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Development and validation of a novel modeling framework integrating ion exchange and resin regeneration for water treatment

Jie Zhang [a], Adib Amini [a], Jeremy A. O'Neal [b], Treavor H. Boyer [b], Qiong Zhang [a], *

[a] *Department of Civil and Environmental Engineering, University of South Florida, 4202 E. Fowler Ave., ENB 118, Tampa, FL 33620, USA*
[b] *Department of Environmental Engineering Sciences, Engineering School of Sustainable Infrastructure & Environment (ESSIE), University of Florida, P.O. Box 116450, Gainesville, FL 32611, USA*

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A B S T R A C T

Models have been developed to simulate the process of ion exchange for water treatment. However the modeling of resin regeneration process, which can predict regeneration efficiency and residual stream for determining technology sustainability, was not incorporated into previous models. Therefore a model integrating both ion exchange and resin regeneration considering regeneration efficiency is needed for evaluating and improving ion exchange technology. This study developed an integrated model aiming to simulate ion exchange and resin regeneration in different configurations (fixed bed, fluidized bed) for the first time. The integrated model has been validated via comparing model predictions with experimental data. The impacts of dimensionless groups (i.e. the Péclet number, the diffusion modulus, and the Biot number) on ion exchange breakthrough curve have been analyzed using this model. In addition, this integrated model has been used to optimize the regeneration frequency to improve the overall performance of ion exchange. It demonstrated this integrated model could be a useful tool for further studies in ion exchange technology.

1. Introduction

Providing safe drinking water is one of grand engineering challenges identified by NAE (Schnoor, 2008). In developed countries, water is typically treated at a central location through a complex treatment train and delivered to users through an extensive distribution network (Crittenden et al., 2012). In developing countries, decentralized treatment prevails at community or household level (Crittenden et al., 2012). Technologies that can be implemented at either centralized or decentralized treatment schemes have unique opportunity to address the challenge of water provision. Ion exchange (IX) is one of such technologies that can be used in water treatment plants or as a point-of-use technology in distribution systems and households. It can be used to remove various contaminants in drinking water and has shown increased adoption in recent years (Ali and Gupta, 2007).

To better understand IX process for IX reactor design, various process models have been developed (Dechapunya, 1981; Schwartz and Milne-Home, 1987; Robinson et al., 1994; Hwang and Lu, 1995; Koh et al., 1995; Kaczmarski et al., 1997; Menoud et al., 1998; Juang et al., 2003; Jia and Foutch, 2004; Lu, 2004; Hokanson, 2004; Fatemi et al., 2007; Boyer et al., 2008, 2010; Vassilis, 2010). The early models were equilibrium models which did not consider intra-particle diffusion in resin (Dechapunya, 1981; Clifford, 1982; Schwartz and Milne-Home, 1987; Aldridge et al., 2004). As Robinson et al. (1994) pointed out that intra-particle diffusion has to be accounted to accurately describe the ion exchange process, most of the later researches considered mass transfer kinetics and intra-particle diffusion in resin. The recent studies on ion exchange process modeling can be categorized into three groups: 1) exploring novel numerical methods or appropriate reactor models (Kaczmarski et al., 1997; Koh et al., 1995; Slizneva and Natareev, 2004). For example, Kaczmarski et al. (1997) developed an orthogonal collocation method based on moving finite elements for simulating ion exchange in fixed-bed; Koh et al. (1995) tried to model the IX process of phenylalanine in fluidized beds using a completely mixed flow reactor (CMFR)-based model and a packed bed model and found the packed bed model had a better performance; 2) improving reactor configurations (Hwang and Lu, 1995; Boyer et al., 2008, 2010; Mazumder et al., 2009). For example, Hwang and Lu (1995) compared the performance of the semi-

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* Corresponding author.
E-mail address: qiongzhang@usf.edu (Q. Zhang).

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fluidized bed, the fluidized bed, and the packed bed by numerical simulations and concluded that the semi-fluidized bed has the highest treatment efficiency; Boyer et al. (2008, 2010) developed process models for the ion exchange in a CMFR configuration for water treatment; 3) applications to different industries such as heavy metals removal (Menoud et al., 1998; Juang et al., 2003), high purity water production (Jia and Foutch, 2004; Hokanson, 2004), metal separation in elution process (Fatemi et al., 2007).

