

Mathematical Modeling of Heat and Mass Transfer in Regenerators with Desiccant Materials

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List of Symbols

\mathcal{A}_p	Flow area
\mathcal{A}_s	Surface area
\mathcal{A}_w	Wall area (perpendicular to flow direction)
c, c_p	Specific heats
\mathcal{D}	Mass-diffusivity
\mathcal{D}_g^T	Soret or thermal-diffusion coefficient
e_{sor}	Fraction by which sorption heat exceeds vaporization heat
f_s	Mass fraction of adsorbent material in felt
h	Convective heat transfer coefficient between felt and process stream
h_m	Convective mass transfer coefficient between felt and process stream
h_w	Heat transfer coefficient between felt and wall
h_π	Mass transfer coefficient between pores and vapor in equilibrium with desiccant
i	Specific enthalpy
\tilde{i}	Specific enthalpy on dry basis
i_{vap}	Latent heat of vaporization
i_{wet}	Differential heat of wetting
Δi_w	Integral heat of wetting
i_{sor}	Heat of sorption
\mathbf{j}''	Mass flux vector
j''	Mass flux component
k	Thermal conductivity
K	Number of sections in regenerator
L	Regenerator length
p	Pressure
\mathcal{P}_s	Wetted perimeter

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\mathcal{P}_w	Contact perimeter at felt-wall interface
$\dot{\mathbf{q}}''$	Mass flux vector
\dot{q}'	Heat flux component
\dot{q}_i''	Heat flux at felt-stream interface
\dot{q}_w''	Heat flux at felt-wall interface
\mathcal{S}	Surface or interface
\mathcal{S}_p	Felt-stream interface
\mathcal{S}_w	Felt-wall interface
\dot{s}_{sor}'''	Volumetric rate of sorption heating
T	Temperature
t	Time
t_f	Total cycle time
W	Concentration in adsorbed phase
Y	Concentration in gas phases

Greek Symbols

ε	Porosity
ϕ	Relative humidity
λ_m	Dufour diffusion coefficient
ρ	Density or specific mass
τ_{dw}	Dwell time
τ_G, τ_S	Tortuosities
ω	Wheel rotation speed
ϕ	Relative humidity

Subscripts

a	Dry air
f	Porous sorbent medium
g	Gas phase of porous medium
i	At or related to the felt-stream interface
k	In a given regenerator section k
l	Adsorbed phase
ls	Saturated liquid
s	Solid phase of porous medium
v	Water vapor

Superscripts

*	Dimensionless quantity
+	Modified quantity

1 Introduction

The phenomenon of Physical Adsorption has been known for over two centuries and extensively studied over the past couple of decades. The fact that porous solids could reversibly take up large volumes of vapor was identified in the late eighteenth century, by the studies of Scheele and Fontana, and the term adsorption appears to have been introduced by Kayser, as mentioned by Gregg and Sing [21]. Nevertheless, it was only several decades later that adsorption technologies gained widespread application to large-scale industrial processes. Among these major applications, regenerative heat and mass exchangers that employ sorbent materials have become an attractive option in a variety of industrial processes.

In HVAC applications, two classes of heat and mass regenerators with sorbent materials are frequently employed: *total heat regenerators*¹ and *regenerative dehumidifiers*. In order to achieve a large surface area in a compact structure, the regenerators are composed of mini-channels, whose walls are partly composed of an adsorbent, which exchanges heat and moisture with the process fluid stream. During operation, two process streams are alternately fed to the channels, resulting in two distinct operating periods, which form a complete cycle. The regenerator channels are arranged in a matrix, which is either of *fixed-bed* (or stationary) type, or *rotary* type. Although both designs can perform equivalently, the fixed-bed type requires two matrices for continuous operation, since each matrix needs to be switched between the two process streams at the beginning of every period. As an alternative, in rotary regenerators, a single rotating matrix allows uninterrupted operation by being continuously cycled between the two process streams.

According to the given application, rotary regenerative exchangers are respectively termed *enthalpy wheels*—used for energy recovery—and *desiccant wheels*—employed in dehumidification. Although this has been the traditional terminology adopted in the literature, an alternative terminology in classifying rotary heat and mass regenerators has been recently proposed [49]. This terminology involves using the term *desiccant wheel* for both types of exchangers; however, enthalpy exchangers are termed *passive desiccant wheels*, since they require no activation energy for regeneration, while dehumidifiers (traditionally referred to as desiccant wheels) are actually termed *active desiccant wheels*, since these, in fact, require an activation energy for regeneration. In this text, the terminology *active desiccant wheel* will be employed for referring to dehumidifiers, whereas *passive desiccant wheel* or simply *enthalpy wheel* will be adopted to denote energy exchangers.

The main difference between an enthalpy wheel and an active desiccant wheel is that the former possesses a low matrix sorbate-capacity, whereas the latter has a high matrix sorbate-capacity. In other words, active desiccant wheels, employ a greater amount of hygroscopic material in their matrix while compared to enthalpy wheels, such that they can uptake a much larger amount of water than enthalpy

¹ Also known as energy or enthalpy exchangers.

exchangers. In regard to operation, dehumidifiers operate at relative low rotation rates, for maximizing the drying potential, while enthalpy exchangers operate at higher rotational speeds, for maximizing heat and mass transfer between the matrix and process streams. In the HVAC industry, a common application of active desiccant wheels is in the so-called *desiccant cooling systems* [22, 33, 48, 50, 71], which rely on water evaporation to meet the required cooling loads. These systems have been gaining popularity over the last decades due to their environmental friendliness, due to the facts that they require no specialized refrigeration fluid and that they can be powered by low-grade energy sources. Also amongst HVAC applications, enthalpy wheels are commonly employed for reducing air-conditioning costs in ventilated buildings by recovering energy from the exhaust air to the supply air [81].

While compared to regenerative sensible heat exchangers [35, 64], or periodic sensible heat exchangers, heat and mass transfer regenerators exhibit similar characteristics. The main difference, is the additional transport phenomena due to the presence of mass transfer, which is highly coupled with heat transfer and conventionally results from normal condensation/evaporation or sorption/desorption. Clearly, the former requires that an adsorbent medium be present. In most formulations of enthalpy wheels and active desiccant wheels, however, the normal condensation and evaporation is not taken into account; nevertheless, this type of phase change is usually unwanted in these devices. Due to the inherent complexity of the phenomena involved in heat and mass regenerators with sorbent materials, a thorough understanding of the transport mechanisms is crucial for obtaining an accurate mathematical formulation; as a consequence, numerous mathematical models for these types of regenerators have been proposed throughout the last decades.

While the mathematical modeling and analysis of sensible heat regenerators can be dated to studies published almost a century ago, such as the works of Hausen [23, 24], models for describing the operation of heat and mass transfer regenerators were only available a few decades later. In addition, the first studies that evaluated the operation of these exchangers were overly simplified. Before periodic solutions were available, the performance of regenerative exchangers with sorbent materials was predicted by models in which the mass transfer breakthrough curves were analyzed. These early models addressed the problem of isothermal mass transfer in fluid flow through an adsorbent porous media. In addition, the transfer rates between the adsorbed phase and the fluid stream were evaluated by considering gas-side resistances, using convective (or film-controlled) transport coefficients. Some formulations also allowed for solid-side resistances, by means of overall (often termed *pseudo*) transfer coefficients. Examples of these models are the studies by Hougen and Marshall [28], and the Schumann-Anzelius solutions, tabulated in [37]. Rosen [52] proposed a model that was probably the first to treat the solid-side transport as an actual diffusional process. He considered a porous medium consisting of spherical particles and applied a linear equilibrium relation. The non-isothermal case of flow through a sorbent porous medium was later considered in the studies by Bullock and Threlkeld [5], and Chi and Wasan [9], in

which the coupled heat and mass transport rates were evaluated using overall transfer coefficients. Meyer and Weber [43] proposed a general treatment for the problem of coupled heat and mass transfer in flow through an adsorbing medium, considering diffusion in spherical particles and using a nonlinear equilibrium relation.

Apparently, until 1970, no provisions had been made to account for flow at the boundaries of the region in which the diffusional transport occurs, as it actually happens in the channeled matrix of a regenerator. The earliest formulation encountered in literature to consider this case was that of Chase et al. [8], who proposed a simple adiabatic two-dimensional linear model with constant coefficients, including the diffusional effects through the thickness of the sorbent medium.

In the 1970s and 1980s, various investigations related to the mathematical modeling of the transport phenomena in periodically operated exchangers were conducted [2, 3, 7, 27, 30–32, 39, 41, 42, 53, 78, 79]. These studies employed one-dimensional formulations in which overall transfer coefficients were used to predict the transfer rates between the two phases, but with the bulk fluid stream flowing through channels rather than the porous media itself. The studies of Close, Banks and Maclaine-Cross [1, 12, 39], presented an approach in which the governing partial differential equations with temperature and humidity ratio as the dependent variables are written in terms of characteristic potentials. This approach leads to a non-linear analogy methodology for predicting the operation of heat and mass transfer regenerators [2, 3]. In addition to these one-dimensional formulation studies, models that accounted for the diffusional processes within the porous material as local phenomena were developed. Ghezelayagh and Gidaspow [18] presented a formulation for the isothermal case considering both micro-pore and macro-pore diffusion mechanisms. Pesaran and Mills [51] proposed a model that allowed for the diffusional process within isothermal spherical particles in fluid flow through an adiabatic sorbent bed, and Charoensupaya and Worek [6] considered the diffusional phenomena within the thickness of the porous sorbent matrix instead of particles and presented periodic solutions for a hypothetical linear equilibrium relationship. Later, Majumdar and Worek [40] proposed a formulation in which the diffusional effects were included in particles and through the sorbent thickness, providing single-blow solutions for nonlinear equilibrium relations curve-fitted from experimental data.

During the 1990s, mathematical formulations were developed for adsorption-based regenerative exchangers, with emphasis on enthalpy wheels. Klein et al. [36] presented one of the first studies dedicated to enthalpy exchangers, and employed the non-linear analogy method presented in [2, 3]. Stiesch et al. [77] analyzed the performance of enthalpy exchangers by a simple approach using curve fitted data from the numerical solution of heat and mass transport equations. Simonson and Besant [67–70] employed a one-dimensional model that includes axial heat diffusion in the matrix, and used the data to develop correlations for predicting the performance of enthalpy exchangers in terms of dimensionless groups; an interesting point observed in these works is that the heating due to adsorption is divided

between the process stream and channel wall. Besides studies focused on enthalpy wheels, new investigations dedicated to modeling and assessing the performance of active desiccant wheels also continued to be developed. Zheng et al. [83–85] employed a simple one-dimensional model without local diffusion transport terms.

