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:

\[
\begin{align*}
\frac{\partial c}{\partial t} + \nabla \cdot (vc - D\nabla c) &= 0, \quad \text{in } \Omega(t), \\
J^{-1}\frac{\partial}{\partial n}(Jc_w) &= (-D\nabla c) \cdot n = k_d(\Lambda(c) - c_w), \quad \text{on } \Sigma(t).
\end{align*}
\]

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 \(\Delta t\).

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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