An Induction Parameter Model for Shock-Induced Hydrogen Combustion Simulations

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An induction parameter model has been constructed for the simulation of shock-induced combustion that incorporates the repro-modeling approach for the description of the energy release phase. The model applies only explicit, algebraic functions for the description of the chemical kinetics. These functions parameterize a set of data calculated from homogeneous combustion simulations using a complete and detailed reaction mechanism. Based on this method a model has been created for the simulation of shock-induced combustion of hydrogen in an argon atmosphere. The parameterized model approximates the results of the full chemistry very closely, but the algebraic functions can be computed in a fraction of the time of the full chemistry solution. We use the parameterized model in one- and two-dimensional reactive flow simulations. The results simulate experimental results well, including transitions to detonations and the propagation of detonation waves.

INTRODUCTION

Computational fluid dynamic (CFD) codes are currently available that can model reactive flows to a high resolution in two- and three-dimensional geometries. The limiting factor for such models is generally the large computational time needed to compute the chemical kinetics. At the same time, chemical kinetic reaction mechanisms are becoming increasingly accurate, but ever larger. Many mechanisms contain hundreds of reactions and a hundred or more chemical species. It is unfortunately not feasible to use these mechanisms in any but the simplest reactive flow models, even using modern supercomputers. For one of the simplest combustion systems, for hydrogen oxidation, typically more than 95% of the computational time used by a reactive flow model is consumed by the chemistry solution. This ratio is much worse for more complicated fuels like hydrocarbons. Most currently available mechanism reduction methods result in a small system of ordinary differential equations (ODEs) or coupled algebraic–differential equations. The solution of these equations is time-consuming and causes similar problems.

One method of overcoming this limitation of reactive flow modeling is to use a parameterized model. Such a model would involve the description of the chemical kinetics by algebraic equations only, these equations being obtained by fitting functions to data obtained by using a detailed mechanism or data obtained from experiments. Such a method would be simple to implement within a CFD code and would be extremely fast to compute compared to systems that require the solution of ODEs.

The structure of most CFD codes lends itself to such an approach, as the method of operator splitting is often used. This means that the chemical changes in the fluid are calculated separately from the advection and diffusion. From the point of view of the code, it is immaterial whether the chemical changes over each time step are calculated by an ODE solver or by algebraic equations.

One such parameterization approach is that of the Induction Parameter Model (IPM). This approach makes use of the fact that combustion reactions have an initial induction time where little energy is released, followed by a shorter period when most of the chemical energy is released and the system variables change rapidly.

The first IPM model was introduced by Korobeinikov et al. [1]. This was a two-variable empirical model which approximated the igni-

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tion delay times in shock waves. This model was used by Taki and Fujiwara [2]. A further development was introduced by Oran et al. [3], who derived a global parameterized model which described the induction time as a function of temperature and pressure. They produced an induction parameter model for the combustion of stoichiometric hydrogen in air and determined the induction times to which the model was fitted by using a detailed chemistry mechanism. This approach was used by Clifford et al. [4], who derived a model describing the shock-induced combustion of ethylene, but the energy release phase of the model was also derived from fitting algebraic functions to data obtained from detailed mechanisms. They demonstrated that an accurate modeling of the energy release phase should be incorporated into an induction parameter model if it is to be used successfully within reactive flow models.

One method of accurately modeling the chemical kinetics during the energy release phase is the "repro-modeling" approach. In a repro-model a complex and computationally expensive model is approximated by a simple empirical model using explicit algebraic functions. The basic idea is that a repro-model will reproduce the output of the complex model for any input within a specified range. In reactive flow modeling, the integration of the chemical kinetic equations is by far the most time-consuming part of the model and therefore is an ideal subject for repro-modeling. Repro-modeling has been applied to traffic control models by Meisel and Collins [5], to atmospheric chemical problems by Dunker [6], Marsden et al. [7], and Spivakovsky [8], to a liquid-phase chemical reaction by Turányi [9], to the simulation of the combustion of wet carbon monoxide (Turányi [10]) and to turbulent flame modeling (Christo et al. [11]).

The repro-modeling approach is theoretically appropriate for modeling the complete combustion process, but the algebraic model would be very large with many variables. After the induction time has elapsed, however, most variables of combustion models become algebraic functions of just a few variables. This is a consequence of the existence of slow manifolds in the combustion space [10], which is a characteristic of all combustion systems (see Maas and Pope [12] and Tomlin et al. [13]). In this region the chemical changes can be described by relatively simple algebraic equations. The combination of an IPM model approach to approximate the induction time period and a repro-model approach to approximate the energy release period would give a simple but accurate parameterized model.

We demonstrate that an accurate and globally applicable parameterized shock-induced combustion model can be created by formulating an induction parameter model which utilizes the repro-modeling approach of Turányi [10] for the description of the energy release phase. We describe a general method for deriving such a model for the combustion of any fuel within any given range of conditions, using a full chemistry reaction mechanism for the calculation of the data. We apply these methods to produce an induction parameter model for the shock-induced combustion of hydrogen. We use the model in two-dimensional reactive flow simulations of a complex system to demonstrate the speed and accuracy of the model and compare the results with experimental data.

APPLICATION OF REPRO-MODELING TO COMBUSTION SIMULATIONS

The method of application of algebraic equations for the description of dynamic phenomena is based on the replacement of a system of ODEs by difference equations

$$Y(t + \Delta t) = F(Y(t)) \tag{1}$$

where Y is the vector of system variables and F is an algebraic expression that predicts the value of the system variables at a time Δt later.

The choice of system variables is dependent on the nature of the problem. For a chemistry model they might be temperature, density, or selected species mass fractions.

