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Effective Surface and Boundary Condition for Heterogeneous Salt Media with Insoluble Material

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Several mechanisms, such as dissolution of salt material or drying of porous media, involve transport from a heterogeneous, rough surface characterized by areas in thermodynamic equilibrium with the surrounding fluid and areas of no flux (insoluble material, solid grains in the porous medium) [1], [2]. In general, the characteristic length-scale of the surface is much smaller than the scale of the process under investigation. To deal with this multi-scale aspect, the engineering practice is to replace the heterogeneous, rough surface by a homogeneous, smooth surface, the "effective" surface, over which is applied the Dirichlet condition corresponding to thermodynamic equilibrium. This idea has been checked partially against direct numerical simulation of the small-scale problem, in particular in the case of drying problems.

In this study, we develop a more complete theory of the concept of effective surface applied to such transport problems. The typical example under investigation corresponds to the laminar flow over a soluble salt medium which contains insoluble materials. To develop the concept of effective surface we apply a multi-domain decomposition approach [3], [4], [5]. We first decompose the system, by introduction of an arbitrary interface Σ_0, into a macro-scale subdomain Ω_0 where the variables are smooth and a series of micro-scale Ω_i subdomains which contain all the roughnesses (cf. Figure 1). We then make estimates of velocity and concentration at the micro-scale with an asymptotic expansion of deviation terms with respect to macro-scale velocity and concentration fields. Closure problems for the deviations are obtained and used to study the position of the effective surface and the related boundary conditions.

After resolution of the closure problems, it is shown that the boundary condition for Navier-Stokes equations is of the Navier type (already known from the literature), and of a mixed reactive type, for the mass balances. The effective surface can be positioned in different places, for instance in order to recover a no-slip condition. The associated surface is denoted Σ_{eff}^v, and the effective boundary conditions are

$$u_0 = 0 \quad \text{at} \ \Sigma_{\text{eff}}^v \qquad (1)$$

$$-n \cdot D\nabla c_0 = k_{\text{eff}}(c_0 - c_{eq}) \quad \text{at} \ \Sigma_{\text{eff}}^v \qquad (2)$$

where u_0 and c_0 denote respectively the velocity and concentration in the first order effective model, while c_{eq} is the thermodynamic equilibrium concentration, n is the normal vector pointing from the fluid towards the solid, D is the diffusion coefficient and k_{eff} is defined as an effective mass exchange coefficient. If one wants to recover the original equilibrium condition, the position of the related effective surface Σ_{eff}^c is different from Σ_{eff}^v. In that case we have

$$c_0 = c_{eq} \quad \text{at} \ \Sigma_{\text{eff}}^c \qquad (3)$$

$$u_0 = n \cdot (w_x^{\ c} - w_x^{\ v})\nabla u_0 \quad \text{at} \ \Sigma_{\text{eff}}^c \qquad (4)$$

where $w_x^{\ c}$ and $w_x^{\ v}$ denote respectively the distance from Σ_0 to Σ_{eff}^c and Σ_{eff}^v. Based on numerical resolution of the closure problems, we investigate the evolution of k_{eff} and the impact of the

effective surface position, for various geometries, Reynolds and Schmidt numbers. Finally, we make a comparison between the numerical results obtained with this effective model and those from direct numerical simulations. This allows us to discuss the practical implementation of the effective surface model, in particular the optimal position of the surface. An example of the obtained concentration fields is shown in Figure 2. Concentration contours from direct numerical simulation and the first order effective model are well superposed, apart from a small entrance region where conditions for upscaling break down, which creates a small but acceptable discrepancy. This demonstrates the interest of using an effective surface model, characterized by a homogeneous, smooth surface, to reproduce in a bulk sense flows over heterogeneous, rough surfaces.
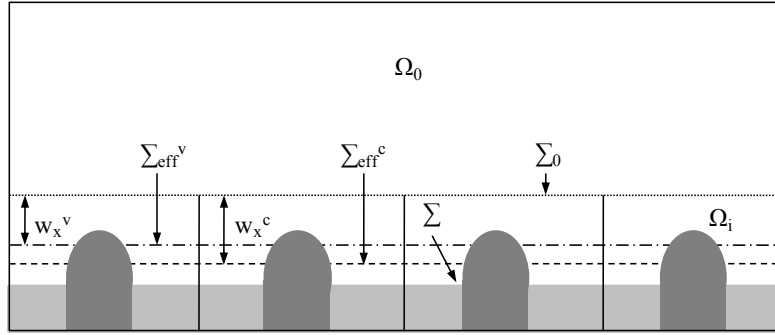

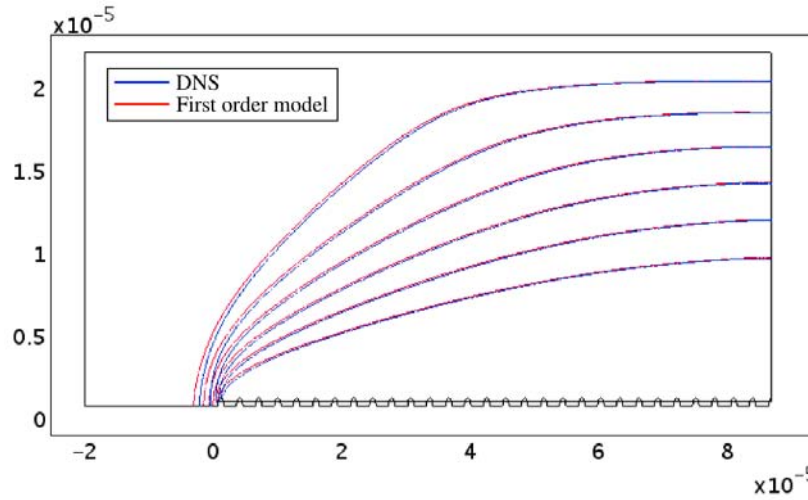Figure 1: Definition of an effective surface.

Figure 2: Concentration field contours for the initial and the effective domain, for a flow entrance velocity of 1m·s⁻¹ and Schmidt number of 1.

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