Simulation of reactive flows using particle methods

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Abstract

We describe a new computational method for the numerically stable particle-based simulation of open-boundary flows, including volume conserving chemical reactions. The novel method is validated for the case of heterogeneous catalysis against a reliable reference simulation and is shown to deliver identical results while the computational efficiency is significantly increased.

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periodic-bc-reactive-flow.pdf available at https://authorea.com/users/368172/articles/487404-simulation-of-reactive-flows-using-particle-methods