

Conditional Moment Closure Modelling for Ignition in Thermally Stratified *iso*-octane/air Mixtures

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Abstract

This paper presents a premixed combustion model based on the first order conditional moment closure (CMC) method for simulation of combustion of *iso*-octane, which is a single stage-ignition hydrocarbon fuel under homogeneous charge compression ignition (HCCI) conditions. The model is implemented into the open source C++ computational fluid dynamic (CFD) code known as OpenFOAM. To evaluate the performance of the CFD-CMC solver, a set of direct numerical simulation (DNS) data is used. The data set includes five cases featuring ignition of thermally stratified *iso*-octane/air mixtures with a mean temperature of 1035 K. The effects of variation of initial temperature fluctuations, turbulence intensity and integral length scale are studied. It is shown that the results from the CFD-CMC solver are in excellent agreement with the DNS for cases in which a low level of conditional fluctuations is present. However, a higher level of these fluctuations leads to an increased deviation of the predicted peak heat release rate and ignition delay time from those of the DNS. A transport equation for the conditional variance is also derived for premixed combustion under HCCI conditions. Assessment of the conditional variance equation using the DNS data shows that correlation between dissipation and conditional fluctuation and correlation between reaction and conditional fluctuations are the dominant sources of conditional fluctuations in the case with a thermal-stratification level of 60 K.

Introduction

Homogeneous charge compression ignition (HCCI) is a fairly recent engine technology developed to alleviate combustion emissions and improve combustion efficiency. In an HCCI engine, a homogeneous mixture of air and fuel, and possibly some combustion products autoignites due to a high compression ratio providing a high diesel-like efficiency with a low level of NO_x and soot emissions. In spite of these favourable features of HCCI, it presents some challenges such as difficulties in controlling the auto-ignition timing and the high rate of heat release and pressure-rise [6]. As reported in the literature, thermal stratification of the charge can spread out the heat release rate profile and therefore reduces the pressure rise rate [6, 11].

From the DNS studies, two combustion modes were found under HCCI conditions; deflagration and spontaneous ignition. In the deflagration mode, importance of molecular transport (diffusion and convection) becomes significant in comparison with

reaction whereas the spontaneous mode presents simultaneous ignition event in which the role of molecular transport is negligible [3, 14, 15]. The DNS were used demonstrated that the deflagration mode was predominant in cases with large thermal stratifications whereas spontaneous combustion mode was found to be prevailing in cases with a low level of temperature inhomogeneities. DNS is able to provide a detailed understanding of ignition characteristics under HCCI conditions while it is not computationally affordable.

HCCI-like conditions have been modelled using various methods such as multi-zone model [1], flamelet-based approaches [4], the G-equation model combined with a multi-zone approach [5], advanced tabulation model [9] and the probability density function (PDF) method [2].

Conditional moment closure (CMC) model was also used to simulate HCCI conditions [10]. A set of transport equations for the conditional moments of some reactive scalars are solved in the first order CMC model. In this method, conditional fluctuations are assumed to be negligible. The choice of a scalar as a conditioning variable in which the fluctuations of species mass fraction and temperature are mainly associated to the scalar fluctuations is a crucial task. Mixture fraction indicating the fuel/oxidiser ratio, is usually chosen as a conditioning variable in non-premixed combustion [8]. However defining a conditioning variable in premixed flames have been found challenging. It is very case dependent and has been defined based on the sensible enthalpy, temperature and fuel or product mass fraction. One of the key challenges for premixed combustion CMC is that with these choices of conditioning variable, it becomes difficult to specify the scalar dissipation rate and the conditioning variables PDF, due to the appearance of thin flamelets.

On the other hand, in HCCI, as discussed in the literature, temperature fluctuations in HCCI engines is about 10-15 K [6] in which HCCI conditions, the spontaneous combustion is the predominant mode and flamelets are less prevalent [3, 15]. Therefore, the combustion process is mainly controlled by thermochemical state prior to ignition. In this situation, total enthalpy can be used as a conditioning variable. Although total enthalpy involves a source term, it spatially fluctuates only by compressible effects, which are small away from knocking conditions.

