Rigorous error control in reacting flow simulations using reduced chemistry models

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Abstract

A method is presented for rigorously controlling the errors introduced by using reduced chemistry models in reacting flow simulations. The method is demonstrated in an Adaptive Chemistry simulation of a simple 1-D laminar premixed methane/air flame. The results are compared with the results of the same calculation performed using the full chemistry model. The Adaptive Chemistry solution satisfies the predicted error criteria.

Keywords: Adaptive Chemistry; Reduced models; Reacting flows; CFD; Error control; Laminar flame

1. Introduction

The challenges of simulating reacting flows with detailed chemistry models are well documented (see [1] for an overview). Research has shown that the bulk of the CPU time is spent evaluating the stiff chemistry terms in these simulations. Consequently, several approaches have been developed to enable a more computationally efficient treatment of chemistry. Since the CPU time of the chemistry evaluations is approximately linear in the number of reactions and quadratic in the number of species in the model, detailed kinetic models are often simplified into reduced models, including only the most important reactions and species. These reduced models are usually faithful to the detailed model over a limited range of reaction conditions. However, they are used at arbitrary conditions, introducing unknown errors because rigorous valid ranges are not defined for the models. In this work we introduce a method to define rigorous valid ranges for reduced models obtained using the method of Bhattacharjee et al. [2]. The method is demonstrated in the context of Adaptive Chemistry.

Adaptive Chemistry has been demonstrated as a method of using reduced models to reduce the CPU time in reacting flow simulations [3,4]. The method exploits the fact that reaction conditions in combustion simulations vary drastically spatially and temporally. Therefore, several smaller locally valid reduced models are used at different regions in the computational domain and at different times during the evolution. A model reduction method was developed to enable the use of optimally reduced models containing the minimum number of reactions necessary to satisfy rigorous reduction criteria locally, with user-specified error tolerances [2]. However, until now it has not been possible to verify the accuracy of Adaptive Chemistry solutions without directly comparing with the corresponding full chemistry solution. In this work we present a method to guarantee a priori the accuracy of Adaptive Chemistry solutions. By defining rigorous valid ranges, we ensure that reduced models are used only when they are guaranteed to satisfy the model reduction tolerances which are set using criteria that guarantee agreement of the final solution at steady state with the full chemistry solution. We demonstrate the method in a simple 1-D laminar premixed methane/air flame simulation.

2. Error control method

The Adaptive Chemistry algorithm works by selecting from a user-supplied library of reduced models, the smallest model that is valid at a given point $\mathbf{x} = (\mathbf{T},\mathbf{P},\mathbf{Y})$. However, the reduced models are strictly known to be valid only at the individual points considered during the reduction. For practical implementation it is necessary to have models that can be used for ranges rather than individual points. Therefore, rigorous valid ranges are

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needed to ensure that the models are used only where they are valid. Furthermore, it is necessary to determine appropriate tolerances for model reduction such that the model truncation errors will not lead to unacceptable errors in the final Adaptive Chemistry solution. These issues are addressed in the following sections.

2.1. Valid ranges of reduced models

As formulated by Bhattacharjee et al. [2], reduced models are required to satisfy the following criteria:

$$E_j(\mathbf{x}) \equiv \left| S_j^{full}(\mathbf{x}) - S_j^{red}(\mathbf{x}) \right| \leq tol_{MR,j} \quad \forall j = 1, \ldots, N_S + 1 \tag{1}$$

where S_j are the time rates of change of temperature and species mass fractions due to kinetics alone (no transport), and tol_{MRj} are the model reduction tolerances. The superscripts indicate the type of model used to evaluate the term. These criteria are required to be satisfied only at the points used for model reduction. Determining the valid range of the reduced model entails finding the largest region $\mathbf{X}$ such that Eq. (1) is satisfied for all $\mathbf{x} \in \mathbf{X}$. This is difficult to do because the functions E_j are nonlinear in $\mathbf{x}$ and the constraints (Eq. (1)) are usually non-convex.

Rather than attempt to characterize the entire valid range of a reduced model we iteratively identify a subset of the full range. The procedure is described below and in Fig. 1.

1. Given a guess range $\mathbf{X}$ containing a point $\mathbf{x}$ used in model reduction, calculate a rigorous upper bound on each $E_j(\mathbf{x})$ in $\mathbf{X}$. A rigorous upper bound $E_{up,j}$ satisfies the criterion $E_{up,j}(\mathbf{X}) \geq E_{max,j}(\mathbf{X})$.
2. Evaluate all $E_{up,j}(\mathbf{X})$ to determine if all satisfy $E_{up,j}(X) \leq tol_{MR,j}$. If so, $\mathbf{X}$ is a rigorous valid range of the reduced model; Otherwise,
3. decrease the size of $\mathbf{X}$ such that the model reduction point remains enclosed in the new guess range, and repeat steps 1 and 2. If a model is desired for the range $\mathbf{X}$, obtain a larger reduced model (larger models are generally valid over wider ranges) and repeat steps 1 and 2.

