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Parametric study of pressure swing adsorption cycle for hydrogen purification using Cu-BTC

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ABSTRACT

Metal organic framework (MOF), for example Cu-BTC, has the characteristics of structure adversity, high pore volume, large surface area and strong selectivity. It is being considered as a new adsorbent in the field of pressure swing adsorption (PSA). A model describing hydrogen mixture flow, heat and mass transfer with multi-component adsorption is developed for predicting breakthrough curves and performance of PSA cycles in the hydrogen purification system using Cu-BTC as adsorbent. The model is implemented on Aspen platform and validated by experiments. Hydrogen purification performances (purity, recovery, productivity) were evaluated, and parametric study on the performance of hydrogen purification has been performed. The results show that the simulated mole fractions, temperature and pressure in the PSA cycles agree with the experiments very well. In general, the variation trend of hydrogen purity is opposite to that of recovery and productivity. As the parametric study shows, within a certain range, higher adsorption pressure, shorter feeding time and lower feeding flow rate lead to higher hydrogen purity, then lower recovery and productivity. Parametric studies help to effectively improve hydrogen purification performance in the Cu-BTC adsorption bed. Furthermore, a multi-objective algorithm is needed to optimize the PSA process.

Introduction

With the heavy use of fossil fuels, environmental pollution is increasing and environmental problems are getting more and more serious. At this time, hydrogen becomes the focus of research because of its many advantages, such as high heat value, no pollution and so on [1]. But now a main reason why hydrogen energy is not widely available is that it is difficult to purify. As pressure swing adsorption technology has been pervasive application in the separation and purification of hydrogen. Some new materials like MOF are valuable to be studied as adsorbents in PSA cycles. Breakthrough experiment is a very important step of PSA cycle, so the study on PSA cycle should start from breakthrough curves. Casas N and his colleagues used activated carbon to do breakthrough experiments of two-component mixture H_2/CO_2 [2]. More experiments were carried out for different parameters such as pressure, temperature and species concentration, then simulations of breakthrough curves were performed using a

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Nomenclature

a_p	particle external specific area, m^{-1}
b_i	extended Langmuir isotherm parameter, bar^{-1}
c_i	molar concentrations of ith component, mol/m^3
c	molar concentrations of mixture, mol/m^3
c_{ps}	specific heat capacity of solid phase, J/kg/K
c_{pw}	specific heat capacity of wall, J/kg/K
C_{pg}	heat capacity of gas phase, J/mol/K
C_{pi}	heat capacity of adsorbed phase, J/mol/K
d_b	internal bed diameter, m
d_p	particle diameter, m
D_L	axial dispersion coefficient, s/m^2
h_{gs}	heat transfer coefficient between gas and solid phase, W/m^2/K
h_{in}	heat transfer coefficient between gas phase and bed wall, W/m^2/K
h_{out}	heat transfer coefficient between wall and environment, W/m^2/K
ΔH_i	heat of adsorption of ith component, J/mol
k_i	mass transfer coefficient of ith component, 1/s
K_{Lg}	thermal conductivity of gas phase, W/m/K
K_{Ls}	thermal conductivity of solid phase, W/m/K
K_w	thermal conductivity of wall, W/m/K
$m_{adsorbent}$	the mass of adsorbent, kg
M_i	molar weight of ith component, kg/mol
n_i^*	equilibrium adsorption amount, mol/kg
n_i	dynamic adsorption amount for each component, mol/kg
n_i^s	saturation adsorption amount for each component, mol/kg
p	pressure, bar
t	time, s
T	temperature of adsorption bed, K
T_g	gas temperature, K
T_s	solid phase temperature, K
T_w	wall temperature, K
v_z	Darcy's velocity, m/s
y_i	gas molar fraction of ith component
z	axial direction, m