Since the turn of the millennium, a number of studies focused on the mathematical modeling and simulation of active desiccant and enthalpy wheels have appeared in the literature. Particularly interesting is the work of Ge et al. [16], who present a review of mathematical models used in different investigations. Dai et al. [14] utilized a two-dimensional model that included diffusion of heat and moisture within the rotary matrix in both axial and angular directions. Niu and Zhang [45], Zhang and Niu [82] adopted a two-dimensional model for the transport phenomena in the sorbent material for analyzing both active and passive desiccant wheels. The model utilized by Gao et al. [15] also included transport terms in the angular direction; however, local diffusion terms were only included in the axial direction within the rotary matrix. Golubovic and Worek [20] considered a simple one-dimensional model, similar to the one employed in [83–85]; however, a modification was included to account for condensation within channels which are prone to occur at higher operating pressures. Later on, Golubovic et al. [19] employed this simple one-dimensional model to predict the performance of rotary regenerators with and without heated purge. Jeong and Mumma [29] utilized a model similar to the one adopted in [67–70] for determining correlations for estimating the performance of enthalpy exchangers. In 2004, Sphaier and Worek proposed a unified formulation that contemplates both enthalpy exchangers and active desiccant wheels. This general formulation considered multi-dimensional heat and mass diffusion within the adsorbent layer. Later on Sphaier and Worek [72], the same authors compared a two-dimensional version of this formulation with a simple one-dimensional counterpart (similar to the one used in most one-dimensional models), and the presented results suggested that one-dimensional models are better suited for active desiccant wheels rather than for enthalpy wheels. The importance of including axial diffusion effects in active desiccant wheels and enthalpy exchangers was analyzed in a separate study Sphaier and Worek [73]. In following studies, the same authors presented a numerical scheme for solving the employed model [74], and presented a generalized effectiveness-NTU approach [75], extending the classical methodology for sensible heat regenerators proposed by Coppage and London [13], to heat and mass transfer regenerators with local diffusion in the rotary matrix.

Over the last half decade, different investigations related to modeling and simulation of heat and mass transfer regenerators have been published. Ruivo et al. [55–61] presented a series of studies regarding to the mathematical modeling simulation of heat and mass exchangers. A one dimensional model was employed in [56] for evaluating the impact of different simplifications mostly related to the diffusion effects in the adsorbent material. A comparison between one- and two-dimensional models, assuming parallel plates channels, was carried out in [57] and the results indicated that a one-dimensional model for the flow in channels (bulk-flow formulation) could be used with small error for channels lengths smaller than

100 mm. A one-dimensional model with axial diffusion in the matrix was also used in [55, 59, 60], and a two-dimensional model for the desiccant matrix, assuming parallel plates-channels, and considering a one-dimensional bulk-flow model for the airstream, was employed in [61]. Chung and Lee [10], Chung et al. [11], and Stabat and Marchio [76] considered a simple one-dimensional model for the airstream and matrix, but included no effects of axial diffusion, and Shang and Besant [65, 66] employed a totally-lumped model. Nóbrega and Brum [46, 47, 49] also employed simple one-dimensional models with no local diffusion phenomena, and considered further simplifications such as negligible heat and mass storage in the airstream. Ge et al. [17] and Heidarinejad and Pasharshahri [25, 26] utilized a one-dimensional model with axial diffusion effects in the matrix. Narayanan et al. [44] also utilized one-dimensional models, but presented a comparison between models with and without axial diffusion effects. Ruan et al. [54] also used a one-dimensional model with axial diffusion effects to analyze an enthalpy wheel with purge air.

As seen from the presented literature review, different mathematical models have been used over the last couple of decades for simulating the operation of heat and mass transfer regenerators. When looking into the differences between these models, one can notice that the main distinctions occur in the heat and mass transport equations for the sorbent material. In this context, the purpose of this chapter is to present different types of mathematical models for heat and mass transfer regenerators, with emphasis on the transport processes within the porous sorbent material. The derivation of these formulations will be discussed, and models with different levels of details in the spatial description of the temperature and humidity concentration in the sorbent material will be presented, from complex multidimensional forms to simple one-dimensional ones.

2 Problem Description and Common Assumptions

The general problem considered in this study is that of a rotary exchanger, which periodically alternates between different process streams, as shown in Fig. 1. The rotary matrix is composed of numerous mini-channels through which the streams flow, transferring mass and energy to the channels' walls, which are composed of porous sorbent materials. The overall process is adiabatic such that during an entire cycle the net energy (as well as mass) transfer rate to the matrix is zero; this means that, if two process streams are employed, for an entire cycle the energy (and mass) removed from one stream is entirely delivered to the other one, and vice versa.

The rotary matrix can be subdivided in K sections, delimited by angles, as shown in Fig. 1. Naturally the sum of all angles add up to 2π :

$$\sum_{k=1}^K \theta_k = 2\pi. \quad (1)$$

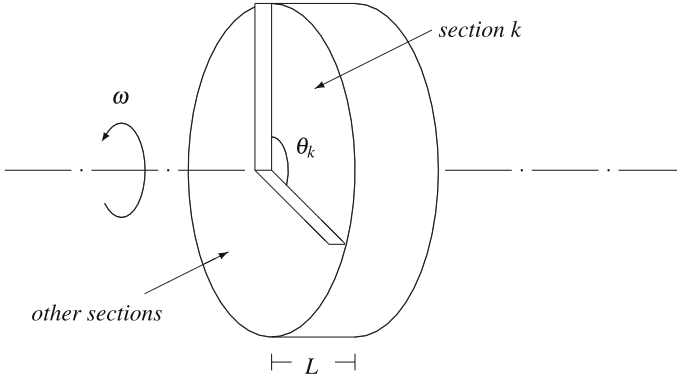


Fig. 1 Rotary exchanger

The wheel operates at a constant angular speed ω , such that if a fixed point is followed as it rotates, each section gives rise to a different operating periods. The duration of these K periods are easily calculated as:

$$\delta t_k = \frac{\theta_k}{\omega}, \quad (2)$$

and the summation of all these periods yield the total cycle time, t_f :

$$\sum_{k=1}^K \delta t_k = t_f. \quad (3)$$

The summation of the δ_k up to a given number of sections smaller than the total sections yield @@@@a partial cycle time:

$$\sum_{p=1}^k \delta t_p = t_k, \quad (4)$$

such that t_K corresponds to the total cycle time t_f .

Despite the rotation, the channels are analyzed as stationary, by choosing a proper reference coordinate system, fixed to a representative channel. The walls of each channel are composed of a porous *sorbent felt*, which may be laid upon an impermeable supporting wall, as displayed in Fig. 2. As shown in this figure, surface \mathcal{S}_p represents the interface between the process stream and the porous sorbent, which is called the *felt-stream interface*. Moreover, surface \mathcal{S}_w represents the interface between the porous sorbent felt and the impermeable structure, termed the *felt-wall interface*. The channels are assumed independent of each other such that the surfaces between adjacent channel-structures are considered adiabatic and impermeable. Due to the actual geometry of these channels, an exact, three-dimensional, representation of the system could be too complex, requiring a prohibitive computational effort for obtaining excessively detailed information.

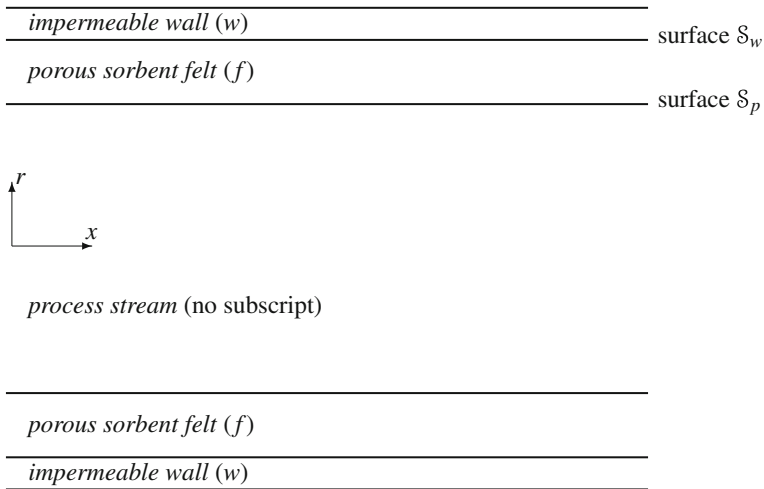


Fig. 2 Single channel-structure

Then again, a one-dimensional description may be overly simplified, and a balance between these two could be required. Different levels of formulations will be presented in this chapter, and the simplifications involved in each case will be discussed, allowing a proper formulation to be chosen according to the considered type of problem.

The porous adsorbent material is modeled as a homogeneous medium composed of a solid portion and pores, in which both gas and adsorbed phases coexist. In order to facilitate the analysis, a subscripting scheme indicating the considered phase is employed. Starting with the solid portion of the material, the subscript s refers to quantities in this solid phase. Conversely, within pores, g is employed for the gaseous phase. The subscript l is employed for the adsorbed phase; nevertheless, since the adsorption occurs on the surface of the solid phase, the subscript s is also employed to describe quantities related to the adsorbed phase, e.g. surface diffusion of the adsorbate. For quantities within the bulk porous material with no required phase distinction, a simple f subscript is used. In the process stream, a single-phase is present, and for the sake of simplicity, no subscript is employed for this phase.