The approximating empirical function needs to be simple to apply, for fast evaluation, but flexible enough to approximate often highly nonlinear systems. A variety of functions have been used in repro models, such as piecewise linear functions [5], second-order polynomials ([6], and [7]) and higher-order polynomials ([8] and [9]).

Application of Orthonormal Polynomials to Repro-Modeling

The algebraic functions that we will use for the parameterization of the calculated data points are high-order polynomials. These functions are suitable for approximating nonlinear systems in a simple way.

One possible drawback of using high-order polynomials is that they can have a large number of coefficients and can be time-consuming to evaluate. Turányi [9] has devised a scheme which produces high-order polynomials with most coefficients set to zero, to parameterize any given set of data points. The fitting procedure involves fitting a series of discrete orthonormal polynomials to the data points, of which there may be tens of thousands. The orthonormal polynomials are fitted using the method of least squares. The sum of these orthonormal polynomials is then converted into a single polynomial. Details of this procedure are given in [9] and [10]. We have made use of these algorithms in the parameterizations described in this paper.

Generation of the Data

The most important part of a repro-model is the generation of the data to which the algebraic functions will be fitted. The first step is to determine the range of validity we wish the repro-model to have. For instance, we may be interested in shock-induced combustion or combustion in jet-stirred reactors in which the pressure and temperature ranges would be very different. We might also wish to produce a repro-model which is valid for varying fuel-to-oxygen ratios and concentrations of nonreactive dilutant gases, or just have a model which is valid for only one particular mixture.

To produce a repro-model for a range of different mixtures, as well as a wide range of pressures and temperatures, a vast number of data points are needed. This problem can be avoided by fitting separate functions in different regions. To fit a number of different functions to data in different regions is no more difficult than to fit one global function and will not penalize performance within a reactive flow code. In fact, a global model would probably be less accurate and more complex, and therefore computationally more expensive than a number of more local models.

The data points to be used in the fitting procedure can be calculated using a chemical kinetics simulation package, such as the package available form Sandia called CHEMKIN (Kee et al. [14]) and an appropriate chemical reaction scheme. To generate the data, we first define an initial gas mixture and choose a pressure and initial temperature, then we integrate a homogeneous reaction going to completion at constant pressure. We record the values of the system variables at intervals of Δt. We repeat this process for a range of pressures, initial temperatures, fuel to oxygen ratios and so on, until we have enough data points to adequately cover the required range. A data point contains the values of the system variables at time t, together with the values of these variables at a time Δt later.

For reasons outlined above, we do not record data points during the induction time for obtaining simple algebraic representations of the chemical kinetics. We generally would achieve this by ignoring all points that fail to conform to some simple criterion. For example, when calculating the data points to be incorporated into the fitting procedure, Turányi [10] ignored all the data points for which the temperature was less then the initial temperature plus 100 K. The exact nature of the criterion depends on the particular problem under consideration.

Choice of Variables

While, in theory, we could choose any number of variables to be the system variables, we have found, in practice, that they have to be carefully chosen for the model to be useful.

Many of the variables in the system, in particular the mass fractions of the chemical species have evolutions that are difficult to model sufficiently accurately using a model that is also numerically stable. The mass fractions tend to change rapidly over a short period of time during some periods of the combustion process and to be nearly constant or only slowly varying during other periods. The gradients of the mass fractions with respect to time have sharp peaks, but also periods where the gradient is almost zero. Different species have these peaks in the gradient at different times. In contrast, the temperature and density vary smoothly and monotonically over the whole of the combustion process.

It is possible to construct a system that models accurately the evolution of all the variables in the system, but this would require a very large number of data points and very high order polynomials. These derived polynomials are extremely sensitive to even very small changes in the values of the system variables and these changes are of lower orders of accuracy than the errors arising in a finite difference hydrodynamic code, and therefore are of little practical use. We have therefore decided not to try to model the species mass fractions but to use temperature and density as our variables.

For any given pressure, however, any data point may not be uniquely defined by the temperature and density alone. These variables would give us no indication of whether the reaction had just started or was nearly complete. We need a progress variable to provide a measure of the progress of the combustion reaction. We can define such a variable by considering the history of the energy release for a single, complete, homogeneous combustion reaction. The total energy per unit mole released by the complete reaction can be written $Q_{\max}$ and the energy released up to any particular point in time of the reaction as $Q(t)$. If we then define a variable $\beta(t)$ to be:

$$\beta(t) = \frac{Q(t)}{Q_{\max}} \tag{2}$$

then we have a suitable rate of reaction variable.

This model does not then attempt to model the evolution of the individual chemical species. This leads to increases in speed of the hydrodynamic code as the species mass fractions, or equivalent, do not have to be stored and advected. It does, of course, mean that the model is not suitable for modeling diffusion, but then any induction parameter model is not suitable for modeling diffusion flames as there is no modeling of species concentrations during the nonexothermic induction time delay phase. Our main interest is in shock-induced combustion.

A REPRO-MODEL FOR THE COMBUSTION OF HYDROGEN

In this section we derive a repro-model which describes the shock-induced combustion of hydrogen. The model is valid for the range of pressures and temperatures that we would expect to find in shock tube combustion (pressures of 0.5 to 10 atm and temperatures of 1100 K to the thermodynamic limit, which is near 3000 K). If the range is too narrow, the model can easily be extended outside this range following the methods described.

We concentrate on just one gas mixture (stoichiometric hydrogen and oxygen diluted by argon at 70% by mole fraction). This mixture has been chosen because we have available some experimental results produced by workers at Aberystwyth University (Sands et al. [15]) in which this particular ratio of gases was used. The model could be extended to encompass any mixture of hydrogen, oxygen, and argon and similar models could easily be constructed for systems containing other inert gases such as nitrogen.