In this paper our CMC-based model [10] is applied for cases in which ignition occurs in a single stage, i.e. *iso*-octane/air mixtures [15]. In order to better understand the sources of con-

ditional fluctuations, we also developed the second conditional moment equations in the context of premixed combustion which is not reported in the literature to the best of our knowledge but could ultimately be used in a second order closure. The contribution of the source terms are then investigated under different conditions.

Conditional Moment Closure

To obtain the CMC equations, a normalised scalar variable is defined as:

$$\theta(x, t) = \frac{h(x, t) - h_{min}(t)}{h_{max}(t) - h_{min}(t)}, \quad (1)$$

where h is enthalpy and h_{min} and h_{max} correspond to minimum and maximum enthalpies in the computational domain, respectively. The conditionally Favre-averaged mass fraction of species α , Y_α , as a function of conditioning variable at time t and location x is then defined as:

$$Q_\alpha(\xi; x, t) = \langle Y_\alpha |_{\theta=\xi} \rangle = \frac{\overline{\rho Y_\alpha(x, t) |_{\theta=\xi}}}{\overline{\rho |_{\theta=\xi}}}, \quad (2)$$

where ρ is the density and ξ is the sample space for normalised enthalpy. The symbols $\overline{(\cdot)} |_{\theta=\xi}$ and $\langle (\cdot) |_{\theta=\xi} \rangle$ refer to the conditional mean and the Favre-conditional mean, respectively. Using the above definition, the species mass fraction equations, can be recast into a set of CMC transport equations. As discussed in Ref. [10], under the assumption of statistically homogeneous cylinder charge, the spatial terms in the physical space are also ignored and conditional mass fractions with high Reynolds assumption then evolve as:

$$\frac{\partial Q_\alpha}{\partial t} = -v_\xi \frac{\partial Q_\alpha}{\partial \xi} + \langle N |_\xi \rangle \frac{\partial^2 Q_\alpha}{\partial \xi^2} + \langle \dot{W}_\alpha |_\xi \rangle, \quad (3)$$

where $\langle \dot{W}_\alpha |_\xi \rangle$ is defined as $\frac{\overline{\dot{\omega}_\alpha |_\xi}}{\rho |_\xi}$ where $\dot{\omega}_\alpha$ is the reaction rate for species α . The scalar dissipation rate, N , is $D \frac{\partial \theta}{\partial x_j} \frac{\partial \theta}{\partial x_j}$ where D is the molecular diffusivity, which is assumed to be equal to the thermal diffusivity. The convective velocity, v_ξ , in the ξ -space is equal to $\langle S_\theta |_\xi \rangle$ where the term S_θ results from the source term of normalised enthalpy, defined as:

$$S_\theta = \frac{1}{h_{max} - h_{min}} \left(\frac{1}{\rho} \frac{Dp}{Dt} - (1 - \theta) \frac{\partial h_{min}}{\partial t} - \theta \frac{\partial h_{max}}{\partial t} \right), \quad (4)$$

where p is the pressure. The conditional reaction rates can be obtained using the first order CMC approximation [10],

Numerical Methods and Test Cases Studied

The open source C++ code known as OpenFOAM was employed to implement the CMC model presented in the previous section. The CFD code implicitly solves the governing equations including continuity, momenta and enthalpy equations for a compressible flow using a pressure-implicit with splitting of operators (PISO) algorithm to treat the pressure-velocity coupling. After advancing the CFD code in time, the conditional scalars are calculated in the conditioning variable space using an efficient search algorithm. In the next step, the conditional mass fraction equations, equation (3), are implicitly solved using an operator splitting method [13] which leads to two sets of equations: non-stiff equations including the progress of diffusion and convection and stiff ones including the progress of chemical reactions which are a set of ordinary differential equations (ODE). Semi-implicit Bullirsch-Stoer (SIBS) method is employed for solving the ODE. After solving equation 3, the

Favre-averaged species mass fractions on the CFD grid are obtained using an assumed Dirac-delta PDF for enthalpy. This is possible in the present case because the flow is deliberately resolved to a DNS level in terms of the conditioning variable, in order to focus only on the effects of the conditioning and not on the models for scalar dissipation and the conditioning variable PDF. (Of course, this approach is not affordable in a real engine.) More details of the numerical methods can be found in Ref. [10].

