A Computer Model of the LiBr-H2O Absorption Cycle for an Absorption Heat Transformer. ⋆

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Abstract: This work presents our progress in the development of a computer model to represent the dynamics of an Absorption Heat Transformer. This heat transformer uses as an absorption mixture LiBr-H2O. The model describes the overall momentum, energy and mass balances in the Generator-Economizer-Absorber. To enhance heat and mass transfer in the generator and in the absorber, both are designed as a helical horizontal exchangers with a falling film. Furthermore, they interact with the refrigerant fluid in the same chamber (as duplex components) to intensify the heat transfer. The Economizer between both components is built as a helical exchanger with concentric pipes. The aim of the model is to represent conditions form a quasi-steady state to load increase, and changes in the concentration of the absorption mixture, thus it can be used to understand the involved process dynamics.

Keywords: Process intensification, Absorption heat transformer, Absorption cycle interaction.

1. INTRODUCTION

Process recycles are difficult to control due to the cascade effect of different dynamics, and the reciprocal interaction between the units involved. A typical case is the reactor-separator-recycle which was presented by Larsson et al. (2003). Bian et al. (2005) developed a dynamic model of an absorption cycle using global models of each operating unit.

Stephan et al. (1997) have developed a dynamic model of a general two-phase absorption vessel used to represent the bulk conditions of an Absorption Heat Transformer, AHT. Jeong et al. (1998) have developed a dynamic model for an absorption heat pump. They use a balance of internal energy, and the heat exchangers are approximated by the Number of Thermal Units, NTU method. Kohlenbach and Ziegler (2008) proposed a bulk model of every vessel of the absorption cycle. They use a mean vessel temperature as a virtual crossover temperature between internal and external temperature levels. Auracher et al. (2008) presented a model of the one horizontal absorption tube to evaluate film thickness and velocity distribution according with the Nusselt assumptions. Iranmanesh and Mehrabian (2013) used an internal energy model with special consideration with the energy masses. They linked the physical properties of EES software with the numerical capabilities of MATLAB. In their study they conclude that generator and condenser are highly dependent of thermal masses of the condenser. Cai et al. (2007) build a model of a refrigeration cycle which considers reverse flow; but it does not include heat transfer equations. This model uses as an absorption mixture ionic liquids. The properties of these fluids are evaluated by an Equation of State.

Matsushima et al. (2010) used an object oriented formulation which allows the change of process configuration.

Once the AHT achieves a steady state it is very stable; therefore the goal of this work is to facilitate the AHT to arrive to a steady state.

2. PROCESS DESCRIPTION

The process is illustrated in Fig. 1. Heat is recovered from a waste stream at a warm temperature by the steam generator which at low pressure evaporates refrigerant from the absorption mixture; thus it produces a concentrated mixture. The concentrated absorption mixture is pumped to an absorber which operates at a higher pressure than the generator. There, when the mixture is in contact with the refrigerant, it releases heat as a product of an exothermic reaction. The economizer is used to recover heat from the hot stream at high pressure and from the cold stream at low pressure.

The geometric characteristics of these vessels appear in Tables 1, 2, and 3. To enhance the heat transfer the absorption mixture descends as a falling-film. In the tube side the warm stream ascends through the helical pipes. Thus turbulence enhances heat transfer between the fluid

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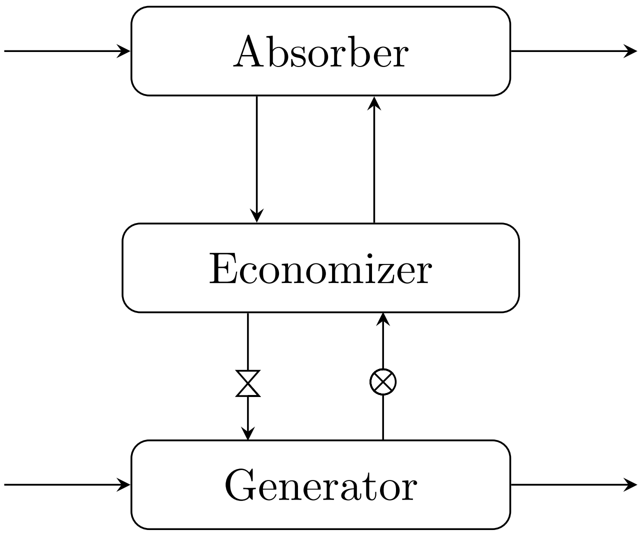

Fig. 1. Schematic view of Absorption Cycle in the AHT

layers. The cycle uses an absorption mixture of aqueous solution of LiBr. Thus, the refrigerant is H_2O.