Calculation of the Data Points

The first step is to find an accurate chemical mechanism. For hydrogen combustion, the reactions are well known and reliable mechanisms are available. We have used a hydrogen oxidation mechanism that was derived from the Leeds Methane Oxidation Mechanism (Clague, A., Hughes, K. J., Pilling, M. G., and Turanyi, T., in preparation) by eliminating all reactions of species containing carbon. This mechanism, which is based on the CEC data collection (Baulch et al. [16]), has been tested against experimental hydrogen combustion data [Clague et al., in preparation]. For the integration of the reactions, and the simulation of homogeneous combustion reactions we have used the CHEMKIN package (see [14]).

An important step is the choice of the time step Δt. This cannot be chosen to be too small, as then the changes in the system variables over a time step would be so small that numerical errors would swamp the solution. If the time step is too large there might not be enough data points to cover the range adequately, and the time step could be larger than the time steps required by the hydrodynamic part of a reactive flow model. Taking all these factors into consideration, we have chosen a time step of 5×10^{-8} s for the current model. A wrong choice of time step could involve the recalculation of all the data points. This step could be important for a model involving the combustion of hydrocarbons, as the recalculation of the data points would require large amounts of computational time, but it is not of major importance when considering hydrogen oxidation.

To generate the data points within our specified range, we started at the lowest pressure, 0.5 atm and lowest temperature 1100 K and let the reaction proceed to completion. We recorded the values of the system variables at intervals of 5×10^{-8} s. We then incremented the initial temperature by 40 K and repeated the process, up to an initial temperature of 2500 K. We then repeated this for a range of pressures between 0.5 and 10 atm. In all, over 4000 initial conditions were used. The calculation of all the data points took about 4 hr using a DEC Alpha 3000 workstation.

For each complete reaction, the criterion at which the recording of data points began was $\beta = 0.04$. We prefer not to use a criterion involving the initial temperature or density as these have meaning only in homogeneous simulations. In a reactive flow model, where the system is heterogeneous, there are no such initial temperature or density values.

When a reaction is almost completed, the system variables do not change by very much over a time step and large numerical errors are observed in the repro-model of these points. We did not attempt to model the very last stage of combustion and we simply ignored all data points for which $\beta > 0.96$.

Fitting Polynomials to the Data

Fourth-order polynomials were fitted to the data points, as we found these to give the most accurate model. The procedure of Turányi [10] was used for computing the coefficients of the polynomials. The accuracy of the polynomials increases as the maximum order increases, but when the model contains higher order polynomials it is numerically unstable.

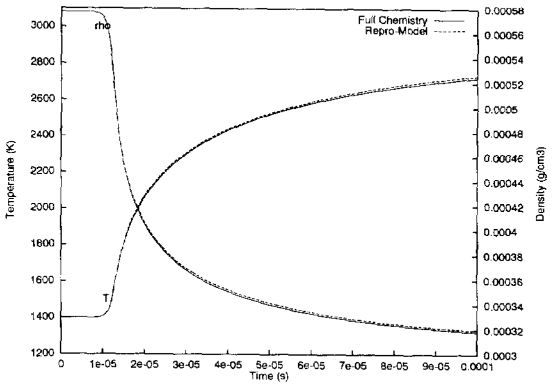

Fig. 1. Time histories of a homogeneous combustion reaction modeled using the full chemistry mechanism and the repro-model. The pressure is 2.1 atm and initial temperature 1400 K. The repro-model covers the range $0.04 < \beta < 0.96$.

There were a very large number of data points used in the fitting procedure and the ranges of pressures and temperatures was wide, so we did not construct a single global model. Instead we constructed four different models for different regions of pressure: 0.5 to 1.0 atm, 1.0 to 2.0 atm, 2.0 to 4.0 atm, and 4.0 to 10.0 atm. Within each pressure range, we found that the accuracy of the model could be increased by constructing separate polynomials in the two regions $\beta < 0.4$ and $\beta > 0.4$. The rates of change with time of the system variables in these two regions have quite different profiles. In the earlier part of the reaction ($\beta < 0.4$) the system variables change rapidly and the gradient profiles have a sharp peak. As the reaction proceeds the gradients are much less and smoothly decrease. Only higher order polynomials can be found to fit the data over the whole region sufficiently accurately, but numerical stability considerations mean that we cannot utilize them. Using separate fourth-order polynomials for the two regions gives us an accurate but numerically stable model.

The fitting procedure produces a number of polynomials with many coefficients. Therefore, we will not print the polynomials that we have derived here, but the full details are available from the authors. A typical polynomial is given below. This polynomial is an algebraic function which predicts the value of $\beta(t + \Delta t)$ given the values of $\beta(t)$, $\rho(t)$, and $T(t)$, where $\Delta t = 5 \times 10^{-8}$, and the pressure is between 2.0 and 4.0 atm and $\beta < 0.4$:

$$
\begin{aligned}
&\beta(t+\Delta t)+1 && =0.65443209 \\
&-0.18543513\times 10^{4}\rho && -0.17866870(\beta+1) \\
&-0.16005639\times 10^{-3}T && +0.53239991\times 10^{6}\rho^{2} \\
&+0.30943999\times 10^{4}\rho(\beta+1) && +0.57495046\rho T \\
&+0.50755934(\beta+1)^{2} && +0.36928071\times 10^{-3}(\beta+1)T \\
&-0.32247408\times 10^{-7}T^{2} && +0.31297814\times 10^{7}\rho^{3} \\
&-0.94859222\times 10^{6}\rho^{2}(\beta+1) && +0.16330922\times 10^{2}\rho^{2}T \\
&-0.12729211\times 10^{4}\rho(\beta+1)^{2} && -0.92100790\rho(\beta+1)T \\
&-0.52114790\times 10^{-5}\rho T^{2} && -0.17427803\times 10^{-3}(\beta+1)^{2}T \\
&+0.14515411\times 10^{-7}(\beta+1)T^{2} && +0.25818106\times 10^{-11}T^{3} \\
&+0.39613347\times 10^{6}\rho^{2}(\beta+1)^{2} && +0.37191443\rho(\beta+1)^{2}T
\end{aligned}
$$

We use $\beta + 1$ in the polynomials instead of β to avoid numerical errors arising in the fitting procedure when β is close to zero.

