Computational Fluid Dynamics in Combustion

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ABSTRACT

Computational fluid dynamics has reached a stage where flow field in practical situation can be predicted to aid the design and to probe into the fundamental flow physics to understand and resolve the issues in fundamental fluid mechanics. The study examines the computation of reacting flows. After exploring the conservation equations for species and energy, the methods of closing the reaction rate terms in turbulent flow have been examined briefly. Two cases of computation, where combustion-flow interaction plays important role, have been discussed to illustrate the computational aspects and the physical insight that can be gained by the reacting flow computation.

Keywords: Computational fluid dynamics, CFD, combustion, composite solid propellant

1. INTRODUCTION

Computational fluid dynamics (CFD) has made a large impact in the understanding of basic fluid flows and in the design of aerospace vehicles and other industrial appliances. CFD has been extended to flows with combustion by solving addition conservation equations for individual species. The additional equations bring significant complications in tackling the problem. In the most basic level, it adds to the number of equations to be solved, an increase of a minimum of a few equations to several tens, or hundreds, of equations. The large heat release during combustion results in large gradients–both spatial and temporal. Chemical reactions bring in source terms which make the equations stiff and the time step required to solve the chemical reactions becomes orders of magnitude smaller than that for solving the fluid flow problem.

2. CONSERVATION EQUATIONS FOR REACTING FLOWS

The conservation equations of reacting flows are the same as those of the non-reacting flows except for the addition of species conservation equations with chemical source terms. The species conservation equations can be written as

$$\frac{\partial Y_i}{\partial t} + \nabla \cdot \varrho u Y_i + \nabla \cdot \mathbf{j}_i = \dot{w}_i''' \tag{1}$$

where Y_i is the mass fraction of the species i, j_i is the diffusive flux of the species i relative to the average mass flux of the fluid, and $\dot{w}_i'''$ is the production of species i due to the chemical reactions. The following constraints apply for the variables of Eqn. (1).

$$\sum_i Y_i = 1 \qquad \sum_i \mathbf{j}_i = 0 \qquad \sum_i \dot{w}_i''' = 0 \tag{2}$$

Summing up Eqn. (1) over all the species and using the constraints Eqn. (2) gives the continuity equation, which is the statement of the conservation of the total mass. The diffusive flux, $\mathbf{j}_i$, is evaluated using the Fick's law of diffusion, which for equal diffusivities of all the species, can be written as

$$\mathbf{j}_i = -\varrho D \nabla Y_i \tag{3}$$

The assumption of equal diffusivities have been made in most of the CFD calculations of multi-component fluids so far, except in one-dimensional computations[1]. Detailed discussion of the diffusive flux including the various effects of unequal diffusivities, pressure diffusion and thermal diffusion are given by Hirschfelder[1], *et al*.

The chemical source term, $\dot{w}_i'''$, is a strong function of temperature and the species concentration. The general expression can be written for a reaction of the $\sum_j v_{ij} A_j = \sum_j v'_{ij} A_j$, where A_j stands for the specie, j, and v_{ij} and v'_{ij} are the stoichiometric coefficients of the reactants and products respectively for the ith reaction. The reaction rate expression is given as

$$R_i = F_i \exp\left(-\frac{E_i}{RT}\right) T^{b_i} \prod_j c_j^{v_{ij}} \tag{4}$$

where R, T, c_j are the universal gas constant, temperature and concentration of jth specie respectively and F_i, b_i, E_i are constants for the particular reaction and are evaluated experimentally. A particular specie could be generated or

consumed in many reactions and the reaction rate of a particular specie can be written as

$$\dot{w}_k''' = \sum_i (v_{ik}' - v_{ik}) M_k R_i \qquad (5)$$

where M_k is the molecular mass of the kth specie. The source term introduced by the above equations make the conservation equations very stiff, and in general, the time step for solving the chemical source terms is several orders of magnitude smaller than that for the conservation equations of momentum and energy. Hence, the chemical reactions are solved as a set of ordinary differential equations taking a large number of fractional time steps for every time step used of the conservation equation. A stiff ODE solver is required for this step. The number of species and reactions in the combustion of a typical hydrocarbon is very large (several hundreds) and simplifying this involves finding minimum number of species and reactions that can represent overall progress of reactions satisfactorily. An extreme step in this direction is to use a single-step reaction between the fuel and the oxidiser to generate the products. In this case, the constants of the rate expression will not have general validity and the exponents of the concentrations in reaction rate expression of Eqn. (4) would not generally be the same as the stoichiometric coefficients, v_{ij}. Another method is the attempt to reduce the number reactions (and species) to a few (tens) by choosing the sensitive steps[2].