Table 1. Geometry of Generator/Condenser.

Sec	D_{Hel} m	Height m	Length m (turns)	D_{Shl} m	D_o m	Pitch m
1	0.177	0.278	9.27 (15.5)	0.305	0.0211	0.0050
2	0.101	0.260	5.50 (15.5)	0.305	0.0211	0.0050

Table 2. Geometry of The Economizer

Length m (turns)	D_o m	D_i m	D_{Hel} m	pitch m
1.8 (3.5)	0.0190	0.0095	0.141	0.025

Table 3. Geometry of the Absorber/ Evaporator

Sec.	D_{Hel} m	High m	Length m(turns)	D_{Shl} m	D_o m	pitch m
1	0.23	0.20	10.11(13)	0.355	0.0127	0.0030

2.1 Instrumentation

Measurements: The generator and the absorber are provided with flow, pressure, and temperature meters. LiBr Concentration is estimated off-line by measurements of the refraction index. Also an eye-hole is provided to detect the level of the absorption mixture.

The *manipulated* variables in the cycle are: input flow to the generator and to the absorber, and flow of the heating stream to the generator.

3. PROCESS OPERATION

When the absorption mixture is heated in the generator, part of the heat is taken to release steam form the absorption mixture and part of it is taken by the more concentrated mixture. The ratio of steam to absorption mixture W_v/W_s is important in the performance of the absorption cycle. The generator operates at low pressure and low temperature. Here, heat transfer limits the separation.

The economizer is a helical heat exchanger. The concentrated solution coming from the generator flows inside the tubes, while the weak solution flows through the annulus.

The absorber produces an exothermic reaction between two streams, i.e. the absorption mixture and the refrigerant. Both input streams must have similar temperatures, and adequate contact to release an optimum amount of heat. The absorber operates at high pressure and high temperature. Mass transfer limits the reaction.

3.1 Start-up Sequence of the Process

- The recirculation pump starts. The absorption mixture flows from the outside of the absorption pipes to the outside of the generator pipes.
- An ejector produces negative differential pressure.
- Heat is *supplied* by a fluid which is pumped inside the generator pipes. As the absorption mixture flows through the generator, the refrigerant is released, and the absorption mixture is concentrated.
- The concentrated mixture flows toward the economizer.
- The cold fluid is preheated and pumped in the absorber pipes.
- The refrigerant is supplied in the absorption chamber. At this condition the regulation of the process switches from level control to flow control.
- The absorption reaction increases pressure and temperature
- Heat is *released* by the absorption process. This heat is taken by the cold stream. This stream is located in the inside of the absorber pipes.

3.2 Operating Range

The process operates in the range shown in Table 4 (Morales (2015))

Table 4. Operating Range of the Absorption Cycle

	Generator	Absorber
P, kPa	3.43 - 14.43	17.47-47.95
W, kg/s	0.002- 0.005	0.0052-0.020
T, ^oC	57.4 - 81.4	78.1-97.0
X, % wt	52 -58	47.68- 57.06
Q kW	0.0.427-0.902	0.0.178-0.668

4. MODEL DESCRIPTION

4.1 Model Assumptions

* There are not heat losses to the environment.
* The expansion valve operates isoenthalpically.
* Bulk conditions are used to estimate the transfer parameters of the model.
* Wetting efficiency is considered during film contact (Jeong and Garimella (2002)).

In a heat pump the generator (where heat is *added* to the cycle) operates at the highest pressure and temperature of the absorption cycle, while in a heat pump the absorber (where heat is *subtracted* from the cycle) operates at the highest pressure and temperature. Thus AHTs has wider applications for energy recovery than heat pumps, due to the temperature increase in the absorber.