Greek symbols

ε_b	bed porosity
ε_p	particle porosity
δ_w	wall thickness, m
μ	dynamic viscosity, m/s
ρ_b	bed density, kg/m^3
ρ_p	particle density, kg/m^3
ρ_s	skeletal density, kg/m^3
ρ_w	wall density, kg/m^3

model with a piping system to describe the distance between the outlet of the adsorption bed and detector [3,4]. They also did some breakthrough curve experiments on MOF and UiO-67/MCM-41 adsorbents to learn about the material adsorption properties [5]. Lopes F V S et al. also did some breakthrough experiments and VPSA (Vacuum Pressure Swing Adsorption) experiments on activated carbon bed but not only just using H_2/CO_2, but also H_2/CO/CO_2 and H_2/CO/CO_2/CH_4/N_2 multicomponent gases [6]. Gomez L F et al. used MIL-53(Al) to do some breakthrough experiments of binary CO_2/CH_4 mixture [7]. Yang J et al. set experiments to study the dynamics of PSA on a zeolite 5A bed using H_2/CO_2 and H_2/CO, and got the best pressure condition in the process of adsorption and desorption [8]. Lee J J et al. improved the structure of adsorption bed and used a dual activated carbon bed to simulate the breakthrough curves of four-component mixture H_2/CO/CO_2/CH_4, they found that the dual bed could not only reduce the spatial occupancy, but also effectively reduce the influence of thermal effect, and improve the purity of hydrogen [9]. Jee J G et al. used activated carbon and zeolite as the layer of adsorbent and studied the influence of adsorption pressure, carbon ratio on breakthrough curves and bed temperatures [10]. There is a lot of heat exchange in PSA process, so Ahn S et al. used activated carbon and zeolite 5A as adsorption beds to set some experiments to make hydrogen recovery from coal gas and study the thermal effects [11]. More breakthrough experiments were performed on a zeolite 5A bed [12], and the layered bed composed with zeolite 5A and activated carbon [13].

On the basis of the breakthrough curves, it is necessary to study the process of PSA cycles to do purification. In order to do pre-combustion CO_2 capture, Casas N et al. also did some PSA experiments and simulations, but it was a little different from PSA experiments for purification because he added two steps before and after pressure equalization step [14,15]. You Y W and his colleagues developed two-bed experiments and did some study on P/F ratio and adsorption pressure in order to purify hydrogen, but simulated temperatures did not fit very well with experiment data [16]. Lopes F V S et al. set five-step fast-cycling VPSA experiments on an activated carbon bed, and got high purity hydrogen with high recovery [17], they also did simulation on step time and flow rates and studied its effects on the purity of hydrogen [18]. And J Y et al. set experiments on two zeolite 5A beds using two components (H_2/CO and H_2/CH_4) and built a mathematical model to do research on the step time of PSA cycles [19]. Cruz P et al. did some research on producing oxygen from air by PSA and VSA (vacuum swing adsorption), moreover, they also did some parametric study [20]. Yavary M et al. built two-bed and six-bed PSA models using zeolite5A, some parametric study were also been done to study the performance of hydrogen purification, but the simulation lacked some experiments for validation [21]. Lee J J et al. developed a spatial occupancy PSA process which can be used in hydrogen station using heat exchange [9]. Experiments and simulations on PSA cycles were also done on layered bed which included zeolite 5A, activated carbon and other adsorbent [22,23]. In addition to activated carbon and zeolite, some new materials are applied to PSA as adsorbents. Chowdhury P et al. studied the adsorption properties of MIL-101 and Cu-BTC [24]. Silva B et al. used the Cu-BTC as adsorbents and carried out a series of experiments of breakthrough curves and PSA cycles, they also evaluated the performance of hydrogen purification through their simulations [25]. Agueda V I and his colleagues did some study on MOF, and they found that multicomponent gas has a longer breakthrough time on MOF compared to traditional adsorption material such as zeolite, and it is more suitable for the application of PSA for hydrogen purification

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