2.1 Common Assumptions

Some common assumptions employed for modeling heat and mass transfer in rotary regenerators can be summarized as:

1. Radiation effects are neglected, as a result of relatively small temperatures.

2. No chemical reaction takes place, nor are there any energy sources within the system.
3. The effects of field forces, such as gravity, on the fluid mixture are negligible.
4. The channel flow is incompressible and viscous dissipation is negligible.
5. The channels are equal and uniformly distributed throughout the wheel.
6. The state properties of each inlet-stream are radially uniform at the inlet face of the wheel; also, the mass flow rate of dry air is constant at each inlet face.
7. Heat and mass transfer between adjacent flow-channels is negligible; heat and mass transfer from the exchanger to the surroundings (besides the channel inflow and outflow) are also negligible.
8. The pressure drop along the axial flow length due to skin friction is small compared to the total pressure, such that thermodynamic properties are unaffected.
9. All sorption phenomena are thermodynamically reversible.
10. Axial diffusion in the process stream is small compared to convective transfer, and is neglected.
11. The channel flow is laminar and fully developed; the convective heat and mass transfer between channels and the felt surface can be evaluated by employing bulk properties and film coefficients.²
12. The gaseous components of the fluid mixture are treated as ideal gases with constant thermo-physical properties.
13. The concentration of fluid other than sorbate in the mixture is assumed constant.
14. The specific heats and thermal conductivities of dry sorbent and adsorbate are assumed constant.
15. The gas mixtures are dilute solutions.
16. The porous felt is assumed to be homogeneous and isotropic, and the concentration of material other than adsorbate is unaffected by sorption.
17. The mass diffusion rate in micro-pores is rapid compared to that of the macro-pores.
18. Thermodynamic equilibrium exists at every point between the sorbate in the gas-phase and on the solid surface (adsorbed phase).
19. No phase change, other than that related to the sorption process, occurs in the exchanger.
20. There is no explicit transfer coupling through *Soret* or *Dufour* effects.

The majority of studies that present mathematical formulations for simulating the operation of active and passive desiccant wheels are based on a list of similar assumptions. Naturally, there are some variations in assumptions that consequently lead to different formulations. The formulations presented in this text are mainly based on the aforementioned assumptions; however, the implications of relaxing some of these assumptions, or even considering additional simplifications, will be

² Convective heat and mass transfer coefficients.

discussed and the modifications in formulations resulting from these considerations will be presented.

3 Concentrations, Enthalpies and Heat of Sorption

Before going into the details of the heat and mass transfer balances that lead to the mathematical model equations, some fundamental quantities are introduced, such as the concentration variables, enthalpies and quantities related to the sorption phenomenon.

3.1 Concentrations

Since it is common practice in enthalpy and active desiccant wheels to assume an invariable density of dry air, it becomes useful to employ dry-basis concentrations. This section introduces the concentration variables used to describe the water concentration in gaseous and adsorbed phases, in both volumetric basis (kg/m^3) and dry basis ($\text{kg water}/\text{kg dry air}$).

The water vapor concentrations in the gas phase, denoted ρ_v (in process stream) and $\rho_{v,f}$ (in void spaces within the sorbent material), are related to the dry-basis concentrations Y and Y_f as:

$$\rho_v = \rho_a Y, \quad \rho_{v,f} = \rho_a Y_f, \quad (5)$$

where ρ_a is the dry air density, which is assumed constant. In this form, the dry basis vapor concentration is equivalent to the traditional *humidity ratio* or *absolute humidity* used in psychrometrics.

In addition, the adsorbed phase concentration, denoted ρ_l is related to its dry-basis counterpart, W , as:

$$\rho_l = \rho_s f_s W, \quad (6)$$

where f_s is the *mass fraction of adsorbent material in the felt*.

While the water vapor concentration $\rho_{v,f}$ is defined per unit volume of pores (excluding dead pores), the adsorbed water concentration ρ_l is given in terms of the actual structural volume of the solid sorbent (including dead pores). As a result, the total mass of water contained in the adsorbent material can be calculated by

$$\int_{\mathcal{V}_f} \varepsilon \rho_{v,f} + (1 - \varepsilon) \rho_l d\mathcal{V}, \quad (7)$$

where \mathcal{V}_f corresponds to the volume of the porous felt and ε to its porosity.

For problems involving active and passive desiccant wheels, the adsorbed phase concentration is generally assumed to be in local equilibrium with the gas phase in the pore space adjacent to it. As a result W is expressed as a function of the temperature and gas-phase concentration of the pore space:

$$\Phi(W, Y_f, T_f) = 0, \quad (8)$$

where Φ is a general function. Many times this relation can be written in an simpler explicit form:

$$W = \Phi(Y_f, T_f). \quad (9)$$

The specific function relation for W is a constitutive equation called an *equilibrium relation* or an *adsorption isotherm*.

3.2 Enthalpies and Heat of Sorption

Since ideal gases are considered, the enthalpies of the gaseous phases depend only on temperature. The dry air and vapor enthalpies are written as:

$$i_a = i_a(T), \quad i_{a,f} = i_{a,f}(T_f), \quad i_v = i_v(T), \quad i_{v,f} = i_{v,f}(T_f), \quad (10)$$

where the subscripts have been included to distinguish between the air and vapor in the felt from those quantities in the process streams (where no subscript is used). The enthalpy of saturated liquid and the solid matrix also depend on temperature only, and are given by:

$$i_{ls} = i_{ls}(T_f), \quad i_s = i_s(T_f), \quad (11)$$

in which no special phase subscript is needed since these only occur within the porous felt. The enthalpy associated with the adsorbed phase is somewhat similar to that of a liquid phase; however, the additional surface attraction associated with the physical adsorption phenomenon imply in enthalpy values that are generally smaller than that of saturated liquid at the same temperature. This enthalpy is defined as:

$$i_l = i_l(T_f, W) = i_{ls}(T_f) + i_{\text{wet}}(T_f, W), \quad (12)$$

where i_{wet} is the *differential heat of wetting*, which is generally a negative value as normally $i_l \leq i_{ls}$. The relations above also reflect the fact that i_{wet} , and consequently i_l , depend on the adsorbed content. The heat of wetting will generally have a larger magnitude for smaller values of W , due to the stronger adsorption forces associated with the first layers of adsorbate on the adsorbent surface.

The heat of wetting also occurs in an integral form, called the *integral heat of wetting* and defined as:

$$\Delta i_{\text{wet}} = \Delta i_{\text{wet}}(T_f, W) = \int_0^W i_{\text{wet}}(T_f, W') dW', \quad (13)$$

where the parenthesis denote the dependence of i_{wet} on the adsorbed content.³ Since the quantity i_{wet} decreases with increasing W , using constant i_{wet} values could lead to overestimated values of Δi_{wet} . Based on the definition of Δi_{wet} , an averaged differential heat of wetting is also defined:

$$\bar{i}_{\text{wet}}(T_f, W) = \frac{\Delta i_{\text{wet}}(T_f, W)}{W} = \frac{1}{W} \int_0^W i_{\text{wet}}(T_f, W') dW', \quad (14)$$

such that the integral heat of wetting for a given adsorbed content W can be simply obtained by multiplying this quantity by \bar{i}_{wet} .

The *heat of vaporization* is defined as the difference between the saturated vapor and saturated liquid enthalpies:

$$i_{\text{vap}} = i_{\text{vap}}(T_f) = i_{v,f}(T_f) - i_{ls}(T_f), \quad (15)$$

in which $i_{v,f}$ equals the saturated vapor enthalpy due to the ideal gas assumption. Similar to the definition of the heat of vaporization, the *differential heat of sorption*⁴ is defined as the difference between the enthalpy of saturated vapor and that of the adsorbed phase:

$$i_{\text{sor}} = i_{\text{sor}}(T_f, W) = i_{v,f}(T_f) - i_l(T_f, W), \quad (16)$$

emphasizing the dependence of i_{sor} on the adsorbed content W . It is useful to know that the difference between the heat of sorption and heat of vaporization leads to the heat of wetting:

$$i_{\text{wet}} = i_{\text{vap}} - i_{\text{sor}}, \quad (17)$$

which implies that i_{sor} is larger than i_{vap} as $i_{\text{wet}} < 0$.

As similarly done for the heat of wetting, an averaged specific enthalpy of the adsorbed phase is also defined:

$$\bar{i}_l = i_{ls} + \bar{i}_{\text{wet}}, \quad (18)$$

such that the enthalpy per mass of dry sorbent of adsorbed water can be simply written as $W\bar{i}_l$.

³ However, the heat of wetting may also depend on temperature.

⁴ For simplicity, the differential heat of sorption is commonly referred to as just *heat of sorption*.

4 Conservation Balances

This section presents heat and mass conservation balances for the process stream and the sorbent material. Although a simple bulk-flow model is presented for the process stream, as employed by the majority of previous investigators, different type of balances will be presented for the transport processes in the sorbent material.

4.1 Conservation Balances for Process Stream

Although a few works may employ more complex formulations for describing the heat and mass transfer within the process streams, most studies employ simple bulk transport equations for describing the heat and mass transfer in the flow. Since the purpose of this text is to present different formulations for the transport within the adsorbent material, simple one-dimensional convection equations, as found in a number of active and passive desiccant wheels studies, are used. Nevertheless, a few nuances that are seen in different literature studies will be commented.

The convective mass transfer in the process stream is described by the mean stream concentration ρ_v , which is obtained from a simple mass balance:

$$\mathcal{A}_p \left(\frac{\partial \rho_v}{\partial t} + u \frac{\partial \rho_v}{\partial x} \right) = \mathcal{P}_s j_i'' , \quad (19)$$

in which \mathcal{P}_s is the wetted perimeter (i.e. based on the heat and mass transfer area at the felt-stream interface), \mathcal{A}_p is the flow area and j_i'' is the mass transfer flux at this interface. Naturally, the adopted convention is that j_i'' be positive when water is transferred from the sorbent felt to the process stream. Using the dry-basis concentration the previous equation may be simplified to:

$$\rho_a \left(\frac{\partial Y}{\partial t} + u \frac{\partial Y}{\partial x} \right) = \frac{\mathcal{P}_s}{\mathcal{A}_p} j_i'' . \quad (20)$$

The convective heat transport equation is also given in terms of a mean stream energy balance:

$$\mathcal{A}_p \frac{\partial}{\partial t} (\rho_a i_a + \rho_v i_v) = - \frac{\partial}{\partial x} (\mathcal{A}_p u (\rho_a i_a + \rho_v i_v)) + \mathcal{P}_s \dot{q}_i'' + \mathcal{P}_s j_i'' i_{v,i} , \quad (21)$$

where i_a and i_v are the mean stream enthalpies of dry air and water vapor, u is the bulk velocity of the flow, and \dot{q}_i'' is the heat flux from the sorbent felt to the process stream. Rearranging Eq. (21) and simplifying yields:

$$\rho c_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = \frac{\mathcal{P}_s}{\mathcal{A}_p} \dot{q}_i'' + \frac{\mathcal{P}_s}{\mathcal{A}_p} j_i'' (i_{v,i} - i_v), \quad (22)$$

in which ρc_p is the volumetric heat capacity of moist air, given by:

$$\rho c_p = \rho_a c_{p,a} + \rho_v c_{p,v} = \rho_a (c_{p,a} + c_{p,v} Y). \quad (23)$$

The vapor enthalpy $i_{v,i}$ represents the specific enthalpy associated with the mass transfer from the sorbent felt. Many studies omit the term involving the enthalpy difference ($i_{v,i} - i_v$) in their formulations, which corresponds to assuming either that $i_{v,i} \approx i_v$ or that the total contribution of the entire energy transfer term due to mass transfer from the felt is negligible.