The pipe manifold where the absorption occurs, is described by a bulk approximation. Described below is the interaction between pressure, temperature and concentration that takes place within the generator and the absorber. Also described below is the pressure and temperature within the economizer. Temperature gradients can switch direction during load changes in the economizer; so, special attention was given while handling its temperature gradients.

Generator The generator was modeled like a heated separator. The conservation, and energy equations for the generator are as follows:

$$\frac{dM_{GE,s}}{dt} = W_{GE,s,i} - W_{GE,s,o} \tag{1}$$

$$\frac{dM_{GE,v}}{dt} = W_{GE,v,i} - W_{GE,v,o} \tag{2}$$

$$\frac{d(HM)_{GE,s,o}}{dt} = Q_{GE,s} - Q_{GE,t} - W_{GE,v,o}H_{GE,abs} \tag{3}$$

$$H_{GE,abs} = H_v - H_s + X(\frac{\partial H_s}{\partial x}) \tag{4}$$

$$\frac{d(XM)_{GE,s,o}}{dt} = (WX)_{GE,s,i} - (WX)_{GE,s,o} \tag{5}$$

Equilibrium relationship see Torres-Merino (1997).

$$X^* = X(P,T) \tag{6}$$

Heating flow Equation

$$MCp_h\frac{dT_h}{dt} = Q_{GE,h} - Q_{GE,t} \tag{7}$$

$$Q_{GE,s} = W_{GE,s}Cp_s(T_{GE,s,i} - T_{GE,s,o}) \tag{8}$$

$$Q_{GE,h} = W_{GE,h}Cp_h(T_{GE,h,i} - T_{GE,h,o}) \tag{9}$$

$$Q_{GE,t} = \eta(UA)_{GE}\Delta T_{lm} \tag{10}$$

η represents the wetting efficiency.

Pressure and flow relationships for momentum balance

$$\begin{aligned} W_s &= Kv_s\Delta P_s/\rho_s \\ W_v &= Kv_v\Delta P_v/\rho_v \end{aligned} \tag{11}$$

ΔP represents the pressure drop with respect to the chamber and the outlet.

Level of the absorption mixture For a cylindrical vessel: $L_s = \frac{M_s}{\rho_s S}$

Economizer The economizer was modeled like a shell-and-tube heat exchanger. During the start-up both input streams of the economizer have the same temperature. When heat is supplied to the generator the concentrated mixture has a *higher* temperature than the weaker mixture. When the exothermic reaction occurs the concentrated mixture has *lower* temperature than the weaker mixture. A robust model of the heat transfer incorporates wall temperature dynamics:

$$M_cCp_c\frac{T_{c,o}}{dt} = W_cCp_c(T_{c,o} - T_{c,i}) + h_oA_o(T_w - T_{c,o}) \tag{12}$$

$$M_wCp_w\frac{T_w}{dt} = h_iA_i(T_{h,o} - T_w) - h_oA_o(T_w - T_{c,o}) \tag{13}$$

$$M_hCp_h\frac{T_{h,o}}{dt} = W_hCp_h(T_{h,i} - T_{h,o}) - h_iA_i(T_{h,o} - T_w) \tag{14}$$

