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On the potential failure of reduced reaction kinetics JOSEPH POWERS, SAMUEL PAOLUCCI, University of Notre Dame — Severe stiffness of equations modeling advection, reaction, and diffusion in combustion systems has motivated many efforts to filter the primary mechanism inducing the stiffness: the simultaneous presence of fast and slow reaction dynamics. Here, it is demonstrated that a common filtering technique for construction of low dimensional reaction manifolds, connection of equilibria by heteroclinic orbits, can fail. While the method is guaranteed to generate an invariant manifold, the local dynamics far from equilibrium may be such that nearby trajectories are in fact carried away from the identified invariant manifold, thus rendering it to be of limited utility in capturing slow dynamics far from equilibrium. An eigenvalue-based method is described to characterize the local behavior of such invariant manifolds. The method provides a diagnostic tool for evaluating whether a candidate manifold has the desirable properties of being both slow and attractive. A simple model system and a realistic hydrogen-air system are examined; method success and failure are demonstrated.

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