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Uncertainty due to Imperfect Models of Chemically Reacting Systems[1]

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In complex phenomena involving chemical reactions, such as detonations and hypersonic shocks, the kinetics of the chemical reactions are critical to the physics. Computational models of the phenomena must therefore reliably represent the chemical kinetics. However, even in relatively simple reactions, there are innumerable chemical reaction pathways involving large numbers of intermediate species and excited states. Development of chemical reaction mechanisms for use in computational models thus requires the modeler to identify and characterize a subset of reactions and species that are deemed most important. Further, in computational models of complex systems, chemical mechanisms may need to be simplified further to reduce computational costs. In either case, there are missing species and pathways, which raises the question of how they impact the reliability of simulations of the phenomena. To address this, we consider representations of the uncertainties due to imperfect kinetics models in terms of stochastic operators, which provide a probabilistic description of the missing species and reactions. The "model inadequacy" representation is formulated to respect constraints imposed by conservation laws and thermodynamics. The approach will be demonstrated on a model of hydrogen-oxygen kinetics in a perfectly stirred reactor.

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