ADIABATIC ABSORBER MODEL FOR THE LIQUID DESICCANT DISTRIBUTION NETWORK AT THE TECHNOLOGY PARK BERLIN ADLERSHOF USING MODELICA

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ABSTRACT

A liquid desiccant distribution network is planned to be installed at the technology park Berlin Adlershof. Liquid desiccant systems provide the ability to connect different temperature levels and to integrate low temperature heat sources like waste heat or solarthermal heat. They have proven to be an energy saving alternative to vapor compression cooling systems to handle latent cooling loads.

To estimate the potential of the distribution network and of liquid desiccant absorber systems at arbitrary locations in general, mathematical models are used to describe the coupled heat- and mass transfer processes. In this paper a modeling approach for adiabatic absorber models for cubic and cylindrical systems in the object-oriented programming language Modelica is presented. The developed model is validated with data from the literature for a cross current flow absorber using lithium chloride as desiccant and shows very good agreement without calibration.

INTRODUCTION

The objective of air conditioning is the manipulation of the room climate to match the human physiological needs, independent of inner and outer disturbances. Besides the air temperature, the air movement, the radiation properties of the enclosing surfaces and the particle load, the air humidity plays an important role.

The control of the air temperature and the humidity divides the cooling load in a sensible and a latent part. While conventional cooling systems can remove the sensible loads very effectively, they lack efficiency at mastering the latent loads. Air is cooled below its dew point temperature and needs reheating before entering interiors. Unlike conventional cooling systems, liquid desiccant systems avoid overcooling and energy savings of up to 40 % can be achieved [Potnis and Lenz, 1996]. Moreover, liquid desiccants have the ability to filter contaminants, bacteria and viruses and provide air of higher quality due to sanitizing effects [Rafique et al., 2016]. Additionally, liquid desiccant systems can be operated at regeneration temperatures below 80 °C, which allows the integration of low temperature heat

sources like solarthermal heat or waste heat [Yin et al., 2014]. Thus, the use of fossil fuels can be further decreased. The dehumidification and regeneration can be executed locally and temporally decoupled, when energy storage is applied. This allows the transfer of the regeneration process to times, where enough heat energy is available. The amount of stored concentrated must be sufficient to bridge the lack of heat supply [Hublitz, 2008].

In the context of the project "Energy Strategy Berlin Adlershof", a small liquid desiccant distribution network will be installed. It gives the opportunity to connect different temperature levels and to save low temperature energy nearly lossless in thermochemical form. Previous investigations showed that the location has high air conditioning demands. This implies considerable energy requirements on cooling machines and therefore significant waste energy potentials. Liquid desiccants reveal a potential to utilize these low-exergetic energy sources and will be demonstrated in air conditioning processes and industrial drying applications as part of the project. Depending on the participants of the distribution network, it will be installed as a grid or as a transport system with containers.

To estimate the potential of the planned distribution network and of liquid desiccant absorber systems at arbitrary locations in general, mathematical models are used to describe the coupled heat- and mass transfer processes.

For the adiabatic process, the mathematical models are roughly classified into three types: the finite volume model, the effectiveness NTU model and simplified models based on fitted algebraic equations. Among those models, the finite volume model proved to provide the most accurate results. The simplified models need to be fitted with experimental data, which restricts their use in a planning tool. They are only valid for specific absorber configurations and operating modes. Figure 1 shows a cross-flow packed bed adiabatic dehumidifier.

Factor and Grossman (1980) suggested a theoretical model to predict the performance of a counter current packed bed dehumidifier. The model discretized the absorber volume one-dimensionally. Gandhidasan et al. (1987) utilized a similar model to study the

influence of the tower height on the air humidity and temperature at the outlet, the mass flow rates and desiccant concentration. Fumo and Goswami (2002) developed a finite difference model that takes insufficient wetting into account. Insufficient wetting cause a considerable reduction of the heat and mass transfer area. Liu et al. (2007) proposed a model for cross current flow absorber. They discretized the volume in two dimensions and described the heat and mass transfer with the dimensionless Le and NTU number. This approach is often chosen in the literature, where Le is assumed to be one and the value of NTU is correlated based on experimental data. Woods and Kozubal (2013) modeled an evaporatively-cooled liquid desiccant dehumidifier. The system is discretized in two dimensions to account for the cross counter flow and uses four fluid streams.

