Optimisation and Bayesian Parameter Estimation of a Kinetic Model of n-Propylbenzene Oxidation in a Shock Tube

Sebastian Mosbach[1], Je Hyeong Hong[1], George P. E. Brownbridge[1], Markus Kraft[1], Soumya Gudiyella[2], and Kenneth Brezinsky[2]

[1] Department of Chemical Engineering & Biotechnology, University of Cambridge, Pembroke Street, Cambridge CB2 3RA, UK, mk306@cam.ac.uk

[2] Department of Mechanical & Industrial Engineering, University of Illinois at Chicago, Chicago, IL 60607, USA, kenbrez@uic.edu

We present an optimised chemical kinetic mechanism for n-propylbenzene oxidation in a shock tube and apply a Bayesian parameter estimation technique to investigate uncertainties in model parameters and responses. The optimisation of the mechanism [1] is carried out in two stages: firstly, a quasi-random global search using a Sobol low-discrepancy sequence is conducted, followed by a local optimisation by means of a hybrid gradient-descent/Newton iteration method. The concentrations of 37 species at a variety of temperatures, pressures, and equivalence ratios are optimised against a total of 2378 experimental targets. We then apply a Bayesian methodology to study the influence of uncertainties in the experimental measurements on some of the Arrhenius parameters in the model as well as some of the predicted species concentrations. Markov Chain Monte Carlo algorithms are employed to sample from the posterior probability densities, making use of polynomial surrogates of higher order fitted to the model responses. The methodology allows analysis of the distributions of model parameters and responses, in particular their uncertainties and correlations.

[1] Gudiyella, S. and Brezinsky, K. *Combust. Flame*, 159(3):940–958, 2012.