A multi-scale model for Transport and Reaction in Heterogeneous Porous Media

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Many practical problems in engineering occur over time and length scales that differ by many orders of magnitude. This makes the application of direct numerical approaches for the prediction of their response impractical. One such class of systems involves heterogeneous porous media in which small spherical porous particles are dispersed within a larger porous domain. We are interested in investigating such systems in which diffusional and convective transport in the continuous phase are coupled with diffusion and reaction/immobilization within the micro-scale inclusions; we develop multi-scale models which enable the prediction of the transient response of such systems taking into account, in a rigorous manner, the transport and reaction at the micro-scale. Immobilized bioreactors [1], ground-water or hydrocarbon flow in fractured rock [2] and ion diffusion in Li-ion batteries [3] are all potential systems of interest.

One example of a process of interest is shown schematically in Fig. 18, where a chemical species is transported by convection and diffusion around and diffuses into a matrix of porous particles, where it also undergoes first order reaction. In the intraparticle space the species concentration is given by Eq. 1, coupled to the local concentration in the bulk fluid by Eq. 2.

$$D_{eff}\left[\frac{\partial^2 C_b}{\partial r^2}+\left(\frac{2}{r}\right)\frac{\partial C_b}{\partial r}\right]-k\varepsilon_p C_b=\varepsilon_p\left(\frac{\partial C_b}{\partial t}\right) \qquad [Eq\ 1]$$

$$-D_{eff}\left(\frac{\partial C_b}{\partial r}\right)_{r=R}=k_e(\beta C_R-C_L) \qquad [Eq\ 2]$$

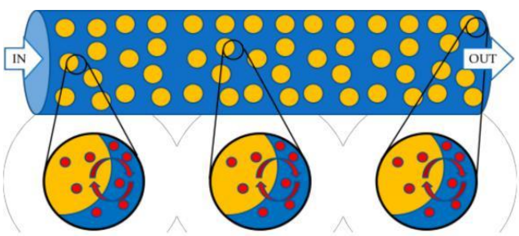
The model involves the spatial discretization of the system into N points, before locally determining the concentration at the particles' surface by using Duhamel's Theorem to solve Eq. 1 and Eq. 2. The result for node i is given by Eq. 3, where the Ψ terms are described by Eq. 4[1]

The system of (2 +) Ordinary Differential Equations is solved easily in MATLAB;

$$\frac{S_i}{\varepsilon D_R}\frac{dC_{Ri}}{dt_R}+\left(\frac{9\phi^2 S_i}{\beta}+\frac{B_m}{2\varepsilon_p}\right)\beta C_{Ri}(t_R)=\frac{B_m}{2\varepsilon_p}C_i(t_R)-\sum_{1}^{n_o}\Psi_i^n(t_R) \qquad [Eq\ 3]$$

$$\frac{d\Psi_i^n}{dt_R}+\varepsilon D_R[(n\pi)^2+9\phi^2]\Psi_i^n(t)=\frac{dC_{Ri}}{dt_R}+9\phi^2\varepsilon D_R C_{Ri}(t) \qquad n=1,2,\ldots..n_o \qquad [Eq\ 4]$$

The system of $N^*(2+n_0)$ Ordinary Differential Equations is solved easily in MATLAB; example simulation results for high and low intraparticle diffusivity conditions are plotted in Fig. 19.



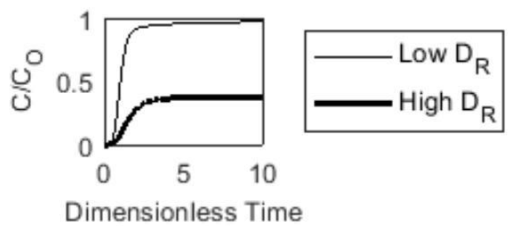


Fig. 18 Schematic of multi-scale system

Fig. 19: Porous-bead bioreactor effluents