The final repro-model produced provides a very accurate approximation of the full chemical reaction mechanism but is very much faster to solve. Figure 1 shows the time histories of the temperature and density for homogeneous combustion simulations using the repro-model and the full chemistry mechanism, at a pressure of 2.1 atm and an initial temperature of 1400 K. The calculation of the data for the repro-model took 0.25 s on an Elonex PC-466 personal computer and the full chemistry solution took 370 s. Similarly, for all temperatures and pressures within the range of validity of the repro-model, the parameterized model is 3 orders of magnitude faster to compute than the full chemistry model. As the results shown in Fig. 1 indicate, the repro-model approximates the data obtained using the full chemistry solution to a very high degree of accuracy for homogeneous combustion simulations within the given range.

INDUCTION PARAMETER MODELS

For any fuel system an induction parameter model can be formulated by determining, for a wide range of initial pressures and temperatures, i) an induction delay time, which corresponds to the time for significant increase in radical concentrations, and ii) an energy release function that describes the release of chemical energy after the induction time has elapsed.

In an induction parameter model the detailed reaction mechanism is replaced by the following reactions:

(1) Nonexothermic Induction Reaction.
The rate of reaction is given by

$$\omega_\alpha \equiv \frac{d\alpha}{dt} = -\frac{1}{\tau_i} \tag{3}$$

where τ_i is the induction time.

The induction time represents the delay between the fluid first experiencing a change in conditions (such as passing through a shock) and the subsequent energy release (as a result of chemical reactions). During the induction period, no energy is released so long as $\alpha > 0$. α represents the fraction of induction time remaining during this period. The chemical composition of the fluid is not assumed to change during the induction period.

The induction time in Eq. 3 is given as a function of temperature and pressure, which is produced by fitting an algebraic function to induction times calculated using a detailed mechanism. The induction time can also be a function of the mole fractions of the initial chemical species, to take into account different initial gas mixtures, as discussed, e.g., in the article of Clifford et al. [4].

(2) Exothermic Reaction.

The energy release phase starts as soon as $\alpha < 0$. Using the repro-model approach for the description of the energy release phase, the rate of reaction is given by:

$$\omega_\beta \equiv \frac{d\beta}{dt} \tag{4}$$

where β is the rate of progress variable as defined previously under "Choice of Variables."

The continuity equation for α (similarly for β) is written as:

$$\frac{\partial(\rho\alpha)}{\partial t} + \nabla \cdot (\rho\alpha\nu) = \omega_\alpha, \tag{5}$$

the solution of which is split into two stages:

(a) Lagrangian phase:

$$\frac{\partial(\rho\alpha)}{\partial t} = \omega_\alpha \tag{6}$$

followed by

(b) Advection phase:

$$\frac{\partial(\rho\alpha)}{\partial t} + \nabla \cdot (\rho\alpha\nu) = 0 \tag{7}$$

and similarly for β.

The energy released (ΔE_{ipm}) at each time step is computed as:

$$\Delta E_{\mathrm{ipm}} = \Delta Q = Q_{\max}\Delta\beta \tag{8}$$

Where $Q_{\max}$ is defined as in the section, "Choice of Variables." In a homogeneous system, $Q_{\max}$ depends on the initial temperature and pressure. But the concept of initial values is not applicable to reactive flow systems. However, using the repro-model approach, we can create polynomial functions which predict the value of $Q_{\max}$ for any given value of the system variables.

Incorporating the Repro-Model into an Induction Parameter Model

During the nonexothermic reaction phase of the induction time model, there is no energy release and β is always zero. At the end of this phase, at the start of the energy release phase β is zero and, for homogeneous combustion, the temperature and density still have their initial values. However, the repro-model that we have derived only models the region where $\beta > 0.04$ and, for homogeneous combustion, the temperature is higher than the initial value and the density is lower than its initial value. The region where $0.04 > \beta > 0.0$ needs to be modelled if we are to incorporate the repro-model into an induction parameter model.

At the end of the induction time period, we do not wish to simply immediately increase β to 0.04 and introduce corresponding changes in temperature and density as this would introduce sharp discontinuities into the system which would lead to unwanted hydrodynamic effects in a reactive flow system. But we could increase β incrementally from 0.0 to 0.04 over a number of time steps and similarly increase and decrease the temperature and density respectively. The simplest way to do this is linearly.