Despite the fact that the process stream balances are written in terms of bulk, or mean stream properties, and the average velocity u is constant, it can assume different values for each stream. As a matter of fact, for counterflow arrangements the velocities will have different signs. In order to work with positive velocity values, the flow transport equations are written as:

$$\rho_a \left(\frac{\partial Y}{\partial t} + (-1)^\gamma u \frac{\partial Y}{\partial x} \right) = \frac{\mathcal{P}_s}{\mathcal{A}_p} j_i'', \quad (24)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + (-1)^\gamma u \frac{\partial T}{\partial x} \right) = \frac{\mathcal{P}_s}{\mathcal{A}_p} \dot{q}_i'' + \frac{\mathcal{P}_s}{\mathcal{A}_p} j_i'' (i_{v,i} - i_v), \quad (25)$$

where $\gamma = 0$ for parallel flow arrangements and $\gamma = 1$ for counterflow arrangements during reversed flow periods.

Another common simplification among formulations for heat and mass transfer in both active and passive desiccant wheels involves assuming that the energy and water vapor storage terms in the fluid flow is negligible compared to the advective term, which leads to the following simplified forms:

$$(-1)^\gamma \rho_a u \frac{\partial Y}{\partial x} = \frac{\mathcal{P}_s}{\mathcal{A}_p} j_i'', \quad (26)$$

$$(-1)^\gamma \rho c_p u \frac{\partial T}{\partial x} = \frac{\mathcal{P}_s}{\mathcal{A}_p} \dot{q}_i'' + \frac{\mathcal{P}_s}{\mathcal{A}_p} j_i'' (i_{v,i} - i_v), \quad (27)$$

4.2 Balance for Impermeable Supporting Structure

As already mentioned, in many cases, the sorbent felt is laid upon an impermeable supporting structure, which will consequently have an influence on the heat and mass transfer in the sorbent material. The impermeability condition only requires that an energy balance be used. This balance can be written in simple one-dimensional form:

$$\mathcal{A}_w \rho_w c_w \frac{\partial T_w}{\partial t} = -\mathcal{A}_w \frac{\partial \dot{q}''_{w,x}}{\partial x} - \mathcal{P}_w \dot{q}''_w, \quad (28)$$

where \mathcal{A}_w is the conduction heat transfer area of the wall (perpendicular to the flow direction), \mathcal{P}_w is the contact perimeter at the felt-wall interface, \dot{q}''_w is the heat flux from the wall to the sorbent material, $\dot{q}''_{w,x}$ is the conduction heat flux in the wall, and $\rho_w c_w$ is the wall thermal capacity. The heat fluxes $\dot{q}''_{w,x}$ and \dot{q}''_w will be introduced in a latter section.

4.3 One-Dimensional Conservation Balances for Sorbent

The simplest formulation for describing active desiccant and enthalpy wheels is a one-dimensional one, which takes into account variations in the flow direction only. These one-dimensional balances are herein presented, and variations between formulations will be discussed according to the application of different simplifying assumptions.

4.3.1 Mass Transport

The mass transport equation is given by the following mass balance for water in the felt:

$$\mathcal{A}_f \left(\varepsilon \frac{\partial \rho_{v,f}}{\partial t} + (1 - \varepsilon) \frac{\partial \rho_l}{\partial t} \right) = -\mathcal{P}_s j''_i - \mathcal{A}_f \frac{\partial j''_{g,x}}{\partial x} - \mathcal{A}_f \frac{\partial j''_{s,x}}{\partial x}, \quad (29)$$

in which \mathcal{A}_f is the frontal area (area perpendicular to the flow direction) of the adsorbent material. The fluxes $j''_{g,x}$ and $j''_{s,x}$ are due to axial mass diffusion in the sorbent material, in the gas-phase (vapor) and adsorbed phase (on the pore surface), respectively. Using the dry-basis concentrations, Eq. (29) can be rewritten as:

$$\varepsilon \rho_a \frac{\partial Y_f}{\partial t} + (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = -\frac{\mathcal{P}_s}{\mathcal{A}_f} j''_i - \frac{\partial j''_{g,x}}{\partial x} - \frac{\partial j''_{s,x}}{\partial x}. \quad (30)$$

Based on the previous equations, the *volumetric rate of sorption*, for the one-dimensional balance, is defined as:

$$\dot{g}'''_{\text{sor}} = (1 - \varepsilon) \frac{\partial \rho_l}{\partial t} + \frac{\partial j''_{s,x}}{\partial x} = (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} + \frac{\partial j''_{s,x}}{\partial x}, \quad (31)$$

representing the actual rate of water adsorption, which comprises for the rate of increase in adsorbed water and less the rate of inflow of adsorbed water through diffusion.

While some investigations consider the axial mass diffusion through the sorbent layer, a common simplification among a number of studies is that the mass diffusion in the axial direction is small compared to the mass transfer in the airstream, such that Eq. (30) could be simply written as:

$$\varepsilon \rho_a \frac{\partial Y_f}{\partial t} + (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = - \frac{\mathcal{P}_s}{\mathcal{A}_f} j_i'' \quad (32)$$

and the rate of sorption is simplified to:

$$\dot{g}_{\text{sor}}''' = (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} \quad (33)$$

More insight on the rate of sorption can be obtained if the mass conservation Eq. (30) is employed to rewrite the rate of sorption as:

$$\dot{g}_{\text{sor}}''' = - \frac{\mathcal{P}_s}{\mathcal{A}_f} j_i'' - \frac{\partial j_{g,x}''}{\partial x} - \varepsilon \rho_a \frac{\partial Y_f}{\partial t} \quad (34)$$

In this form, if one considers that the convective mass transfer to the process stream is much larger in magnitude than the storage in gas-phase and the gas-phase diffusion transfer, the rate of sorption could be alternatively simplified to:

$$\dot{g}_{\text{sor}}''' = - \frac{\mathcal{P}_s}{\mathcal{A}_f} j_i'' \quad (35)$$

This simplification is considered by different investigators and generally also implies that vapor storage effect in the gas-phase is small compared to that of the adsorbed phase. For these cases, one could simplify Eq. (32) to:

$$(1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = - \frac{\mathcal{P}_s}{\mathcal{A}_f} j_i'' \quad (36)$$

Nevertheless, while this could be a good approximation for some active desiccant wheels, when enthalpy wheels are considered, the fraction of adsorbent material in the felt (f_s) may assume small values, and this approximation could lead to incorrect results.

4.3.2 Energy Transport

With the assumptions of small pressure variation, the energy transport equation can be obtained from an enthalpy balance within the sorbent felt:

$$\begin{aligned}
& \mathcal{A}_f \frac{\partial}{\partial t} \left(\varepsilon (\rho_a i_a + \rho_{v,f} i_{v,f}) + (1 - \varepsilon) \left(\rho_s i_s + \int_0^{\rho_l} i_l d\rho_l \right) \right) \\
&= -\mathcal{A}_f \frac{\partial \dot{q}_{f,x}''}{\partial x} - \mathcal{P}_s \dot{q}_i'' - \mathcal{P}_s j_i'' i_{v,i} + \mathcal{P}_w \dot{q}_w'' - \mathcal{A}_f \frac{\partial (i_{v,f} j_{g,x}'')}{\partial x} - \mathcal{A}_f \frac{\partial (\bar{i}_l j_{s,x}'')}{\partial x},
\end{aligned} \tag{37}$$

which can also be written in terms of the dry-basis concentrations:

$$\begin{aligned}
& \mathcal{A}_f \frac{\partial}{\partial t} \left(\varepsilon \rho_a (i_a + Y_f i_{v,f}) + (1 - \varepsilon) \rho_s \left(i_s + \int_0^w i_l dW' \right) \right) \\
&= -\mathcal{A}_f \frac{\partial \dot{q}_{f,x}''}{\partial x} - \mathcal{P}_s \dot{q}_i'' - \mathcal{P}_s j_i'' i_{v,i} + \mathcal{P}_w \dot{q}_w'' - \mathcal{A}_f \frac{\partial (i_{v,f} j_{g,x}'')}{\partial x} - \mathcal{A}_f \frac{\partial (\bar{i}_l j_{s,x}'')}{\partial x},
\end{aligned} \tag{38}$$

where $\dot{q}_{f,x}''$ is the conduction heat flux in the sorbent material. The integrated enthalpy of adsorbed water needs to be used due to the dependence of the enthalpy of the adsorbed phase (i_l) on the adsorbed concentration, which occurs due to the nature of the heat of wetting.

Another point worth noting is that the energy transfer associated with the diffusion in the adsorbed phase is written in terms of the averaged enthalpy \bar{i}_l . Hence, the enthalpy of the diffused amount is the averaged value of all adsorbed layers, which implies an assumption that the diffusion is equally distributed among different adsorbed layers. Indeed, the ‘‘exact’’ value of the specific enthalpy of the diffused adsorbed water would involve an integral over the different diffusion rates associated with different adsorbed layers. On the other hand, using i_l instead of \bar{i}_l involves an assumption that the amount of diffused water, regardless of its quantity, will have an enthalpy value of the last adsorbed layer. Although \bar{i}_l is herein adopted as the enthalpy of the diffused layer, one could easily modify the formulation if a better approximation or the actual enthalpy of the diffused adsorbed water is available.

