Assessment of conditional moment closure for ignition in compositionally and thermally stratified mixtures

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Abstract

A conditional moment closure (CMC) model is developed to simulate auto-ignition in compositionally and thermally stratified mixtures. The performance of the CMC model is examined in *a priori* and *a posteriori* manners. Two-dimensional direct numerical simulations (DNSs) are performed to generate the data required for *a priori* and *a posteriori* tests. The DNS cases simulate the conditions similar to a stratified charge compression ignition (SCCI) combustion mode with compositionally and thermally stratified *n*-heptane/air mixtures in a constant volume. The cases feature two different levels of stratification with three mean temperatures. The CMC model is implemented into an open source computational fluid dynamics (CFD) package known as OpenFOAM®. The CMC solver is used to simulate the DNS cases using exactly the same initial conditions as the DNS data.

An excellent agreement between the CMC solver and DNS is observed for the cases with low levels of stratification, whereas deviations from DNS are observed in cases which exhibit high level of stratifications. *A priori* analysis reveals that the reason for disagreement is failure of the first-order closure hypothesis in the CMC model. It is also shown that in the cases with a high level of stratification, even the second-order estimation of the reaction rate source term cannot provide a reasonably accurate closure. Double conditioning using mixture fraction and sensible enthalpy, however, provides an accurate first-order closure to the reaction rate source term. A detailed analysis of the DNS data suggests that conditional fluctuations of temperature lead to the breakdown of the first-order closure when a single conditioning variable is used.

1 Introduction

Homogeneous charge compression ignition (HCCI) engines have shown a great potential for achieving high-efficiency with low level of pollutant emissions; however, the main challenge is how to address the large pressure rises caused by homogeneous-like ignition in such engines. One solution is to introduce inhomogeneities in the mixture, commonly referred to as stratification. The stratification may involve temperature and/or composition of the charge [1, 2]. This has motivated a vast body of work in the literature to understand the ignition mechanism in stratified mixtures, e.g. [3-7]. Direct numerical simulation (DNS) is a means that can provide a detailed understanding of the ignition mechanism in such mixtures since all time and length scales are fully resolved. However, considering this level of resolution, simulating a real engine is by far out of reach for DNS. This makes other simplified and inexpensive modelling approaches more attractive.

Conditional moment closure (CMC) is one of the alternatives to DNS. This method was originally developed for non-premixed flames, and extensively validated for such flames [8]. The extension to premixed flames, however, is arguably scarce in the literature [9]. In non-premixed applications of CMC, mixture fraction is usually taken as conditioning variable, while in premixed CMC, a wider variety of conditioning scalars have been proposed [10]. Stratified HCCI, moreover, is neither categorised neatly under non-premixed nor premixed combustion. Given that the charge in HCCI

combustion is nearly homogeneous, it tends to ignite almost simultaneously. Upon ignition, the charge burns rapidly which leaves almost no time for mixing between unburned, burning, and burned regions. Consequently, it is expected the combustion behaviour mainly depends on the thermo-chemical state prior to ignition. Therefore, if an appropriate choice of conditioning variable is made to represent the initial state, conditional fluctuations during burning are expected to be negligible.

In the present study, the performance of the CMC model is investigated for cases featuring ignition in thermally and compositionally stratified mixtures. Six two-dimensional (2D) cases of lean *n*-heptane/air mixtures with two levels of stratification and three mean temperatures are set up. Local temperatures and species are specified as a function of mixture fraction. As a result, all scalars are *initially* a function of mixture fraction only, suggesting that mixture fraction would be a natural choice for conditioning scalar. The CMC model is then investigated in *a priori* and *a posteriori* against the DNS data.

2 Numerical methodology

In this section the CMC equation is introduced. Then the implementation of the CMC model into OpenFOAM® is briefly explained. This is followed by briefly discussing the DNS solver and finally the test cases and initial conditions are introduced.

