The Retrieval of Chemical Reaction Rates Using Genetic Algorithms

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Abstract

A general inversion procedure for determining the optimum rate coefficients for chemical kinetic schemes, based upon limited net species production data, using Genetic Algorithm techniques is presented. The objective of the optimisation process is to derive rate parameters such that the given net species production rates at various conditions are simultaneously achieved by searching the parameter space of the rate coefficients in the generalised Arrhenius form of the reaction rate mechanisms.

1 PROBLEM DESCRIPTION

The chemistry of combustion may be modelled using a system of chemical reactions for which the rates of each reaction are known. Databases which give measurements of reaction rate parameters are commercially available but a large uncertainty in the reaction rates at all temperatures is generally observed.

In this initial study, Genetic Algorithms are used to predict the reaction rate parameters for hydrogen/oxygen/nitrogen flames to enable confidence in the technique to be generated before the possible progression on to higher-order hydrocarbon scheme optimisations. CHEMKIN's Perfect Stirred Reactor (PSR) computer program (see Glarborg *et al.* (1988)) is used to determine the net species concentrations of each product based upon different reactor conditions.

It is assumed that each reaction proceeds according to the law of mass action and the forward rate coefficients are in modified Arrhenius form

$$\text{rate}, \quad k_{f_i} = A_i T^{\beta_i} \exp\left(-\frac{E_i}{RT}\right) \tag{1}$$

where T is the temperature and R is the universal gas constant. It is the possibility of the determination of the three parameters A_i, β_i and E_i for each reaction, based upon outlet species mass fractions alone, which is investigated in this study.

The Genetic Algorithm process optimises a fitness evaluation function which measures the accuracy of the net product species concentrations at some set of reactor conditions against known (simulated or experimental) measurements. We employ k-Tournament Selection and Two-Point Crossover.

2 RESULTS AND CONCLUSIONS

A sensitivity analysis of the problem has shown that the retrieval of the Arrhenius coefficients within a single reaction equation is possible based upon measurements of a single product species. However, from the results of a series of inversion calculations based upon product measurements at a sequence of reactor conditions, we have concluded that, for a number of simultaneous competing reactions, we must, in general, specify measurement data for all product species.

The Genetic Algorithm inversion process promises the ability to enable the accurate prediction of emission characteristics, stable species concentrations and flame characterisation. Such predictive capabilities are of paramount importance in many industries.

References

Glarborg, P., Kee, R.J., Grcar, J.F. and Miller, J.A. (1988), PSR: A FORTRAN Program for Modeling Well-Stirred Reactors, *Sandia National Laboratories Report SAND86-8209.*