Using this procedure reduced models with rigorous valid ranges are obtained. The ranges are defined geometrically as N-dimensional hyperrectangles ($\mathbf{X} = [\mathbf{x}_{lo}, \mathbf{x}_{hi}]$ such that $x_{lo,j} \leq x_j \leq x_{hi,j}$ for all x_j in $\mathbf{X}$). Rigorous upper bounds are calculated using interval extensions of remainder Taylor expansions of $E_j(\mathbf{x})$. The interested reader is referred to the following sources for more information on interval extensions and remainder Taylor expansions [5,6]. The current implementation uses

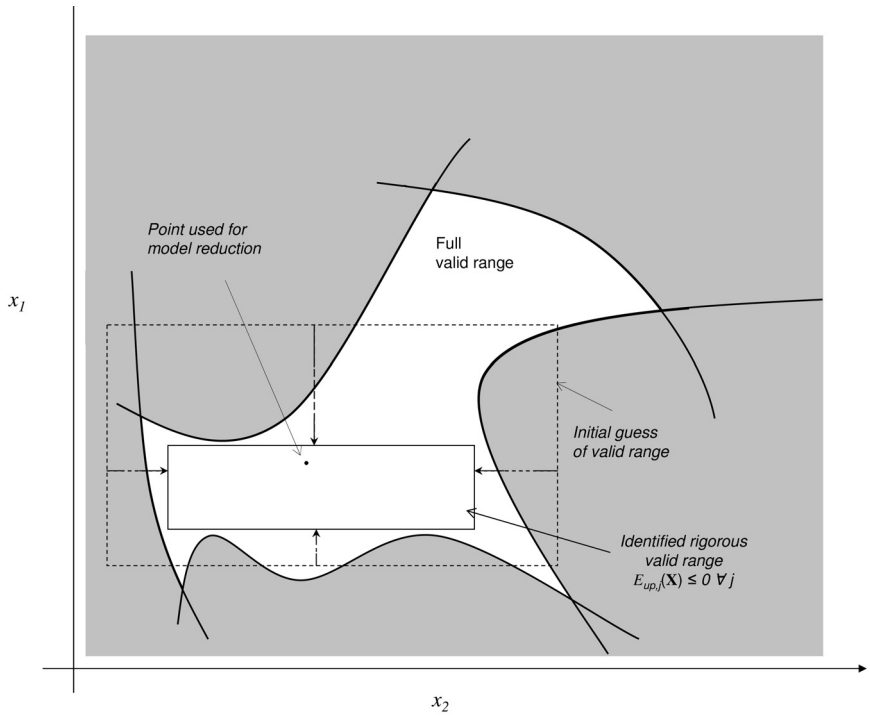


Fig. 1. Identifying valid ranges by iteratively seeking the guess range in which validity can be rigorously verified. Note that this illustration is shown in only two dimensions for clarity. The method actually identifies valid ranges of temperature and concentrations of all species using the full N-dimensional hyperrectangle.

the DAEPACK library [7] to evaluate rigorous upper bounds as described above.

Other methods have been used to estimate valid ranges [8,9,10]. This method is unique in that it guarantees rigorous valid ranges.

2.2. Model reduction tolerances

For steady-state calculations, we set model reduction tolerances to ensure that the Adaptive Chemistry solution will remain unchanged if refined using the full chemistry model, making it a valid solution of the full model problem. This criterion is derived below.

The N species and energy conservation equations can be separated into two parts:

$$F_j(\mathbf{x}) = T_j(\mathbf{x}) + S_j(\mathbf{x}) \tag{2}$$

where T_j contains the transport terms and S_j the kinetic source terms. The simulation is considered to be at steady state when:

$$\begin{aligned} |F_j^{full}(\mathbf{x}_{ss}^{full})| &\le \delta_j^{full} \quad \forall j = 1, \ldots, N \\ |F_j^{adap}(\mathbf{x}_{ss}^{adap})| &\le \delta_j^{adap} \quad \forall j = 1, \ldots, N \end{aligned} \tag{3}$$

Here the superscripts denote the method used in the simulation, $\mathbf{x}_{ss}^{full}$ is the steady state solution obtained using the full model and $\mathbf{x}_{ss}^{adap}$ is the steady-state solution using Adaptive Chemistry. Rigorous valid ranges ensure that Eq. (1) is satisfied whenever a reduced model is used, therefore at the Adaptive Chemistry solution,

$$|F_j^{full}(\mathbf{x}_{ss}^{adap})| \le \delta_j^{adap} + tol_{MR,j} \quad \forall j = 1, \ldots, N \tag{4}$$

