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Rigorous upscaling of the reactive flow through a pore, under dominant Peclet and Damkohler numbers

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In this talk we present a rigorous derivation of the effective model for enhanced diffusion through a narrow and long 2D pore. The analysis uses a singular perturbation technique. Starting point is a local pore scale model describing the transport by convection and diffusion of a reactive solute. The solute particles undergo a first order reaction at the pore surface. The transport and reaction parameters are such that we have large, dominant Peclet and Damkohler numbers with respect to the ratio of characteristic transversal and longitudinal lengths (the small parameter epsilon). We give a rigorous mathematical justification of the effective behaviour for small epsilon. Error estimates are presented in the energy norm as well as in L-infinity and L-1 norms of the space variable. They guarantee the validity of the upscaled model. As a special case, we recover the well-known Taylor dispersion formula. It is important to note presence of both chemical reactions and dispersion effects in the upscaled coefficients. Under dominant Peclet and Damkohler numbers, hydrodynamics and chemistry effects are strongly coupled.