The energy equation written in terms of total energy remains unchanged between reacting multi-component fluid and non-reacting fluid. Neglecting potential energy of the fluid, the energy conservation equation can be written as

$$\frac{\partial \varrho(e + u^2/2)}{\partial t} + \nabla \cdot [\varrho u(e + u^2/2)] + \nabla \cdot (pu) + \nabla \cdot q + \nabla \cdot (u \cdot \tau) = 0 \quad (6)$$

The energy of the fluid at a given temperature, T, can be expressed in terms of enthalpy or internal energy as

$$h = \sum_i h_i Y_i \qquad h_i = \left\{ h_{i0} + \int_{T_0}^{T} c_{pi} dT \right\} \qquad e = h - p/\varrho \qquad (7)$$

where h_i is the standard heat of formation of the specie, i. The term, q, in Eqn. (6) is the flux of energy due to molecular transport, which for a multi-component fluid, can be written as

$$q = -\lambda \nabla T + \sum_i h_i j_i \qquad (8)$$

where λ is the thermal conductivity of the fluid. With the assumption of equal diffusivities for all the species and unity Lewis number, $Le \ (= D\varrho c_p/\lambda)$, the energy flux can be expressed using Eqn. (3) as

$$q = -\frac{\lambda}{c_p} \nabla h \qquad (9)$$

2.1 Handling Turbulent Flow

The Reynolds averaged Navier-Stokes equations are used to compute the mean flow variables in the case of non-reacting fluids. With reactions present and the consequent large temperature and density variations in the field, Favre (density weighted) averaging has advantage in reducing the number of terms to be modelled. The turbulent transport of energy and species are modelled using similarity among momentum, energy, and mass transport. However, there are situations in flow with combustion (e.g., premixed flames, discussed later) where the gradient transport is not obeyed. The Favre averaged equation of species conservation is

$$\frac{\partial \bar{\rho} \tilde{Y}_i}{\partial t} + \nabla \cdot \bar{\rho} \tilde{\mathbf{u}} \tilde{Y}_i + \nabla \cdot \overline{\rho \mathbf{u}'' Y_i''} + \nabla \cdot \bar{\mathbf{j}}_i = \bar{\dot{w}}_i''' \qquad (10)$$

The reaction rate term, being a nonlinear function of temperature and species concentrations, on averaging leaves unclosed terms that need to be modelled for solving the equations. Unfortunately, there are no universal models that can be applied to various situations even with approximate validity. The approach so far has been to use different models for pre-mixed and non-premixed flames. Of the two, the non-premixed flames has been more extensively studied because of its importance in a large number of practical applications. A detailed excellent review is provided by Veynante and Vervisch[3], but the methods are briefly described below.

2.1.1 Models for Turbulent Non-premixed Flames

The approach used in most models is to solve for one more conserved scalar and to obtain the species mass fraction using some assumptions on the reaction rate. The conserved scalar is a linear combination of the mass fractions chosen such that the reaction rate term vanishes. With equal diffusivities of the species, the equations for conserved scalars reduce to simple convection-diffusion balance with coupling only to the velocity field. Mixture fraction, defined as the fraction of one of the streams (usually fuel) in the fluid at any point within the domain, is one such conserved scalar extensively used in simulating the reacting non-premixed flows.