For any homogeneous combustion simulation, let τ_c be the time at which $\beta = 0.04$ and let T_c and ρ_c be the values of the temperature and pressure at this point. If, starting at some induction time τ_i, which we have not yet defined, we let β increase as a linear function of time from 0.0 to 0.04 so that it reaches the value 0.04 at the time τ_c, then:

$$\beta(t) = \frac{0.04}{\tau_c - \tau_i}(t - \tau_i). \tag{9}$$

If we also let the temperature and density be linear functions of time in this region then:

$$T(t) = \frac{T_c - T_i}{\tau_c - \tau_i}(t - \tau_i) + T_i \tag{10}$$

and

$$\rho(t) = \frac{\rho_c - \rho_i}{\tau_c - \tau_i}(t - \tau_i) + \rho_i. \tag{11}$$

From the data calculated using the full chemistry solution we know what the time derivative of β is at time τ_c. Let us call this value β'_c. If we then impose the condition that the gradient of the function defined in Eq. 9 is equal to β'_c then this defines the induction time τ_i. Explicitly:

$$\tau_i = \tau_c - \frac{0.04}{\beta'_c}. \tag{12}$$

An example of this is shown in Fig. 2. For a homogeneous combustion simulation with a pressure of 3.5 atm, and an initial temperature of 1400 K, we show the repro-model solution, starting at $\beta = 0.04$ together with the linear function as defined above, tangent to the repro-model curve at the point $\beta = 0.04$. The time at which the linear line crosses the time axis is then the induction time τ_i and we have a model that can simulate the complete combustion reaction.

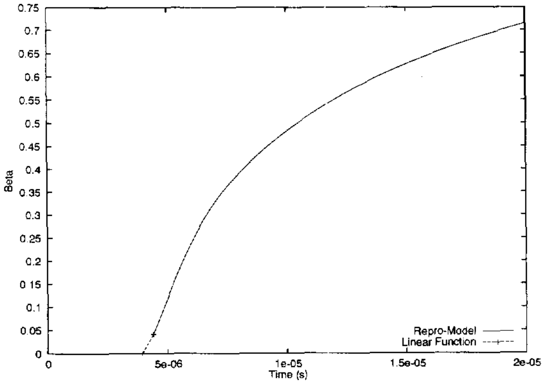

Fig. 2. Time history of a homogeneous combustion reaction modeled using the repro-model. The pressure is 3.0 atm and initial temperature 1600 K. The repro-model covers the range $0.0 < \beta < 0.96$. The range $0.0 < \beta < 0.04$ is modeled using a linear function of time which is tangent to the curve at $\beta = 0.04$.

It is not entirely straightforward to generalize this to a global model as the gradients of the linear functions depend upon the initial conditions. But there is an easily applicable way of incorporating these linear functions into a global induction parameter model. For each homogeneous combustion simulation performed for calculating the data points for the repro-model we follow the above procedure for producing the linear functions as given in Eqs. 9 to 11. We then use the linear functions to calculate additional data points in the region $0.04 > \beta > 0.0$. These data points are then included in the repro-model fitting procedure and a global model applicable at all points for $\beta < 0.96$ is constructed.

This procedure also gives us the values of the induction times from Eq. 12. These induction times are used as the data points in the construction of the parameterized model of the induction times. We have used polynomials for this parameterization and an example of an induction time model is given below where τ_i is the induction time, P the pressure in atmospheres, and T the temperature. The example is for pressures between 2.0 and 4.0 atm:

$$\begin{array}{ll}
\log(\tau_i) & =0.40232532 \times 10^{2} \\
-0.14024303\, T & +0.27390845 \times 10^{2} \log(P) \\
+0.16271496 \times 10^{-3}\, T^{2} & -0.64229296 \times 10^{-1}\, T \log(P) \\
-0.96842484 \times 10^{-7}\, T^{3} & +0.53500828 \times 10^{-4}\, T^{2} \log(P) \\
+0.10426885 \log(P)^{3} & +0.28796042 \times 10^{-10}\, T^{4} \\
-0.19704248 \times 10^{-7}\, T^{3} \log(P) & +0.45043245 \times 10^{-6}\, T^{2} \log(P)^{2} \\
-0.57000508 \times 10^{-3}\, T \log(P)^{3} & +0.21037739 \log(P)^{5} \\
-0.33934508 \times 10^{-14}\, T^{5} & +0.26533476 \times 10^{-11}\, T^{4} \log(P)
\end{array}$$

After following these procedures, we have now constructed a complete induction parameter model (for $\beta < 0.96$) and some representative results are given in Fig. 3. This shows the data calculated using the detailed reaction mechanism for a homogeneous simulation at 2.5 atm and with an initial temperature of 1500 K together with the data obtained from the same simulation using the IPM model.

APPLICATION OF THE INDUCTION PARAMETER MODEL IN REACTIVE FLOW SIMULATIONS

Having derived the parameterized model it is necessary to see if it will work within a reactive flow model, which it was ultimately designed to do. In this section we will first introduce the reactive flow code that we use. Then we describe some one-dimensional reflected shock simulations using this model with the full chemistry solution and with the IPM model. These seemingly simple one-dimensional simulations are actually a very good test of the model as they involve many different reactive flow phenomena including a transition to detonation and the propagation of detonation waves. We then use the IPM model within two-dimensional simulations of a shock wave interacting with a cuboid obstacle.

For both geometries the results obtained using the IPM model give remarkably good

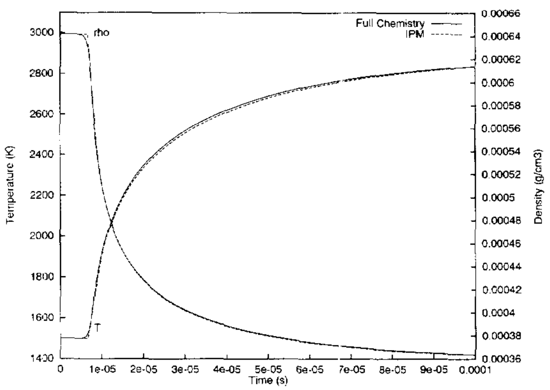

Fig. 3. Time histories of a homogeneous combustion reaction modeled using the full chemistry mechanism and the IPM model. The pressure is 2.5 atm and initial temperature 1500 K. The IPM covers the range $0.0 < \beta < 0.96$.

agreement with the results of the same simulations made using the full chemistry solution, but the IPM model requires only a fraction of the computational time.

