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ABSTRACT:

Concentration Dependency of Diffusivity in Non-isothermal Miscible Displacements

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Estimating an effective diffusion coefficient in binary miscible systems remains a challenging task because diffusion is inherently composition dependent. A particularly important example of such systems arises in solvent-heavy oil mixtures. In these systems, solvent molecules diffuse into bitumen, altering its composition, viscosity, and volume [1,2]. The situation becomes more complex in thermal recovery processes, where temperature gradients evolve during operation. In this work, a non-isothermal model coupling discrete element simulations with continuum fluid flow modeling is developed. Eulerian predictions are compared with corresponding Lagrangian results to quantify diffusional behavior. The model incorporates not only Brownian-motion-induced transport and classical Fickian diffusion, but also particle-particle interaction forces. In addition, swelling of the in-place fluid caused by solvent dissolution is accounted for through a moving mesh formulation. As solvent molecules diffuse into bitumen, the bitumen swells and its volume increases. This volumetric expansion generates a pressure gradient that induces bulk flow of the mixture in the direction opposite to the diffusive flux. Results show that, in addition to the swelling effect, the concentration dependency of diffusion in solvent-heavy oil systems can also be attributed to non-Fickian behavior arising from interparticle interaction forces. The proposed framework provides a basis for fitting available experimental data and extrapolating transport behavior to new heavy oil systems when direct measurements are limited or unavailable. Such a description is particularly useful for optimizing solvent-assisted thermal recovery processes, with the broader goal of reducing greenhouse gas emissions, and supporting sustainable energy recovery strategies.

[1] P. Babak, A.M. Mendoza and A. Kantzas, Chemical Engineering Science, 181, 286-297 (2018).
[2] S.K. Das, and R.M. Butler, The Canadian journal of chemical engineering, 74(6), 985-992 (1996).