The rearrangement of Eq. (38) leads, after simplification, to:

$$\begin{aligned}
\rho_f c_f \frac{\partial T_f}{\partial t} + j_{g,x}'' \frac{\partial i_{v,f}}{\partial x} + j_{s,x}'' \frac{\partial \bar{i}_l}{\partial x} &= -\frac{\partial \dot{q}_{f,x}''}{\partial x} - \frac{\mathcal{P}_s}{\mathcal{A}_f} \dot{q}_i'' \\
&\quad - \frac{\mathcal{P}_s}{\mathcal{A}_f} j_i'' (i_{v,i} - i_{v,f}) + \dot{s}_{\text{sor}}''' + \frac{\mathcal{P}_w}{\mathcal{A}_f} \dot{q}_w'',
\end{aligned} \tag{39}$$

where \dot{s}_{sor}''' is the *volumetric rate of sorption heating*, which, for the one-dimensional balance, is defined as:

$$\dot{s}_{\text{sor}}''' = (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} (i_{v,f} - i_l) + \frac{\partial j_{s,x}''}{\partial x} (i_{v,f} - \bar{i}_l), \tag{40}$$

and the *volumetric thermal capacity of the felt* includes contributions from the moist air in pores, the solid adsorbent and the adsorbed water:

$$\rho_f c_f = \varepsilon \rho_a (c_{p,a} + c_{p,v} Y_f) + (1 - \varepsilon) \rho_s (c_s + f_s W c_l), \quad (41)$$

in which the specific heat of the adsorbed phase is defined by

$$W c_l = \frac{\partial}{\partial T_f} \left(\int_0^W i_l dW \right)_W \quad \text{or} \quad c_l = \left(\frac{\partial \bar{i}_l}{\partial T_f} \right)_W, \quad (42)$$

where the subscript W indicates differentiation holding W constant. Equation (41) shows that the energy storage term in Eq. (39) represents the combined energy storage in all three phases present at a point in the sorbent material.

Observing the left-hand-side of Eq. (39), one notices that besides the energy storage term, there are two advective energy transport terms due to the water motion in gas and adsorbed phases. Since these mass transfer rates are due to diffusion, these terms are assumed negligible and removed from the transport equation. Finally, with the introduction of the heat of sorption from Eq. (16), one obtains:

$$\rho_f c_f \frac{\partial T_f}{\partial t} = - \frac{\partial \dot{q}_{f,x}''}{\partial x} - \frac{\mathcal{P}_s}{\mathcal{A}_f} \dot{q}_i'' - \frac{\mathcal{P}_s}{\mathcal{A}_f} J_i'' (i_{v,i} - i_{v,f}) + \dot{s}_{\text{sor}}''' + \frac{\mathcal{P}_w}{\mathcal{A}_f} \dot{q}_w'', \quad (43)$$

Introducing the definition of the heat of sorption (16) in Eq. (40) leads to:

$$\dot{s}_{\text{sor}}''' = (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} i_{\text{sor}} + \frac{\partial J_{s,x}''}{\partial x} (i_{v,f} - \bar{i}_l). \quad (44)$$

The sorption heating can be also written in terms of the rate of sorption:

$$\dot{s}_{\text{sor}}''' = \dot{g}_{\text{sor}}''' i_{\text{sor}} + \frac{\partial J_{s,x}''}{\partial x} (i_l - \bar{i}_l), \quad (45)$$

in which the last term represents an additional contribution due to diffusion in the adsorbed layers. An example of the manifestation of this term is a situation in which no adsorption occurs, but due to a difference in surface concentration, there is movement in the adsorbed phase, thereby resulting in a redistribution of adsorbate within different adsorbed layers. The enthalpy difference associated with different layers will produce a heating or cooling effect, which is represented by the last term in equation. Naturally, if there is no surface diffusion, \dot{s}_{sor}''' is simply given by:

$$\dot{s}_{\text{sor}}''' = \dot{g}_{\text{sor}}''' i_{\text{sor}} = (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} i_{\text{sor}}. \quad (46)$$

Finally, since three dependent variables appear in the heat and mass balance, an extra equation is needed. This equation is the sorption isotherm, or equilibrium relation, as generally defined by Eq. (8) or (9), such that W is calculated directly

from the properties (T_f and Y_f) of the gas-phase in the void spaces of the sorbent felt.

4.4 Multidimensional Conservation Balances for Sorbent

The derivation of the mass and energy transport equations for a multidimensional formulation in the sorbent can also be easily obtained, as demonstrated in this section. As presented for the one-dimensional formulation, variation in equations arising from different simplifications are also discussed. A specific modification that will be shown is due to the inclusion of additional transport rates due to Soret and Dufor effects. This modification was not included in the one-dimensional sorbent equations to avoid repetition. Nevertheless, one can easily modify the one-dimensional transport equation for the sorbent material as similarly shown for the multi-dimensional formulation to include these effects.

4.4.1 Mass Transport

Considering a control volume \mathcal{V} with a bounding surface \mathcal{S} , within the sorbent material, an integral mass balance yields:

$$\frac{d}{dt} \int_{\mathcal{V}} (\varepsilon \rho_{v,f} + (1 - \varepsilon) \rho_l) d\mathcal{V} = - \int_{\mathcal{S}} (\mathbf{j}_g'' + \mathbf{j}_s'') \cdot \mathbf{n} d\mathcal{S}, \quad (47)$$

where \mathbf{j}_g'' and \mathbf{j}_s'' represent the mass flux vectors corresponding to diffusion of vapor in the gas-phase and adsorbed water on the surface of the pores, respectively. Then, applying Gauss' Divergence Theorem finally leads to:

$$\varepsilon \frac{\partial \rho_{v,f}}{\partial t} + (1 - \varepsilon) \frac{\partial \rho_l}{\partial t} = -\nabla \cdot \mathbf{j}_g'' - \nabla \cdot \mathbf{j}_s'', \quad (48)$$

which correspond to a statement that the water storage in gaseous and adsorbed form result from the net mass inflow due to gas-phase and surface diffusion, which are assumed to occur in parallel. Using the dry-basis concentration variables, Eq. (48) can be simplified to:

$$\varepsilon \rho_a \frac{\partial Y_f}{\partial t} + (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = -\nabla \cdot \mathbf{j}_g'' - \nabla \cdot \mathbf{j}_s''. \quad (49)$$

This is probably the most common form of the mass conservation equation used in multidimensional formulations for solid sorbents in active and passive desiccant wheels.

The equation can naturally be modified if some effects are considered unimportant. A common modification seen among literature studies involves assuming

that the adsorbed phase storage is much higher than that of the gas-phase storage, such that Eq. (49) is modified to the following form:

$$(1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = -\nabla \cdot \mathbf{j}_g'' - \nabla \cdot \mathbf{j}_s''. \quad (50)$$

While the last modification simplifies Eq. (49), additional modifications can be made to include other phenomena. For instance, if the hypothesis of no *thermo-diffusion* is relaxed, this equation should be modified to include an additional transport term:

$$\varepsilon \rho_a \frac{\partial Y_f}{\partial t} + (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = -\nabla \cdot \mathbf{j}_g'' - \nabla \cdot \mathbf{j}_s'' - \nabla \cdot \mathbf{j}_T'', \quad (51)$$

where \mathbf{j}_T'' represents the mass flux vector due to thermo-diffusion, also known as *thermophoresis* or simply as Soret effect.

4.4.2 Energy Transport

As similarly carried out for the mass balance, an integral energy balance with a control volume \mathcal{V} yields:

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{V}} \left(\varepsilon (\rho_a i_a + \rho_{v,f} i_{v,f}) + (1 - \varepsilon) \left(\rho_s i_s + \int_0^{\rho_l} i_l d\rho_l \right) \right) d\mathcal{V} \\ = - \int_S \dot{\mathbf{q}}_f'' \cdot \mathbf{n} d\mathcal{S} - \int_S \left(i_{v,f} \mathbf{j}_g'' + \bar{i}_l \mathbf{j}_s'' \right) \cdot \mathbf{n} d\mathcal{S}, \end{aligned} \quad (52)$$

where $\dot{\mathbf{q}}_f''$ is the effective heat flux vector in the porous felt. Then, employing Gauss' Divergence Theorem and using the mass conservation Eq. (48) leads, after simplification, to:

$$\rho_f c_f \frac{\partial T_f}{\partial t} + \mathbf{j}_g'' \cdot \nabla i_{v,f} + \mathbf{j}_s'' \cdot \nabla \bar{i}_l = -\nabla \cdot \dot{\mathbf{q}}_f'' + \dot{s}_{\text{sor}}''', \quad (53)$$

where the last term on the right hand side of Eq. (53) represents the heating effects associated with the sorption phenomenon. The volumetric rate of sorption for the multidimensional formulation is given by:

$$\dot{s}_{\text{sor}}''' = (1 - \varepsilon) \frac{\partial \rho_l}{\partial t} + \nabla \cdot \mathbf{j}_s'', \quad (54)$$

and the rate of heating due to sorption is given by:

$$\dot{s}_{\text{sor}}''' = (1 - \varepsilon) \frac{\partial \rho_l}{\partial t} i_{\text{sor}} + (\nabla \cdot \mathbf{j}_s'') (i_{v,f} - \bar{i}_l) = \dot{g}_{\text{sor}}''' i_{\text{sor}} + (\nabla \cdot \mathbf{j}_s'') (i_l - \bar{i}_l), \quad (55)$$

as analogously defined for the one-dimensional formulation by Eqs. (31) and (44), respectively. Naturally, if the contribution of surface diffusion is negligible to the sorption heating term, one arrives at:

$$\dot{s}'_{\text{sor}} = \dot{g}'_{\text{sor}} i_{\text{sor}}. \quad (56)$$

As previously discussed, as the advective heat transport terms due to the diffusion mass fluxes can generally be assumed negligible compared to the other energy transport terms, Eq. (53) is simplified to give:

$$\rho_f c_f \frac{\partial T_f}{\partial t} = -\nabla \cdot \dot{\mathbf{q}}'_f + \dot{s}'_{\text{sor}}, \quad (57)$$

which is also a traditional form found in the literature for multidimensional heat transfer in sorbents of active and passive desiccant wheels. As done for the mass transport equation, modifications to Eq. (57) may be easily accomplished. If an additional heat transfer rate due to Dufour effects are considered, an additional transport term is incorporated:

$$\rho_f c_f \frac{\partial T_f}{\partial t} = -\nabla \cdot \dot{\mathbf{q}}'_f - \nabla \cdot \dot{\mathbf{q}}'_f + \dot{s}'_{\text{sor}}, \quad (58)$$

where $\dot{\mathbf{q}}'_f$ represents the heat flux due to the diffusion thermo-effect, or simply to the Dufour effect. Although boundary conditions are required for solving the presented heat and mass balance equations, an extra relation is needed due to the presence of three unknown dependent variables. As mentioned in the one-dimensional formulation, an equilibrium isotherm, such as Eqs. (8) and (9), is required for relating W with Y_f and T_f .