A Description of the CFD Code

To model reactive flows we use a hydro-code named EDEN (Boulton [17], Milne [18]) which incorporates finite-rate nonequilibrium chemistry into a two-dimensional hydro-code. The complete time cycle is divided into different phases and the changes in the fluid variables due to only some of the terms in the hydrodynamic equations are then calculated in each phase. The changes in the variables over a whole time step are then found by summing the changes in each phase. The chemistry solution is thus a self-contained package and solved separately from the other routines. This means that we can easily incorporate different chemistry models into the reactive flow code.

The code solves the following reactive flow conservation equations:
Mass continuity:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) \tag{13}$$

Continuity of number density of species i, n_i (for each $i = 1, \ldots N$)

$$\frac{\partial n_i}{\partial t} = -\nabla \cdot (n_i \mathbf{v}) + \omega_i \tag{14}$$

where ω_i represents the chemical production (or loss) rate of the species i. For reasons outlined above, diffusion velocities have been ignored.
Momentum conservation:

$$\frac{\partial (\rho \mathbf{v})}{\partial t} = -\nabla \cdot (\rho \mathbf{v}\mathbf{v}) - \nabla \cdot P \tag{15}$$

where P is the pressure scalar.
Energy conservation:

$$\frac{\partial (\rho \epsilon)}{\partial t} = -\nabla \cdot (\rho \epsilon \mathbf{v}) - P\nabla \mathbf{v} - \nabla \cdot (q) + \Delta E \tag{16}$$

where ϵ is the specific internal energy and ΔE is the chemical energy released due to combustion. The last term is determined during the chemistry phase and added as a source term to the hydrodynamic phase. When full chemistry is being solved, the energy release is given by the difference in enthalpies due to chemical kinetics over the chemical time step (calculated at constant volume):

$$\Delta E_{\mathrm{kin}} = H_0(T_0) - H_1(T_0) \tag{17}$$

where T_0 is the temperature at the start of the time step. For the IPM model, ΔE_{kin} is replaced by ΔE_{ipm}, and α and β are advected with the fluid.

In the full chemistry solution routine, the change in mass fractions of the species and the energy released (or absorbed) as a result of the reactions are calculated. For the IPM solution, the energy released over the time step is calculated and the chemical species are updated as explained below. This is the first stage of the calculation. The initial chemistry time step is taken as the hydro time step determined from Courant conditions and is reduced if the energy release during this phase is too large. This revised chemistry time step then becomes the hydro time step. The energy released is then used as a source term in the second, Lagrangian phase, in which the velocity and energy are calculated based on acceleration effects due to pressure gradients. The final phase is a Van Leer advection phase, into which the species mass densities from the chemical phase are input and the momentum and energy are transported.

Chemical Species Approximations in the IPM Model

In the reactive flow code the pressure and temperature are not independent variables, but are calculated using the following thermodynamic relationships:

$$P = (\gamma - 1)\rho\epsilon \tag{18}$$

and

$$T = \frac{(\gamma - 1)\epsilon\bar{\mu}}{R}, \tag{19}$$

where ϵ is the internal energy. For the full chemistry solution the mean molecular weight $\bar{\mu}$ and the value of γ are calculated using the CHEMKIN (Kee et al. [14]) package as the mass fractions of the chemical species are known, being updated at the end of the chemistry phase.

In the IPM model we do not have information about the chemical species. However, we can make a simple, but useful approximation to the chemical species using the model as it stands. Information that is available is the initial gas mixture and the current mean molecular weight, which is given by:

$$\bar{\mu} = \frac{R\rho T}{P}. \tag{20}$$

At the end of any IPM time step, we know the values of the pressure, temperature, and density, so therefore we know the mean molecular weight of the mixture from Eq. 20.

From the initial mixture, we know how many moles of each element must be present in the mixture. If the initial mean molecular weight is μ_i, then we can produce a mixture with the correct mean molecular weight by combining stoichiometrically some of the fuel and oxygen to produce H_2O in the correct proportion.

For example, for an initial mixture of H_2, O_2, and Ar in the ratio 2:1:7 by mole fraction, the mean molecular weight of the initial mixture is given by:

$$\mu_i = 0.2W_{H2} + 0.1W_{O2} + 0.7W_{AR} \tag{21}$$

where W_K is the molecular weight of the species K. If the mole fraction of H_2O is $2X$, then

$$\mu = (0.2 - 2X)W_{H2} + (0.1 - X)W_{O2} + 2XW_{H2O} + (0.7 + X)W_{AR}. \tag{22}$$

The value of X can be calculated by using Eq. 20 so that the mean molecular weight at the end of an IPM time step is correct.

If we then use these chemical species values in the CHEMKIN routines for calculating γ, the values of γ will be very nearly the same as for the full chemistry solution. Failure to carry out this procedure leads to large errors in the predicted hydrodynamic motions.

One-Dimensional Reflected Shock Simulations

We have used the reactive flow code to simulate reflected shocks in a shock tube, using both the IPM and full chemistry submodels. The geometry for such a simulation is simple, having a single row of cells with a perfectly reflecting boundary at one end, but the range of dynamic behavior is wide.

To calculate the initial conditions, we specify the conditions in the unshocked gas and the Mach number of the incident shock, then we calculate the conditions behind the incident shock using the CHEMKIN package [14]. We then let most of the cells initially have the incident shock conditions, so that we are representing a shock that has almost reached the reflecting wall. At the other boundary we have inflow conditions that are continuous with the incident shock variable values.

