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Hydrodynamic modelling of complex fixed bed geometries in simulated moving bed adsorption processes

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HIGHLIGHTS

- CFD model coupling Brinkman–Forchheimer and k–ε turbulence models validated.
- RTD obtained through stationary simulations.
- Accurate 1D model developed based in the spatial distributions of two moments.

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ABSTRACT

Hydrodynamics inside industrial simulated moving bed (SMB) adsorption columns can be complex due to the presence of internal distribution devices. They have to be taken into account in SMB numerical models to scale-up processes. In the present work, CFD is used as an intermediate step to develop a 1D model simple enough to be used for cyclic SMB simulations while being able to represent realistic hydrodynamics. First, a mock-up representative of an industrial SMB is used to perform residence time distribution (RTD) experiments and to provide validation data. Experiments are well predicted by a CFD model including porous media and turbulent zones, allowing to consider CFD simulations as references to fit simpler models. The moments of internal age distribution are characterized following the calculation method developed by Liu and Tilton, 2010. AIChE J. 56(10), 2561–2572, which allows to estimate the degree of mixing (Liu, 2012. Chem. Eng. Sci. 69(1), 382–393) inside adsorption beds. A major result is that RTD and degree of mixing inside adsorption beds are well described by a 1D multi-exit model, unlike classical dispersed plug flow models (Ruthven and Ching, 1989) that were generally used to simulate SMB processes. Additionally, a numerical method was developed which is able to reproduce the RTD with steady state simulations.

1. Introduction

1.1. SMB processes

Simulated moving bed (SMB) is a cyclic adsorption process used to separate molecules that are hardly separable by distillation, solvent extraction or other classical operation units (Ruthven and Ching, 1989). Several industrial applications are known. A classical one is the separation of xylene isomers (Minceva and Rodrigues, 2007; Bergeot et al., 2010; Laroche et al., 2011) operated in adsorption columns up to 10 m of diameter. SMB comprises a set of superposed fixed bed adsorbers which present several hydrodynamic heterogeneities, as pipes and beams placed in the porous media, the packing itself and non-ideal injection and collecting devices, as shown in Fig. 1. Such heterogeneities generate significant deviations from the desired plug flow. As far as transport limitations inside (diffusion) or outside (external mass transfer) adsorbent particles generate major dispersion in the process, the impact of hydrodynamic discrepancies is not significant. However, when low dispersive adsorption media is used, hydrodynamics can become the most dispersive phenomenon of the process. In this context, it is crucial to study correctly hydrodynamics inside adsorption beds and its effect on adsorption performances.

1.2. Residence time distribution and CFD

In order to model industrial processes, a classic approach for chemical engineers consists in studying the RTD (Danckwerts, 1953) and estimating the global axial dispersion resulting from

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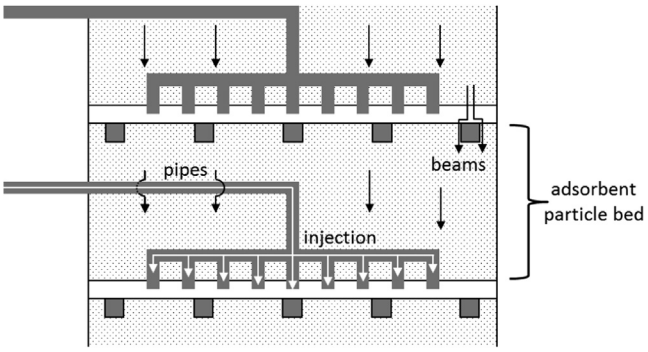

Fig. 1. Schematic view of an example of one SMB geometry.

internal flow patterns (Van Baten et al., 2001; Moustiri et al., 2001). Despite being a very powerful tool for hydrodynamics characterization, the RTD only gives overall information and does not take into account the quality of the mixing or dispersive phenomena in the flow. The lack of information on internal hydrodynamics can lead to inappropriate modelling and important errors on the calculation of performances (Shinnar, 1993). For this reason, Danckwerts (1958) and Zwietering (1959) introduced the concept of degree of mixing (J). Zwietering showed for example that reactors with the same RTD but different J can lead to different performances in case of chemical reactions with non-linear kinetics (for instance, of order $n \neq 1$). Other studies have been recently done to fill in the gaps of classical RTD methods, as Smart RTD (Simcik et al., 2012) and the reactive-mixing index analysis (Yablonsky et al., 2009). Yet, Claudel et al. (2003) and Hocine et al. (2008) developed simple hydrodynamic models through the RTD by making some assumptions about the internal information of the systems in study.