2.1 Conditional moment closure (CMC)

If the entire computational fluid dynamics (CFD) domain is taken as one CMC cell, the full form of the CMC equation (Eq.(103) in Ref.[8], for example) reduces to a spatially zero-dimensional formulation called the 0D-CMC model. By neglecting the terms associated with the conditional fluctuations (Eq.(105) in Ref.[8]), the 0D-CMC equation for a given species mass fraction can be written as

$$\frac{\partial \widetilde{Y}_\xi}{\partial t} = -\widetilde{v}_\xi \frac{\partial \widetilde{Y}_\xi}{\partial \xi} + \frac{1}{(\Delta\Theta)^2} \widetilde{N}_\xi \frac{\partial^2 \widetilde{Y}_\xi}{\partial \xi^2} + \frac{\dot{\omega}_\xi}{\rho_\xi} \, , \tag{1}$$

where ρ_ξ and $\dot{\omega}_\xi$ represent conditional mean of density and reaction rate, respectively. Furthermore, $\widetilde{Y}_\xi$ and $\widetilde{N}_\xi$ are conditional Favre mean (CFM) of the given species mass fraction and scalar dissipation rate. The scalar dissipation rate is defined using the mixture fraction, *Z*, as $N \equiv D(\nabla Z)^2$, where *D* is the thermal diffusivity. The Lewis number is assumed to be one. In Eq.(1), ξ is the sample variable in conditional space of the *normalised* mixture fraction, $\overline{Z} = (Z - Z_{min})/(Z_{max} - Z_{min})$, where Z_{min} and Z_{max} represent the extremes of *Z* and are only a function of time, *t*. The normalised mixture-fraction space is used since in the present HCCI cases, unlike typical non-premixed flames, the mixture fraction range, $\Delta\Theta = Z_{max} - Z_{min}$, is smaller than unity. The variable $\widetilde{v}_\xi$ in Eq.(1) may be expressed using $\Delta\Theta$, time derivatives of Z_{min} and Z_{max}, and the CFM of $\overline{Z}$, $\langle \rho \overline{Z} | \xi \rangle / \rho_\xi$, viz.

$$\widetilde{v}_\xi = -\frac{1}{\Delta\Theta}\left[\frac{\partial Z_{min}}{\partial t} + \frac{\langle \rho \overline{Z} | \xi \rangle}{\rho_\xi} \frac{\partial(\Delta\Theta)}{\partial t} \right], \tag{2}$$

2.2 OF-CMC solver

The CMC model, Eq.(1), is implemented in OpenFOAM® which is an open source CFD package written in C++ language [11]. The implementation is referred to as OF-CMC here. In this implementation the CMC equations are solved in association with the governing equation for density, pressure, velocity and enthalpy. Because mixture fraction is chosen as conditioning scalar, a transport equation for *Z* is also solved. In the CMC solver, Eq.(1) is solved using the first-order closure

hypothesis for reaction rate source term, i.e. $\dot{\omega}_\xi = \dot{\omega}\left(\widetilde{T}_\xi, \widetilde{Y}_\xi, \overline{p}\right)$. This yields a one-dimensional (1D) vector of updated $\widetilde{Y}_\xi$ values for each species as a function of normalised mixture fraction. Then using a Dirac's delta probability density function (PDF) for mixture fraction and spline-fitted $\widetilde{Y}_\xi$, the species mass fraction, Y, is obtained on the CFD grid based on the local value of Z. By having the mass fraction field, other parameters such as velocity, enthalpy, density, and pressure are calculated in the CFD domain. This completes one time-step iteration of the OF-CMC solver. Viscosity is found using Sutherland's formula. Prandtl number and Lewis number are 0.705 and 1, respectively. The OF-CMC is efficiently parallelised, both in the CFD domain and in the CMC solver using MPI libraries. One should note that in the OF-CMC solver, the equations in the CFD domain are solved using the DNS grid. Therefore, it is assumed that mixing effects are simulated as accurate as DNS. This allows for validation of the core of the implementation, that is the CMC model equation.

2.3 DNS solver

S3D, an explicit DNS solver developed in Fortran language at the Combustion Research Facility at Sandia National Laboratories is used [12]. S3D is a high-order yet low-dissipation numerical solver. It utilises a Cartesian grid to solve Navier-Stokes, species mass-fraction transport and total energy equations. The governing equations are discretised using a central, 8th order finite differencing scheme for spatial derivatives and a 6 stage, 4th order explicit Runge-Kutta scheme for time integration. CHEMKIN software libraries are linked to S3D to evaluate thermo-physical properties and reaction rates. The same transport model as the OF-CMC solver is implemented into S3D in the present study.

2.4 Test cases and initial conditions

Six two dimensional test cases, with their details outlined in Table 1, are simulated using S3D and the OF-CMC solver. Initial conditions for these cases are taken from Ref. [7]. The difference of DNSs in the present study to those of Ref. [7] is that here Le=1 is imposed to be consistent with the derivation of the CMC equation and the transport model used in the OF-CMC implementation. Three mean temperatures of 850 K, 950 K, and 1000 K are chosen to initialise the temperature field. These temperatures correspond to the negative temperature coefficient (NTC) regime of a homogeneous *n*-heptane/air mixture with the mean stoichiometric fuel air equivalence ratio of $\phi_0 = 0.3$ and pressure of $p = 40\,\text{atm}$ [13].