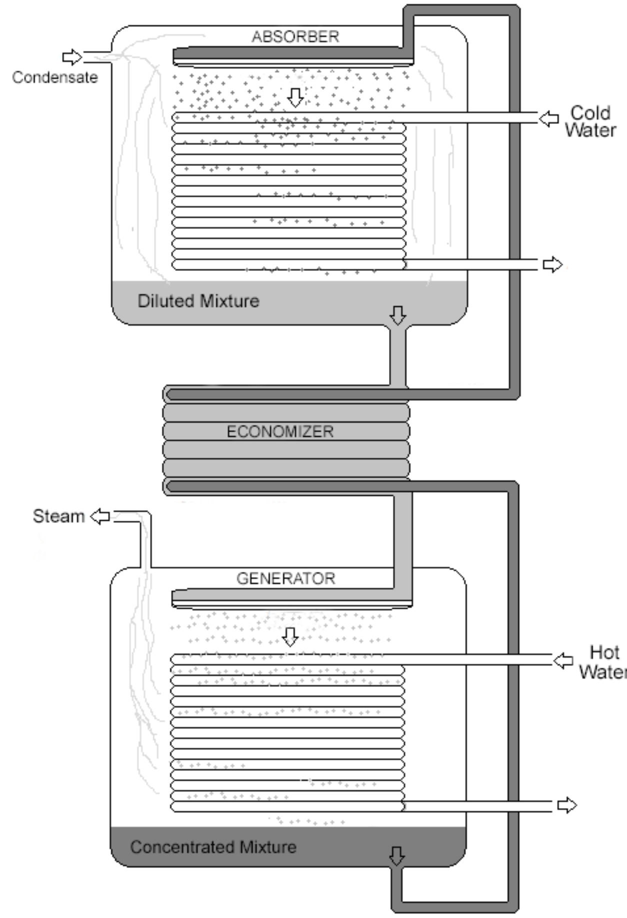

Fig. 2. Interaction between the streams of Absorption Cycle in the AHT

The wall temperature dynamics was included to allow gradients with fluctuation in its direction. This differential equation includes the wall inertia.

Absorber The absorber is modeled like a cooled exothermic reactor. In the exterior of the helical pipes the concentrated mixture flows. When it is in contact with the refrigerant it releases absorption heat. The weak mixture is collected at the bottom. The heat released is used to increase the temperature of the fluid inside the helical pipes which ascend to the top of the absorber.

While in the Generator the process is dominated by the temperature gradients, in the absorber the process is dominated by the concentration gradients

$$\frac{d(M\ X)_{AB}}{dt} = Kx_{AB}(X_{AB} - X^*) \tag{15}$$

Thermo-physical properties of the absorption mixture were evaluated from correlations of Yuan and Herold (2005). The physical properties of water were evaluated from correlations coded by Holmgren (2003). The properties of the fluid ρ and μ are closely related with momentum transport, while Cp and κ are closely related with energy transport, and H_{abs} is closely related with the conveyed heat from the absorber to the refrigerant fluid. Each of this properties are temperature and composition dependent.

4.2 Tuning Parameters

From typical values, the following parameters were fitted in the model: Kv, Valve coefficient, U, overall heat transfer of every unit, Kx, Mass transfer coefficient, and η, wetting efficiency.

5. MODEL DYNAMICS

Fig 2. shows the absorption-economizer-generator's layout.

5.1 Sensitivity Analysis in the Pressure-Temperature Relationship in the Absorption/Generator chamber

Using a) the total volume conservation $V_T = M_s\hat{v}_s + M_v\hat{v}_v$, and b)the overall internal energy, $H - PV$, the partial derivatives can be obtained as a function of the temporal variation of pressure, P, and steam enthalpy, H_v. Remaining as the dominant terms:

$$M_v\frac{\partial\hat{v}_v}{\partial P}\frac{dP}{dt} \propto -\hat{v}_s\frac{dM_s}{dt} - \hat{v}_v\frac{dM_v}{dt}$$
$$-V_T\frac{dP}{dt} + \left(M_s\frac{Cp_s}{Cp_v} + M_v\right)\frac{dH_v}{dt} \propto -Hs\frac{dM_s}{dt} - Hv\frac{dM_v}{dt}$$

At sub-atmospheric conditions

$$\frac{\partial\hat{v}_v}{\partial P} = -\frac{RT}{MWP^2} \quad (16)$$

and

$$\frac{\partial\hat{v}_v}{\partial H_v} = \frac{\partial\hat{v}_v}{\partial T}\frac{1}{Cp_v} = \frac{R}{MWPCp_v} \quad (17)$$

Since $P_{AB} > P_{GE}$, and $\left|\frac{dM_s}{dt}\right| >> \left|\frac{dM_v}{dt}\right|$, then:

* In the generator, *enthalpy* (temperature) fluctuations depend more on fluctuations of absorption mixture holdup, M_s, than on the absorber.
* In the absorber, *pressure* fluctuations depend more on fluctuations of absorption mixture holdup M_s than in generator.

