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Computational Efficiency and Accuracy of the Two Forms of the Rate-Controlled Constrained-Equilibrium Method FATEMEH HADI, Northeastern University, REZA SHEIKHI, 61124602 — In this study, the Rate-Controlled Constrained-Equilibrium (RCCE) method in constraint potential and constraint forms have been investigated in terms of accuracy and numerical performance. The RCCE originates from the observation that chemical systems evolve based on different time scales, dividing reactions into rate-controlling and fast reactions. Each group of rate-controlling reactions imposes a slowly changing constraint on the allowed states of the system. The fast reactions relax the system to the associated constrained-equilibrium state on a time scale shorter than that of constraints. The two RCCE formulations are equivalent mathematically; however, they involve different numerical procedures and thus show different computational performance. In this work, the RCCE method is applied to study methane oxygen combustion in an adiabatic, isobaric stirred reactor. The RCCE results are compared with those obtained by direct integration of detailed chemical kinetics. Both methods are shown to provide very accurate representation of the kinetics. It is also evidenced that while the constraint form involves less numerical stiffness, the constraint potential implementation results in more overall saving in computation time.

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