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MODELING AND SIMULATION OF THE ABSORBER OF AN ABSORPTION REFRIGERATION SYSTEM

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Abstract. *The increasing energy demand and use of HVAC-R equipment make the use of absorption refrigerators an excellent alternative in the quest for sustainability. In addition, they allow for the use of waste heat as energy input, therefore becoming potentially more efficient than the vapor compression refrigeration cycle. Thus, in order to became absorption refrigerators increasingly commercially competitive, both economically and thermodynamically, this study presents a transient mathematical modeling and the computational simulation of the absorber of an absorption refrigeration system. The model equations were based on the application of the mass and energy conservation principles in a transient regime for this component. The absorber was modeled as a single control volume. Finally, with the developed mathematical model, a computational code was elaborated in Fortran® 95 language, which allowed obtaining the numerical and transient concentration responses of the chemical species present in this absorption refrigerator component. The mathematical model resulted in a system of ordinary differential equations which were integrated at time and using the* $4^{th}/5^{th}$ *order Runge-Kutta Fehlberg method. As a result, the proposed model can be a useful tool for simulation of the absorber in absorption refrigeration systems with transient operation because presents the concentration distribution over time and that, subsequently, used for testing different conditions of operation and optimization procedures.*

Keywords: *Absorber Component, Absorption Refrigeration System, Mathematical Modeling, Fortran® Programming and Numerical Simulation.*

1. INTRODUCTION

According to the latest National Energy Balance released by the Ministry of Mines and Energy in 2016, the industrial sector accounted for approximately 37.6% of Brazil's electricity consumption in 2015, followed by residential (25.1%) and commercial (17.5%). If these three sectors are taken into account together, it is possible to affirm that they consume more than 80% of all electricity consumed in the country. In these sectors, refrigeration systems account for a significant portion of total electricity consumption. Taking into account only the residential and commercial sectors data, it is possible to affirm that, approximately, 11.8% of the total electricity consumption in Brazil is destined to the several refrigeration systems, e.g., HVAC-R (Brazil MME, 2016).

Therefore, any technological-scientific measure with the aim of reducing the energy consumption of HVAC-R systems will represent an unequivocal contribution to the search for solutions to the growing world energy demand (Cardoso and Nogueira, 2007). Thus, in the saving and reducing electricity consumption context and taking into account the high energy consumption of HVAC-R and refrigeration systems, we highlight the refrigeration systems that use alternative sources of energy as, for example, the absorption refrigeration systems that can be fed by residual heat and solar energy, thus dispensing with the use of energy considered traditional and in most cases causing damage to the environment.

In absorption systems, a physicochemical process replaces the mechanical process of the vapor compression system by using energy in the form of heat rather than mechanical work (Moran and Shapiro, 2009). The absorption refrigeration ammonia-water cycle has some attractive features when compared to conventional compression cycle, e.g. no use of oil; if there is waste heat available, operating costs drop considerably; little consumption of electric energy and it produces no noise other than pumps (Hudson, 2002). The disadvantages of the absorption refrigeration systems include: higher capital investment is needed, the hardware is more complex and more space required. In Brazil the installed absorption refrigeration capacity is relatively small, despite the potential for it in different economy sectors (Cortez, Muhle and Silva, 1994).

Regarding the scientific and technical literature, there are several studies developed in order to mathematically model and computationally simulate the dynamic behavior of absorption refrigeration systems. For example, Vargas et al. (2000) developed a dimensionless mathematical model and internally reversible, i.e., when there are no internal irreversibility's or when the same are in the boundary of the system, of an absorption refrigeration unit thermally driven through a fuel burner. Chua, Toh and Ng (2002) developed a stationary model taking into account the irreversibility's of an absorption refrigeration system, as well as a careful thermodynamic analysis applied to the generator, the rectifier and the absorber, since in these components the liquid and the vapor are not in thermodynamic equilibrium.

Among dynamic simulation models, recently, Kim and Park (2007) presented a model for a particular type of absorption chiller, therefore not general for all types of single effect absorption refrigeration systems. Vargas et al. (2009) proposed a mathematical model, based on empirical and fundamental correlations, in addition to the principles of classical thermodynamics and heat and mass transfer, in order to simulate the behavior, in transient and permanent regimes, of a cogeneration system developed to, simultaneously, generate heating and cooling, under different design and operation conditions. Finally, Martinho et al. (2016) proposed a semi-transient dimensionless mathematical model to analyze the dynamic behavior of single-stage absorption refrigeration systems according to several geometric and operation parameters.