One of the earliest model for turbulent diffusion flames has been proposed by Spalding[4], called the eddy breakup model. This model assumes that the reaction takes place in thin zones, which occupy negligible fraction of the volume of the domain with the reaction rate limited by the dissipation time scale of the turbulent eddies. A related model was proposed by Magnussen and Hjertager[5] and the reaction rate can be expressed in terms of the rate at which the species are transported to the flame zone as

$$\bar{\dot{w}}_f''' = -\bar{\varrho} A \frac{\varepsilon}{k} \min \left(\bar{Y}_f, \frac{\bar{Y}_o}{s}, \frac{\bar{Y}_p}{1+s} \right) \qquad (11)$$

where f stands for fuel, o for oxidiser, p for products, s the stoichiometric oxidiser-to-fuel ratio, and k and ε the turbulent kinetic energy and dissipation, respectively, $\bar{\varrho}$ is the mean density and A is a model constant. This model has been used extensively for computation of turbulent flows. The single-step, finite rate chemistry has been accounted by taking the turbulent reaction time scale as the sum of chemical reaction time scale and the dissipation time scale[5].

This concept has been extended to the multi-step detailed chemistry assuming the reaction to be taking placing in a fraction of the volume of the fluid, which can be treated a stirred reactor and the mass exchange between the reacting fluid and the surrounding fluid being treated as that in the fast chemistry model.

Another model, which has been used extensively is the laminar flamelet model, proposed by Peters[6], in which it is assumed that the turbulent diffusion flame can be considered as an ensemble laminar diffusion flamelets. The laminar diffusion flamelet behaviour is assumed to be the same as that of a laminar counter-flow diffusion flame and is decided by the mixture fraction and the scalar dissipation rate. The conservation equation for mixture fraction is solved and the distribution of species is obtained from the stored flamet library and the assumed or computed probability distribution of the scalar dissipation rate and the mixture fraction.

The conditional moment closure (CMC) is another model proposed to model turbulent non-premixed flames[7-9]. The conditional mean of a variable such as the mass fraction of a specie, is defined as the mean of the variable at a given mixture fraction. The conservation equations of the conditional mean variables are solved over domain at different fixed values of the mixture fraction. The conditional averaging of the conservation equations introduces unclosed terms for which closure models have been proposed. It is assumed that the conditional mean of the reaction rate is the same as the reaction rate calculated with the conditional mean of the variables. The mean variables are obtained by averaging the conditional means over the mixture fraction space.

2.1.2 Pre-mixed Combustion Models

Unlike in non-premixed combustion, mixture fraction cannot be used in the case of pre-mixed combustion since the mixture fraction remains constant in the field. The reaction progress variable, which is essentially a normalised mass fraction of the deficient reactant, is sometimes used in its place; but this is not a conserved scalar. As in the case of non-premixed flames, many models utilise the laminar flame to characterise the fine structure of the turbulent flame.

The Eddy break up (EBU) model was one of the earliest models proposed for pre-mixed combustion[4] based on the consideration that the fluid at any instant is either completely unreacted or fully reacted mixture assuming that the flame thickness is very small. Under these conditions, the reaction rate is assumed to be mainly controlled by the mixing time scale, $\tau_t = k/\varepsilon$, and in terms of the fluctuations in the progress variable, the reaction rate of the fuel can be expressed as

$$\bar{w}_f''' = -C_{EBU}\,\bar{\rho}\,\frac{\widetilde{c''^2}}{\tau_t}$$ (12)

Under the assumption of thin flame, c can take only the values either 0 or 1, and hence, $\overline{\rho c''^2}$ can be shown to be equal to $\bar{\rho}\tilde{c}(1-\tilde{c})$.

Bray[10-12], et al. proposed a fairly comprehensive model for turbulent combustion, popularly known as BML model, and obtained expression similar to Eqn. (12) with a formal derivation with the assumptions clearly stated. The analysis stresses the presence of counter gradient of the scalars in pre-mixed flames.

Many models of turbulent pre-mixed combustion are based on flame surface density (FSD), defined as the flame surface area per unit volume. Based on the flame surface density, the reaction rate can be expressed as

$$\bar{w}''' = \rho_0 S_L \Sigma$$ (13)

where Σ is the flame surface density, S_L the laminar flame speed, which could be modified by stretch effects, and ρ_0 is the density of the unburnt mixture. Methods vary depending on the method of determining Σ, In BML model, an algebraic expression for Σ is used to obtain the expression for $\bar{w}'''$. A conservation equation for flame surface density can be written in the form

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\mathbf{u}\Sigma) = \nabla \cdot \left(\frac{\nu_t}{\sigma_\Sigma} \nabla \Sigma \right) + S_1 + S_2 - D$$ (14)

where ν_t is the turbulent viscosity, σ_Σ is the flame surface turbulent Schmidt number, S_1, S_2 are the source terms due to strain rate acting on the surface and induced by the surface, the strain rate due to turbulent motion, respectively and D describes consumption of flame area. These production and destruction terms need to be modelled and several closure terms are proposed by various authors[13,17]. These models have been used for computing flows in IC engines and in closed vessels[14,18].

