Is Darcy's Law Applicable for Modeling of Multicomponent Mixtures in Porous Media when Diffusion Is Not Neglected?

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Abstract: Proper modeling of transport of several chemical species in porous media is an important problem with many applications in environmental engineering, science, and industry. Examples of applications are e.g. nuclear waste storage, remediation of contamined sites, enhanced oil recovery or geological CO_2 sequestration. In all these problems the transport of chemical species is described by a set of partial differential equations expressing the mass (or mole) balance of each component. These equations are supplemented by additional constitutive relationships and initial and boundary conditions. The constitutive relationships typically include Darcy's law to describe convection of the mixture and Fick's law to describe diffusion of the mixture components and possibly other equations describing other processes (e.g. compressibility, chemical reactions, etc.) depending on the application.

In this presentation we will focus on the modeling of transport of several chemical components in porous media via convection and diffusion only. We will discuss in detail the usual formulation of the miscible displacement problem and show that once the diffusion is taken into account, the modeling of convection using Darcy's law can be ambiguous. The principal issue here is that it is not clear what kind of velocity is provided by Darcy's law when it is applied to the multicomponent mixture. Is it the mass average velocity or the mole average velocity? Both assumptions can be found the literature but it seems that there is no physical argument for any of these two choices.

Another issue is how to model the diffusion coefficients in the generalized Fick's law. These coefficients generally depend on temperature and concentrations of the mixture components in a complicated way. A systematic way to derive these coefficients is based on the use of the Maxwell-Stefan model. This model can be used only if there is no pressure gradient in the system. The ususal Maxwell-Stefan formulation therefore cannot be applied in porous media in the presence of convection.

The main goal of this talk is to discuss the issues mentioned above and to propose an extension of the Maxwell-Stefan formulation describing the transport of several chemical components in porous media and treating both the convection and diffusion altogether in a thermodynamically consistent way.

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