However, resin regeneration process was not incorporated or over-simplified in previous IX process models. Regeneration is an integral part of IX process and the disposal of the waste streams generated in regeneration process has been a challenge for IX processes. A common treatment for resin regeneration in the previous ion exchange models is to assume 100% of regeneration efficiency. Such assumption is not realistic and results in the overestimate of the treatment performance. Without integrating resin regeneration process in the model, it is impossible to assess the residual stream which is the primary obstacle for promoting ion exchange technology. Three studies attempted to integrate resin regeneration process to IX process model: Guter et al.'s model for nitrate removal considered regeneration (Guter, 1984; Guter and Hardan, 1985; Liang et al., 1999). However this model was not widely used since it is a proprietary program and the governing equations used in the model are not clear. Gomes et al. (2001) modeled the processes of ion exchange and resin regeneration for gold recovery. However two processes are modeled separately and not linked as an integrated framework. Besides, no intra-particle diffusion was considered in the models and the results predicted by the regeneration model were not in alignment with the experimental data. Mazumder et al. (2009) developed an integrated model for the Liquid–Solid Circulating Fluidized Bed (Lan et al., 2002) in which IX and resin regeneration operates simultaneously in continuous mode. However this model cannot be applied to the commonly used configurations (i.e. fixed bed and fluidized bed) in which resin regeneration operates in batch mode. Thus it is necessary to develop a model integrating both ion exchange and resin regeneration for the fixed bed and fluidized bed.

The objective of this study is to develop a process model integrating ion exchange and resin regeneration for the most commonly used reactor configurations (i.e., the fixed bed and fluidized bed). With this model, it is able to predict ion exchange performance, regeneration efficiency, and residual stream information. And the operation parameters, such as regeneration frequency, can be optimized to maximize the economic and environmental sustainability of water systems.

2. Model development

Ion exchange process involves the mass transfer of ions and the exchange of ions in the aqueous phase for ions in the resin phase. In general, the ion exchange process can be described by an advection–dispersion equation at macroscale and a mass transfer equation for resin particle at microscale, as illustrated in Fig. 1. Common assumptions made in previous models (Hwang and Lu, 1995; Koh et al., 1995; Chowdiah and Foutch, 1995; Boyer et al., 2008, 2010; Sengupta and Pandit, 2011) include constant flow rate; uniform flow velocity profile in reactor; homogeneous effective intra-particle diffusion; and negligible resistance to mass transfer across the boundary layer surrounding the sorbent particle; The local liquid-phase mass transfer is described by the linear driving force approximation and local equilibrium between liquid and resin phases at resin surface. Those assumptions have been employed in the integrated model developed in this study. The modeling of resin regeneration is similar to that of ion exchange but with different initial and boundary conditions. Details will be provided subsequently.

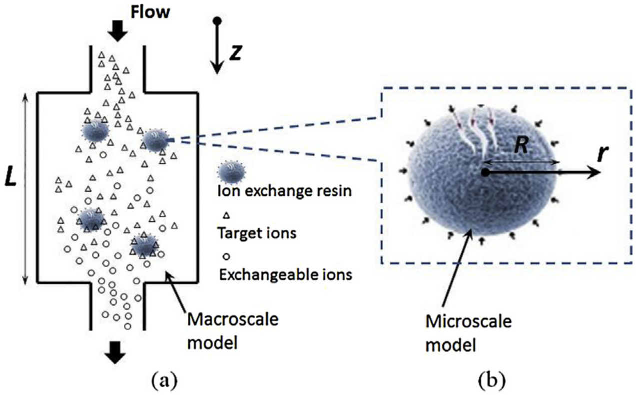

Fig. 1. Illustration of modeling ion exchange process for drinking water: (a) macroscale model describing flow and (b) microscale model showing particle.

2.1. Governing equations and models for ion exchange process

The general mass balance equation for each contaminant species in the fixed bed (macro-scale model) is

$$\frac{\partial C}{\partial t} = \frac{\rho_b}{\varepsilon}\frac{\partial \langle q \rangle}{\partial t} - u\frac{\partial C}{\partial z} + D_z\frac{\partial^2 C}{\partial z^2} \tag{1}$$

$$\langle q \rangle = \frac{3}{4\pi R^3}\int_{r=0}^{r=R} q(r)\cdot 4\pi r^2 dr \tag{2}$$

Initial condition:

$$C(t=0,z) = 0 \tag{3}$$

$$\langle q \rangle(t=0,z,r) = \begin{cases} 0, & \textit{for the initial cycle} \\ \langle q \rangle_{reg}(z,r), & \textit{for the rest cycles with regeneration} \end{cases} \tag{4}$$

Boundary conditions:

$$C(t,z=0) = C_{in} \tag{5}$$

$$\left.\frac{\partial C}{\partial z}\right|_{z=L} = 0 \tag{6}$$

where C is concentration in bulk liquid phase, q is the average resin-phase concentration, $q(r)$ is the resin-phase concentration at coordinate r in resin, u is velocity of fluid, z is axial coordinate, L is the length of the bed, r is radical coordinate for resin, t is time, D_z is the liquid axial dispersion or diffusion coefficient, ρ_b is the bulk density of the bed, kg/m3, ε is porosity of bed or liquid holdup, C_{in} is influent concentration. D_z can be estimated by a modified empirical model (Chung and Wen, 1968)

$$\frac{D_z \rho}{\mu}(X) = \frac{\varphi Re}{0.20 + 0.011 Re^{0.48}} \tag{7}$$

valid for $Re \in (1 \times 10^{-3}, 1 \times 10^{3})$.where ρ is density of fluid, μ is viscosity of fluid, φ is a constant fitted to be 1.7 for this study, Re is Reynolds number which is calculated as