Considering these technical works and scientific studies presented above, it is possible to affirm that, according to the survey carried out by the authors, no articles were found that take into account a fully transient mathematical analysis of absorption refrigeration systems. In this way, it is possible to define the objective of this study as an initial mathematical modeling and computational simulation, in a transient regime of operation, programmed in Fortran® 95 for the absorber of absorption refrigeration systems.

2. MATHEMATICAL MODEL

2.1 The Physical Problem

The physical problem constitutes the configuration of the absorber of an absorption refrigeration system as the division of the component in only one control volume, but considered five volume elements to analyze all chemical constituent present in this component, as showed in Fig. (1). Figure (1) shows the schematic representation of the absorber, a component responsible for absorbing vapor produced in the evaporator by an ammonia-water solution, poor/weak in ammonia, producing a rich/strong ammonia solution with heat release, once that the absorption process, represented by the chemical reaction $NH_3 + H_2O \rightleftarrows NH_4^+ + OH^-$, is exothermic.

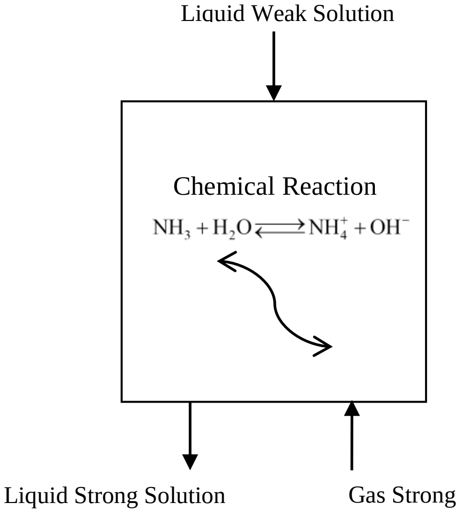

Figure 1. Schematic Representation of the Absorber with the Chemical Reaction.

2.2 Mathematical Equations

In the absorber occurs the absorption process of ammonia in the form of superheated vapor from the evaporator by the weak solution exiting of a regenerative heat exchanger. Thus, within this control volume there are two phases in contact producing a liquid solution concentrated in ammonia (Martinho et al., 2016). The absorber was considered to be a single control volume, and this was subdivided into five volume elements. Taking into account that the chemical reaction that occurs in the absorber can be expressed by:

$$NH_3 + H_2O \rightleftarrows NH_4^+ + OH^- \tag{01}$$

it is possible to determine, based on the mass balance, the concentration-time variation equations of five chemical components present in the absorber and, each of them, being considered one element of volume: ammonia in the liquid phase, ammonia gas, liquid water, water vapor and ion ammonium (considerable product in the reaction). The concentration variation of the ammonia in the liquid phase ($[NH_{3,liq}]$) can be expressed by:

$$\frac{d[NH_{3,liq}]}{dt} = C_1 + C_2 - C_3 \tag{02}$$

where:

$$C_1 = \frac{q_{liq}}{V_{liq}}\left([NH_{3,liq,in}] - [NH_{3,liq}]\right) \tag{03}$$

$$C_2 = \frac{kLa^{Abs}_{NH_3}\left(x^*_{Abs,NH_3} - x_{Abs,NH_3}\right) \cdot n_{tot} \cdot \bar{M}_{NH_3}}{V_{liq}} \tag{04}$$

$$C_3 = K_{NH_3} \cdot [NH_{3,liq}] \cdot [H_2O_{liq}] \tag{05}$$

where q_{liq} is the volumetric flow of liquid, V_{liq} represents the volume of liquid in the absorber, $[NH_{3,liq,in}]$ denotes the initial liquid ammonia concentration in the CV, $kLa^{Abs}_{NH_3}$ is the mass transfer coefficient for ammonia in the absorber, x^*_{Abs,NH_3} represents the ammonia molar fraction in this CV, n_{tot} corresponds to total moles number of the solution present in the absorber, $\bar{M}_{NH_3}$ is the molar mass of ammonia and K_{NH_3} represents the chemical reaction constant of ammonia.