For any of these simulations, where the temperatures and pressures behind the reflected shock are within the range of validity of the IPM model, the same general behavior is observed. At the reflecting boundary we observe an induction time, the duration of which depends upon the strength of the shock, followed by a rapid release of energy. This produces a sharp increase in pressure near to the wall which initiates a reactive wave which propagates away from the wall. This reactive wave rapidly catches up with and passes through the reflected shock front, then steepens into a detonation wave.

We have performed a number of these simulations for a variety of Mach numbers (the unshocked gas being at 300 K and 0.1 atm) and in each case the results are very similar for both

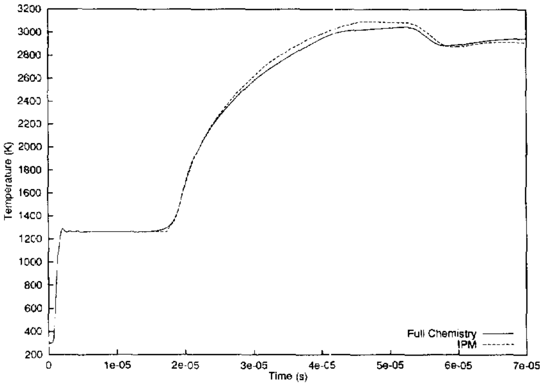

Fig. 4. The time histories of the temperature at the reflecting wall for one-dimensional reactive flow simulations using the full chemistry and the IPM models for the chemistry. These results are for an incident shock with Mach = 2.49.

the IPM and full chemistry models. The induction time and energy release at the reflecting boundary are always modeled well (as in Fig. 4). We would expect the IPM model to model this region well, as the conditions are very similar to a homogeneous combustion simulation. However, the transition to detonation and the propagation of the detonation wave, where conditions are far from homogeneous, are also modeled well (see Fig. 5). The computational time taken for the full chemistry model was 1 hr 7 min and the time for the IPM model was 3 min 50 s, using a DEC Alpha 3000 workstation. These one-dimensional models are a very good test of the accuracy and usefulness of the IPM model and the results are very encouraging.

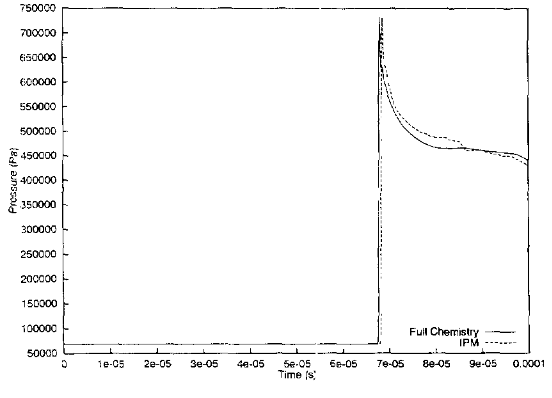

Fig. 5. Pressure time histories 49 mm from the reflecting wall for a shock of Mach = 2.49. The spatial resolution is 4 cells per mm.

Two-Dimensional Reactive Flow Simulations

We present here some results of two-dimensional simulations of shock interactions with a rectangular obstacle. This geometry has been chosen so that the results can be compared with experimental data produced at Aberystwyth (Sands et al. [15]). The gas mixture and range of validity of the IPM model described in this paper have also been chosen with these experimental results in mind.

Experimental Details

The shock tube used consists of three horizontal sections—a driver, buffer, and test section. The driver section is filled with helium up to 20 bar. The buffer section is filled with an inert gas mixture and allows the incident shock to stabilize before it enters the reactive test gas. The test section is 0.31 m long and 76 mm high. The test and buffer gases are matched acoustically so that the incident shock propagates from the buffer section into the test section without any changes in the transmitted pressure and velocity. The test and buffer sections have the same initial pressure and are separated by a slide valve, the valve being opened at the same time as the shock is initiated in the drive gas by the bursting of a diaphragm that separates the driver and buffer gases.

A cuboid obstacle of height 38 mm (half the tube height) and width 25 mm is placed in the test section, which produces a wide range of gas-dynamic conditions as part of the shock is reflected from the obstacle and part is diffracted around it.

Numerical Results

To model the above experimental setup, we just need to know the conditions in the unshocked test gas and the Mach number of the incident shock in this region. We can then calculate the conditions behind the incident shock and let these be the initial conditions to within a few cells of the reflecting wall. The obstacle boundaries and the upper and lower walls of the tube are modeled as perfectly reflecting surfaces. At the end of the test region where the shock enters, we prescribe inflow boundary conditions that model the incident shock.

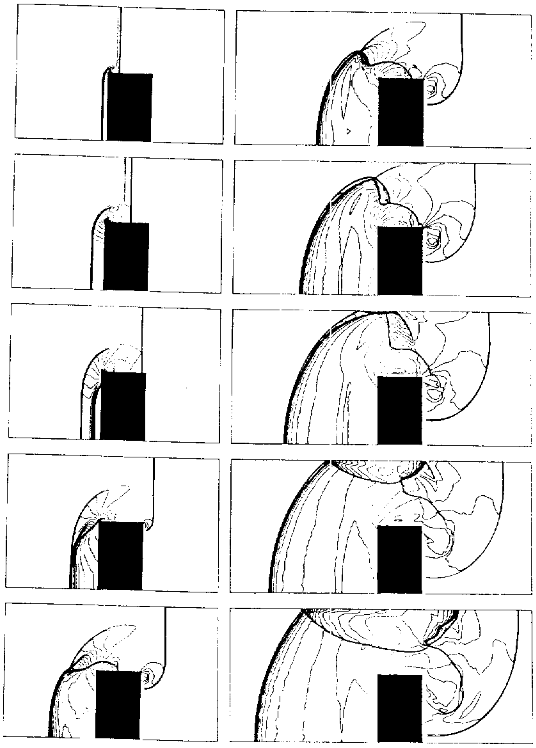

Fig. 6. Temperature contours showing the evolution of the system after the shock hits the obstacle for Mach 2.49. The shock hits the obstacle at 0/mus. The first contour plot is for a time of 10/mus and the time interval between each picture is 10/mus. The spatial resolution is 4 cells per mm.