A set of DNS data including ignition of *iso*-octane/air mixtures with thermal stratifications in a constant volume were used to examine the performance of the CFD-CMC solver [15]. A 99-species reduced chemical mechanism [15] was employed in both DNS and CMC. All the DNS cases were initialised with a uniform mixture composition field with an equivalence ratio of 0.3 and an initial uniform pressures of 20 atm. As shown in table 1 [15], five cases with the mean temperature of 1035 K and temperature fluctuations of 15-60 K were considered. The homogeneous ignition delay time, $\tau_{ig,0}$, corresponding to the mean temperature is 2.5 ms [15].

A uniform two-dimensional CFD grid of 160×160 was employed for all cases, compared with the DNS grid of 640×640. The CMC domain included 101 equally spaced grid points. The time-step used in the CFD-CMC solver was 2.5 μ s while the DNS time-step was 2.5 ns. The initial and boundary conditions for the CFD-CMC were the same as the DNS cases.

Case	T' (K)	u' (m/s)	l_e (mm)	Er.(HRR) %	Er. (τ_{ig}) %
1	15	0.5	1.25	1.1	0.40
2	30	0.5	1.25	2.61	0.20
3	60	0.5	1.25	9.70	12.5
8	15	2.5	1.25	0.64	1.20
9	15	0.5	0.25	1.96	1.23

Table 1. Physical parameters of the DNS and CMC cases and error percentages of peak heat release and ignition delay time.

Results

Figure 1 presents the mean heat release rate and pressure versus time obtained from the CFD-CMC solver in comparison with the DNS data. Time is normalised by the homogeneous ignition delay time of 2.5 ms. As can be seen, the CMC model predicts the ignition delay time and the peak heat release rate with good accuracy for cases with $T' = 15$ and 30 K whereas for the case with a high level of temperature inhomogeneities (case 3 with $T' = 60$ K), the agreement is not as good as the other cases (but still reasonable).

Figure 2 presents error percentage of the peak heat release rate and ignition delay time versus T' for all cases in comparison with the DNS results. The errors are also shown in table 1. It can be seen that the error percentage of both peak heat release rate and ignition delay time is less than 3% for cases with $T' = 15$ and 30 K while case 3 with the highest temperature fluctuation has maximum errors of peak heat release rate (9.7%) and ignition delay time (12.5%).

It is also observed that case 8 exhibits a lower error value for the peak heat release rate compared with case 1. The only difference between these two cases is that case 8 has a larger u' . As discussed in Ref. [15], turbulence has a key role to homogenise the mixture. Therefore, a higher level of homogenisation in case 8 leads to a less error percentage in prediction of the peak heat release rate. Comparison of cases 9 and 1 shows worse agreement for case 9 with a lower initial l_e which has a

shorter turbulence time scale. This may at first seem counter-intuitive. However, as discussed by Yoo et al [15], since l_e in case 9 is smaller than the length scale of temperature fluctuations, a higher level of mixture homogenisation for the mixture is not achieved. Therefore, a better agreement for case 9 is not expected although it has a shorter turbulence time scale.

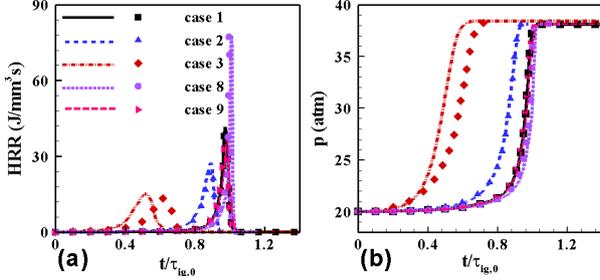


Figure 1. Temporal evolution of the a) mean heat release rate and b) pressure obtained using CFD-CMC solver (lines) in comparison with DNS (symbols).

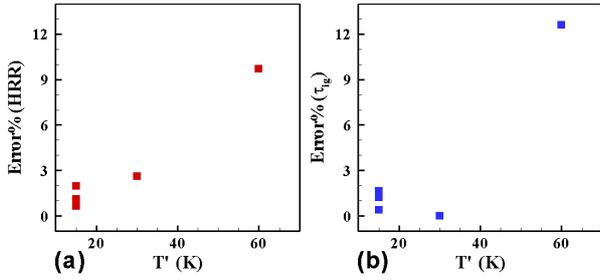


Figure 2. Percentages of error for prediction of a) maximum of mean heat rate and b) ignition delay time.