Similarly to that developed for liquid ammonia in Eq. (02), the concentration variation of the water in the liquid phase ($[H_2O_{liq}]$) can be expressed by:

$$\frac{d[H_2O_{liq}]}{dt} = C_4 + C_5 - C_6 \tag{06}$$

where:

$$C_4 = \frac{q_{liq}}{V_{liq}}\left([H_2O_{liq,in}] - [H_2O_{liq}]\right) \tag{07}$$

$$C_5 = \frac{kLa^{Abs}_{H_2O}\left(x^*_{Abs,H_2O} - x_{Abs,H_2O}\right) \cdot n_{tot} \cdot \bar{M}_{H_2O}}{V_{liq}} \tag{08}$$

$$C_6 = K_{H_2O} \cdot [NH_{3,liq}] \cdot [H_2O_{liq}] \tag{09}$$

where $[H_2O_{liq,in}]$ denotes the initial liquid water concentration in the CV, $kLa^{Abs}_{H_2O}$ is the mass transfer coefficient for water in the absorber, x^*_{Abs,H_2O} represents the molar fraction of water in this CV, $\bar{M}_{H_2O}$ is the molar mass of water and K_{H_2O} represents the reaction constant of water. In addition, the equations showing the time concentration variation of the ammonium ion ($[NH^+_{4,liq}]$), the water vapor ($[H_2O_{gas}]$) and gaseous ammonia ($[NH_{3,gas}]$) can be described, respectively, by:

$$\frac{d[NH^+_{4,liq}]}{dt} = C_7 + C_3 \tag{10}$$

$$\frac{d[H_2O_{gas}]}{dt} = C_8 - C_9 \quad (11)$$

$$\frac{d[NH_{3,gas}]}{dt} = C_{10} - C_{11} \quad (12)$$

where:

$$C_7 = \frac{q_{liq}}{V_{liq}}\left([NH^+_{4,liq,in}] - [NH^+_{4,liq}]\right) \quad (13)$$

$$C_8 = \frac{q_{gas}}{V_{gas}}\left([NH_{3,gas,in}] - [NH_{3,gas}]\right) \quad (14)$$

$$C_9 = \frac{kLa^{Abs}_{NH_3}\left(x^*_{Abs,NH_3} - x_{Abs,NH_3}\right)\cdot n_{tot}}{V_{gas}} \quad (15)$$

$$C_{10} = \frac{q_{gas}}{V_{gas}}\left([H_2O_{gas,in}] - [H_2O_{gas}]\right) \quad (16)$$

$$C_{11} = \frac{kLa^{Abs}_{H_2O}\left(x^*_{Abs,H_2O} - x_{Abs,H_2O}\right)\cdot n_{tot}}{V_{gas}} \quad (17)$$

and C_3, utilized in Eq. (10), is calculated through Eq. (05). Besides it, the terms n_{tot}, x_{Abs,NH_3}, x_{Abs,H_2O}, x^*_{Abs,NH_3} and x^*_{Abs,H_2O} can be obtained through:

$$n_{tot} = n_{NH_3} + n_{H_2O} + n_{NH_4^+} \quad (18)$$

$$x_{Abs,NH_3} = \frac{n_{NH_3}}{n_{tot}} \quad (19)$$

$$x_{Abs,H_2O} = \frac{n_{H_2O}}{n_{tot}} \quad (20)$$

$$x^*_{Abs,NH_3} = 0.067 \cdot p_{sat,NH_3} + 0.245 \quad (21)$$

$$x^*_{Abs,H_2O} = \frac{[H_2O_{gas}]\cdot R \cdot T_{emp}}{p_{sat,H_2O}} \quad (22)$$

with:

$$p_{sat,NH_3} = 10^{A_{NH3} - \frac{B_{NH3}}{T_{emp} + C_{NH3}}} \quad (23)$$

$$p_{sat,H_2O} = 10^{A_{H2O} - \frac{B_{H2O}}{T_{emp} + C_{H2O}}} \quad (24)$$

where all numerical terms are considered constant for the absorber are shown in Table 1.

Table 1. Numerical Constants used in Absorber Component Simulation.