3. APPLICATION OF CFD TO REACTING FLOW COMPUTATIONS

Computation of reacting flows have been made extensively in the last two to three decades. A range of applications from low-speed to high-speed flows have been computed using the methods discussed in the earlier sections. In this section, some examples of computation of reacting flows have been discussed to illustrate the various aspects discussed above. In particular, those cases which provide significant physical insight from the computational results have been chosen.

3.1 Combustion of Composite Solid Propellants

The composite propellants essentially consists of a crystalline oxidiser embedded in a polymeric fuel. The size of particles of propellants are of the order of about 100 m and the spaces between the oxidizer particles are filled with the polymeric fuel. There are other additives in the propellant; but these are not considered at present. To understand the behaviour better, a two-dimensional analogue of the propellant has been experimentally investigated in the literature[19,20]. A schematic of this is shown in Fig. 1.

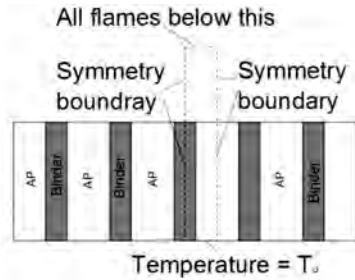The sandwich propellant consists of a series of slabs

Figure 1. Schematic of the sandwich propellant along with the computational domain.

of polymeric fuel and ammonium perchlorate (AP), a commonly used solid oxidiser. Ammonium perchlorate-burns as a mono-propellant without any fuel above a pressure of 20 bar, but gets quenched below this pressure, known as the low-pressure deflagration limit (LPDL). With the addition of fuel, the burning rate behaviour of the propellant becomes different from that of pure AP. There are many experimental observations regarding the burning behaviour of this propellant, which remained unexplained before the CFD analyses were made on the burning propellant[21]. The typical dimensions of the binder and AP thickness are about 20 μm and 200 μm respectively. The flow in the vicinity of the propellant remains laminar. There are mainly three types of flames on the propellants of this kind[22]: the decomposition flame close to the AP surface, the primary diffusion flame near the interface between the AP and the fuel between the fuel vapour and the pyrolysis products of AP, and the final diffusion flame between the fuel vapour and the products of AP decomposition flame.

The computational domain includes both the gas and the condensed phases. The interface evolves during the computation because of the evaporation of the surface due to the decomposition of the solid and the heat transfer from the gas. The problem is inherently unsteady and there is a large difference between the time scales of the condensed phase and the gas phase. This difference in time scales causes unstable behaviour in the system and can cause spontaneous quenching of the propellant for certain combinations of properties. It was observed during the initial phase of the computations that the values of the surface pyrolysis parameters, which have been considered well-known and standard for several decades, were in the unstable regime, and hence, not correct. This observation could be made because of the computations with both condensed phase and the gas phase in the unsteady mode. Though the stability boundaries were known for a long time[23], the pyrolysis properties were proposed without verifying the validity of these from stability considerations.

Several other interesting results also were obtained from these computations.

Figure 2 shows the temperature and the reaction rate contours of various reactions at two pressures namely, 1.4 MPa and 2.1 MPa. These two pressures were chosen because these are below and above the LPDL of AP respectively. The reaction rate contours show the regions where the

three reactions are taking place. As can be seen, at pressure above LPDL, the primary diffusion flame is very small; but its importance becomes large at low pressure since the burning rate of AP becomes low and the surface dips significantly at the fuel-AP interface because of the heat released in the primary diffusion flame. The temperature contours also show the variation in flame structure with pressure. At high pressure, the fuel surface protrudes above the AP surface and vice-versa at low pressure. This feature was observed experimentally earlier and with the computations, prediction of several observations became possible.

