Applied Energy 163 (2016) 167–179

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

A dual-scale analysis of a desiccant wheel with a novel organic–inorganic hybrid adsorbent for energy recovery

Huang-Xi Fu [a], Li-Zhi Zhang [a,b,*], Jian-Chang Xu [a], Rong-Rong Cai [a]

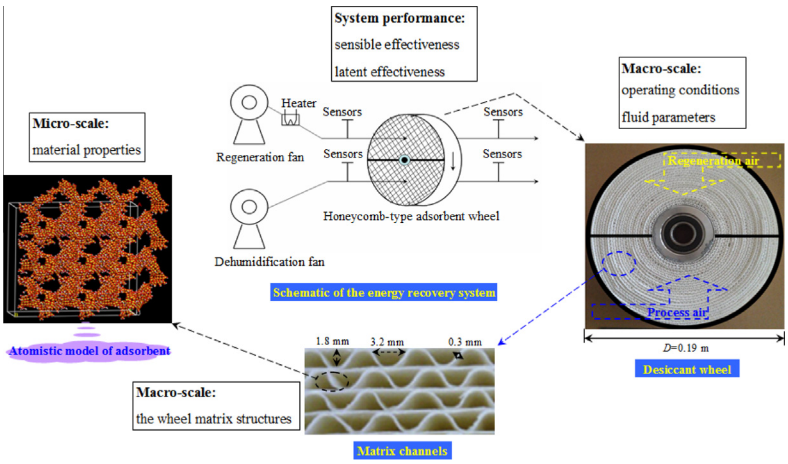
[a] Key Laboratory of Enhanced Heat Transfer and Energy Conservation of Education Ministry, School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, PR China
[b] State Key Laboratory of Subtropical Building Science, South China University of Technology, Guangzhou 510640, PR China

HIGHLIGHTS

- A dual-scale modeling approach was proposed for a desiccant wheel.
- It includes a micro-scale molecular dynamics (MD) sub-model for adsorbent material.
- It also includes a macro-scale sub-model for heat and mass transfer in matrix channels.
- The system can be designed from perspectives of "material-performance-system".

GRAPHICAL ABSTRACT

The dual-scale modeling of desiccant wheels.



ARTICLE INFO

Article history:
Received 7 May 2015
Received in revised form 29 September 2015
Accepted 30 October 2015

Keywords:
Multi-scale modeling
Desiccant wheel
Energy recovery
Molecular dynamics simulation
Hybrid adsorbent

ABSTRACT

Desiccant wheels have been extensively used for energy recovery of ventilation air from buildings. Performance of these wheels is influenced by many factors like the material properties, wheel matrix structures, operating conditions and fluid parameters. Previous studies only involved the macro-scale heat and mass transfer in the wheels and the system performance, by neglecting the micro-scale properties of wheel materials. In this study, a dual-scale modeling approach was proposed for a desiccant wheel with a novel organic–inorganic hybrid adsorbent (HA) material which combines high adsorption capability with good mechanical durability. The proposed dual-scale model included a micro-scale molecular dynamics (MD) sub-model for adsorbent material, a macro-scale sub-model for heat and mass transfer in matrix channels and system performance evaluation. The two sub-models were linked together through information exchange to form the dual-scale model. Through modeling, the effects of the micro physical–chemical properties of materials and macro structure of wheels, as well as the operating parameters on system performance were investigated. With the dual-scale model as a design tool,

---

* Corresponding author at: Key Laboratory of Enhanced Heat Transfer and Energy Conservation of Education Ministry, School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, PR China. Tel./fax: +86 20 87114264.

