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CONDITIONAL MOMENT CLOSURE MODELLING FOR HCCI FEATURING COMPRESSION HEATING AND EXPANSION COOLING

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ABSTRACT

This paper presents a conditional moment closure (CMC) model for ignition of a lean ethanol/air mixture under homogeneous charge compression ignition (HCCI) conditions. A set of direct numerical simulations (DNSs) presented by Bhagatwala *et al.* (2014) is used to evaluate the performance of the CMC model. The DNS data includes five cases with a mean temperature of 924 K and three different levels of thermal stratification. The effect of compression heating and expansion cooling is considered in the first three cases with $T' = 15$, 25 and 40 K. For this purpose, an inert mass source term is added to the governing equations. However, the other two cases with $T' = 15$ and 40 K do not consider compression heating and expansion cooling. The results show a better agreement between the CMC and DNS for cases in which compression heating and expansion cooling is considered. Further investigation of the DNS data shows that the contribution of the diffusion term in the CMC equations, representing the importance of deflagration mode, is only significant for the case which has the largest level of thermal stratification and does not involve compression heating and expansion cooling.

INTRODUCTION

Internal combustion engines are central to energy generation in the transportation sector. However, combustion results in emissions of pollutants, such as nitrogen oxides (NO_x) and carbon monoxide (CO), which are harmful to human health. In order to reduce the formation of these pollutants and their adverse impacts on human health and the environment, the development of cleaner combustion technologies is required.

Homogeneous charge compression ignition (HCCI) have been introduced to develop an engine type with high efficiency of diesel engines and very low emissions of gasoline engines. In an HCCI engine, extremely low levels of NO_x and soot formation are achieved while the thermal efficiency is still very high. In spite of these favourable features, HCCI is still in the phase of laboratory research since it presents considerable challenges such as difficulties in controlling the auto-ignition timing, especially during transients, and the high rate of pressure rise at high load (Dec, 2009).

Thermal stratification, which naturally happens in HCCI engines is one of the strategies to overcome these difficulties. As discussed in the literature, thermal stratifications can reduce the pressure rise and heat release rates (Dec, 2009; Snyder *et al.*, 2011) in HCCI engines. Effects of thermal stratification on ignition have been studied by direct numerical simulation (DNS) for various mixtures under HCCI conditions (Hawkes *et al.*, 2006; Yoo *et al.*, 2011, 2013; Talei & Hawkes, 2015). These DNS studies showed that there are two combustion modes under HCCI conditions: deflagration and spontaneous ignition. In the deflagration mode of combustion, the ignition front propagates due to both reaction and molecular transport while the spontaneous mode presents a cascade of ignition events in which the molecular transport has an insignificant role. The deflagration combustion mode is dominant in cases with large temperature inhomogeneities while the cases with a low level of thermal stratification present a prevalence of the spontaneous combustion mode.

The conditional moment closure (CMC) (Klimenko & Bilger, 1999) is an approach can be used to model combustion process in HCCI. The basic idea behind the CMC model is that errors in the evaluation of the unclosed reaction source term can be significantly reduced if its evaluation is conditioned on another variable upon which the reaction rate mainly depends. In our previous work, a model based on the CMC method was developed to study effects of temperature inhomogeneities on the ignition process under HCCI conditions (Salehi *et al.*, 2015*b*). The model was then evaluated using different sets of DNS data for ignition process of a lean *n*-heptane/air mixture (Yoo *et al.*, 2011) and a lean *iso*-octane mixture (Yoo *et al.*, 2013) with different mean temperatures and various levels of temperature fluctuations (Salehi *et al.*, 2015*b*,*a*). It was found that the CMC model predicted the ignition process very well for cases with low and medium levels of thermal stratification. However, the agreement between the CMC and the DNS for cases with large thermal stratification was not as good as other cases. It was also shown that since the deflagration mode was dominant in cases with large temperature inhomogeneities, the conditional fluctuations were high and hence the first-order CMC model was not able to predict the ignition process very well in these cases. In a separate study, we derived a transport equation for the conditional variance for premixed combustion (Salehi *et al.*, 2015*a*). An assessment of the conditional variance equations using the DNS data revealed that the correlation between dissipation rate fluctuations and conditional mass fraction fluctuations played an important role to generate conditional mass fraction fluctuations (Salehi *et al.*, 2015*a*).

Our previous works (Salehi *et al.*, 2015*b*,*a*) focused on constant volume ignition of lean mixtures with temperature inhomogeneities. However, in a real HCCI engine, combustion is affected by the piston motion due to compression heating of the mixture before the top dead center (TDC), and expansion cooling after TDC. In the present paper, the effects of compression heating and expansion cooling on the ignition process in a thermally stratified mixture are therefore studied using the CMC model in Ref. (Salehi *et al.*, 2015*b*). To evaluate the performance of the CFD-CMC solver in this condition, a set of DNS data reported in Ref. (Bhagatwala *et al.*, 2014) is used.

