WENO scheme on characteristics for the equilibrium dispersive model of chromatography with generalized Langmuir isotherms

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Abstract: Column chromatography is a laboratory and industrial technique used to separate different substances mixed in a solution. Mathematically, it can be modeled using non-linear partial differential equations whose main ingredients are the adsorption isotherms, which are non-linear functions modeling the affinity between the different substances in the solution and the solid stationary phase filling the column.

In this talk, we consider multicomponent adsorption isotherms which are generalizations of the multicomponent *Langmuir* isotherms. Following the techniques in [1], we will prove that, for this family of functions, there is a smooth bijection between the concentrations of the solutes in the liquid phase and the conserved variables that allows us to write the model as a well-posed system of conservation laws with diffusive corrections. We will show that this correspondence allows us to numerically recover the characteristic information of the Jacobian matrix of the convective fluxes and use it to design an implicit-explicit scheme that uses characteristic-based numerical fluxes for the fifth-order WENO reconstruction technique. Finally, some numerical examples will be displayed to reinforce that the proposed numerical technique is a reliable and robust tool for numerically solving this model [2].

References:

[1] R. Donat, F. Guerrero, P. Mulet, *Implicit-explicit WENO scheme for the equilibrium dispersive model of chromatography*, Appl. Numer. Math. 123 (2018) 22-42.

[2] R. Donat, M.C. Martí, P. Mulet, *WENO scheme on characteristics for the equilibrium dispersive model of chromatography with generalized Langmuir isotherms*, Appl. Numer. Math. 201 (2024) 247–264.