Pressure Swing Adsorption Modeling

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Contributor: Donghui Zhang ,

The pressure swing adsorption (PSA) process has been considered a promising method for gas separation and purification. However, experimental methods are time-consuming, and it is difficult to obtain the detailed changes in variables in the PSA process.

PSA numerical modelling optimization

1. Introduction

Pressure swing adsorption (PSA) is a typical cyclic process, in which multiple columns are interconnected and operated according to a specified sequence to realize gas separation and purification [1]. As a commercial, robust and flexible separation unit, PSA has been widely applied in the fields of air separation, hydrogen purification, carbon dioxide capture, biogas upgrading, low-concentration syngas enrichment and so on [2][3][4][5][6].

According to the principle of gas separation, the adsorption and desorption behavior of adsorbate—adsorbent pairs is closely related to the separation performance. Therefore, most efforts in PSA technology have focused on the use of adsorbents with high selectivity (material science), and the design/operation of efficient processes (engineering) [7]. Fabian et al. conducted a CO_2-PSA warm gas separation technology with a ZnO sorbent for IGCC power plants, wherein the cost of electricity would reach up to 127.2 $/MWh within one year [8]. The practical cost of hydrogen production from steam reforming with a vacuum PSA unit was around 5 EUR/kg of hydrogen as well [9]. The naturally dynamic character and complexity of the PSA process occurring there required high investment and tedious features for experimental investigations [10]. In contrast, numerical simulations are recognized as the dominant method for research and optimization work at a reduced cost [11]. The numerical modeling and simulation of the PSA process has been established in a series of mathematical models comprising mass, momentum, and energy conservation, as well as thermodynamics and kinetics [12][13], which can be described by a set of second-order partial differential and algebraic equations (PDAEs) with initial conditions and boundary conditions. The formation of a more complete model means an increase in the number of differential equations and functional dependencies by which the model coefficients are calculated [14]. Hence, to describe different PSA processes, some variants of mathematical models needed to be taken into account, such as heat transfer between a gas and adsorbent, gas intra-diffusion transfer in an adsorbent and mass and heat transfer coefficients during sorption. Considering that the reliability of simulation results is fundamentally determined by the description and establishment of the adsorption behavior and mathematical models, it is necessary to analyze the advantages and disadvantages of model assumptions and the scope of their use.

Various commercial numerical platforms have been applied for the modeling of the PSA process, such as Aspen Adsorption [15], gPROMS [16][17], MATLAB [18] and FLUENT [19]. The common approach used by the numerical calculations is the method of lines (MOL), which can discretize spatial derivatives to convert PDAEs to differential-algebraic equations (DAEs) or algebraic equations (AEs) and then solve them through different solvers. For the simulation and optimization of the PSA process with complex models and cyclic features, the solution of AEs is difficult to converge and will produce different calculation results. In addition, numerical integration of the DAEs system is complicated and time-consuming, to guarantee the performance accurately and capture the process' dynamic features simultaneously [20], especially dealing with highly nonlinear isotherms, due to numerical dispersion (smearing) and oscillation. All that has also greatly increased the difficulty of process optimization [21].To reduce the computation amounts for simulation and optimization, researchers have proposed a variety of different surrogate models, such as the polynomial surface response model (PRSM) [22], Kriging model [23], proper orthogonal decomposition [24][25][26], polynomial regression model (PNR), support vector regression, and artificial neural network (ANN) model [27][28]. The surrogate model is essentially a black-box model, which is built from a known sample of input–output data points, and can be used to predict the output response at untried points/configurations [25][29]. Limited by the number of samples, the accuracy and feasibility of the surrogate model still need further verification and benchmarking studies to extend its application.

After determining the process model, it is also necessary to optimize the PSA process to find the best design parameters and operating variables to improve process efficiency. The optimization of the PSA process is a multi-objective optimization problem, which generally includes various process performance indicators, such as product purity, recovery rate, production capacity, process energy consumption, etc. For decades, various optimization strategies and algorithms have been continuously developed, which can be roughly divided into deterministic and metaheuristics algorithm. Gradient-based deterministic algorithms include sequential quadratic programming (SQP), reduced space sequential quadratic programming (rSQP), the interior point method, the efficient set method, the trust region efficient algorithm, etc. [30][31][32]. Novel metaheuristic and artificial-intelligence-based optimization algorithms, including the genetic algorithm (GA), particle swarm optimization (PSO), the ant colony algorithm, the annealing algorithm, etc. Among these, GA and PSO are typical metaheuristic algorithms, which have demonstrated superior performance and efficiency in multiple reports [31][33][34]. Currently, the research on PSA process optimization shows a clear trend toward a more intelligent, easier, and integrated direction. The combination of deep-learning technology with artificial-intelligence-based optimization algorithms will be new task for PSA industrial application. In addition, in actual industrial production, there are inevitably some uncertain factors that cause disturbance to the PSA process, such as feed flow, concentration and temperature deviating from the operation set, which make it take a long time to recover, resulting in suboptimal results of the entire process. Therefore, it is necessary to develop and design the control system to minimize impact and achieve stable operation. Researchers have actively explored the control system for a PSA unit, including the proportional-integral-derivative control strategy (PID) and model-predictive control strategy (MPC) [17][35].