To ensure that the Adaptive Chemistry solution would satisfy the steady-state criteria for the full chemistry problem then, it is sufficient to require that:

$$\delta_j^{adap} \le \delta_j^{full} + tol_{MR,j} \quad \forall j = 1, \ldots, N \tag{5}$$

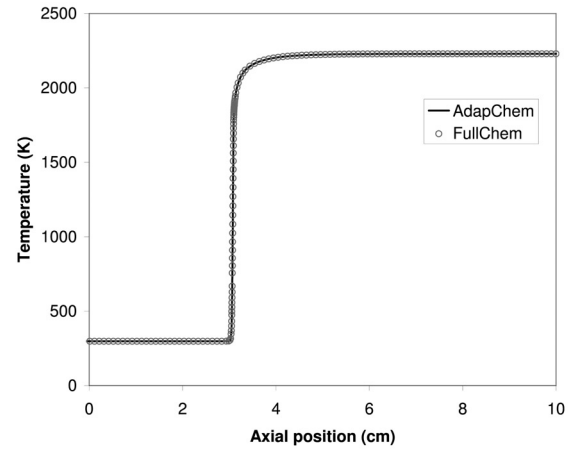
Essentially, by accounting for model reduction error by using stricter numerical error tolerances we can ensure a priori that the steady state solution of the Adaptive Chemistry simulation will be a valid solution of the full chemistry model.

2.3. Results and discussion

The error control ideas presented in the previous sections are now demonstrated in a 1-D laminar premixed methane/air flame simulation. The flame simulated is a freely propagating flame under stoichiometric conditions. The problem configuration is based on the example of a freely propagating flame included in PREMIX in the CHEMKIN II package [11]. The problem was simulated to steady state using a modified version of TWOPNT [12] that solves the time-dependent conservation equations until the steady state residuals

Table 1
Summary of full chemistry and adaptive chemistry simulations for 1-D methane/air flame

Conserved quantity		Full chemistry	Adaptive chemistry
Tolerances – Steady state convergence (δ)			
Enthalpy (K/s)		100	50
Species (s^{-1})		100	50
Tolerances – Model reduction (tol_{MR})			
Enthalpy (K/s)		–	50
Species (s^{-1})		–	50
Model library			
Models {Number of reactions}		% of rate evaluations performed using models	
2 models for pre-ignition chemistry	0 reactions	–	35%
	8 reactions		
1 model for exhaust chemistry	67 reactions	–	33%
4 models for flame-front	106 reactions	–	5%
	181 reactions		
	259 reactions		
	272 reactions		
Full model:	325 reactions	100%	26%



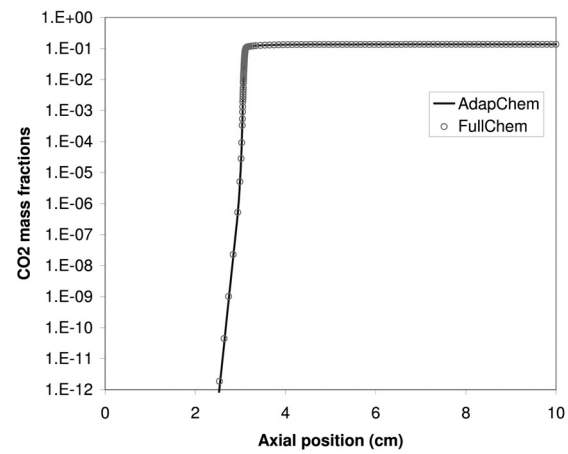
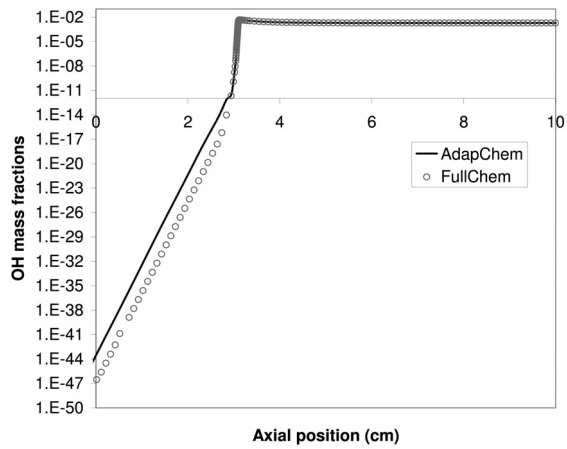


Fig. 2. Comparing Adaptive Chemistry and full chemistry solutions.



