Equation-Based Adsorption Modeling For Aqueous Inorganic Species In Cylindrical Porous Media

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Abstract

Numerous adsorptive media have been evaluated for the removal of inorganic contaminants in water, such as harmful heavy metals, toxic oxyanions, and radioactive species. Due to the complexity of water chemistry and chemical reactions at adsorptive media surface, lab-scale adsorption isotherm data are often inconsistent with pilot-scale three-dimensional column or filtration tests. The discrepancy makes it hard for scientists/engineers to estimate and compare the actual performance of an adsorbent to other materials. While traditional approach is through trial-and-error testing that can be repetitive and inefficient, in the current study, we used COMSOL Multiphysics® with the Chemical Reaction Engineering Module for simulating the transport and adsorption of inorganic contaminants on a number of adsorptive media with different base material and surface characteristics including point-of-zero charge (PZC), total surface area, total pore volume, etc. To overcome the inconsistency from batch experiments to product tests, the theoretical adsorption maximum (c_(p,max)) and the pseudo-second-order rate constant (K_2) were carefully obtained from each kinetic experiment. The adsorption rate is plugged into the surface reaction equation as a source/sink term in the Chemical Reaction Engineering Module. A mass-transport equation, in the form of Partial-Differential Equation (PDE), was used to describe the concentration of contaminant in the fluid (c_f) and on the adsorptive material surface (c_p). As a result, the equation must be solved numerically using the built-in PDE interfaces. In addition to the equation-based numerical analysis, axisymmetric PDE simulation tips in a curvilinear coordinate system for compensating the conservative flux term will be discussed during the presentation. For model validation, the simulated adsorption results in an axisymmetric model were compared against pilot-scale filtration results which were tested at two pH values (6.5 & 8.5) per the industry standard protocol, NSF/ANSI Standard 53. The simulated results successfully explain how material's embedded kinetic characteristic, in terms of adsorption rate, plays an important role in the filtration performance of adsorptive media.

Figures used in the abstract

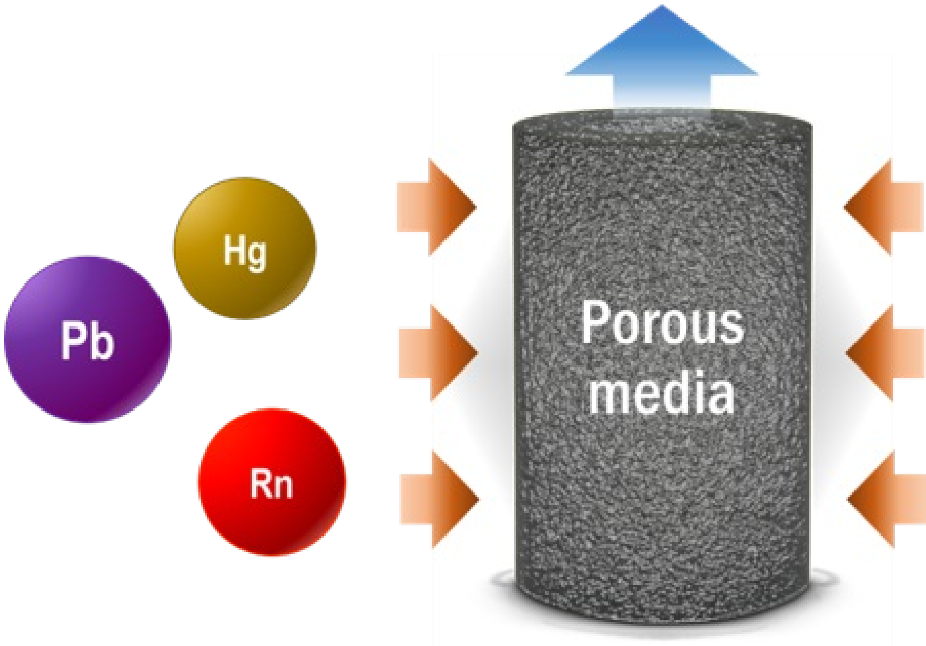

Figure 1 : Figure 1. Heterogeneous porous media.

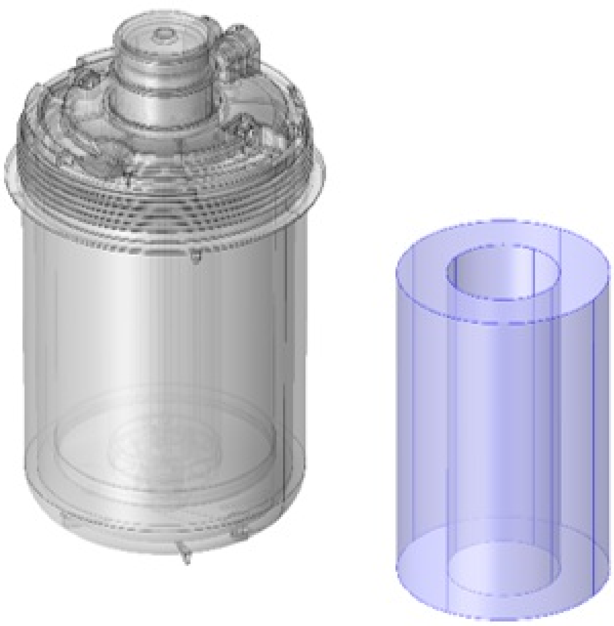

Figure 2 : Figure 2. Pilot-scale filtration device and molded adsorptive media.

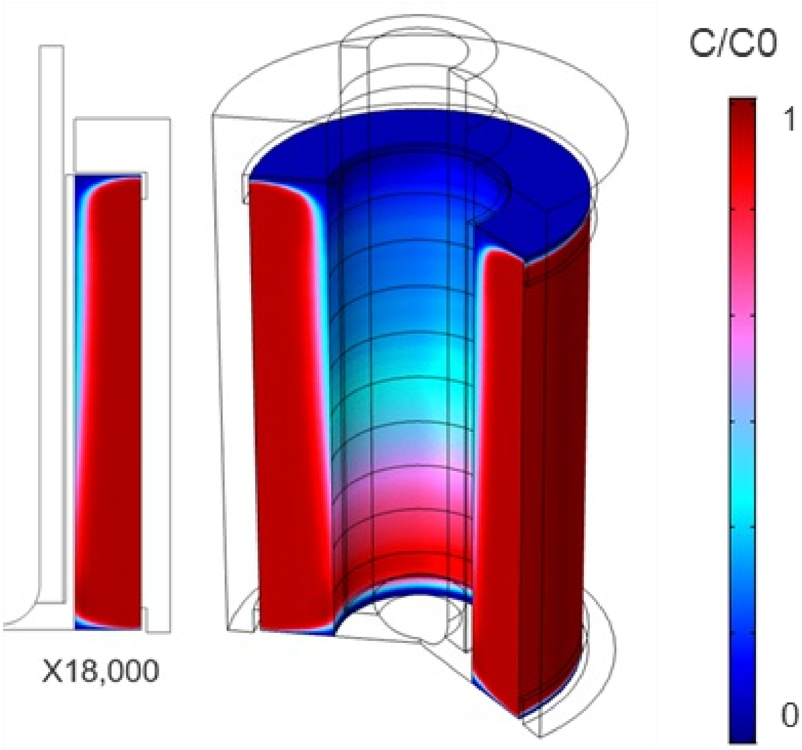

Figure 3 : Figure 3. Concentration (c) change in the adsorptive media: Time-dependent transport study (tds) with partial differential equation (g) interfaces. View: Revolution 2D.