Equations (48) through (50) assume no mass transfer resistance between the water vapor in pores and the gaseous phase that is in equilibrium with the adsorbed phase, such that these two quantities are the same. Under some circumstances, however, it could be important to consider such resistances. One example would be in a desiccant material having larger and smaller pores. In this type of situation the vapor in the smaller pores (and near the surfaces of larger pores) could be in equilibrium with the the adsorbed phase, but the vapor in the larger pores would have a different concentration.

A relatively simple formulation for this case can be obtained if Eq. (49) is split into two parts:

$$\varepsilon \rho_a \frac{\partial Y_f}{\partial t} + \nabla \cdot \mathbf{j}''_g = j''_{\pi}, \quad (59)$$

$$(1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} + \nabla \cdot \mathbf{j}''_s = -j''_{\pi}. \quad (60)$$

Naturally, the addition of these two equations lead to Eq. (49). The mass flux j''_{π} will depend on the concentration at the pore Y_f , and another concentration Y_{π} , representing the vapor state that is in equilibrium with the adsorbed state:

$$j''_{\pi} = j''_{\pi}(Y_f, Y_{\pi}). \quad (61)$$

The other modification is that W be related to the temperatures and concentration in a different way:

$$W = W(T_f, Y_{\pi}), \quad (62)$$

so that W is in equilibrium with Y_{π} instead of Y_f . Note, however, that if $Y_{\pi} = Y_f$, the previous formulation is obtained. Finally, one must mention that this formulation still considers that there is thermal equilibrium between these two states, such that they possess the same temperature.

5 Constitutive Equations

5.1 Expressions for Heat and Mass Fluxes

The heat and mass diffusion fluxes within the sorbent felt, needed for the multi-dimensional formulation, are given in terms of Fourier's Law of heat conduction

$$\dot{\mathbf{q}}''_f = -k_{\text{eff}} \nabla T_f, \quad (63)$$

where, the heat diffusion in the solid desiccant also is given in terms of an apparent property: the effective thermal conductivity k_{eff} . However, different than the thermal capacity, there are a number of models available in the literature for expressing k_{eff} in terms of the different components found in the porous adsorbent material [38]. For the one-dimensional formulation, only the axial component of the flux is needed:

$$\dot{q}''_{f,x} = -k_{\text{eff}} \frac{f}{\partial x}. \quad (64)$$

Similar to the heat diffusion flux, the mass diffusion fluxes are given by Fick's Law expressions:

$$\mathbf{j}''_g = -\rho_a \mathcal{D}_{g,\text{eff}} \nabla Y_f, \quad (65)$$

$$\mathbf{j}''_s = -\rho_s f_s \mathcal{D}_{s,\text{eff}} \nabla W, \quad (66)$$

where the effective Fick diffusion coefficients account for tortuosities in the sorbent material, being given by:

$$\mathcal{D}_{g,\text{eff}} = \frac{\varepsilon \mathcal{D}_g}{\tau_G}, \quad \mathcal{D}_{s,\text{eff}} = \frac{(1 - \varepsilon) \mathcal{D}_s}{\tau_S}. \quad (67)$$

Many works model the gas-phase mass diffusion as a combination of molecular diffusion and Knudsen diffusion. These are assumed to be parallel processes [80],

such that the gas-phase diffusion coefficient is calculated from a combination of a molecular diffusion coefficient \mathcal{D}_M and a Knudsen diffusion coefficient \mathcal{D}_K :

$$\frac{1}{\mathcal{D}_g} = \frac{1}{\mathcal{D}_M} + \frac{1}{\mathcal{D}_K}. \quad (68)$$

The molecular diffusion coefficient can be obtained from expressions for binary air–water gas mixtures.

As analogously mentioned for the conduction flux, for the one-dimensional sorbent formulation only the axial components of the mass fluxes in the felt are needed. These are simply given by:

$$j_g'' = -\rho_a \mathcal{D}_{g,\text{eff}} \frac{\partial Y_f}{\partial x}, \quad (69)$$

$$j_s'' = -\rho_s f_s \mathcal{D}_{s,\text{eff}} \frac{\partial W}{\partial x}. \quad (70)$$

If Soret and Dufour effects are taken into account, additional expressions for these fluxes are needed. In a general way, the diffusion flux due to the Soret effect may be written as [4, 34]:

$$\mathbf{j}_T'' = -\mathcal{D}_{g,\text{eff}}^T \nabla(\log T) = \frac{\mathcal{D}_{g,\text{eff}}^T}{k_{\text{eff}} T} \dot{\mathbf{q}}_f'', \quad (71)$$

where \mathcal{D}_g^T is *thermal diffusion coefficient*. In a similar fashion, the heat flux due to a concentration difference, comprising the Dufour effect, may be expressed as [34]:

$$\dot{\mathbf{q}}_m'' = \lambda_m \mathbf{j}_g'', \quad (72)$$

in which λ_m is a coefficient that relates the heat flux due to concentration difference to the mass flux \mathbf{j}_g'' . Although Soret and Dufour effects were discussed and expressions for the associated heat and mass fluxes were presented, apparently no models found in the literature related to active and passive desiccant wheels include these effects. Since the inclusion of these terms involve simple modifications to the transport equations, and since no literature studies include these effects in simulations of heat and mass transfer regenerators, they will be assumed negligible from this point on for the sake of simplicity.

The convective heat flux from the sorbent felt to the process stream is given by Newton's Cooling Law:

$$\dot{q}_i'' = h (T_i - T), \quad (73)$$

where h is the convective heat transfer coefficient, and T_i is the temperature at the felt-stream interface. The value of T_i will depend on the type of formulation employed; for the one-dimensional sorbent formulation it is the actual sorbent temperature $T_s(x, t)$, whereas for the multidimensional sorbent model it is the sorbent temperature $T_s(\mathbf{x}, t)$ evaluated at the felt-stream interface.

Traditionally, the convective mass flux from the sorbent felt to the process stream is written in terms of a concentration difference, similarly to Newton's Cooling Law:

$$j_i'' = h_m \rho_a (Y_i - Y), \quad (74)$$

where h_m is a convective mass transfer coefficient and Y_i is the vapor concentration in the felt, at the interface. As similar to T_i , this concentration can assume different values depending on the type of formulation employed for the adsorbent material; it will be simply given by $Y_i = Y_f(x, t)$ for the one-dimensional sorbent formulation and by $Y_i = Y_f(\mathbf{x}, t)$ with \mathbf{x} evaluated at the felt-stream interface for the multi-dimensional model.

The mass flux j_π'' used in the multidimensional formulation with an additional mass transfer resistance within the felt can also be written as a Newton's Law-type expression:

$$j_\pi'' = h_\pi \rho_a (Y_\pi - Y_f), \quad (75)$$

where, h_π is the mass transfer coefficient across the additional resistance. Naturally, higher h_π values will lead to a lower mass transfer resistance, and in the limit with $h_\pi \rightarrow \infty$ this resistance becomes negligible.

The conduction heat flux in the supporting wall is simply given by Fourier's Law:

$$\dot{q}_{w,x}'' = -k_w \frac{\partial T_w}{\partial x}. \quad (76)$$

Moreover, the heat flux from the impermeable wall to the sorbent felt (at the felt-wall interface), can be given in terms of a contact heat transfer coefficient:

$$\dot{q}_w'' = h_w (T_w - T_{fw}), \quad (77)$$

in which T_{fw} is the temperature of the sorbent material at the felt-wall interface. For the one-dimensional sorbent formulation T_{fw} is the actual temperature of the sorbent felt T_f ; however, for a multi-dimensional sorbent formulation T_{fw} is the temperature of the felt evaluated at this position.

5.2 Adsorption Isotherm and Heat of Sorption

A number of relations for expressing the equilibrium between water in adsorbed form and vapor in the air-water mixture in contact with it can be found in the literature. A commonly used simple isotherm is the explicit separation-factor based relation:

$$W = \frac{\phi_f W_{\max}}{r + (1 - r)\phi_f}, \quad (78)$$

where r is the separation factor and ϕ_f is the relative humidity of air in the pore space, i.e. $\phi_f = \phi_f(T_f, Y_f)$. As one can observe, this isotherm combines the temperature and absolute humidity dependence of W into a single parameter: the relative humidity. Equation (78) is further simplified if $r = 1$:

$$W = W_{\max} \phi_f, \quad (79)$$

which is known as the linear isotherm.

Equations (78) and (79) naturally apply to the case without the extra mass transfer resistance between the gas-phase and the layer in equilibrium with the adsorbed phase. For cases with the additional resistance, ϕ_f should be substituted by $\phi_\pi = \phi_\pi(T_f, \phi_\pi)$.

Another traditional isotherm relation is the Langmuir model:

$$W = W_{\max} \frac{bp_{v,f}}{1 + bp_{v,f}}, \quad (80)$$

where $p_{v,f}$ is the vapor partial pressure of the gas-phase in pores and b is a coefficient, which generally depends on temperature. The quantity W_{\max} represents the maximum water uptake by the desiccant, which can also depend on temperature.

