Asociación Argentina
de Mecánica Computacional

Mecánica Computacional Vol XXXIX, págs. 665-665 (resumen)
F.E. Dotti, M. Febbo, S.P. Machado, M. Saravia, M.A. Storti (Eds.)
Bahía Blanca, 1-4 Noviembre 2022

A FINITE-VOLUME TOOLBOX FOR COMPREHENSIVE SIMULATION OF FLUID FLOW AND MASS TRANSPORT PHENOMENA IN PAPER-BASED MICROFLUIDICS

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Keywords: Unsaturated flow, Reactive transport, Paper-based microfluidics, Porous media.

Abstract. This work introduces porousMicroTransport, a new numerical toolbox for simulating flow and reactive transport in porous media, aimed at the study and design of paper-based microfluidic devices. The software is able to solve problems that involve the simultaneous coupling of (1) saturated (single-phase) or unsaturated (multiphase) fluid flow; (2) advection–diffusion–dispersion transport in porous media encompassing any number of concurrently transported species; and (3) a set of chemical reactions involving such species. porousMicroTransport adopts a macroscopic, Darcy-based approach for modeling fluid flow, with unsaturated cases fully described with the help of unsaturated flow models. The built-in library of unsaturated flow models offers implementations of various known constitutive relations, including the LETd model, which has been proposed specifically for paper-based microfluidics. After the flow equation is solved at each timestep, reactive transport equations are solved to update the concentration fields of every species. The transport stage considers concentration changes by advection, molecular diffusion, (an)isotropic mechanical dispersion effect dependent on the flow velocity, and arbitrary reaction terms as defined by a reaction model, which by default can express power-law kinetic reactions of integer or fractional order. The toolbox, developed for the OpenFOAM finite-volume platform, uses a configuration scheme that purposely follows the conventions of other numerical tools for multiphase flow in porous media. It is worth noting that, so far, none of the computational tools available for OpenFOAM have been able to deal simultaneously with these phenomena in unsaturated porous media, and neither are the existing tools tailored towards microfluidic problems and substrates. The new software is validated by means of an automated test suite, and includes a set of tutorial cases.