Table 1: Parameters of simulated cases

Case	LS1	LS2	LS3	HS1	HS2	HS3
T_0 [K]	850	950	1000	850	950	1000
T' [K]	15	0	15	60	0	60
Z'	0.005	0.005	0.005	0.02	0.02	0.02

While three cases are set up to have low stratification levels (LS1, LS2, LS3) in composition and temperature, the other three have high stratification levels (HS1, HS2, HS3). Two cases (LS2, HS2) have initial stratifications in mixture only with temperature field initialised uniformly at 950 K. This is to see if mixture fraction can succeed as conditioning variable in the absence of initial temperature stratifications. The remaining four cases are initialised with initial temperature fluctuations being *negatively* correlated to those of mixture composition. All six cases have the same initial mixture fraction field with a mean mixture fraction equal to $Z_0 = 0.0195$, corresponding to $\phi_0 = 0.3$. A reduced chemical mechanism for *n*-heptane/air with 58 species and 387 reactions developed for HCCI-like conditions is employed [13]. To reduce the computational cost, considering the size of the chemical mechanism, a domain size of $3.2 \times 3.2\,\text{mm}^2$ is chosen. The grid spacing is set at 640×640 for the LS cases and 1280×1280 for the HS cases. The chosen grid sizes are found sufficient to fully resolve the flame. Periodic boundary conditions are imposed in all directions. All six cases have the same initial velocity field with further details outlined in Ref. [7].

3 Results and discussions

Figure 1 shows the mean heat release rate (HRR) as a function of time using different approaches[1]. The first row shows a comparison between the mean HRRs obtained from DNS, $\langle \omega_T \rangle_{dns}$, and the mean HRR calculated by the OF-CMC solver, $\langle \omega_T \rangle_{OF\text{-}cmc}$, for the LS cases only. As can be seen a very good agreement between DNS and CMC results is observed for these cases.
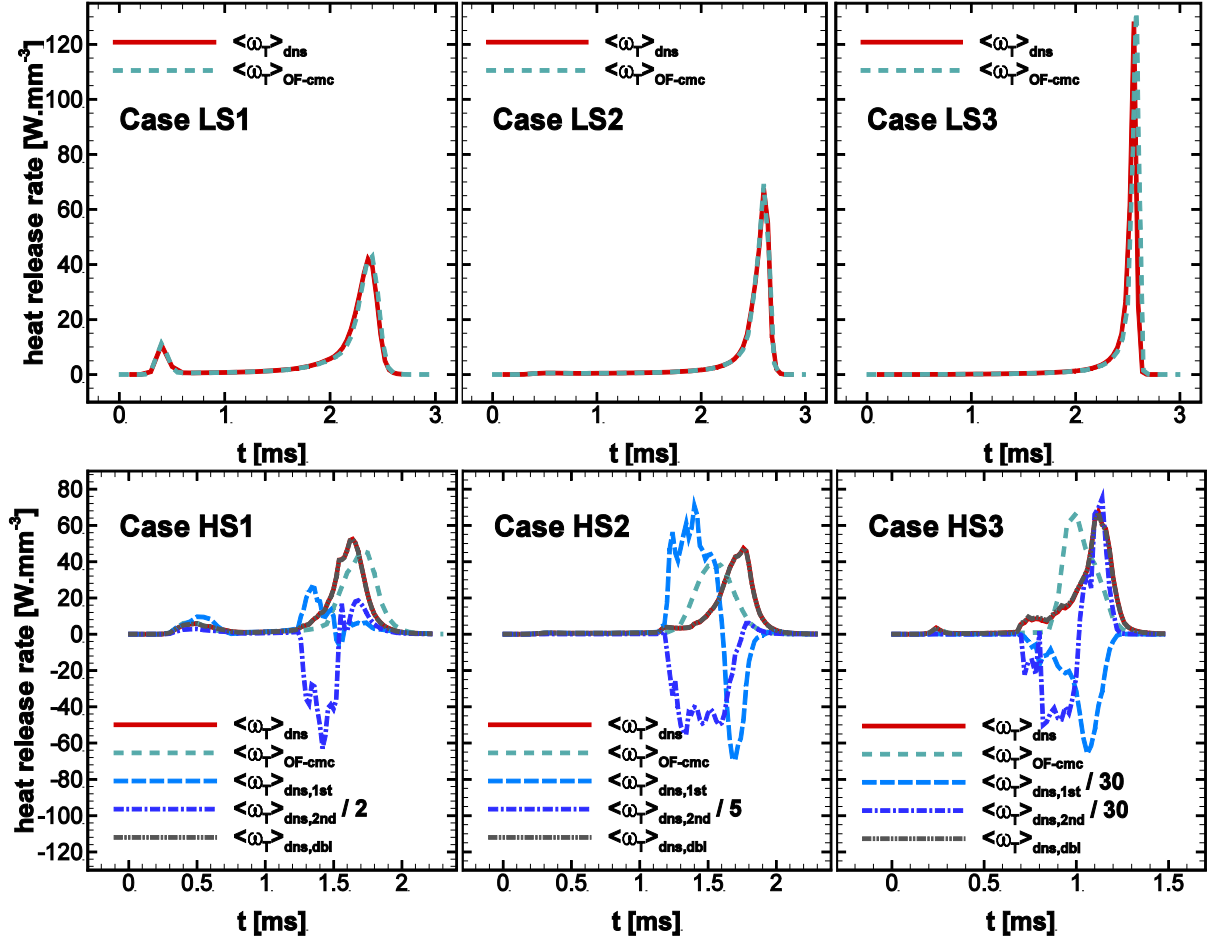