3.2 Combustion in IC Engine Cylinder

The computation of flow in an IC engine cylinder throws up several challenges. The computational domain is continuously changing due to the movement of the piston, and the change in volume from the bottom to top dead centre is very large. This cause the mesh quality to become bad with the piston movement. Figure 3 shows the computational domain and the grids before the ignition. The flame surface density model with the source terms being computed using the model proposed by Candel and Poinsot[24] was used to model the chemical reactions. The modifications were required because the proposed model had a constant length scale and the length scale was changing significantly in the present case. Turbulence was modelled using the k-ε model. The computations were made using CFX-10 software.

The predicted p-θ curves at an ignition advance of 12° along with the fringe plot of product mass fraction is shown in Fig. 4.

The product mass fraction shows how the flame is spreading within the chamber after the ignition. The ignition process was not properly modelled and hence it was necessary
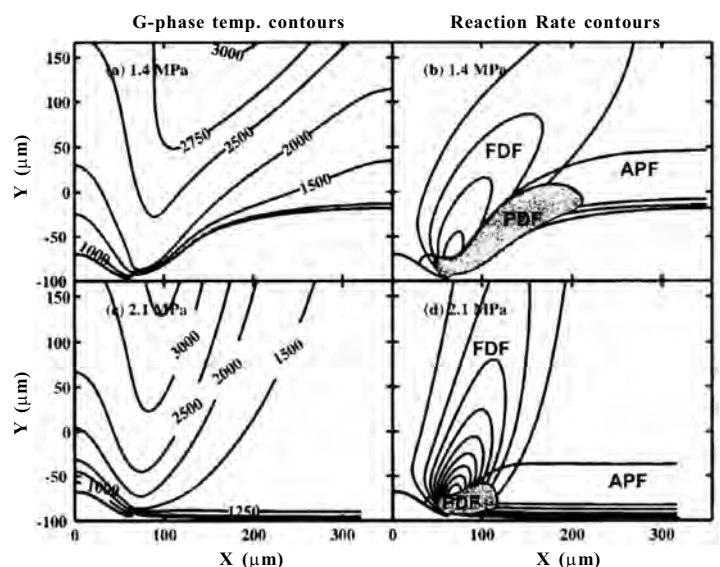

Figure 2. Temperature and reaction rate contours in the gas phase of burning sandwich propellant at two pressures.
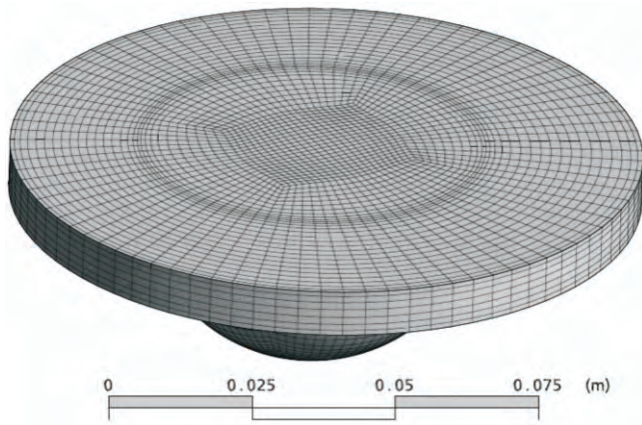
Figure 3. **Computational domain when the piston is near the top dead centre before ignition.**
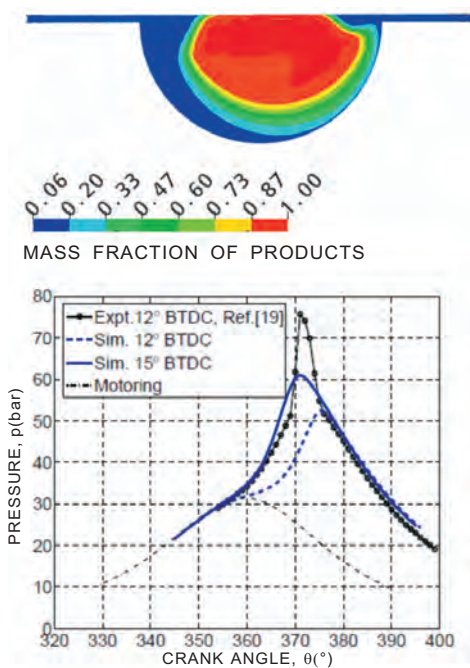