As discussed in Ref. [15], the deflagration mode of combustion is predominant in case 3 with $T' = 60$ K. In our previous work [10], it was shown that conditional fluctuations became significant due to importance of deflagration mode in cases with large thermal stratifications. It was also discussed that dissipation rate fluctuations generated conditional fluctuations which in turn caused a breakdown of the first order closure hypothesis. To further investigate the cause of the conditional fluctuations, the conditional expectations of the second moments of reactive scalars [8] are considered in the following. The conditional covariance $G_{\alpha\beta}$ of species α and β is defined as $G_{\alpha\beta} = \langle K_{\alpha\beta} | \xi \rangle$ where $K_{\alpha\beta} = Y''_{\alpha} Y''_{\beta}$. The variable Y''_{α} is the conditional mass fraction fluctuation of species α and is defined as $Y''_{\alpha} = Y_{\alpha} - \langle Y_{\alpha} | \xi \rangle$. The conditional covariance/variance equations for non-premixed combustion were investigated in the literature [8, 12, 7], however, to the best of our knowledge the conditional covariance/variance equations for premixed flames has not been reported. Here, an equation for the conditional variance, $G_{\alpha\alpha}$, using the decomposition method [8] with the assumption of statistically homogeneous charge is derived from equation (3). By neglecting the spatial derivatives, the equation for the conditional variance may be written as follows,

$$\begin{aligned} \frac{\partial G_{\alpha\alpha}}{\partial t} &= \langle N | \xi \rangle \frac{\partial^2 G_{\alpha\alpha}}{\partial \xi^2} - \langle S_{\theta} | \xi \rangle \frac{\partial G_{\alpha\alpha}}{\partial \xi} \\ &+ 2 \langle \dot{W}_{\alpha}'' Y''_{\alpha} | \xi \rangle + 2 \langle N'' Y''_{\alpha} | \xi \rangle \frac{\partial^2 Q_{\alpha}}{\partial \xi^2} \end{aligned}$$

$$- 2 \langle S_{\theta}'' Y''_{\alpha} | \xi \rangle \frac{\partial Q_{\alpha}}{\partial \xi}, \quad (5)$$

where $(\cdot)'' = (\cdot) - \langle (\cdot) | \xi \rangle$. The source terms in equation (5) consist of $2 \langle \dot{W}_{\alpha}'' Y''_{\alpha} | \xi \rangle$ representing the correlation between reaction rate and mass fraction fluctuations, $\langle N'' Y''_{\alpha} | \xi \rangle \frac{\partial^2 Q_{\alpha}}{\partial \xi^2}$ representing the correlation between dissipation rate and mass fraction fluctuations and $-2 \langle S_{\theta}'' Y''_{\alpha} | \xi \rangle \frac{\partial Q_{\alpha}}{\partial \xi}$ representing the correlation between source term in conditioning variable equation and mass fraction fluctuations.

All terms on the right hand side of equation (5) for fuel mass fraction variance obtained from the DNS data are presented at different instants in figure 3. The derivatives with respect to ξ appeared in equation (5) are obtained by fitting a ninth-order polynomial to the appropriate conditional mean and covariance. Swaminathan and Bilger [12] showed that this method was able to capture the derivatives accurately.

It can be seen that the source term due to $\langle S_{\theta}'' Y''_{\alpha} | \xi \rangle$ is small at all instants. The contribution of the convective term, $\langle S_{\theta} | \xi \rangle \frac{\partial G_{\alpha\alpha}}{\partial \xi}$, is also insignificant, hence S_{θ} representing the effects of the temporal evolution of pressure in the normalised enthalpy domain, does not have any role to generate conditional fluctuations. The importance of the diffusion term, $\langle N | \xi \rangle \frac{\partial^2 G_{\alpha\alpha}}{\partial \xi^2}$, is also found to be minor in comparison with the source terms, $\langle \dot{W}_{\alpha}'' Y''_{\alpha} | \xi \rangle$ and $\langle N'' Y''_{\alpha} | \xi \rangle \frac{\partial^2 Q_{\alpha}}{\partial \xi^2}$.

