1016/S0360-5442(99)00007-9).
- [37] C. Martin, "Study of cooling production with a combined power and cooling thermodynamic cycle," Ph. D. Thesis, University of Florida, USA. 2004.
- [38] Y. M. El-Sayed, and M. Tribus, "Thermodynamic properties of water ammonia mixtures theoretical implementation for use in power cycles analysis," Special publication AES (1) New York, ASME, pp. 89-95, 1985.
- [39] P. C. Gillespie, W. V. Wilding, and G. M. Wilson, "Vapor-Liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K," *AIChE Symp Ser*, vol. 83(256), pp. 97-127, 1987.
- [40] B. Ziegler, and Ch. Trepp, "Equation of state for ammonia-water mixtures," *Int J Refrig*, vol. 7 (2), pp. 101-106, Mar. 1984. DOI: [http://doi.org/10.1016/0140-7007\(84\)90022-7](http://doi.org/10.1016/0140-7007(84)90022-7).
- [41] A.A. Hasan, and D. Y. Goswami, "Exergy analysis of a Combined Power and Refrigeration Thermodynamic Cycle Driven by a Solar Heat Source," *Journal of Solar Energy Engineering*, vol. 125 (1), pp. 55-60, 2003. DOI: <http://doi.org/10.1115/1.1530628>.
- [42] D. Boer, B. H. Gebreslassie, M. Medrano, *et al.*, "Effect of internal heat recovery in ammonia-water absorption cooling cycles: exergy and structural analysis," vol. 12(1), pp. 17-27, Mar. 2009.
- [43] I. Vera-Romero and Ch. L. Heard-Wade, "Desarrollo de una aplicación para el cálculo de las propiedades de la mezcla amoniaco-agua," *Revista Ingeniería Investigación y Desarrollo*, vol. 17(2), pp. 58-72, Jun. 2017. DOI: <http://doi.org/10.19053/1900771X.v17.n2.2017.7185>.