Figure 4. **Distribution of products in the cylinder at 5° after top dead centre and the p-θ curve obtained by computation and from the experiment.**

Figure 5. **Flow distribution inside the cylinder at different instances: comparison between motoring without ignition and with ignition. (a) & (b) θ = 5° BTDC, and (c) & (d) θ = 5° ATDC). Spark is at 12° before TDC.**

to provide a 3° advance for the ignition in the computation compared to the experiments in order to predict the pressure rise reasonably. However, even then, the peak pressure could not be predicted accurately and it was inferred that there could be spontaneous end gas ignition in the experiments, which was also inferred from the large $dp/d\theta$ values observed in the experiments.

Interesting insights into the flow field could also be obtained from these computations. Since the piston has a bowl, during the compression stroke, as the piston approaches the top dead end (TDC), the fluid from the sides flows into the bowl and is known as squish flow. During the expansion process when the piston is moving away from the TDC, the fluid from the bowl region moves to the 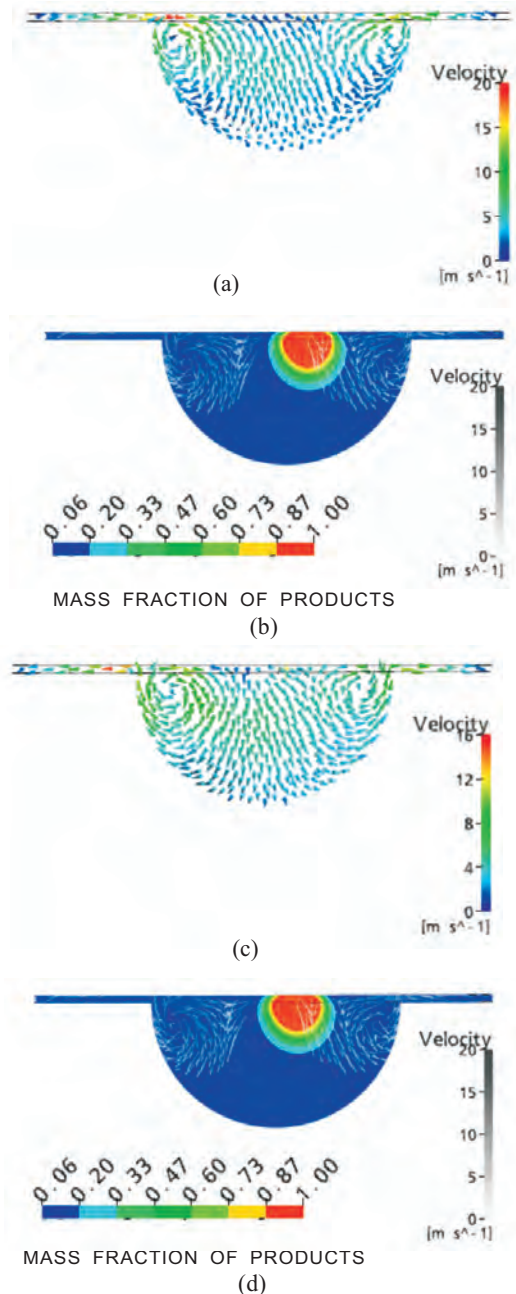sides and this flow is known as the reverse-squish flow. The flow field during motoring, when there is no burning, and with ignition at −12° from TDC are shown in Fig. 5 for comparison.

The product mass fraction distribution is also shown in the figures in the case with ignition and flame position can be seen from the distribution of the products. The flow distribution is not affected significantly at 5^0 before TDC since flame is still small. During the reverse-squish period, the flow velocity is significantly increased, the maximum velocity ratio reaching a value of 2.3 at about 8° after TDC. This causes significant distortion of the

flame shape from spherical and increases the speed of propagation of the flame. The reverse effect is possible at lower ignition advance.

4. CONCLUSION

The study has briefly looked into the issues in computing reacting flows and has examined some of the methods used for closing the reaction rate term in the conservation equation for turbulent flows. The computation of reacting flow is reasonable matured and most commercial CFD codes currently come with several of the reaction rate closure model in-built. Two-phase flow with liquid injection is an important field in combustion; but this has not been examined in this study

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