MODELING

This paper presents a mathematical absorber model with only a few parameters that have to be specified. Generally, the detailed heat and mass transfer is not known to the user and all he can provide are the geometrical data and information about the structure. Therefore the model needs correlations to describe the coupled heat and mass transfer without further knowledge of the process itself. Furthermore, the desired liquid desiccant is not fixed to the system and should be exchangeable.





Modelica is a multi-domain modeling language, that fulfills the requirements very well. It is objectoriented and was developed for the modeling of transient physical systems. The main benefits over other languages are non-causal programming and polymorphism, which is a special form of inheritance. Polymorph objects have the same interface, but can have very different properties. This allows the exchange-ability of sub-models and the implementation of different modeling approaches for the same physical problem.

Thermodynamic properties

The most common used liquid desiccants are LiCl, LiBr and CaCl₂. The dehumidification and regeneration process depend strongly on the choice of the substance. The most important parameters are the vapor pressure reduction, the heat of absorption and the caloric properties of the aqueous solution. The thermodynamic properties do not only depend on the pressure and temperature, but mostly on the composition.



Figure 2: Class diagram of the media model

The Modelica Standard Library (MSL) defines interfaces to access fluid properties. As part of this work a new interface for aqueous solutions is developed, which extends the existing interface PartialMixtureMedium. The new interface PartialBrineMedium implements new functions for liquid desiccants and expands already declared ones. The associated class diagram is shown in Figure 2. Every liquid desiccant medium model expands this class with equations that are specifically valid for that substance.

For the calculation of the thermodynamic properties of moist air, the model from the Modelica Buildings Library of the Lawrence Berkeley National Laboratory is used [Wetter et al. 2014]. Models for LiBr and LiCl are based on the work of Pàtek and Klomfar (2006, 2008). They analyzed experimental studies about the thermodynamic properties and developed equations of state. For LiBr they specify thermal, caloric and entropy equations of state, that are valid from 273 to 500 K in temperature and from 0 to 75 wt.-% LiBr in concentration. For LiCl they developed a Gibbs free energy equation, that allows the calculation of all thermodynamic properties, including the saturation attributes. The fundamental equation of state is valid from 273 to 400 K in temperature and from 0 to 50 wt.-% LiCl in concentration. Both media models use the new interface PartialBrineMedium, with implementations of the equations of state.

During dehumidification, water vapor molecules are absorbed by the liquid desiccant. Condensation occurs inside the liquid volume and energy in the form of absorption enthalpy is released.

$$\Delta h_{\rm abs} = \Delta r_0 + \Delta h_{\rm b} \tag{1}$$

It consists of the condensation enthalpy of pure water Δr_0 and the binding enthalpy of the liquid desiccant $\Delta h_{\rm b}$. The binding enthalpy can be calculated from the caloric equation of state of the real fluid.

Heat and mass transfer

Several modeling approaches exist to describe the heat and mass transfer:

- The detailed diffusion model takes the liquid and gaseous resistances into account. This should especially be done, when a variation of the film thickness is considered.
- A first simplification considers a gas side controlled transfer process. This simplified approach is often utilized in open adsorption processes or in process engineering to calculate packed beds [Casas, 2005].
- A second simplification considers pseudo gas side controlled transfer processes, which are mathematically identical to the previous case. The difference lies in the interpretation of the transfer coefficients. They are represented by an effective coefficient that combines the gaseous and liquid resistances.

The presented model neglects the influence of the desiccant distribution and assumes a constant and homogeneous film thickness. Liquid resistances are neglected and the transfer processes are characterized by effective coefficients.

Correlations for the heat and mass transfer of adiabatic absorber units are investigated by several researchers. The mass transfer coefficients must be associated with the liquid desiccant. Therefore universal equations are not available and studies for different configurations and desiccants are carried out. Onda et al. (1968) developed empirical correlations to determine the mass transfer in random packings using organic desiccants. Gandhidasan et al. (1986) provided heat and mass transfer correlations for CaCl₂ solutions used in packed towers. Chung et al. (1996) analyzed random and structured packings and developed heat and mass transfer correlations for LiCl solutions. Potnis and Lenz (1996) studied random and structured packings using LiBr. Ertas et al. (1991) compared heat and mass transfer coefficients of CaCl₂, LiCl and a liquid desiccant

mixture (CELD) in a packed column. The suggested correlations are valid for different packings.

In this paper, the study of Chen et al. (2016) is used. They investigated an adiabatic absorber with a structured packing and LiCl as the desiccant in a cross flow configuration.

