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Modeling the removal of dissolved organic carbon by ion exchange in a completely mixed flow reactor

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ABSTRACT

A mathematical model was developed to describe removal of dissolved organic carbon (DOC) by a macroporous, strong-base anion exchange resin in a completely mixed flow reactor with resin recycle and partial resin regeneration. The two-scale model consisted of a microscale model describing the uptake of DOC by the resin coupled with a macroscale model describing the continuous-flow process. Equilibrium and kinetic parameters were estimated from batch laboratory experiments. The model was validated using continuous-flow data from two pilot plant studies. Model predictions were found to be in good agreement with the observed pilot plant data.

1. Introduction

During drinking water treatment, dissolved organic carbon (DOC) reacts with chlorine to form halogenated organic disinfection byproducts (DBPs), e.g., trihalomethanes, haloacetic acids, haloacetonitriles, haloketones, halonitromethanes, and haloaldehydes (Krasner et al., 2006). Health risks, such as bladder cancer and adverse reproductive outcomes, have been attributed to consumption of water that contains these and other DBPs (Villanueva et al., 2007). A common strategy for reducing the formation of DBPs is to remove the DBP precursors (i.e., DOC) prior to disinfection via processes such as enhanced coagulation, granular-activated carbon adsorption, nanofiltration, lime softening, and ion exchange (Thompson et al., 1997; Karanfil et al., 1999; Bolto et al., 2002). Of particular interest in the present work is a magnetic ion exchange (MIEX) resin that has been extensively studied for removal of DOC from raw drinking waters (Drikas et al., 2003; Fearing et al., 2004; Johnson and Singer, 2004; Mercer et al., 2004; Boyer and Singer, 2005, 2006; Humbert et al., 2005; Singer et al., 2007). The MIEX resin is a macroporous, polyacrylic, strong-base anion exchange resin. The resin is used in a suspended manner in a completely mixed flow reactor (CMFR) in which a majority of the resin is recycled and a fraction of the resin is regenerated; Fig. 1 shows a schematic of the continuous-flow process. Continuous-flow studies have shown that pre-treatment with MIEX resin results in a substantial removal of DOC, thereby decreasing subsequent chemical requirements (i.e., coagulant and chlorine) and reducing the formation of DBPs (Mercer et al., 2004; Boyer and Singer, 2006; Singer et al., 2007). Due to the variability in raw drinking water quality, however, bench-scale batch experiments in combination with pilot-scale continuous-flow studies are often required on a site-specific basis to assess the efficacy of ion exchange treatment for the removal of DOC. An alternative to extensive pilot-scale testing is to use a model that would predict process performance in different waters under varying operating scenarios and inform the direction of experimental testing.

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Nomenclature

c	concentration of removable solute in pore fluid (M/L^3)
C	effluent concentration of removable solute (M/L^3)
C'	effluent concentration of total solute (M/L^3)
C_e	effluent concentration of removable solute at equilibrium (M/L^3)
C_0	influent concentration of removable solute (M/L^3)
C'_0	influent concentration of total solute (M/L^3)
D_a	apparent diffusivity (L^2/T)
D_l	free-liquid diffusivity (L^2/T)
$D_{p,e}$	effective pore diffusion coefficient (L^2/T)
$E(t)$	residence time distribution of resin (1/T)
F	microscale mass flux ($M/L^2\,T$)
f_N	non-removable fraction of solute (dimensionless)
f_R	resin regeneration ratio (dimensionless)
$g(t_a)$	particle age probability density function (dimensionless)
$h(R)$	particle size probability density function (dimensionless)
K_D	linear distribution coefficient (L^3/M)
m'	rate of addition/removal of resin (M/T)
m_s	mass of solid phase (M)
M^{s-a}	interphase mass exchange (M/T)
N_{age}	number of resin particle age-classes (dimensionless)
N_{size}	number of resin particle size-classes (dimensionless)
q	solid-phase solute concentration (M/M)
Q	volumetric flow rate (L^3/T)
r	radial distance from center of particle (L)
R	resin particle radius (L)
t	time (T)
t_a	resin particle age (T)
V	reactor volume (L^3)
X_R	volume fraction of resin (L^3/L^3)
ε_p	resin porosity (L^3/L^3)
$\kappa(t)$	residence time function (1/T)
ρ_a	apparent resin density (M/L^3)
ρ_s	solid-phase density (M/L^3)
τ	resin tortuosity (dimensionless)
τ_H	hydraulic residence time (T)
τ_S	solids residence time (T)

Accordingly, the objective of this research was to formulate a mathematical model to describe DOC removal by ion exchange in a CMFR with resin recycle and partial resin regeneration. The two-scale model consisted of a microscale model describing uptake of DOC by the resin coupled with a macroscale model describing the continuous-flow process. The transport equations were solved numerically using a finite-element scheme. Equilibrium and kinetic parameters were estimated from laboratory experiments using three raw drinking waters. The model was evaluated by comparing predictions from the model to results obtained from two continuous-flow pilot plant studies (Mercer et al., 2004; Boyer and Singer, 2006).

2. Materials and methods

2.1. Experimental procedures

Three raw drinking waters were evaluated in this work. The waters were taken from North Bay Aqueduct (NBA) near Vacaville, CA, Sweetwater Lake (SL) in San Diego County, CA, and Durham, NC (see Boyer and Singer, 2005, 2006). Equilibrium and kinetic tests were conducted following the bottle-point isotherm procedure (Randtke and Snoeyink, 1983). Briefly, varying amounts of MIEX resin (Orica Watercare, Watkins, CO) were added to the test water and mixed end-over-end at 25 revolutions per minute for a pre-determined length of time. Following this contact period, all samples were filtered through a pre-rinsed 0.45-μm membrane filter (Supor-450, Pall Corp., Ann Arbor, MI), and analyzed for DOC using a Shimadzu TOC-5000 Total Organic Carbon Analyzer (Shimadzu Corp., Atlanta, GA).

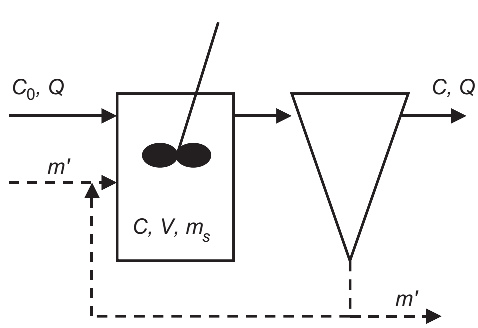

Fig. 1 – Continuous-flow process schematic.

Data from two continuous-flow pilot plant studies were used to evaluate the predictive accuracy of the model (see Mercer et al., 2004; Boyer and Singer, 2006). The configuration of the pilot plants was similar to the process shown in Fig. 1. Tables 1 and 2 list the operating conditions tested at North Bay Aqueduct and Durham, respectively. At each process-operating condition, multiple influent and effluent samples were collected and analyzed for DOC at Durham and total organic carbon (TOC) at North Bay Aqueduct. For most waters, DOC accounts for greater than 90% of TOC (Thurman, 1985). In addition, ion exchange only removes dissolved species. Therefore, all subsequent discussions will refer to the organic carbon concentration as DOC. It was assumed that all samples were collected at steady state.

2.2. Model formulation

A substantial amount of research has been devoted to the mathematical modeling of the sorption kinetics of completely mixed systems (Najm, 1996; Traegner et al., 1996; Bautista et al., 2000; Campos et al., 2000; Soriano et al., 2002). Common