5.2 Results

The numerical results were obtained with an Euler explicit method for Ordinary Differential Equations implemented with Matlab. The time step $\Delta t = 0.001$ s. The transient last for 5000 s. This method was used to treat physical constraints related with gradients and values of physical properties. Fig. 3 shows the start-up of the process modeled.

The absorption mixture starts at 50^oC in both generator and absorber, while heating water to the generator is maintained at 80^oC. When the absorption mixture is steadily heated it produces steam after $t = 3000s$. Then, the condensate returns from the refrigerant cycle and is introduced in the absorber. Later, this refrigerant is evaporated and comes in contact with the concentrated mixture, and, as a result, the absorption mixture delivers reaction heat. Thus, the absorber increases the temperature of its absorption mixture, while the generator maintains the temperature of its absorption mixture.

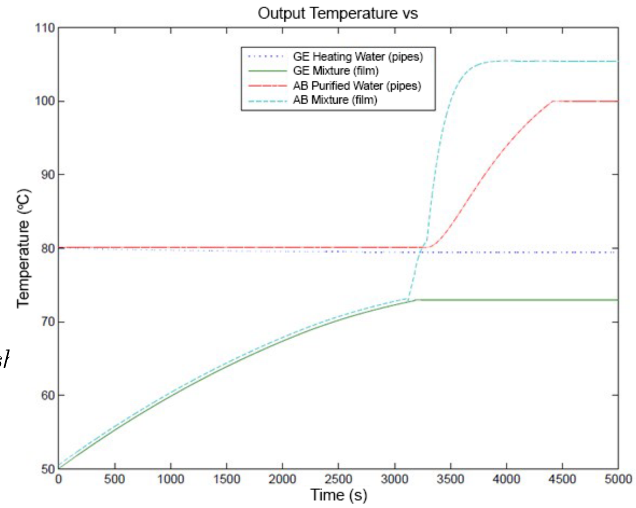

Fig. 3. Behavior of Model Temperatures along the Absorption Cycle in the AHT

The water flowing inside the absorber pipes increases steadily around 20^oC. During this transient pressure in the absorber changes, and as result the flow from the absorber increases. So to attain steady state it is necessary to appreciate the conditions at which the regulation switches from level to flow control.

6. CONCLUSIONS

Among the advantages of this model there is its prediction capability with respect to the operating variables. Specifically, the close relationship between the pressure and the temperature in the absorption/desorption chamber was observed, and the sensitivity of these properties on the mass holdup of the absorption mixture. The model has flexibility to implement similar absorption cycles with the design characteristics and to change the absorption mixture with the appropriate correlations of the thermodynamic and transport properties subject to their valid operating range.

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7. NOTATION

AHT = Absorption Heat Transformer
A = Area, m^2
Cp = Heat capacity, kJ/kg^oC
D = Diameter, m
g = Acceleration of gravity,m^2/s
H = Enthalpy, kJ/kg
h = Heat transfer coefficient, kW/m^2oC
Kx = Transfer coefficient kg/s
Kv = Valve coefficient , $N/kg-m$
L = Level, m
M = Mass, kg
MW = Molecular weight, kg/mol
P = Pressure, kPa
Q = Heat, kJ/s
S = Cross section area, m^2
T = Temperature, K
t = Time, s
U = Overall heat transfer coefficient, kW/sm^2oC
$\hat{v}$ = Specific volume, m^3/kg
V = Volume, m^3
W = Flow, kg/s
X = Concentration, % LiBr

Superscripts

$*$ = Equilibrium
a = Annulus side
AB = Absorber
abs = Absorption
blk = Bulk
c = Cold stream
d = Distributor
EC = Economizer
$film$ = Film
GE = Generator
h = Hot stream
Hel = Helical
i = Internal, inlet condition
lm = Logarithmic mean
m = Mass
o = Outer, outlet condition
p = Pipe
r = Recollector
s = Absorption mixture
T = Total
t = Transfer
v = Steam
w = Wall

Greeks
Δ = increment
δ = film thickness, m
η = wetting efficiency, [-]
γ = flow per unit length, $kg/m-s$
μ = viscosity, $kg/m-s$
ρ = density, kg/m^3