Variables	Numerical Value	Units
$\bar{M}_{NH_3}$	17	[g.mol^{-1}]
$\bar{M}_{H_2O}$	18	[g.mol^{-1}]
q_{liq}	5.0	[Lh^{-1}]
q_{gas}	2000	[Lh^{-1}]
V_{liq}	0.1	[L]
V_{gas}	0.01	[L]
R	0.082057338	[ATM.L.mol^{-1}.K^{-1}]
T_{emp}	300	[K]
A_{NH_3}	4.86	[-]
B_{NH_3}	1113.9	[-]
C_{NH_3}	-10.409	[-]
A_{H_2O}	4.65	[-]
B_{H_2O}	1435.2	[-]
C_{H_2O}	-64.840	[-]
$kLa_{NH_3}^{Abs}$	3.0	[s^{-1}]
$kLa_{H_2O}^{Abs}$	3.0	[s^{-1}]
K_{NH_3}	100	[Ls^{-1}g^{-1}]
K_{H_2O}	100	[Ls^{-1}g^{-1}]

2.3 Numerical Method

The numerical results were produced with a code written in Fortran®-based mathematical model described in Section 2.2 and the system of ordinary differential and algebraic equations was numerically integrated in time using the 4th-5th order Runge-Kutta method with some initial conditions, as showed in Table 2.

Table 2. Initial Conditions for Absorber.

Variables	Numerical Value	Units
$[NH_{3,liq,in}]$	25	[gL^{-1}]
$[H_2O_{liq,in}]$	950	[gL^{-1}]
$[NH^+_{4,liq,in}]$	25	[gL^{-1}]
$[NH_{3,gas,in}]$	0	[gL^{-1}]
$[H_2O_{gas,in}]$	0	[gL^{-1}]

3. NUMERICAL RESULTS AND DISCUSSIONS

The results presented for the absorber are the variations of the concentrations over time of the reactants and products of the chemical reaction occurring in this component, as shown in Eq. (01). Such reagents and products are: ammonia in the liquid phase, water in the liquid phase, ion ammonium and gaseous ammonia. The simulation time of the absorber was conducted during 0.5 hours. All the analyzed chemical components reached the stead state at times inferior to the one of computational simulation. Figure (2) shows the variation of the ammonia concentration in the liquid phase with respect to time. As a simulation condition, the initial concentration of [$NH_{3,liq}$] was assumed to be 25 [gL^{-1}]. After the simulation began, this concentration dropped dramatically to 0.3 [gL^{-1}] and, after 0.10 [h], reached a steady state at 0.789 [gL^{-1}].

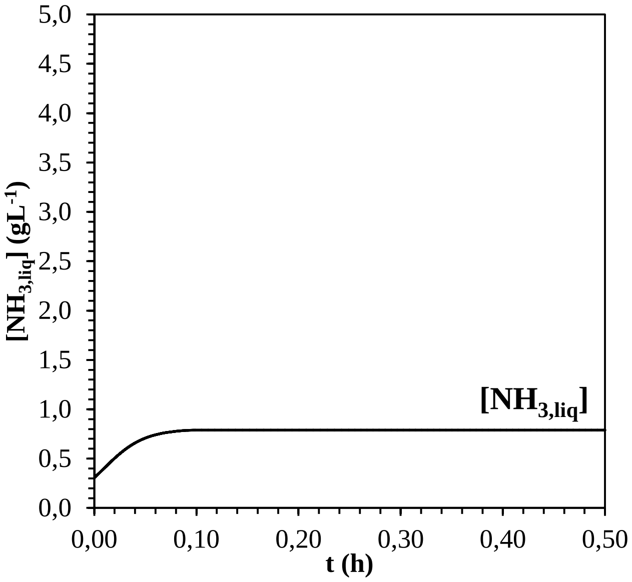

Figure 2. Concentration Distribution of $NH_{3,liq}$ in Absorber.

Figure (3) shows the variation of the water concentration in the liquid phase with respect to time. As a simulation condition, the initial concentration of [H_2O_{liq}] was assumed to be 950 [gL^{-1}]. After the computational simulation began, this concentration reached a steady state at 348.82 [gL^{-1}] in 0.01 [h]. As in the case of liquid ammonia ([$NH_{3,liq}$]), shown in Fig. (2), the liquid water concentration ([H_2O_{liq}]) is also reduced, since both chemical components are the reactants of the reaction shown in Eq. (01).

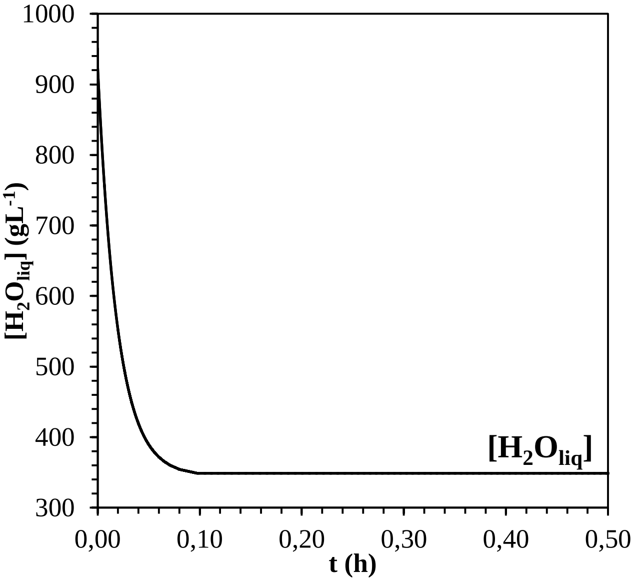

Figure 3. Concentration Distribution of H_2O_{liq} in Absorber.