However, in many applications, including adsorption processes, RTD has been extensively used to estimate overall axial dispersion coefficients. Dispersion coefficients are then used in dispersed plug-flow (DPF) models to take into account the effect of hydrodynamics on the separation (Ruthven and Ching, 1989). When low dispersion coefficients are involved, DPF models are very close to a cascade of N Continuous Stirred-tank Reactors (NCSTR). In the following, DPF and NCSTR models are considered as equivalent ($Pe = 2N$ for $Pe > 50$, Schweich, 2001). Augier et al. (2008) estimated the impact of obstacles within porous media on the dispersion of concentration fronts by measuring the resulting variance, allowing to further adjust equivalent DPF models. Notwithstanding, asymmetric RTD curves were already found, pointing out the relative unsuitability of DPF models, which may lead to strong discrepancies in the scenario discussed above. Kwapinski et al. (2010) had already shown the inadequacy of the plug flow model for the representation of the impact of adsorber packed bed hydrodynamics and thermal effects on the breakthrough curves.

Otherwise, CFD has well been known for more than 20 years as a pragmatic and reliable tool to describe local hydrodynamics in various reactors and separation processes. It can be used as a "stand-alone" numerical tool to solve simultaneously hydrodynamics, transfer and kinetics at any point of a geometry. Madeira et al. (2004) used a CFD code to solve the problem mentioned by Brunier et al. (1984): they simulated a tracer experiment in order to obtain the RTD and compute the mean residence times of the reservoirs in study.

Zheng et al. (2010) performed CFD simulations to study a Pressure Swing Adsorption cyclic process successfully. In the present SMB processes, it is still unrealistic to consider this direct approach that can be very time consuming. A more pragmatic method consists in studying hydrodynamics with CFD and deducing a simpler hydrodynamic model that can be easily coupled with other physics. This last method is the one used in the present work. CFD can be used for example to simulate RTD. This kind of calculation is important but fastidious because long physical times have to be solved to simulate the transport of a passive tracer inside the process, and lastly does not give quantitative information on internal mixing phenomenon as previously pointed out. Recently, Liu (2012) proposed to use CFD to access the internal information inside reactors. Based on the transport of the first and second moments of the internal age distribution, Liu developed a method to calculate the degree of mixing J introduced five decades ago but used, up to now, as a theoretical concept. Furthermore, this method is based on steady-state, i.e. inexpensive CFD simulations.

The method is sufficient to estimate the variance (2nd moment) of a RTD, and then the equivalent number of CSTR N. Nevertheless it is hardly usable to reconstruct the RTD curve. Indeed, the reconstruction of a distribution from its moments is an impossible task since even the knowledge of all the moments up to infinity can lead to different functions (John et al. 2007).

1.3. Objectives of the study

Based on the recent advances of flow characterisation by CFD, it is proposed to characterize in detail hydrodynamics of a SMB process, and then to deduce a simple but robust 1D model that can be used in cyclic simulations. For this, a new method is proposed that can, under some assumptions, calculate RTD only by transporting the first and second moments of the internal age inside the studied configuration.

The study is divided in four steps:

- RTD experiments in a laboratory setup representative of a SMB fixed bed.
- CFD calculations, simulation of RTD and comparison with experimental results as a validation of hydrodynamics modelling.
- CFD simulation of the transport of the moments of the age distribution and computation of the degree of mixing.
- 1D modelling of one bed of a SMB process resulting from the previous step. Validation of the 1D model by comparing the obtained results with those obtained from the CFD.

Sections 2 and 3 present the experimental setup and the numerical modelling respectively. The validation of the CFD approach is presented in Section 4. Finally in Section 5, CFD-based moment calculations are used to reconstruct the RTD, and a 1D model is proposed to represent complex hydrodynamics of adsorption beds.

2. Experimental setup

The dispersion caused by the different factors introduced above was studied using a cold mock-up representative of a slice of a SMB bed, whose dimensions are shown in Fig. 2. The plates of the distribution system of the SMB are divided into panels that withdraw the flow from the bottom of the packed bed and mix it with an injected feed from the distribution network in order to send it to the packed bed below (see for example the patent US20110303602 A1, Augier and Hotier, 2011).

The experimental setup comprises a packed bed of glass spheres, within which a cylinder or a square prism can be placed as obstacles, with a free flow chamber above the bed and another one below it (see Fig. 2). Above and below the packed bed a tight grid is placed to avoid the movement of the packing due to the motion of the fluid. The inlet pipe ($R = 0.021$ m as for the outlet