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Chaotic flow and the finite-time Lyapunov exponent: Competitive autocatalytic reactions in advection-reaction-diffusion systems
RICHARD M. LUEPTOW, CONOR P. SCHLICK, PAUL B. UMBANHOWAR, JULIO M. OTTINO, Northwestern University — We investigate chaotic advection and diffusion in competitive autocatalytic reactions. To study this subject, we use a computationally efficient method for solving advection-reaction-diffusion equations for periodic flows using a mapping method with operator splitting. In competitive autocatalytic reactions, there are two species, B and C, which both react autocatalytically with species A ($A+B\rightarrow 2B$ and $A+C\rightarrow 2C$). If there is initially a small amount of spatially localized B and C and a large amount of A, all three species will be advected by the velocity field, diffuse, and react until A is completely consumed and only B and C remain. We find that the small scale interactions associated with the chaotic velocity field, specifically the local finite-time Lyapunov exponents (FTLEs), can accurately predict the final average concentrations of B and C after the reaction is complete. The species, B or C, that starts in the region with the larger FTLE has, with high probability, the larger average concentration at the end of the reaction. If species B and C start in regions having similar FTLEs, their average concentrations at the end of the reaction will also be similar. Funded by NSF Grant CMMI-1000469.

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