2. PSA Modeling

At present, the numerical simulation based on adsorption theory is a promising method for PSA-process design. It can analyze the continuous distribution of physical quantities that is difficult to obtain through experiments and explore process-design variables more quickly. The fundamental of simulation is the mathematical model; as PSA is a periodic, cyclic, and dynamic process, its mathematical models are quite complex. Li et al. [12] summarized the mathematical modeling pathway map, which comprised the correspondence between the real physical scenario and mathematical model for carbon capture by adsorption (CCA). A typical mathematical model for the adsorption bed contains a mass-transfer model, energy-transfer model and momentum-transfer model to describe the transfer process that occurs between gas and adsorbent. In addition to the above three models, strict adsorption-bed models also include the adsorption-kinetics model and adsorption-equilibrium model. Among them, the mass-transfer model strictly includes diffusion in the axial and radial directions, but the radial diffusion coefficient is difficult to measure and estimate. Adsorption kinetics is to study the adsorption process of external diffusion, internal diffusion and surface-adsorption behavior; the adsorption-equilibrium model describes the static-adsorption equilibrium of a single component or multicomponent on the surface of a solid adsorbent after the external diffusion and internal diffusion of gas. Different adsorption-equilibrium-isotherm models will produce different predictions, and the selection of a suitable model can help to improve the accuracy of numerical calculations. A complete process simulation also needs to consider the auxiliary module models such as tank, the valve, pump, and pipeline and performance indicators such as purity, recovery and energy consumption. Exceptionally, for a system with simple cycle schedules such as air separation, the virtual moving-bed modeling methodology, which considers only mass and energy balances and adsorption isotherms, can be employed to describe the cyclic steady state [3]. To avoid complicated numerical computations, some key assumptions frequently used will be discussed, as follows.

2.1. Adsorption-Kinetics Model

In the aspect of kinetic models, three representative adsorption-kinetic models are taken into consideration. First, a homogeneous-solid or pore-diffusion model (HSDM) has been used to describe intraparticle mass transfer [36]. This model assumes that the adsorbent is homogeneous and that the adsorption process occurs at the external surface, followed by the diffusion of the adsorbate into the interior of the adsorbent particles [37]. The mathematical expression for intraparticle diffusion is shown in Equation (1).

$$\frac{\partial q_i}{\partial t} = \frac{D_e}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial q_i}{\partial r}\right) \tag{1}$$

The pore-diffusion model further shows that the microstructure of particles consists of very small pores and that diffusion occurs in the internal void fraction [38]. A simplified model was proposed to calculate the amount of the mass variation of the adsorbed gas component over time, as shown in Equation (2) [12]. Although the HSDM model is much closer to the real state, the complex solving process limits its practical applications.

$$\frac{dq}{dt} = 6q^{*} \sum_{n=1}^{\infty} \frac{D_c}{r_0^2} \exp\left[-(n\pi)^2 \frac{D_c}{r_0^2} t\right] \tag{2}$$

Second, the local equilibrium model is proposed for the strong-adsorbed component on the adsorbent material, which assumes that the mass transfer between solid adsorbent particles and external gas instantaneously completes, regardless of the mass transfer resistance. Thus, the second model only works for some ideal states, such as CO_2/N_2 separation on activated carbon.

Finally, a first-order linear-driving-force (LDF) model was proposed by Lagergren [39], which suggests that the uptake rate of a species into the adsorbent is proportional to the linear difference between the concentration of the species at the outer surface of the particle (equilibrium adsorption capacity) [40]. The average concentration within the particle is expressed as:

$$\frac{\partial q}{\partial t} = k_1 \left(q_e - q\right) \tag{3}$$

where k is the rate constant (1/s), which can be approximated by $15D_e/r^2c$, and D_e/r^2c is the diffusion-time constant. The LDF mass transfer coefficient plays a considerable role in the flow and adsorption process through a breakthrough experiment. Ma et al. [41] found that a lower LDF mass transfer reduced the appearance time of the breakthrough point but extended the completion time of the adsorption process. Moreover, the conventional LDF equation is verified to underestimate the adsorption rate in the initial stage. Li et al. [40] proposed an improved LDF equation derived from the parabolic concentration profile for the intraparticle adsorbate, to eliminate the flaw of the conventional LDF concentration profile assumption, expressed as:

$$\frac{\partial q}{\partial t} = \frac{15D_e}{R^2}\left(q_e + 0.2789 q_e e^{-\frac{q}{2q_e}} - q\right) \tag{4}$$

2.2. Pressure-Drop Model

A continuous PSA process is implemented through circulating changes in pressure. Thus, a pressure drop in the adsorption bed will directly affect the recovery and purity of the product. However, in a situation of low adsorption pressure or short cycle time, several computational studies indicate that the pressure drop has a limited effect on the overall process performance. Aaron [42] experimentally confirmed that the effect of a pressure drop was negligible on process performance in the flow regime; namely, the pressure drop concerns were not reasonable for small-scale air separation processes using similar column lengths (9.8–19.6 cm) and particle sizes (0.5 mm). When considering the energy consumption of the process, the pressure drop model is a key concern, since a higher pressure drop leads to a lower energy-storage efficiency [43]. The Darcy model assumes that the pressure drop is proportional to the flow rate, as expressed by Equation (5).

