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Investigation of Mixing and Chemical Reaction Interactions Using Rate-Controlled Constrained-Equilibrium 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 applied to study the interaction between mixing and chemical reaction in a constant pressure Partially-Stirred Reactor (PaSR). The objective is to understand the influence of mixing on RCCE predictions. The RCCE is a computationally efficient method based on thermodynamics to implement the combustion chemistry. In the RCCE the dynamics of reacting systems is described by a small number of rate-controlling reactions and slowly-varying constraints. The method is applied to study methane combustion via 12 constraints and 133 reaction steps. Simulations are carried out over a wide range of initial temperatures and equivalence ratios. The RCCE predictions are assessed by comparing with those of detailed kinetics model, in which the same kinetics, involving 29 species and 133 reaction steps, is integrated directly. Chemical kinetics and mixing interactions are studied for different residence and mixing time scales. Results show that the RCCE accurately represents the effect of mixing with different mixing strengths. An assessment of numerical performance of the RCCE is also performed. It is shown that the method is effective to reduce the stiffness of the kinetics and thus allows simulations with much lower computation costs.

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