Physics > Chemical Physics

Advanced quasi-steady state approximation for chemical kinetics

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Computational feasibility of turbulent reacting flows hinges on the reduction of large chemical kinetics systems to smaller more manageable reaction sets. Recently, several sophisticated reduction techniques have been developed but they continue to be computationally prohibitive for practical three-dimensional unsteady computations. For such applications, the classical quasi-steady state assumption (QSSA), despite serious shortcomings, continues to be popular due to its conceptual clarity and computational simplicity. Starting from invariant manifold description, we develop an advanced quasi-steady state assumption which (i) is independent of the choice of the retained (slow) species; (ii) possesses much improved physical and mathematical characteristics; and (iii) can be specialized for any objective function.

Comments: I will submit a different work in this topic
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