ARTICLE IN PRESS

Applied Mathematical Modelling xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Applied Mathematical Modelling

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

Simulation study on the effect of gas permeation on the hydrodynamic characteristics of membrane-assisted micro fluidized beds ☆

Lianghui Tan [1], Ivo Roghair [1], Martin van Sint Annaland *

Chemical Process Intensification, Multiphase Reactors Group, Department of Chemical Engineering & Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

ARTICLE INFO

Article history:
Received 26 July 2013
Received in revised form 26 March 2014
Accepted 17 April 2014
Available online xxxx

Keywords:
Membrane
Discrete particle model
Micro fluidized beds
Gas permeation
Gas by-passing

ABSTRACT

Recent research has shown the potential of membrane-assisted fluidized bed reactors for various applications, and for ultra-pure hydrogen production in particular. Due to the excellent mass transfer characteristics of fluidized beds, concentration polarization (i.e. mass transfer limitation) can be overcome and the production capacity of membrane-assisted fluidized bed reactors could be further improved by maximizing the installed membrane area per unit volume, leading to the concept of a micro-structured membrane-assisted fluidized bed reactor. In this study, numerical simulations have been systematically carried out with a discrete particle model to investigate in detail the effects of gas addition and extraction through the confining porous membrane walls on the hydrodynamic characteristics of a single membrane-assisted micro fluidized bed compartment. In particular, the effect of the permeation ratio (amount of gas permeated through the membrane relative to the amount fed) and the installed membrane area on the hydrodynamics was investigated. Gas addition or extraction via the porous membrane walls confining the emulsion phase was simulated via inward or outward directed fluxes of the gas phase, which was found to have a very pronounced influence on the bed hydrodynamics. The effects of gas permeation on the solids circulation pattern, solids holdup distribution and porosity probability density function in membrane-assisted micro fluidized beds have been discussed in great detail. It has been found that gas permeation can have an adverse effect on the bed expansion caused by gas by-passing either through the bed center for the case of gas extraction or close to the membrane walls for the case of gas addition. In addition, the formation of densified zones (increased solids holdup) close to the membrane wall that was observed in case of gas extraction may increase the bed-to-membrane mass transfer resistance. These effects may strongly decrease the gas–solid contacting and the gas residence time, which may deteriorate the reactor performance. On the other hand, it is shown that these problems caused by gas permeation may be avoided by properly tuning the gas velocity through the membrane via membrane area and other design parameters and operating conditions.

☆ This article belongs to the Special Issue: *Topical Issues on CFD in the Minerals and Process Industries drawn from CFD2012*.

* Corresponding author. Tel.: +31 (0)40 247 2241; fax: +31 (0)40 247 5833.
E-mail address: m.v.sintannaland@tue.nl (M. van Sint Annaland).
[1] Tel.: +31 (0)40 247 2241; fax: +31 (0)40 247 5833.

http://dx.doi.org/10.1016/j.apm.2014.04.044

Nomenclature

d_p	particle diameter (m)
D	distribution function
e_n, e_t	normal and tangential coefficient of restitution
f	volume fraction
f_a	volume fraction of a particle in a grid cell
$\mathbf{F}_{contact,a}$	contact force of particle (N)
$\mathbf{g}$	gravitational acceleration (m/s^2)
H	bed height (m)
$\mathbf{H}$	rotational matrix
I	moment of inertia (kg m)
$\mathbf{I}$	unit matrix
k_n	normal spring stiffness (N/m)
k_t	tangential spring stiffness (N/m)
K_N	number of steps during one contact
m_{ab}	effective mass (kg)
m_a	particle mass (kg)
$\mathbf{n}_{ab}$	normal unit vector
V_a	particle volume (m^3)
M_g	molar mass of gas (kg/mol)
N	number specified by subscript
P_g	gas pressure (kg/m^2 s)
Q	mass flux (kg/m^2 s)
$\mathbf{r}$	position (m)
R	gas constant (J/mol K)
Re_p	particle Reynolds number
$\mathbf{S}_p$	particle drag source term (N/m^3)
$\mathbf{t}_{ab}$	tangential unit vector
t	time (s)
T_g	gas temperature (K)
$\mathbf{T}_a$	torque (N m)
u_g	superficial gas velocity (m/s)
$\mathbf{u}_g, \mathbf{v}_a$	gas and solid velocity (m/s)
$\mathbf{v}_{ab}$	relative velocity at the contact point (m/s)
V_{cell}	volume of the cell (m^3)

Greek symbols

β	inter-phase momentum exchange coefficient (kg/m^3 s)
δ	displacement (m)
ε	volume fraction
η	damping coefficient (N s/m)
λ_g	gas phase bulk viscosity (kg m/s)
μ_g	gas phase shear viscosity (kg m/s)
μ	friction coefficient
ρ	density (kg/m^3)
ω	angular velocity (rad/s)

Subscripts

0	prior to collision
a, b, p	particle
cell	computational grid cell
g	gas
n	normal direction
t	tangential direction

Abbreviations

CFD	computational fluid dynamics
DNS	direct numerical simulation
DPM	discrete particle model
MAFB	membrane-assisted fluidized bed

Please cite this article in press as: L. Tan et al., Simulation study on the effect of gas permeation on the hydrodynamic characteristics of membrane-assisted micro fluidized beds, Appl. Math. Modell. (2014), http://dx.doi.org/10.1016/j.apm.2014.04.044