Figure 1. Mean heat release rate as predicted by OF-CMC and DNS.

In the second row of Figure 1, in addition to $\langle \omega_T \rangle_{dns}$ and $\langle \omega_T \rangle_{OF\text{-}cmc}$, the HRR calculated from the DNS using the first-order closure hypothesis, $\langle \omega_T \rangle_{dns,1st}$, second-order closure, $\langle \omega_T \rangle_{dns,2nd}$, and finally first-order closure using two conditioning variables, i.e. sensible enthalpy and mixture fraction, $\langle \omega_T \rangle_{dns,dbl}$, are also plotted for the HS cases. In these cases, the agreement between the DNS and CMC results is reasonable for case HS1 but not satisfactory for cases HS2 and 3. Interestingly, both first- and second-order closure fail to reproduce the correct behaviour whereas double conditioning provides an excellent match with the DNS results.

Table 2 presents the error percentage for the ignition delay time, τ_{ig}, and combustion duration, τ_{dur}, when the CMC model is used. Ignition delay, τ_{ig}, is defined as the time needed for half of the total heat to be released. Combustion duration, τ_{dur}, is defined as the time elapsed between 10 percent to 90 percent of the total heat release. The LS cases in the table demonstrate a very good agreement with

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[1] The total heat release rate is calculated using the enthalpy of formation for each species.

DNS which is consistent with Figure 1, showing that the first-order closure is an adequate model in these cases. For the HS cases, however, high levels of error in τ_{dur} are observed. The observations in Figure 1 suggest that the reason for this disagreement is the breakdown of the first-order hypothesis, because the only difference is that the OF-CMC results are obtained using *a posteriori* approach.

Table 2: Relative error in percentage for τ_{ig} and τ_{dur} predicted by OF-CMC.

Case	LS1	LS2	LS3	HS1	HS2	HS3
τ_{ig}	0.8	0.2	0.8	4.6	9.1	7.2
τ_{dur}	2.9	1.5	0.7	11.0	17.7	40.7