The heat of sorption is commonly expressed in terms of the heat of vaporization:

$$i_{\text{sor}} = (1 + e_{\text{sor}})i_{\text{vap}}, \quad (81)$$

where e_{sor} is the fraction by which the heat of sorption exceeds the heat of vaporization. This implies that e_{sor} is related to the differential heat of wetting as:

$$e_{\text{sor}} = -\frac{i_{\text{wet}}}{i_{\text{vap}}}. \quad (82)$$

Jurinak and Mitchell [30] argument that a reasonable expression for water vapor being adsorbed on silica gel, based on the experimental data, is given by:

$$e_{\text{sor}} = \Delta e \frac{\exp(W^* \kappa) - \exp(\kappa)}{1 - \exp(\kappa)}, \quad (83)$$

in which $W^* = W/W_{\max}$. The parameters Δe and κ are constants, with $\kappa < 0$. It is interesting to note that, if $W = W_{\max}$, $e_{\text{sor}} = 0$ and the heat of sorption is reduced to the latent heat of vaporization. This reflects the fact that any change of phase (in the direction of moisture removal from the airstream) beyond this point can only occur by simple condensation. For illustration purposes, for a linear isotherm with $W_{\max} = 0.5$ kg water/kg sorbent, possible values for the constants are $\Delta e = 0.3$, $\kappa = 0.5$.

San and Hsiau [62, 63] also use a similar expression for silica-gel and water, in which e_{sor} is given by:

$$e_{\text{sor}} = 0.2843 \exp(-10.28W). \quad (84)$$

6 Equations in Terms of Temperature and Concentration

After the introduction of heat and mass fluxes, the transport equations arising from the presented conservation balances are written in terms of temperature and concentration.

6.1 Process Stream and Impermeable Wall

Starting with the process stream, the governing equations are given by:

$$\rho_a \left(\frac{\partial Y}{\partial t} + (-1)^\gamma u \frac{\partial Y}{\partial x} \right) = \frac{\mathcal{P}_s}{\mathcal{A}_p} h_m \rho_a (Y_i - Y), \quad (85)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + (-1)^\gamma u \frac{\partial T}{\partial x} \right) = \frac{\mathcal{P}_s}{\mathcal{A}_p} h (T_i - T) + \frac{\mathcal{P}_s}{\mathcal{A}_p} h_m \rho_a (Y_i - Y) (i_{v,i} - i_v). \quad (86)$$

By inspecting these equations, one notices that although T_i and Y_i are clearly defined, the value of $i_{v,i}$ is unclear. Physically, it must be within the values of the vapor enthalpy in the process stream i_v and the vapor enthalpy in the sorbent felt $i_{v,f}$. In order to facilitate matters, the parameter φ is introduced:

$$\varphi = \frac{i_{v,i} - i_v}{i_{v,f} - i_v}, \quad 1 - \varphi = \frac{i_{v,f} - i_{v,i}}{i_{v,f} - i_v}. \quad (87)$$

In addition, $i_{v,f} - i_v$ can be written in terms of a temperature difference:

$$i_{v,f} - i_v = c_{p,v} (T_i - T), \quad (88)$$

where T_i has been used for representing the temperature associated with the felt enthalpy because, $T_i = T_f$ for the one-dimensional sorbent balances and $T_i = T_f$ at the felt-stream interface for the multi-dimensional case. With Eq. (87) the energy Eq. (86) can be rewritten as:

$$\begin{aligned} \rho c_p \left(\frac{\partial T}{\partial t} + (-1)^\gamma u \frac{\partial T}{\partial x} \right) &= \frac{\mathcal{P}_s}{\mathcal{A}_p} h (T_i - T) \\ &+ \frac{\mathcal{P}_s}{\mathcal{A}_p} h_m \rho_a \varphi c_{p,v} (Y_i - Y) (T_i - T). \end{aligned} \quad (89)$$

The energy equation for the impermeable wall is given in terms of its temperature as:

$$\rho_w c_w \frac{\partial T_w}{\partial t} = k_w \frac{\partial^2 T_w}{\partial x^2} - \frac{\mathcal{P}_w}{\mathcal{A}_w} h_w (T_w - T_{fw}). \quad (90)$$

6.2 One-Dimensional Sorbent Equations

For the sorbent felt, if the one-dimensional balances are employed, one obtains the following equations:

$$\begin{aligned} \varepsilon \rho_a \frac{\partial Y_f}{\partial t} + (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = & -\frac{\mathcal{P}_s}{\mathcal{A}_f} h_m \rho_a (Y_f - Y) \\ & + \rho_a \frac{\partial}{\partial x} \left(\mathcal{D}_{g,\text{eff}} \frac{\partial Y_f}{\partial x} \right) + \rho_s f_s \frac{\partial}{\partial x} \left(\mathcal{D}_{s,\text{eff}} \frac{\partial W}{\partial x} \right), \end{aligned} \quad (91)$$

$$\begin{aligned} \rho_f c_f \frac{\partial T_f}{\partial t} = & k_{\text{eff}} \frac{\partial^2 T_f}{\partial x^2} - \frac{\mathcal{P}_s}{\mathcal{A}_f} h_m (T_f - T) \\ & + \frac{\mathcal{P}_s}{\mathcal{A}_f} h_m \rho_a (1 - \varphi) c_{p,v} (Y_f - Y) (T_f - T) + \dot{s}'_{\text{sor}} + \frac{\mathcal{P}_w}{\mathcal{A}_f} h_w (T_w - T_{fw}), \end{aligned} \quad (92)$$

where, naturally, if mass diffusion through the porous felt is negligible, Eq. (91) can be simplified to:

$$\varepsilon \rho_a \frac{\partial Y_f}{\partial t} + (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = -\frac{\mathcal{P}_s}{\mathcal{A}_f} h_m \rho_a (Y_f - Y). \quad (93)$$

It is interesting to note that, if rate of sorption term can be written in the form of Eq. (35), one arrives at:

$$\dot{s}'_{\text{sor}} = -\frac{\mathcal{P}_s}{\mathcal{A}_f} h_m \rho_a (Y_f - Y). \quad (94)$$

Then, if one further considers that the effects of surface diffusion are negligible to the sorption heating term, the energy equation can be written in the following form:

$$\rho_f c_f \frac{\partial T_f}{\partial t} = k_{\text{eff}} \frac{\partial^2 T_f}{\partial x^2} - \frac{\mathcal{P}_s}{\mathcal{A}_f} h_m (T_f - T) + \dot{s}'_{\text{sor}} i_{\text{sor}}^+ + \frac{\mathcal{P}_w}{\mathcal{A}_f} h_w (T_w - T_{fw}), \quad (95)$$

where i_{sor}^+ is a modified heat of sorption, defined as:

$$i_{\text{sor}}^+ = i_{\text{sor}} + (1 - \varphi) c_{p,v} (T_f - T), \quad (96)$$

which also involves a sensible heating portion.

It is also interesting to note that combining Eqs. (89), (90) and (92) leads to

$$\begin{aligned} \mathcal{A}_p \rho c_p \left(\frac{\partial T}{\partial t} + (-1)^\gamma u \frac{\partial T}{\partial x} \right) + \mathcal{A}_f \rho_f c_f \frac{\partial T_f}{\partial t} + \mathcal{A}_w \rho_w c_w \frac{\partial T_w}{\partial t} = \mathcal{A}_f k_{\text{eff}} \frac{\partial^2 T_f}{\partial x^2} \\ + \mathcal{A}_w k_w \frac{\partial^2 T_w}{\partial x^2} + \mathcal{P}_s h_m \rho_a c_{p,v} (Y_f - Y) (T_f - T) + \mathcal{A}_f \dot{s}'_{\text{sor}}, \end{aligned} \quad (97)$$

which actually represents the energy balance for the entire system, including the process stream, felt and supporting structure. From this equation, one notices that regardless of the value of φ , the complete system will have the same heating effect, which is represented in the last two terms of this equation. The last term represents the latent heating due to sorption, whereas the next-to-last term represents a sensible heating. Its interesting to note that depending on the signs of $T_f - T$ and $Y_f - Y$, the sensible heating term can assume positive or negative values, representing a heating or even a cooling effect. Finally, comparing Eqs. (89) and (92) it becomes clear that the φ parameter determines which medium is directly affected by the sensible heating term. If $\varphi = 1$ the sensible heating is entirely delivered to the process stream; on the other hand, if $\varphi = 0$ it is entirely delivered to the sorbent felt. Any other value will lead to a fraction of this effect being delivered to each of these media. A similar consideration is done in [67]; however, it is also considered that the latent fraction of the sorption heating effect can be delivered partly to the felt and partly to the process stream.

Equation (92) considers the effect of a thermal resistance between the impermeable structure and sorbent felt. This is actually a general case that can be used for other simple situations. For instance, if there is no impermeable wall, one can simply equal h_w to zero, removing the wall from the problem. On the other hand, if perfect contact is assumed between the wall and sorbent, h_w goes to infinity and the temperature difference $T_w - T_f$ goes to zero. As both the wall and felt are at the same temperature for this special case, Eqs. (90) and (92) can be combined into a single form:

$$\begin{aligned} \left(\rho_f c_f + \rho_w c_w \frac{\mathcal{A}_w}{\mathcal{A}_f} \right) \frac{\partial T_f}{\partial t} = \left(k_{\text{eff}} + k_w \frac{\mathcal{A}_w}{\mathcal{A}_f} \right) \frac{\partial^2 T_f}{\partial x^2} - \frac{\mathcal{P}_s}{\mathcal{A}_f} h_m (T_f - T) \\ + \frac{\mathcal{P}_s}{\mathcal{A}_f} h_m \rho_a (1 - \varphi) c_{p,v} (Y_f - Y) (T_f - T) + \dot{s}'_{\text{sor}}, \end{aligned} \quad (98)$$

which shows, for the perfect thermal contact, that the wall contributes to augmenting the thermal capacity and thermal conductivity of the felt.