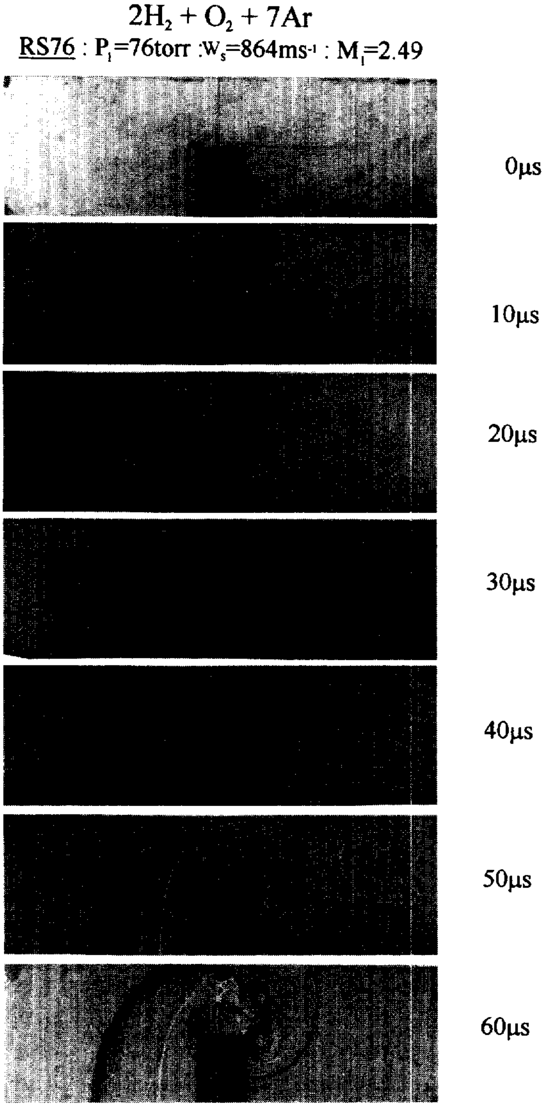

Fig. 7. Schlieren photographs obtained by Williams, Sands, and Thomas (Aberystwyth) of a shock of Mach 2.49 at 10-μsec intervals.

The evolution of the system for a simulation using the IPM model for the chemistry, with an incident shock of Mach 2.49, with an unshocked pressure of 0.1 atm and temperature of 300 K is shown in Fig. 6, where the resolution used was 4 cells per mm. We do not need to model the whole of the experimental test region, but can restrict ourselves to the central 200-mm section, to save computational time and reduce memory requirements.

The behavior observed in the simulation is the same as that seen in the experiments. After the shock hits the obstacle, the unrestricted upper part passes over the top of the obstacle and expands into the region behind it. The lower part of the incident shock is reflected by the obstacle. Conditions behind the reflected shock produce a reaction along the leading edge of the obstacle with an observable induction time. The subsequent reactive wave propagates outwards from the wall and steepens to form a detonation wave which passes through the reflected shock front and reflects form the upper surface of the tube.

The good agreement between these numerical results and the experimental results can be seen from photographs like those shown in Fig. 7. These Schlieren photographs clearly show that the reactive flow simulation incorporating the IPM model can model the physical behavior of the system to a remarkably high degree. More experimental results are described in [15]. The total computational time for the complete simulation was about 30 hr on a DEC Alpha 3000 workstation. Equivalent numerical results using the full chemistry solution would take weeks to produce on conventional computers, even for the relatively small chemical reaction mechanism required for hydrogen combustion reactions.

CONCLUSIONS

We have described a method for the formulation of a parameterized model for the description of shock-induced combustion reactions. The model is an induction parameter model which uses a repro-modeling approach for the energy release phase of the model. Such a model is derived by fitting algebraic functions (in this case high-order polynomials) to data calculated from homogeneous combustion simulations using complete chemical kinetic reaction mechanisms. The induction parameter model is computationally much faster to solve than a full chemistry system and provides a relatively simple, accurate and, above all, fast method to incorporate combustion reaction modeling into a reactive flow code.

We follow these methods to produce a model for the combustion of hydrogen under shock tube conditions for one initial mixture of hydrogen, oxygen, and argon. We use the resulting model in a reactive flow simulation of a shock over a rectangular obstacle. The results compare very well with experimental results.

Following these methods, we can construct similar parameterized models for the combustion of hydrocarbons, under a variety of conditions, using full chemistry models for the calculation of the data points, which would be extremely fast and easy to use in reactive flow models but would give accurate results, provided that the full reaction mechanism is a good model of the real physical system. For the hydrogen combustion model described in the paper, the IPM model was approximately 3 orders of magnitude faster to compute than the full chemistry model. For the combustion of hydrocarbons, where the chemical mechanism describing the reactions are usually larger than that for hydrogen (the hydrogen combustion mechanism usually being a subset of these mechanisms), even for reduced mechanisms, the increase in speed could be many times greater still. Following the methods described, similar models can easily be constructed for different mixtures under different conditions.

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