It is noted that, in Figure 1, even though OF-CMC is using first-order assumption, $\langle \omega_T \rangle_{\text{OF-cmc}}$ yet is not as bad as $\langle \omega_T \rangle_{\text{dns,1st}}$. This implies that the *a posteriori* time integration tends to damp rather than magnify accumulated errors. One possible reason for this is that both the DNS and OF-CMC solutions are rapidly attracted as time advances towards a underlying low-dimensional manifolds in thermochemical state-space, upon which the state varies slowly. In the OF-CMC this manifold is by definition only two dimensional (mixture-fraction and time), whereas in the DNS it can be much higher dimensional while evidence in practice shows that typical manifolds in combustion can be represented quite accurately with only a few dimensions [14]. In contrast in the *a posteriori* test, the averaged state-space variables can lie significantly off the underlying manifold (except in the trivial case where the manifold is planar) and therefore reaction rates can be significantly different to those that would exist on the manifold. A simple example of this would be a bi-modal conditional temperature distribution, discussed below, where real states are either burning or not burning, but the averaged state is an unphysical state somewhere in between.
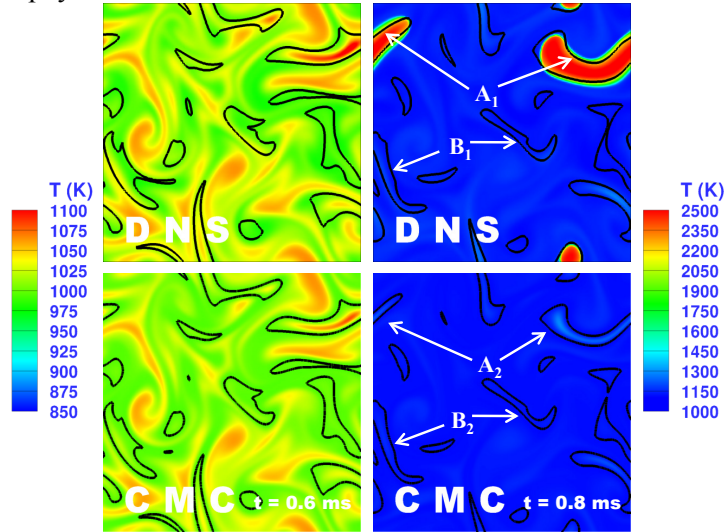
Figure 2. Instantaneous temperature field (colour-flooded) with iso-contour lines of $Z = 0.035$.

Figure 2 explains why double conditioning in Figure 1 can provide a closure for reaction rate. Up to $t = 0.6\,\text{ms}$ very good agreement is observed between OF-CMC and DNS. This shows that OF-CMC captures mixing effects very well while the first-order closure assumption holds. At $t = 0.8\,\text{ms}$, however, OF-CMC is showing delay in auto-ignition. This could be explained by iso-contour lines of mixture fraction at $Z = 0.035$. While at $t = 0.6\,\text{ms}$, all $Z = 0.035$ lines share almost the same background temperatures, in $t = 0.8\,\text{ms}$, at the same $Z = 0.035$, two extremes of hot and cold temperatures co-exist in the DNS results. They are labeled A_1 and B_1, respectively. This bi-modal distribution of temperature leads to conditional mean of temperature to be around 1750 K which is *not* representative of either of cold (1000 K) or hot (2500 K) zones. Evaluating reaction rate with first-

order or even second-order at this *fictitious* mean temperature would lead to non-physical results for $\langle \omega_T \rangle_{dns,1st}$ and $\langle \omega_T \rangle_{dns,2nd}$ witnessed previously in Figure 1. Double conditioning with mixture fraction and sensible enthalpy, however, provides a very good first-order closure, as illustrated in Figure 1. This is because sensible enthalpy can differentiate different temperatures co-existing in a given mixture fraction. The last point to be made from Figure 2 is that both A_2 and B_2 have the same background temperature. This is because OF-CMC treats both A_2 and B_2 identically through the Dirac's delta PDF of mixture fraction. Due to *self-sustainability* of OF-CMC, first-order closure does not lead to catastrophic over-predictions observed for $\langle \omega_T \rangle_{dns,1st}$ and $\langle \omega_T \rangle_{dns,2nd}$ in Figure 1.

4 Conclusions

A CMC model is developed to address the auto-ignition in *n*-heptane/air mixtures with temperature and composition stratifications under HCCI-like conditions. Two levels of stratifications with three different mean temperatures are investigated. Two dimensional DNS is performed to generate the data necessary for *a priori* and *a posteriori* analysis of the model. The CMC model is implemented in OpenFOAM® and its performance is assessed by comparison to the DNS data.

Excellent agreement between OF-CMC and DNS is observed for the low stratification cases. In the high stratification cases, while a strong disagreement between exact reaction rates from DNS and those obtained using the first-order closure in an *a priori* study is observed, the OF-CMC predictions of reaction rates are not as bad. This is attributed to *a posteriori* nature of OF-CMC where the solution in the CFD domain *adapts* itself to evolve along an underlying low-dimensional manifold which is similar to a somewhat higher dimensional manifold observed in the DNS. Using *a priori* analysis, it is shown that in the HS cases even second-order estimation of reaction rate cannot provide an adequate closure. Double conditioning with mixture fraction and sensible enthalpy, however, provides a first-order closure to reaction rate. Conditional fluctuations of temperature are shown to be the reason for the breakdown of the first-order closure with a single conditioning variable.

Acknowledgement

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