Based on 153 experimental runs, correlations for the Nu and Sh number are developed as a function of the inlet parameters of moist air and desiccant solution by nonlinear regression. The effective gas phase heat and mass transfer correlations are:

$$Nu = 4.7756 e^{-5} Re_{a}^{1.7936} Pr_{a}^{0.3333} \left(\frac{\dot{m}_{d}}{\dot{m}_{a}}\right)^{-1.001} \left(1 - \frac{x_{d,eq,in}}{x_{a,in}}\right)^{0.8198} \left(\frac{T_{d,in}}{T_{a,in}}\right)^{0.3846}$$
(2)

$$Sh = 7.3492 e^{-7} R e_{a}^{2.1576} S c_{a}^{0.3333} \left(\frac{\dot{m}_{d}}{\dot{m}_{a}}\right)^{0.5235} \left(1 - \frac{x_{d,eq,in}}{x_{a,in}}\right)^{-0.8986} \left(\frac{T_{d,in}}{T_{a,in}}\right)^{0.2376}$$
(3)

The Reynolds number Re is calculated as a function of the volumetric air flow rate per column cross section v and the void fraction of the packing ε .

$$Re = \frac{v_a \rho_a d_{\rm eq}}{\eta_a \varepsilon} \tag{4}$$

The heat and mass transfer coefficients are expressed as the dimensionless numbers Nu and Sh.

$$Nu = \frac{\alpha d_{\rm eq}}{\lambda_{\rm a}} \tag{5}$$

$$Sh = \frac{\beta d_{\rm eq}}{D_{\rm a}} \tag{6}$$

Equation (7) yields the diffusion coefficient of water vapor in air in m²/h. The pressure p is in kp/m² and $T_0 = 273.15$ [Gröber et al. 1988].

$$D_{\rm a} = \frac{805}{p} \frac{T^{1.8}}{T_0} \tag{7}$$

Assumptions

In order to simplify the complexity of the model, several assumptions are used:

- The dehumidification process is adiabatic and no energy in the form of heat is exchanged with the environment.
- The heat and mass transfer occurs only in the flow direction. Heat conduction and mass diffusion in the transverse direction are neglected.
- The dehumidifier is flooded equally and the heat transfer area equals the mass transfer area.

- The moist air and the liquid desiccant at the interface are in equilibrium with respect to the temperature and humidity.
- Radiation heat transfer is neglected, due to small temperature differences in the process.
- The release of the absorption heat happens completely inside the desiccant.
- The diffusion process acts as the limiting factor and the absorption kinetics can be neglected.

Balance equations

The fluid flow of the moist air and the liquid desiccant are described with one-dimensional flow models. The distribution of composition and temperature is uniform inside a control volume, as internal heat conduction and mass diffusion are neglected. The air and desiccant control volumes are represented by the same model and the balance equations are independent of the used fluid.

Figure 3 shows the energy and mass balance of the moist air and desiccant phase in an adiabatic absorber. For a one-dimensional flow along the coordinate y, the mass balance simplifies to

$$\frac{\partial \rho}{\partial t}V + \frac{\partial (\rho v)}{\partial y}V = \dot{m}_{\rm v} \tag{8}$$

for the total mass and to

$$\frac{\partial \rho_k}{\partial t} V_k + \frac{\partial (\rho v)_k}{\partial y} V_k = 0 \tag{9}$$

for the independent mass fractions, respectively. The energy balance consists of a latent and a sensible heat flow term.

$$\frac{\partial(\rho u)}{\partial t}V + \frac{\partial(\rho v u)}{\partial y}V = \dot{Q}_{\rm S} + \dot{Q}_{\rm L} \tag{10}$$

The partial derivatives with respect to time are handled by the Modelica compiler. The partial derivatives with respect to y are solved with the finite volume method. Therefore the one-dimensional flow model is discretized in n equally sized control volumes. The partial differential equations are transformed to algebraic expressions and solved for every individual fluid segment. The negligence of heat conduction and mass diffusion simplifies the mathematical system greatly, as no second partial derivative appears. The flow model is based on the pipe model from the Buildings Library [Wetter et al. 2014]. Each control volume is equipped with heat and mass transfer connectors to exchange information with other models.