As can be seen, not surprisingly, at early stages of ignition, all terms are small while at later stages they become substantial. It can be seen that from $t/\tau_{ig} = 0.3$ to $t/\tau_{ig} = 0.8$, the source terms become considerable for a wider range of normalised enthalpies. It is interesting to note that as the peak of the source terms move from the region of high to low enthalpies, source terms appear in a wider region in the enthalpy domain. This can be due to the increasing contribution of the deflagration mode as the flame propagates into the unburned region. Once deflagrations appear, they can propagate in directions which are not necessarily aligned with the conditioning variable, thus generating more conditional fluctuations. Another point to note is that the terms never balance across the whole of the enthalpy space, suggesting that transport equations would need to be solved for the conditional second moments rather than attempting to devise an algebraic model from a balance of modelled source terms.

It is also demonstrated that the term due to N -fluctuations acts as a sink (positive values) in regions with low enthalpies while it acts as a source in regions with high enthalpies; for instance, at $t/\tau = 0.8$ about $\xi = 0.45$. It should be noted that the correlation between conditional dissipation and mass fraction fluctuations, $\langle N'' Y''_{\alpha} | \xi \rangle$, embedded in this term is negative across all enthalpies (not shown here). Therefore, the second derivative, $\frac{\partial^2 Q_{\alpha}}{\partial \xi^2}$ should be negative and positive for $\xi < 0.45$ and $\xi > 0.45$, respectively. A similar trend for the second derivative, $\frac{\partial^2 Q_{\alpha}}{\partial \xi^2}$, was also found in Ref. [4] for a thermally stratified H_2 /air mixture. This term therefore transports conditional fluctuations from burned to igniting regions. On the other hand, $\langle \dot{W}_{\alpha}'' Y''_{\alpha} | \xi \rangle$ acts more prevalently as a production term, but also tends to destroy fluctuations in the burned gases. It can be seen that the terms due to $\langle \dot{W}_{\alpha}'' Y''_{\alpha} | \xi \rangle$ and $\langle N'' Y''_{\alpha} | \xi \rangle$ are respectively the most and second most dominant terms in equation (5), in particular at later stages of ignition.

Conclusions

The CMC model presented in Ref. [10] was applied to a set of DNS data featuring thermal stratifications in a lean *iso*-octane/air mixture. The results for the cases with $T' = 15$ and 30 K show an excellent performance of the CFD-CMC solver while the results for case 3 with $T' = 60$ K show a reasonable

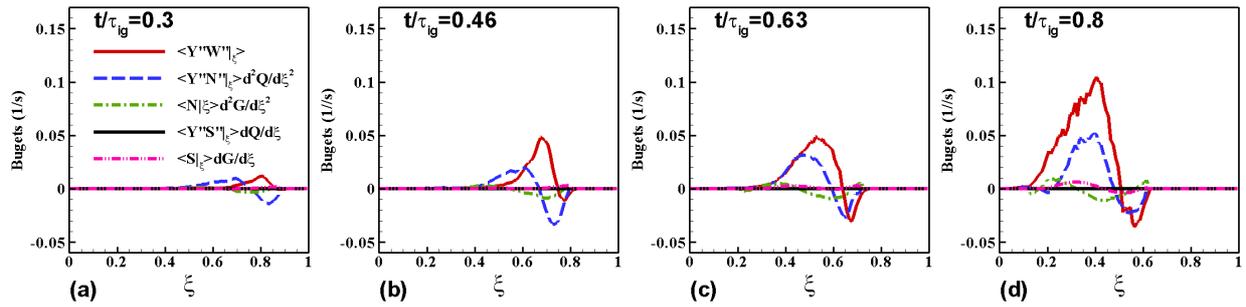


Figure 3. Balance of terms in conditional variance equation (5) for case 3 with $T' = 60$ K at $t/\tau_{ig} = 0.3, 0.46, 0.63$ and 0.8 .

accuracy of the CMC model. Case 3 ($T' = 60$ K) with the highest level of temperature fluctuations, presented maximum percentage of error for the peak heat release rate and the ignition delay time.

To investigate the cause of conditional fluctuations, the transport equation for the conditional variance was derived and studied using the DNS data. The source term due to the correlation between mass fraction and dissipation rate fluctuations and the source term due to the correlation between mass fraction and reaction rate fluctuations were found to be the cause of significant conditional fluctuations in case 3 which has a large thermal stratification level.

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