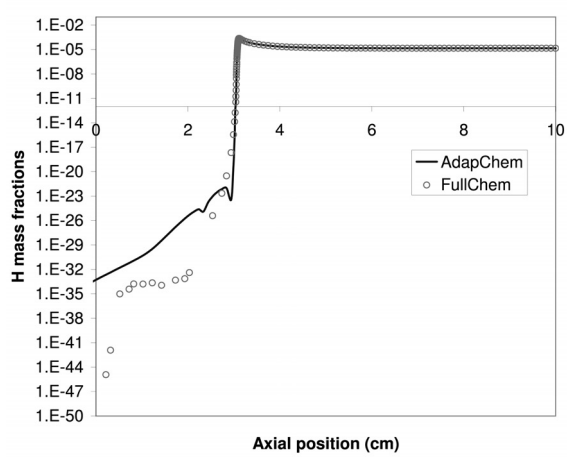


Fig. 3. Comparing Adaptive Chemistry and full chemistry solutions.

fall below specified tolerances δ_j. Thermal properties, transport properties and all reaction rates were calculated using the CHEMKIN II library.

GRI-Mech version 3.0 [13] with 53 species involved in 325 elementary reactions was used as the full model. A library of seven reduced models with rigorous valid ranges was generated to span the range of conditions encountered near steady state in the full model simulation. The range of conditions near steady state in the full model simulation was used as an estimate of the set of conditions encountered over the entire simulation. With this model library the same flame simulation was then performed using Adaptive Chemistry. Relevant statistics from both simulations are presented in Table 1.

Using the converged Adaptive Chemistry steady-state solution as the initial value, the problem was re-solved using the full model and as expected, the solution did not change. As shown on Figs. 2 and 3, there is excellent agreement between the Adaptive Chemistry solution and the full model solution even at reasonably high precision. The differences are noticeable only at the very low values which can be approximated as zero.

The Adaptive Chemistry simulation was almost twice as fast as the full model simulation in this simple problem. Greater speeds have been achieved in the past using Adaptive Chemistry. Particularly, greater speeds are expected in higher dimensions (2-D and 3-D problems), especially if a fine mesh is used to resolve complex flow and if the chemistry is complex. In such problems smaller reduced models (relative to the full model) can be used over a greater number of the grid points.

3. Conclusions

A method has been introduced for rigorously controlling errors in reacting flow simulations using reduced chemistry models. Rigorous valid ranges for reduced models ensure that the model reduction constraints are satisfied whenever a model is used. Rigorous criteria are used to set model reduction tolerances to ensure that a steady-state solution obtained using reduced models will be a valid solution of the full model problem. The method has been successfully demonstrated in a 1-D laminar premixed methane/air flame simulation using Adaptive Chemistry. The simulation was almost twice as fast as the full model simulation and, as expected, the solution was a valid solution of the full model problem.

References

[1] Okino MS, Mavrovouniotis ML. Simplification of mathematical models of chemical reaction systems. Chem Rev 1998;98(2):391–408.

[2] Bhattacharjee B, Barton PI, Schwer DA, Green WH. Optimally-reduced kinetic models: reaction elimination in large-scale kinetic mechanisms. Combustion and Flame 2003;135(3):191–208.

[3] Green WH, Schwer DA. Adaptive chemistry. In: Bathe KJ, editor, Computational Fluid and Solid Mechanics. Oxford: Elsevier Science, 2001.

[4] Schwer DA, Lu Pisi, Green WH. An adaptive chemistry approach to modeling complex kinetics in reacting flows. Combustion and Flame 2003;133(4):451–465.

[5] Ratschek H, Rokne J. Computer Methods for the Range of Functions. Chichester, UK: Ellis Horwood Limited, 1984.

[6] Berz M, Hoffstatter G. Computation and application of Taylor polynomials with interval remainder bounds. Reliable Comput 1998;4:83–97.

[7] Tolsma J, Barton PI. The DAEPACK library. http://yoric.mit.edu/daepack.

[8] Sirdeshpande AR, Ierapetritou MG, Androulakis IP. Design of flexible reduced kinetic mechanisms. AIChE J 2001;47(11):2461–2473.

[9] Pope SB. Computationally efficient implementation of combustion chemistry using in situ adaptive tabulation. Combustion Theory Modelling 1997;(1):47–63.

[10] Tonse SR, Moriarty NW, Brown NJ, Frenklach M. PRISM: Piecewise Reusable Implementation of Solution Mapping. An economical strategy for chemical kinetics. Israel J Chem 1999;39(1):97–106.

[11] Kee RJ, Rupley FM, Miller JA. CHEMKIN-II: A FORTRAN chemical kinetics package for the analysis of gas-phase chemical kinetics. Sandia National Laboratories, SAND89–8009, 1990.

[12] Grcar JF. The Twopnt program for boundary value problems. Sandia National Laboratories, SAND91–8230, 1992.

[13] Smith GP, Golden DM, Frenklach M, Moriarty NM, Eiteneer B, Goldenberg M, Bowman CT, Hanson RK, Song S, Gardiner WC, Lissianski VV, Qin Z. GRI-Mech 3.0. http://www.me.berkeley.edu/gri_mech/