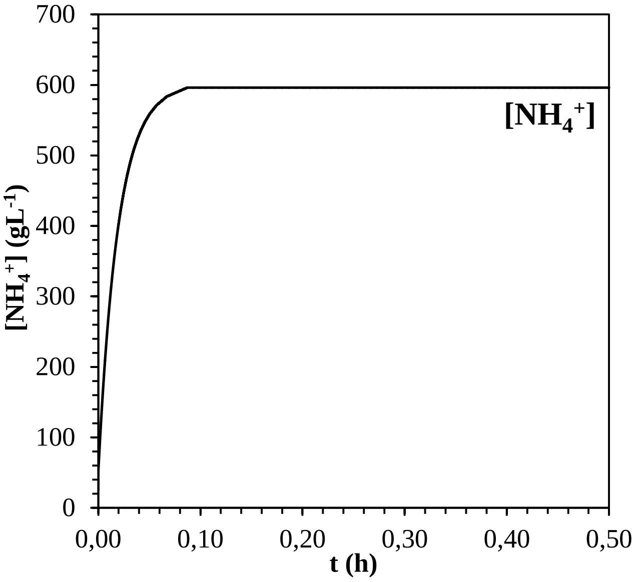

Figure 4. Concentration Distribution of NH_4^+ in Absorber.

Figure (4) shows the variation of the ammonium ion concentration with respect to time, the main product of the chemical reactions that occurs in the absorber. As a simulation condition, the initial concentration of $[NH_4^+]$ was assumed to be 25 [gL^{-1}]. After the computational simulation began, this concentration increases and reaches the steady state at 596.14 [gL^{-1}] in 0.01 [h]. Similarly to Fig. (2), (3) and (4), the Fig. (5) shows the variation of the ammonia concentration in the vapor phase with respect to time. After the computational simulation began, this concentration increases and reaches the steady state at 0.00728 [gL^{-1}] in 0.01 [h].

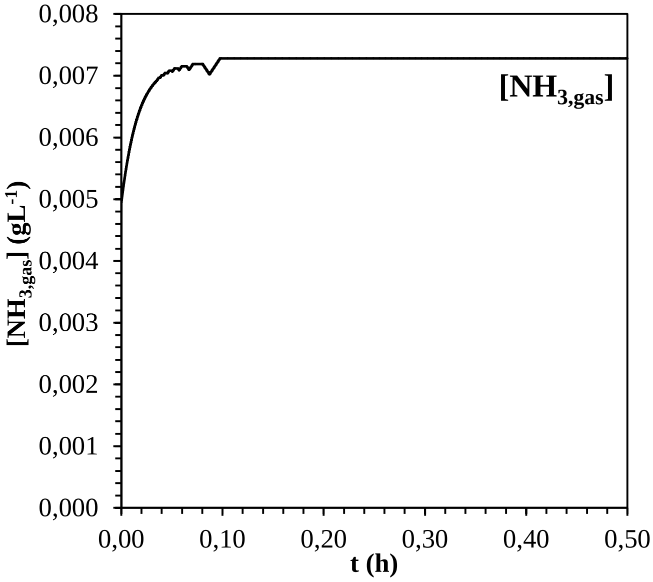

Figure 5. Concentration Distribution of $NH_{3,gas}$ in Absorber.

4. CONCLUSIONS

This study presents a transient mathematical model and computational simulation, developed through the application of the mass and energy conservation principles, for the absorber of absorption refrigeration systems that uses ammonia and water as work fluids. Through the computational simulations of the mathematical model developed in this study, for the absorber, the main result is the time concentration variation of ammonia, water and ammonium ion when this component is operating in a transient regime. In general, the numerical results have been consistent with the experimental data, showing the effectiveness of the model for procedures of simulation, design and optimization of the absorber component of an absorption refrigeration system.

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