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Diffusion and dispersion with heterogeneous reaction in homogeneous porous media: The macroscale models revisited

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Mass transport combined with heterogeneous reaction in homogeneous porous media is a common process encountered in chemical engineering that is of major concern for many applications ranging from packed bed reactors to porous electrodes. In these systems, reactants are transported by diffusion (and eventually by advection) inside the pores where chemical reactions take place at the solid-fluid interfaces. Modelling the macroscopic behavior of these mechanisms is of prime importance and has been the subject of numerous studies [1, 2, 3, 4]. However, in almost all the analyses reported in the literature, the Kinetic number, Ki, referred to as the ratio between the characteristic time associated to diffusion and the characteristic time associated to reaction at the pore-scale, is considered to be exceedingly small compared to unity. Many industrial processes are indeed operating in this range of Ki, but this constraint is however not always fulfilled. Under these circumstances, the purpose of the present work is focused on the development of macroscopic models in a range of Ki $\leq$1, relaxing the above mentioned restriction.

The study is focused on single-phase transport of a single chemical species undergoing a first-order heterogeneous reaction in rigid and homogeneous porous media. In addition, the advection problem is assumed to be decoupled from the transport/reaction mechanisms. Macroscopic models are derived, with and without advection, using the volume averaging method and the associated closure problems are provided to compute the effective diffusion (or dispersion) and reaction-rate coefficients. In order to elucidate the impact of the Kinetic number on the coefficients involved in the upscaled equations, a Maclaurin expansion in Ki is carried out, yielding models for which the corrections at the successive orders in Ki and the necessary closure problem to compute them are clearly highlighted and numerically solved in periodic unit cells. Validations of the macroscopic models are carried out from comparisons with direct numerical simulations and a discussion is provided on the impact of the corrections. In particular, it is shown that the impact of the Kinetic number is significant on the effective reaction-rate coefficient as well as on the convective macroscopic term in the average transport equation when the Péclet number is non zero but that Ki has a completely negligible contribution to the effective diffusion (or dispersion) tensor.

Keywords: Diffusion, Heterogeneous reaction, Upscaling

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