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# Comparative assessment of the linear driving force and pseudo-gasside-controlled models for the prediction of mass transfer in desiccant matrices



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#### ABSTRACT

Simplified and realistic simulation models are of great relevance for industrial development of components and systems. The simplified approaches based on the pseudo-gas-side-controlled model and on the linear driving force model are investigated in the simulation of the mass transfer phenomena between the airflow and the channel wall of a solid desiccant matrix. The differences between the two approaches lie in the mass transfer coefficient and potential that are considered in the conceptual equation.

The investigation is centred on the behaviour of an elemental cell of desiccant matrices. The reference data are provided by the results of a detailed model.

The response of the desiccant wall to a step change in the airflow state is simulated, for both adsorption and desorption processes. For each approach, a mass transfer coefficient is estimated after the time evolutions predicted by the detailed model. It is concluded that, when adopting a constant mass transfer coefficient: (i) the pseudo-gas-side-controlled model with an adsorption—desorption averaged value is more suitable for predicting the behaviour of matrices with lower thickness desiccant wall and (ii) the linear driving force model is more appropriate for higher thickness desiccant wall if using a mass transfer coefficient of the specific sorption process.

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#### 1. Introduction

The mathematical modelling of cyclic sorption processes such as those occurring in desiccant wheels requires the use of models that describe the coupled heat and mass transfer in both gas and solid sides. The internal mass transport is commonly assumed to occur by vapour diffusion and by surface diffusion of the adsorbed water, and both mechanisms can be assumed as Fickian type diffusion.

The linear driving force model (LDFM), which was originally proposed by Gleuckauf and Coates [1,2], is often used to describe mass transfer in several sorption processes [3–8]. It is a simple and physically consistent method [3,4], but it has not often been used for modelling the behaviour of desiccant wheels [9–12]. Most authors have adopted a gas-side-controlled model (GSCM), by

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assuming negligible mass transfer resistance in the desiccant layer [13–18], a hypothesis that is valid only for cases with a relatively low desiccant wall thickness. The pseudo-gas-side-controlled model (PGSCM) can be seen as a modified version of the GSCM that takes into account the solid-side mass transfer resistance. It has also been used in few works [19].

Like the PGSCM, the use of the LDFM avoids the need of solving the more rigorous Fickian diffusion equations in the solid domain. The main difficulty in using those simplified approaches lies in the estimation of the mass transfer coefficient, since the manufacturer of a desiccant matrix usually does not provide such data. The range of validity of such simplified models can be investigated by conducting experimental tests [20] or by numerical modelling [21,22].

The detailed numerical modelling of the behaviour of a wall channel element of a hygroscopic matrix has been conducted with the main purpose of investigating the validity of simplified methods [23–25] and providing guidelines for the optimisation of the wheel performance. The investigation conducted by Ruivo et al. [25] on the validity of the PGSCM for predicting the behaviour of silica gel matrices was focused on the response of a channel