Figure 3: Energy and mass balance of air and desiccant phase

The sensible heat transfer occurs due to the temperature difference between the moist air and the liquid desiccant. It can be expressed as

$$\dot{Q}_{\rm S} = \alpha A (T_{\rm a} - T_{\rm d}) \quad . \tag{11}$$

The latent heat transferred from the air to the desiccant is released together with the binding enthalpy inside the desiccant.

$$\dot{Q}_{\rm L} = \dot{m}_{\rm v} \Delta h_{\rm abs} \tag{12}$$

The absorbed water vapor is calculated from the difference in water concentration between the core flow $X_{\rm a}$ and the moist air at the surface of the desiccant $X_{\rm eq}$. The air at the surface is assumed to be in equilibrium with the desiccant.

$$X_{\rm eq} = \frac{M_{\rm w}}{M_{\rm a}} \frac{1}{\frac{p}{p_{\rm sat}} - 1 + \frac{M_{\rm w}}{M_{\rm a}}}$$
(13)

The mass transfer can then be calculated according to

$$\dot{m}_{\rm v} = \rho \beta A (X_{\rm a} - X_{\rm eq}) \quad . \tag{14}$$

The model doesn't investigate pressure losses and therefore no impulse equations are implemented.

Flow configurations

To create the final absorber model, multiple instances of the described flow model need to be connected with each other. The connections and quantities of flow models depend on the flow configuration. Counter and direct flow configurations use a single flow model for the moist air and the liquid desiccant, respectively. Figure 4 shows the connections of the flow models for a discretization of n = 4. The fluids enter at the first control volume and leave at the last one. In every control volume heat and mass according to (11), (12) and (14) are exchanged. The resulting absorber model is one-dimensional.



Figure 4: Schematic of direct and counter current flow configuration

The generation of the cross flow configuration requires more modeling effort, as the flow needs to be described in two dimensions. Therefore another discretization parameter m is introduced. It represents the number of parallel desiccant flow models as shown in the example in Figure 5 with m = 2 and n = 4. This yields two parallel desiccant flow models with a discretization of four and four parallel air flow models with a discretization of two. The flow configuration is implemented as a parameter in the absorber model and all connections between the control volumes are applied automatically according to the discretization parameters.

The model supports both cubic and cylindrical constructions. The cubic construction permits all three flow configurations, while the cylindrical profile is only valid for counter and cross current flow.



Figure 5: Schematic of cross current flow configuration

VALIDATION

The developed medium models are validated with property values provided by Pàtek and Klomfar (2006, 2008) for different temperatures and solution concentrations. The calculated values match their results precisely, so simulation errors with respect to medium properties can be excluded.

The validation of the absorber model was performed with experimental data from Chen et al. (2016). They selected lithium chloride aqueous solution as the desiccant and used a Celdek structured packing in the dehumidifier. The structural properties of the packing are presented in Table 2. The void fraction and the correct height of the absorber were provided by the authors. Experimental errors were not attributed in their paper.

Table 1: Inlet parameters and comparison of predicted and experimental values from Chen et al. (2016)

	T /°C	m /(m/lrm)	$\dot{m} / (lrg/g)$	T /°C	¢ /07.	m /(leg/g)	$T_{\rm a,out}/{\rm ^{o}C}$		$x_{\rm a,out}$	$x_{\rm a,out}/({\rm g/kg})$		$T_{\rm d,out}/{\rm ^{o}C}$	
	$I_{\rm a,in}/$ U	$x_{a,in}/(g/kg)$	m _{a,in} /(kg/s)	$I_{\rm d,in}/$ C	$\zeta_{\rm d,in}/\gamma_0$	$m_{\rm d,in}/({\rm kg/s})$	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	
1	25.6	16.2	1.85	14.9	23.00	2.61	19.2	18.74	9.1	9.29	21.3	20.19	
2	28.6	20.2	1.87	18.2	24.00	2.63	22.9	22.26	11.6	11.41	25.2	24.45	
3	27.5	18.1	1.92	17.7	25.50	2.65	21.9	21.44	9.9	10.08	24.3	23.69	
4	30.0	17.7	1.89	18.9	26.00	2.66	23.5	22.95	9.7	10.22	25.8	24.74	
5	27.6	16.4	1.92	17.3	27.00	2.67	21.6	21.04	8.7	9.03	23.7	23.10	
6	21.7	10.8	2.04	9.5	25.13	2.93	14.1	13.27	5.7	5.81	14.6	14.13	
7	22.7	15.3	1.97	12.6	26.00	2.76	16.5	16.17	7.7	7.75	18.6	18.38	
8	24.7	15.3	1.96	15.5	27.00	2.77	19.2	18.87	8.0	8.07	21.6	20.95	
9	23.3	14.3	1.99	14.7	28.50	2.80	18.1	17.87	7.2	7.21	20.3	20.10	
10	24.0	15.2	1.94	16.8	29.61	2.82	20.1	19.79	7.5	7.62	23.1	22.09	
11	24.2	16.0	1.98	17.7	30.07	2.85	20.9	20.65	7.7	7.88	23.9	23.22	
12	25.1	15.2	1.94	18.1	30.52	2.90	21.3	21.05	7.5	7.61	24.1	23.27	
13	25.2	14.3	1.95	17.8	31.82	2.85	21.1	20.79	6.9	7.02	23.9	23.08	
14	25.9	15.9	1.99	19.2	32.15	2.86	22.6	22.24	7.7	7.68	25.8	24.97	
15	25.6	14.3	1.93	18.4	33.12	2.88	21.6	21.38	6.6	6.84	24.5	23.72	