6.3 Multi-Dimensional Sorbent Equations

Employing the more general model that includes an extra mass transfer resistance, the governing equations in terms of temperature and concentrations are given by:

$$\varepsilon \frac{\partial Y_f}{\partial t} - \nabla \cdot (\mathcal{D}_{g,\text{eff}} \nabla Y_f) = h_\pi (Y_\pi - Y_f), \quad (99)$$

$$(1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} - \rho_s f_s \nabla \cdot (\mathcal{D}_{s,\text{eff}} \nabla W) = -h_\pi \rho_a (Y_\pi - Y_f), \quad (100)$$

$$\rho_f c_f \frac{\partial T_f}{\partial t} = \nabla \cdot (k_{\text{eff}} \nabla T_f) + \dot{s}'_{\text{sor}}, \quad (101)$$

remembering that $W = W(T_f, Y_\pi)$. As previously mentioned, if $h_\pi \rightarrow \infty$, $Y_f = Y_\pi$, and Eqs. (99) and (100) can be combined into a single from:

$$\varepsilon \rho_a \frac{\partial Y_f}{\partial t} + (1 - \varepsilon) \rho_s f_s \frac{\partial W}{\partial t} = \rho_a \nabla \cdot (\mathcal{D}_{g,\text{eff}} \nabla Y_f) + \rho_s f_s \nabla \cdot (\mathcal{D}_{s,\text{eff}} \nabla W). \quad (102)$$

Regardless of the value of h_π , the heating rate due to sorption is given by:

$$\dot{s}'_{\text{sor}} = \rho_s f_s \left[\left((1 - \varepsilon) \frac{\partial W}{\partial t} - \nabla \cdot (\mathcal{D}_{s,\text{eff}} \nabla W) \right) i_{\text{sor}} - \nabla \cdot (\mathcal{D}_{s,\text{eff}} \nabla W) (i_t - \bar{i}_t) \right], \quad (103)$$

which for no surface diffusion is simply reduced to:

$$\dot{s}'_{\text{sor}} = \rho_s f_s (1 - \varepsilon) \frac{\partial W}{\partial t} i_{\text{sor}}. \quad (104)$$

7 Boundary and Periodicity Conditions

7.1 Process Stream and Impermeable Wall

The heat and mass convection equations for the process streams and the impermeable wall heat balance equation require boundary conditions in the axial direction only. For the supporting wall, convection heat transfer conditions can be written at $x = 0$ and $x = L$:

$$\dot{q}''_{w,x} = h_0 (T_0 - T_w), \quad \text{at } x = 0, \quad (105)$$

$$\dot{q}''_{w,x} = h_L (T_w - T_L), \quad \text{at } x = L, \quad (106)$$

where h_0 and h_L are convective heat transfer coefficients at the boundaries, and T_0 and T_L are the fluid temperatures at $x = 0$ and $x = L$, respectively. Nevertheless, it is generally considered that the heat transfer through these boundaries is insignificant compared to that exchanged with the sorbent felt, such that insulated conditions can be applied:

$$\dot{q}''_{w,x} = 0, \text{ at } x = 0 \text{ and } x = L. \quad (107)$$

For the process stream, the presence of first order spatial derivatives only require a single boundary condition for each dependent variable. These are the inlet conditions of the different process streams:

$$T(\gamma_k L, t) = T_{in,k} \text{ and } Y(\gamma_k L, t) = Y_{in,k}, \text{ for } t_{k-1} \leq t < t_k, \quad (108)$$

for $k = 1, 2, \dots, K$, where $\gamma_k = 0$ for streams flowing in the positive x direction and, whereas $\gamma_k = 1$ for streams that flow in the opposite direction.

7.2 Sorbent Material

The remaining required boundary conditions involve the sorbent material. Since two types of balances were employed, different sets of boundary conditions will be used. At $x = 0$ and $x = L$, the boundary conditions will be the same for both one-dimensional and multi-dimensional balances. As similarly considered for the impermeable wall, the mass and energy transfers at the boundaries $x = 0$ and $x = L$ are negligible compared to the transfer rates to the process stream and wall, such that insulated and impermeable boundaries may be assumed. This leads to the following result

$$\dot{q}''_{f,x} = 0, \text{ at } x = 0 \text{ and } x = L, \quad (109)$$

$$j''_{g,x} = 0, \text{ at } x = 0 \text{ and } x = L, \quad (110)$$

$$j''_{s,x} = 0, \text{ at } x = 0 \text{ and } x = L, \quad (111)$$

which can also be expressed in terms of temperature and gas-phase concentration:

$$\frac{\partial Y_f}{\partial x} = \frac{\partial T_f}{\partial x} = 0, \text{ at } x = 0 \text{ and } x = L. \quad (112)$$

For the one-dimensional sorbent balance, these are actually the only boundary conditions required. In fact, if axial diffusion through the supporting structure is assumed negligible, no boundary conditions are required at all.

For the multi-dimensional balances, additional conditions at the remaining interfaces are needed. At the felt-stream interface a mass balance yields the following boundary condition:

$$\left(\mathbf{j}_s'' + \mathbf{j}_g''\right) \cdot \mathbf{n} = j_i'' \text{ for } \mathbf{x} \in \mathcal{S}_p, \quad (113)$$

noting that in this case the interface concentration Y_i is given by the value of Y_f at the interface. Although thermodiffusion was not considered in this equation, one could easily modify it to include this effect. In a similar fashion, an energy balance can be written at the felt-stream interface:

$$\left(\bar{i}_l \mathbf{j}_s'' + i_{v,f} \mathbf{j}_g'' + \dot{\mathbf{q}}_f''\right) \cdot \mathbf{n} = \dot{q}_i'' + j_i'' i_{v,i} \text{ for } \mathbf{x} \in \mathcal{S}_p. \quad (114)$$

A simplified equation can be obtained if the mass balance at the interface is used, leading to:

$$\dot{\mathbf{q}}_f'' \cdot \mathbf{n} = \dot{q}_i'' + j_i'' (i_{v,i} - i_{v,f}) + (i_{v,f} - \bar{i}_l) \mathbf{j}_s'' \cdot \mathbf{n} \text{ for } \mathbf{x} \in \mathcal{S}_p, \quad (115)$$

where the last two terms on the right-hand-side are generally assumed negligible among most literature studies leading to

$$\dot{\mathbf{q}}_f'' \cdot \mathbf{n} = \dot{q}_i'' \text{ for } \mathbf{x} \in \mathcal{S}_p, \quad (116)$$

which implies that the heat conduction into the sorbent material is solely due to the sensible heat transfer from the process stream. As similarly mentioned for the interface mass balance, T_i [appearing in the definition of \dot{q}_i'' , Eq. (73)] is the value of T_f evaluated at this interface. In terms of concentration and temperature, the boundary conditions given by Eqs. (113) and (115) are written as:

$$-(\rho_a \mathcal{D}_{g,\text{eff}} \nabla Y_f + f_s \rho_s \mathcal{D}_{s,\text{eff}} \nabla W) \cdot \mathbf{n} = h_m \rho_a (Y_f - Y), \quad (117)$$

$$-k_{\text{eff}} \nabla T_f \cdot \mathbf{n} = h (T_f - T) +$$

$$+ h_m \rho_a (Y_f - Y) (i_{v,i} - i_{v,f}) - (i_{v,f} - i_l) \rho_s f_s \mathcal{D}_{s,\text{eff}} \nabla W \cdot \mathbf{n}, \quad (118)$$

At the felt-wall interface, the impermeability condition must hold:

$$\left(\mathbf{j}_s'' + \mathbf{j}_g''\right) \cdot \mathbf{n} = 0 \text{ for } \mathbf{x} \in \mathcal{S}_w. \quad (119)$$

In a similar fashion, an energy balance can be written at same interface:

$$\left(\bar{i}_l \mathbf{j}_s'' + i_{v,f} \mathbf{j}_g'' + \dot{\mathbf{q}}_f''\right) \cdot \mathbf{n} = -\dot{q}_w'' \text{ for } \mathbf{x} \in \mathcal{S}_w, \quad (120)$$

and this equation can be simplified by using the mass boundary condition (119):

$$\dot{\mathbf{q}}_f'' \cdot \mathbf{n} = -\dot{q}_w'' + (i_{v,f} - \bar{i}_l) \mathbf{j}_s'' \cdot \mathbf{n} \text{ for } \mathbf{x} \in \mathcal{S}_w. \quad (121)$$

Finally, in terms of concentration and temperatures, the boundary conditions given by Eqs. (119) and (121) are written as:

$$-(\rho_a \mathcal{D}_{g,\text{eff}} \nabla Y_f + f_s \rho_s \mathcal{D}_{s,\text{eff}} \nabla W) \cdot \mathbf{n} = 0, \quad (122)$$

$$-k_{\text{eff}} \nabla T_f \cdot \mathbf{n} = -h_w (T_w - T_f) - (i_{v,f} - \bar{i}_l) \rho_s f_s \mathcal{D}_{s,\text{eff}} \nabla W \cdot \mathbf{n}, \quad (123)$$

In the absence of a supporting structure, the surface \mathcal{S}_w is treated as impermeable and adiabatic. For these cases, it is easy to show that the boundary conditions at this interface are reduced to:

$$\nabla T_f \cdot \mathbf{n} = \nabla Y_f \cdot \mathbf{n} = 0 \quad \text{for } \mathbf{x} \in \mathcal{S}_w. \quad (124)$$

7.3 Periodicity Conditions

Although the regenerative exchanger problem associated with active and passive desiccant is transient, its solution is periodic, such that the following periodicity conditions must be satisfied:

$$T(x, t) = T(x, t + t_f), \quad (125)$$

$$Y(x, t) = Y(x, t + t_f), \quad (126)$$

$$T_f(\mathbf{x}, t) = T_f(\mathbf{x}, t + t_f), \quad (127)$$

$$Y_f(\mathbf{x}, t) = Y_f(\mathbf{x}, t + t_f), \quad (128)$$

$$T_w(x, t) = T_w(x, t + t_f), \quad (129)$$

remembering that t_f is the total operation period, as defined by Eq. (3). The position vector \mathbf{x} was used for the sorbent temperature and vapor concentration, since in the multi-dimensional formulation it can depend one more than one spatial variable.

8 Concluding Remarks

This chapter presented a detailed description of different mathematical models that can be applied for simulating the operation of both active and passive desiccant wheels. Following a trend seen in the vast majority of literature studies, the transport equations for the airstream were treated in a simple bulk-form, and most of the presented features were focused on the transport phenomena that occur within the porous desiccant material. The simplifying assumptions and required steps for obtaining the governing equations were properly discussed, and some of the resulting formulations are very similar to models available in the literature. In addition, suggestions for modifications in current literature models for this type of problem were also presented, as an attempt to motivate the development of new studies related to modeling and simulation of heat and mass transfer regenerators,

such as active and passive desiccant wheels. The presented set of equations are very general such that a variety of configurations can be simulated. As expected, due to the coupling and non-linearities involved, one should seek a numerical scheme for solving such equations. Nevertheless, such numerical schemes are readily available in the literature related to heat and mass transfer regenerators.

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