E-mail address: lzzhang@scut.edu.cn (L.-Z. Zhang).

http://dx.doi.org/10.1016/j.apenergy.2015.10.175

Nomenclature

A_{ij}	L–J 9-6 potential parameters
B_{ij}	L–J 9-6 potential parameters
b, b_0	chemical bond length and equilibrium bond length, respectively
b', b'_0	same to b and b_0
C	constant in sorption curve
c_p	specific heat (kJ kg^{-1} K^{-1})
D	diffusivity (m^2 s^{-1}), diameter of the adsorbent wheel (m)
D_h	hydrodynamic diameter of a channel (m)
d_p	mean pore diameter of adsorbent (nm)
f	desiccant content, fugacity
$F_{bb'}$	elastic constant of stretch–stretch coupling
$F_{b\theta}$	elastic constant of stretch–bending coupling
$F_{\phi\theta\theta'}$	elastic constant of torsion–bending–bending coupling
$F_{\theta\theta'}$	elastic constant of bending–bending coupling
H_2, H_3, H_4	elastic constants of angle
k_B	Boltzmann constant
K_2, K_3, K_4	elastic constants of bond stretch
K_χ	elastic constant of out-of-plane bending
K_p	partition coefficient [(kg water/kg material)/(kg vapor/kg air)]
P_{heater}	maximum power of the regeneration heater (kW)
L	length of a wheel channel (m)
L_v	latent heat of water vapor (kJ kg^{-1})
$\dot{m}$	mass flow rate (kg s^{-1})
m_d	mass of the wheel (kg)
M	molar mass (g mol^{-1})
n	number of ducts in a wheel
N_A	Avogadro constant (mol^{-1})
q_i, q_j	charges of atoms
q_{st}	adsorption heat (kJ kg^{-1})
r_{ij}	distance between two atoms
t	time (s)
T	temperature (K)
u_a	air velocity (m s^{-1})
V	volume (m^3)
V_1, V_2, V_3	elastic constants of torsion angle
w	water uptake in adsorbent (kg water/kg dry adsorbent)
W_{max}	maximum water uptake of adsorbent (kg kg^{-1})
x	axial coordinate (m)
z	thickness coordinate (m)

Greek letters

χ	angle of out-of-plane bending
ϕ	relative humidity, dihedral angle among the four adjacently connected atoms that are not in a same plane
ϕ^0	initial phase shift of dihedral angle
λ	thermal conductivity (kW m^{-1} K^{-1})
ε	effectiveness, effective dielectric constant
ε_t	porosity
θ, θ_0	bond angle and equilibrium angle, respectively
ρ	density (kg m^{-3})
δ	half thickness of solid wall (m)
ω	humidity ratio (kg moisture/kg dry air)

Subscripts

a	air
ad	adsorption
c	cell
cyc	cycle
d	desiccant wall
de	desorption
eq	equilibrium
gf	glass fiber paper
i	inlet
L	latent
max	maximum
min	minimum
o	outlet
p	process air (fresh air)
r	regeneration air (exhaust air)
s	surface, sensible, solid
v	vapor
w	water
z	thickness

material compositions were optimized. The moisture adsorption capacity of the material was two times higher than that of silica gel B at high relative humidities. Consequently the sensible and latent effectiveness were improved by 12% and 30% respectively.

1. Introduction

Desiccant wheels have been extensively used in recent years for energy recovery from ventilation air. A unique advantage of rotary wheels is their capability to recover both sensible and latent heat [1]. One of the earliest investigations of rotary wheel recovery was performed by Sauer and Howell [2]. They used the AXCESS program to evaluate the energy requirements of a desiccant wheel for a two-story office building located in St. Louis on an hour-by-hour basis. Their results showed that the energy recovered by the rotary wheel was around 2.5 times greater than that by a sensible heat exchanger.

Recent work has been concentrated on theoretical and experimental studies of heat and mass transfer in wheels. Zhang and Niu [3] presented a two-dimensional, dual-diffusion transient heat and mass transfer model to investigate the effects of rotary speed, the number of transfer units, and the specific area on the performance of the wheel for air dehumidification and enthalpy recovery. Later, Zhang et al. [4] noticed that the length scale in flow direction ($L = 0.1$ m) was much larger than that in wall thickness ($\delta = 0.15$ mm). The heat conduction and moisture diffusion resistance in solid along longitudinal direction were several magnitudes lower than those along transverse (thickness) direction. Therefore they can be neglected. Consequently, they proposed a one-dimensional, transient heat and mass transfer model which was much quicker in solution without much sacrifice in precision. Using this 1-D model, they compared the performance of honeycomb-type adsorbent beds (wheels) for air dehumidification with various desiccant wall materials. Stabat and Marchio [5,6] developed a desiccant wheel parametric model. This model has