Table 2: Physical characteristics of the packing

Properties	Value
Surface area (m ² /m ³)	450
Void fraction (-)	0.90
Equivalent diameter (m)	0.01
Height (m)	1.50
Width (m)	0.75
Length (m)	0.75

Table 1 shows the inlet parameters for the simulation and a comparison of the calculated values with the experimental data. The results were obtained with a discretization of n = 10 and m = 10. The maximum deviation of the air outlet temperature is -5.90 % with a mean deviation of 2.07 %. The calculations of the absolute outlet air humidity yield a maximum deviation of 5.33 % and a mean deviation of 1.95 %. Both properties define the specific air outlet enthalpy with a maximum deviation of -2.15 % and a mean deviation of 0.69 %. These results are very close to the experimental data and show compliance with the overall energy balance of the model. The simulated desiccant outlet temperature has a maximum deviation of -5.23 % and a mean deviation of 3.08 %.



Figure 6: Simulation of case 2 with the maximum deviation

The results are obtained without any calibration of the model and agree very well with the available experimental data. The absorber model is therefore able to predict the outlet states of moist air and the desiccant. Figure 6 and Figure 7 show the least and the most accurate simulated cases in a Mollier diagram with respect to the specifc enthalpy. The round mark on the right represents the measured air inlet state. The round mark on the left characterizes the measured air state at the outlet of the dehumidifier and the red diamond shows the air outlet state calculated by the model.



Figure 7: Simulation of case 13 with the minimum deviation

CONCLUSION

This paper presents a model to predict the thermodynamic behavior of an adiabatic absorber. It is written in Modelica and compatible to popular Modelica libraries. The model allows the technical design and the estimation of the potential of liquid desiccant dehumidification systems at arbitrary locations. Coupled with models for building systems, the energetic advantages can be investigated. In addition, Modelica allows the integration of control strategies.

The presented model is not fixed to specific configurations, but can be used for cubic or cylindrical absorber systems with direct, counter or cross current flow. Its object-oriented construction allows the use of different medium models for the desiccant and moist air. The heat and mass transfer correlations are implemented as replaceable and new correlations can be added according to the developed interfaces. These features ensure that the model can be applied to different desiccants and configurations very easily.

The validation showed that the model agrees very well with the available data from Chen et al. (2016) and needs no calibration at all. The derived results depend on accurate media models and correct correlations to describe the heat and mass transfer. As the available heat and mass transfer correlations are only valid for very limited cases, new correlations have to be added for other investigations.

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NOMENCLATURE

Latin symbols

A	m^2	Surface area
d	m	Diameter
D	m^2/s	Diffusion coefficient
h	J/kg	Spec. enthalpy
$\Delta h_{\rm abs}$	J/kg	Spec. absorption enthalpy
$\Delta h_{\rm b}$	J/kg	Spec. binding enthalpy
\dot{m}	$\rm kg/s$	Mass flow rate
M	mol	Molar mass
Nu	_	Nusselt number
p	Pa	Pressure
\dot{Q}	W	Heat flow rate
Δr_0	J/kg	Spec. condensation enthalpy
Re	_	Reynolds number
Sh	_	Sherwood number
Т	Κ	Temperature
u	J/kg	Spec. internal energy
v	m/s	Velocity
V	m^3	Volume
x	$\rm kg_w/kg_a$	Humidity ratio
X	kg/kg	Water concentration

Greek symbols

α	$\mathrm{W}/\mathrm{m}^{2}\mathrm{K}$	Heat transfer coefficient
β	m/s	Mass transfer coefficient
ε	_	Void fraction
η	Pa s	Dynamic viscosity
ξ	_	Desiccant concentration
ρ	kg/m^3	Density

Subscripts

a	Air
d	Desiccant
eq	Equilibrium
in	Inlet
L	Latent
S	Sensible
sat	Saturation
V	Vapor
W	Water

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