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An Assessment of the RCCE for Computationally Efficient Combustion Simulations with Detailed Kinetics FATEMEH HADI, Northeastern University, MOHAMMAD JANBOZORGI, University of Southern California, REZA H. SHEIKHI, HAMEED METGHALCHI, Northeastern University — The Rate-Controlled Constrained-Equilibrium (RCCE) method is assessed for detailed kinetics simulations in combustion. The method describes the reacting system dynamics by a relatively small number of rate-controlling reactions and slowly-varying constraints. The unconstrained chemical species are assumed to be in a temporary constrained-equilibrium state and their compositions are determined by maximizing the entropy. The RCCE is applied to predict methane combustion in a constant pressure Partially-Stirred Reactor (PaSR) using 12 constraints and 133 reaction steps. Simulations are carried out over a wide range of initial temperatures and equivalence ratios. The RCCE predictions are compared with those obtained from direct integration of detailed kinetics. It is demonstrated that the set of constraints chosen, accurately represents the methane oxidation kinetics. The effect of mixing on reaction is studied for different residence and mixing time scales. Results show that the RCCE provides accurate prediction of reaction dynamics with various levels of mixing. The RCCE is also shown to significantly reduce the stiffness and the overall computational cost associated with detailed kinetics.

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