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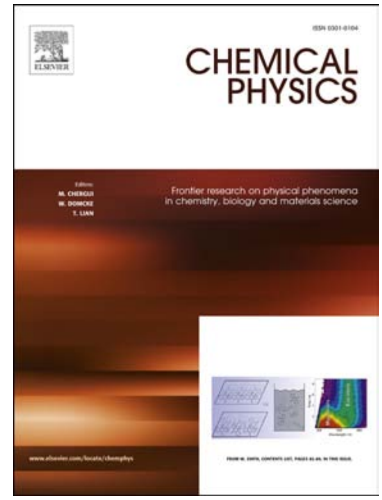

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Uncertainty Quantification and Robust Predictive System Analysis for High Temperature Kinetics of $HCN/O_2/Ar$ Mixture

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Abstract

In this paper, a stochastic system based Bayesian approach is applied to quantify the uncertainties involved in the modeling of the $HCN/O_2/Ar$ mixture kinetics proposed by Thielen and Roth [1]. This enables more robust predictions of quantities of interest such as rate coefficients of HCN + Ar → H + CN + Ar and O_2 + CN → NCO + O by using a stochastic Arrhenius form calibrated against their experimental data. This Bayesian approach requires the evaluation of multidimensional integrals, which cannot be done analytically. Here a recently developed stochastic simulation algorithm, which allows for efficient sampling in the high-dimensional parameter space, is used. We quantify the uncertainties in the modeling of the $HCN/O_2/Ar$ mixture kinetics and in turn the two rate coefficients and the other relevant rate coefficients. The uncertainty in the error including both the experimental measurement error and physical modeling error is also quantified. The effect of the number of uncertain parameters on the uncertainties is investigated.

Keywords: Bayesian approach, Stochastic system, Uncertainty quantification, Robust predictive analysis, Arrhenius form, Deterministic

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