A NONLINEAR ALE-FCT SCHEME FOR NON-EQUILIBRIUM REACTIVE SOLUTE TRANSPORT IN MOVING DOMAINS

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Abstract. We consider the reactive transport of chemical solutes in a deformable channel. This is modeled by the following convection-diffusion equation with wall adsorption-desorption equation:

$$\partial_t c^f + \nabla \cdot (\boldsymbol{v} c^f - D \nabla c^f) = 0, \text{ in } \Omega(t),$$
$$J^{-1} \partial_t (J c^w) = (-D \nabla c^f) \cdot \boldsymbol{n} = k_d(\Lambda(c^f) - c^w), \text{ on } \Sigma(t).$$

We present a conservative, positivity-preserving, high-resolution nonlinear ALE-flux-corrected transport (FCT) scheme for the above model. The reactive transport is characterized by dominant Péclet and Damköhler numbers, a phenomenon that often results in non-physical negative solutions. The scheme presented here is proven to be mass conservative in time and positive at all times for a small enough Δt. Reactive transport examples are simulated using this scheme for its validation, to show its convergence, and to compare it against the linear ALE-FCT scheme. The nonlinear ALE-FCT is shown to perform better than the linear ALE-FCT schemes for large time steps.

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