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Model for the simulation of reaction-mixing processes at boundary layers

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Reactive boundary conditions are employed to model an increasingly wide range of transport scenarios. While the capability of a variety of computational schemes for reliable description of such reaction-diffusion processes at the boundary of a given domain has been assessed in the literature, the effects of hydrodynamic processes on the rates of reactions taking place at the boundary are still largely unexplored.
We present a computational algorithm to model the turbulent mixing and transport of scalars through a channel in the presence of reactive boundary conditions, and obtain a pdf of their concentrations through time and space. A Lagrangian stochastic particle technique is used to model scalar transport. We consider a system with a partially adsorbing boundary condition modelled through the coarse-graining of small scale linear reactions. We observe a nonlinear dependence of the boundary reaction (i.e., sorption) rate on the turbulent frequency.

Participation

In-Person

References

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Primary authors: SOPPITT, Alisdair (University of Warwick); MOUSAVI NEZHAD, Mohaddeseh (Associate Professor); Dr HUDSON, Thomas (Warwick Mathematics Institute, University of Warwic)

Presenter: SOPPITT, Alisdair (University of Warwick)

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