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An inverse method to estimate adsorption kinetics of light hydrocarbons on activated carbon

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ABSTRACT

An inverse algorithm to estimate the adsorption kinetics inside the spherical particles in a constant molar flow (CMF) gas adsorber reservoir by measuring the bulk pressure is developed. The formulation includes Knudsen diffusion, surface diffusion, slip and viscous flows. To obtain an efficient algorithm, the conjugate gradient method (CGM) for optimization procedure and the incremental differential quadrature method (IDQM) for solving the governing equations are adopted. The results show that the Knudsen diffusion, surface diffusion, slip and viscous flows effects depend on the type of adsorbate and adsorbent gases. It is shown that the effective diffusivity is not constant and goes through a minimum at an intermediate pressure. Also, it is found that the Knudsen diffusion and the viscous flow are the dominant parts of the mass transfer process at low and high pressure, respectively, and despite the viscous flow, the Knudsen diffusion is highly sensitive to temperature change.

1. Introduction

Separation, purification, and storage of gases in industrial level is widely used by physical adsorption and kinetics plays a key role in these processes (Bastos-Neto et al., 2005; Kalyanaraman et al., 2015; Pirngruber et al., 2014; Vizhemehr and Haghighat, 2014; Siahpoosh et al., 2009; Civan, 2010). Although there is a significant amount of adsorption investigations in literature, there are still some uncertainties on the modeling aspects of adsorption kinetics and its interaction with mass diffusion at adsorbent particles. On the other hand, now days by development of the numerical methods, the simplified assumptions in modeling the physical phenomenon can be reduced and consequently, the results of simulation improved.

Presence of the mass transfer resistances inside the adsorbent particles is confirmed by the estimated effective diffusivity (Castillo-Araiza et al., 2015). The kinetics describes mechanisms of interparticle mass transfer such as, Knudsen diffusion, surface diffusion, slip and viscous flows. To simulate adsorption or desorption processes, it may be possible to choose rigorous or approximate methods. In the rigorous methods, mass balance formulation inside the particle is taken into account, while in the approximation methods, a parabolic concentration inside the particle is considered (Liaw et al., 1979). In approximate methods, mass transfer is described by a lumped coefficient and a linear driving force or alternate forms is considered as the difference among fluid or solid-phase concentrations (Siahpoosh et al., 2009). Conversely, both of the rigorous and approximate methods require the estimation of internal effective diffusivity. On the other hand, parameter estimations in dynamic are complicated because molecules both diffuse through pores and interact with the wall surface.

There are different methods to study the surface diffusion in porous media, such as the differential adsorption bed, time lag, constant molar flow and differential permeation methods (Medved and Cerny, 2011). However, due to limited available data for the surface diffusivity, researchers ignored the surface diffusion in modeling the adsorption phenomenon (Siahpoosh et al., 2009). This drawback can be improved by using an inverse solution together with an effective diffusivity (Do et al., 2000; Do et al., 2001).

The inverse problem solutions have numerous related applications in engineering and science. In the inverse problems, the initial conditions, boundary conditions, physical properties or geometrical parameters of the system can be unknown and should be estimated by measuring other physical parameter (s) of the system at some limited locations (Alifanov, 1974). A lot of efforts have been devoted

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Nomenclature

a_H	Surface area per unit volume of particle
$A^{(i)}$	The first-order weighting coefficients ($i = r,t$)
$B^{(r)}$	The second-order weighting coefficients
b	Affinity constant
b_0	Affinity constant at T_0
C_μ	Dimensionless adsorbed phase concentration
$\bar{C}_\mu$	Adsorbed phase concentration
$C_{\mu s}$	Maximum adsorbed concentration
D_i	The i-th dimensionless parameters (Eq. (24a-e))
D_{eff}	Effective diffusivity
D^0_μ	Surface diffusivity
$D^0_{\mu,0}$	Surface diffusivity at T_0
E_μ	Activation energy of surface diffusion
F	Inlet molar flow rate of gas
F_o	Dimensionless parameter, (Eq. (24f))
k_m	External mass transfer coefficient
K_n	Knudsen number
M	Molecular weight
m_p	Mass of the adsorbent
N	Total gas flux
N_K	Knudsen flux
N_S	Slip flux
N_V	Viscous flux
N_μ	Surface flux
P_b	Dimensionless bulk pressure
$\bar{P}_b$	Bulk pressure
P_0	Reference pressure
P_r	Dimensionless pore pressure
$\bar{P}_r$	Pore pressure
Q_0	Heat of adsorption
r	Dimensionless coordinate variable
$\bar{r}$	Coordinate variable
r_p	Pore radius
R_p	Adsorbent particle radius
t	Dimensionless time
$\bar{t}$	Time
t_f	Final time of adsorption
$\bar{T}$	Temperature
T_0	Reference temperature
V_b	Bulk volume of the gas adsorber reservoir
Y	Desired bulk pressure

Greek symbols

ε_p	Adsorbent particle porosity
$\hat{\varepsilon}$	A small value number
φ	Wall-molecule collision probability function
γ	Conjugate coefficient
λ_b	Lagrange multiplier in bulk
λ_r	Lagrange multiplier in pore
μ_0	Gas viscosity at reference temperature
ρ_p	Adsorbent particle density
σ	Collision diameter
σ_s	Standard deviation
τ_f	Tortuosity factor

to estimation of the boundary conditions and heat source intensities in heat conduction problems as well as thermal properties and geometrical parameters in such diffusive processes (Huang and Wang, 1999; Huang and Lo, 2005; Lee et al., 2013; Hong et al., 2010; Rahideh et al., 2012; Medi et al., 2013; Khajehpour et al., 2013). In the our previous work, we developed an inverse algorithm to estimate equilibrium adsorption isotherm in a gas storage vessel by using the dynamic transient internal pressure and through the solved cases study, it was shown that the presented approach has the ability to accurately predict the equilibrium isotherms with very low effort in computational time (Rahideh et al., 2015). However, to the best of authors' knowledge, there are only limited works on the inverse