$$\nabla p=-\frac{\mu}{\alpha}v \tag{5}$$

where μ is the kinetic viscosity and α is the permeability, which is an important consideration in this model. Furthermore, the Ergun equation combines the description of pressure drops by the Carman–Kozeny equation for laminar flow and the Burke–Plummer for turbulent flow, which is more appropriate in packed adsorbing columns, as expressed by Equation (6) [44].

$$-\frac{\partial P}{\partial z}=\frac{150\mu_{\mathrm{g}}(1-\varepsilon_{\mathrm{b}})^{2}u}{\varepsilon_{\mathrm{b}}^{3}d_{\mathrm{p}}^{2}}+\frac{1.75\rho_{\mathrm{g}}\,(1-\varepsilon_{\mathrm{b}})u^{2}}{\varepsilon_{\mathrm{b}}^{2}d_{\mathrm{p}}} \tag{6}$$

2.3. Fluid-Flow Model

Fluid-flow models in a fixed bed include plug flow, plug flow with axial dispersion, and 2-dimensional (2D) radial dispersion flow, while the last term can be ignored because the adsorption bed diameter is much larger than that of particles.

Currently, most PSA process numerical simulations are governed by 1-dimensional (1D) models, without radial variation in the gas concentration, temperature and pressure. As the development of available powerful computer resources raises, there is an interest in extending these 1D adsorption modeling approaches into 2D/3D configurations. Compared to the 1D model, the 2D/3D models seem to be more accurate in terms of heat- and mass-transfer results, as more flow directions are taken into consideration [45]. In addition, it is more intuitive to reflect the distribution of some parameters (mole fractions, temperature, pressure and so on) in the adsorption bed. Moreover, a 3D model can be used in complex bed geometries or perform research on the equipment in the column, such as gas distributor optimization [46]. However, with the increase in dimensions, the number of computations is increased, meaning that it should take a long time to run the required simulations.

2.4. Special Treatments for Energy Balance

2.4.1. Heat of Adsorbed Phases and the Heat of Adsorption

The heat of the adsorbed phases for each component is a function of the loading and the temperature in the solid phases, the adsorbed phase heat capacity, and the solid density, as shown in Equation (7). Wang et al. found that the adsorbed phase would influence the effective thermal conductivity of an adsorption bed, but this effect could be ignored under certain temperature conditions [47].

$$H_i = \rho_s C_{pai} w_i \frac{\partial T_s}{\partial_t} \tag{7}$$

The rate of heat generation by the adsorption of each component *i* per unit mass of solid, depends on the local rate of mass transfer:

$$HT_i = \frac{\partial w_i}{\partial t} \Delta H_i \tag{8}$$

These rates are held in vectors, *HT*, and summed for all components, to obtain the total rate of heat generation by adsorption per unit volume of solid:

$$\rho_s \sum_i (-HT_i) \tag{9}$$

2.4.2. Non-Isothermal Conditions and Thermal Equilibrium

For non-isothermal conditions, an additional heat transfer coefficient resistance between the adsorbent and gas introduces what can be calculated as follows:

$$rate\ of\ heat\ transferred\ per\ \mathrm{m}^3\ of\ bed = HTCa_p\left(T_g - T_s\right) \tag{10}$$

When gas and solid are in thermal equilibrium, $T_g = T_S$.

2.4.3. Adiabatic, Thin-Wall, and Rigorous Models of Heat Transfer to Environment

Adiabatic condition means no heat transfer occurs between the bed and the wall. For a thin wall, the heat exchange between the gas in the bed and the environment is included in the gas-phase energy balance as:

$$\frac{4H_w}{D_B}(T_g - T_{amb}) \qquad (11)$$

A rigorous model includes a wall-energy-balance equation that contains the following terms: heat transfer from the gas in the bed to the inner wall; heat transfer from the outer wall to the environment (including the influence of any insulating material); axial thermal conduction along the wall; and heat accumulation within the wall material. The governing equation is:

$$-k_w \frac{\partial^2 T_w}{\partial z^2} + \rho_w c_{pw} \frac{\partial T_w}{\partial t} - H_w \frac{4D_B}{(D_B + W_T)^2 - D_B^2}(T_g - T_w) + H_{amb} \frac{4(D_B + W_T)^2}{(D_B + W_T)^2 - D_B^2}(T_w - T_{amb}) = 0 \qquad (12)$$

Abd et al. studied the three heat transfer models mentioned above on CO_2 separation properties in a biomethane-upgrading system. The result showed that highest methane purity of 97% was presented in the rigorous model, followed by thin-wall (93%) and adiabatic (92%) systems. The rigorous model can help in the design of a new PSA system that can recuperate heat during the adsorption and desorption steps, for effective adsorption and regeneration.

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