Chemeca 2025 and Hazards Australasia
28 – 30 September, Adelaide, South Australia

Analytical modeling and exact upscaling for solute transport with adsorption in micro-heterogeneous chromatographic columns.

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ABSTRACT

Single-phase flow with adsorption in porous media exhibiting heterogeneity is crucial in gradient and tandem chromatographic columns, heterogeneous chemical reactors, and the transport of solutes or contaminants in geological aquifers. This study examines one-dimensional transport of solutes with a sorption isotherm that varies along the linear coordinate of the chromatographic column. The coordinate-dependency corresponds to the heterogeneity exhibited at the microscale, while the macroscale refers to the entire homogenised column. An exact solution is developed, enabling the formulation of an exact upscaling (homogenization) method, replacing the coordinate-dependent desorption isotherm with a uniform one, while preserving the breakthrough concentration history. Laboratory tests on single-phase flow with adsorption were performed in two uniform columns with significantly different desorption isotherms, as well as in a composite column consisting of these two sections. The fully predictive analytical model for the composite-column breakthrough, based on data from the individual columns, shows excellent agreement with experimental results, confirming the validity of the upscaling procedure. According to the exact solution, breakthrough concentration and upscaled concentration profiles in composite columns composed of uniform sections are independent of the order of columns when arranged in series. This finding is validated by analytical modeling at the micro and macro scales.

KEY WORDS

Adsorption; Solute transport; Porous media; Composite column; Exact solution; Upscaling

BIOGRAPHY

Kofi Ohemeng Kyei Prempeh is a highly skilled PhD candidate in Petroleum and Reservoir Engineering at the University of Adelaide. His current research focuses on advanced computational methods, optimization, and modeling to solve complex challenges in the energy and chemical industry. Specifically, his research involves the development of upscaled mathematical models for solute transport in chromatographic columns as well as CO_2 storage in heterogeneous porous media, with a primary emphasis on the optimization of storage capacity and ensuring the long-term safety of CO_2 storage sites.

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