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Nomenclature		Greek : Δt	symbols time step
	specific transfer area of the matrix	$\delta X_0$	error indicator
$a_{\rm s}$	specific transfer area of the matrix		
$c_{p,p}$	specific heat of the desiccant wall	$\varepsilon_{ m m}$	matrix porosity
$D_{ m s,eff}$	effective coefficient of surface diffusion (of adsorbed water)	$arphi_{V}$	vapour mass fraction of the gas mixture inside the porous medium
$E_{\rm p}$	thickness of the desiccant layer	$\varphi_{v,f}$	vapour mass fraction of the airflow
$H_{\rm c}$	half-thickness of the channel	$\varphi_{V,i}$	vapour mass fraction of the gas mixture at the interface
$H_{\rm p}$	half-thickness of the desiccant layer	$\varphi_{ m v,p}$	average vapour mass fraction of the gas mixture in the
$h_{\mathrm{ads,p}}$	heat of adsorption	•	wall
$h_{ m h}$	convection heat transfer coefficient	$\kappa_{ m m}$	mass transfer coefficient in the pseudo-gas-side-
$h_{\rm m}$	convection mass transfer coefficient, m $\rm s^{-1}$		controlled model (PGSCM)
K <sub>m</sub>	mass transfer coefficient in the linear driving force	$\overline{\kappa}_{\mathrm{m}}$	average mass transfer coefficient in the PGSCM
	model (LDFM)	$\widehat{\kappa}_{\mathbf{m}}$	mass transfer coefficient in the PGSCM that minimizes
$\overline{K}_{\rm m}$	average mass transfer coefficient in the LDFM		the error indicator
$\widehat{K}_{\mathrm{m}}$	mass transfer coefficient in the LDFM that minimizes	$\lambda_{\mathbf{p}}$	thermal conductivity of the porous medium
	the error indicator	$ ho_{ exttt{d}}^{st}$	apparent density of the dry desiccant
$j_{ m h}$	convective heat flux	$ ho_{ m d,p}^{st}$	average apparent density of the dry desiccant
$j_{ m m}$	convective mass flux	$ ho_{ m f}$	density of the airflow
$S_{\rm ads}$	source-term in the energy conservation equation		
$S_{v-\ell}$	source-term in the mass conservation equation	Superscripts	
T	temperature	*	apparent density; adsorption—desorption averaged
$T_{\rm i}$	temperature of the interface		value of the mass transfer coefficient
$T_{\mathrm{f}}$	temperature of the airflow		
$T_{\rm p}$	average temperature of the wall	Subscripts	
$T_0$	initial temperature in the porous medium	0	initial condition
t	time	ads	relative to the adsorption phenomenon
$U_{\rm m}$	pseudo mass transfer coefficient	d	dry desiccant
$w_{\rm v}$	water-vapour content of moist air (d.b.)	des	relative to the desorption phenomenon or process
$w_{\rm v,f}$	water-vapour content of the airflow (d.b.)	eff	effective quantity
$X_{\ell}$	adsorbed water content (d.b.)	eq	equilibrium conditions
$X_{\ell,p}$	average adsorbed water content (d.b.)	f	airflow; final
$X_{\ell,\mathrm{eq}}$	average adsorbed water content at equilibrium (d.b.)	h	heat
$X_{\ell,i}$	adsorbed water content at interface (d.b.)	i	solid—airflow interface
$X_{\ell,0}$	initial adsorbed water content in the porous medium	m	mass; model
y ,	spatial coordinate	p	porous medium
1	- -	•	-

element both in an adsorption process and in a desorption process, from an initial state up to a final equilibrium state given by the assigned constant airflow conditions. It was concluded that the simplified approach using constant transfer coefficients is feasible only for layer half-thicknesses lower than 0.1 mm, approximately.

In the present work, the numerical modelling of the behaviour of a layer of a desiccant matrix is addressed, considering the complete set of governing equations for the local sorption, heat conduction and mass diffusion phenomena within the porous medium. The desiccant layer belongs to the channel wall of a compact matrix. The hypothesis of one-dimensionality assumed in this study — a plane and short element of the desiccant layer — is mainly intended (i) to achieve a constant value of the mass transfer coefficients required for PGSCM and LDFM and (ii) to perform a comparison between the results predicted by the numerical model and those provided by both simplified approaches.

#### 2. Modelling a channel element of a desiccant matrix

### 2.1. Detailed numerical model

The study here conducted applies to desiccant matrices with a honeycomb channel structure. A cross section of a hygroscopic matrix of a desiccant wheel with four representative cells is depicted in Fig 1. Laminar airflow inside the matrix is usually observed for common operation of desiccant wheels due the relatively low hydraulic diameter of each channel and the moderate airflow velocity values found in practice.

For the purposes of the present work, an element of the channel wall is investigated, as represented in Fig. 2. The performance of the solid-side domain is simulated by considering that the transport phenomena occur only in the y direction [23–25].

This assumption simplifies significantly the analysis of the heat and mass transfer phenomena inside the porous medium, towards

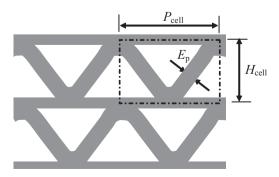


Fig. 1. Cross-section of a hygroscopic matrix with four representative cells.

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