The structure of the paper is as follows. The governing equations in addition to the CMC model are first introduced. The numerical method and test cases are then presented. The performance of the CMC model is next investigated using the DNS data. To shed light on the differences between cases with and without compression heating and expansion cooling in the concept of the CMC modelling, further investigations using the DNS data are also presented.

BALANCE EQUATIONS

An inert mass source term, $\dot{M}_c$, is added to the governing equations to simulate effects of compression heating and expansion cooling due to the piston motion (Bhagatwala *et al.*, 2014). By considering this term, the continuity and momentum can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_j}{\partial x_j} = \dot{M}_c, \tag{1}$$

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial \rho v_i v_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \dot{M}_c v_j, \tag{2}$$

where ρ, v_j, p, τ_{ij} are the density, the velocity component in j-th coordinate director, the pressure, and the viscous stress tensor, respectively. Similarly, transport equations for mass fraction of species α and enthalpy are as follows:

$$\frac{\partial \rho Y_\alpha}{\partial t} = -\frac{\partial \rho v_j Y_\alpha}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial Y_\alpha}{\partial x_j}\right) + \dot{\omega}_\alpha + \dot{M}_c Y_\alpha, \tag{3}$$

$$\frac{\partial \rho h}{\partial t} = -\frac{\partial \rho v_j h}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial h}{\partial x_j}\right) + \frac{Dp}{Dt} + \dot{M}_c h, \tag{4}$$

where Y_α, $\dot{\omega}_\alpha$, and h are the mass fraction for species α, the reaction rate for species α, and the enthalpy, respectively. The inert mass source term is defined as:

$$\dot{M}_c = \frac{\partial \bar{\rho}}{\partial t}, \tag{5}$$

where $\bar{()}$ refers to the mean value in the cylinder. In HCCI engines, volume is varied due to the piston motion and hence the density is changed whereas the total mass is constant. In this study, it is assumed that the volume is constant while the total mass is varied to account for the change in the mean density. Therefore, assuming the ideal gas low, the inert mass source term can be written as:

$$\dot{M}_c = \frac{\partial}{\partial t}\left(\frac{m_e}{V_e(t)}\right) = \frac{\partial}{\partial t}\left(\frac{m_s(t)}{V_s}\right) = -\frac{\bar{\rho}}{V_e(t)}\frac{\partial V_e(t)}{\partial t}, \tag{6}$$

where (t) indicates the parameters are a function of the time and subscript e and s refer to the values in the real engine and simulation, respectively. The crank-slider relationship for the engine volume, V_e, is (Heywood, 1988):

$$\frac{V_e}{V_c} = 1 + \frac{r_c - 1}{2}\left(r + 1 - \cos\Theta - \sqrt{r^2 - \sin^2\Theta}\right), \tag{7}$$

where V_c, r_c, r and Θ are the clearance volume, compression ratio, ratio of connecting rod length to crank radius and crank angle, respectively. If $\Theta = \Omega t$ where $\Omega = 2\pi RPM$, the term dV_e/dt, can readily be obtained.

CONDITIONAL MOMENT CLOSURE

In HCCI, the combustion process is mainly controlled by the thermochemical state prior to ignition. Therefore, total enthalpy is used as a conditioning variable which represents the thermochemical variables to which ignition delay is sensitive (Salehi *et al.*, 2015*b*). Then, the species mass fraction equations, Eq. 3, can be recast into the set of CMC equations using the following definition for the conditionally Favre-averaged mass fraction of species α:

$$Q_\alpha(\xi; x, t) = \langle Y_\alpha|_{\theta=\xi}\rangle = \frac{\overline{\rho Y_\alpha(x,t)|_{\theta=\xi}}}{\overline{\rho|_{\theta=\xi}}}, \tag{8}$$

where ξ is the sample space for a normalised scalar variable defined as:

$$\theta(x,t) = \frac{h(x,t) - h_{min}(t)}{h_{max}(t) - h_{min}(t)}, \tag{9}$$

and where h_{min} and h_{max} correspond to minimum and maximum enthalpies in the computational domain, respectively. It may be shown that the source terms in Eq. (3) and (4), representing compression heating and expansion cooling effects do not appear in the non-conservative form of these equitations. Since the CMC equations are derived, using a decomposition method (Klimenko & Bilger, 1999), from non-conservative form of Eq. (3) and (4), the CMC equations remain the same as what previously reported in Ref. (Salehi *et al.*, 2015*b*,*a*). Therefore, the CMC equations are as follows:

$$\frac{\partial Q_\alpha}{\partial t} = -v_\xi \frac{\partial Q_\alpha}{\partial \xi} + \langle N|_\xi \rangle \frac{\partial^2 Q_\alpha}{\partial \xi^2} + \langle \dot{W}_\alpha|_\xi \rangle, \tag{10}$$

where $\dot{W}_\alpha$ is $\overline{\dot{\omega}_\alpha|_\xi}/\overline{\rho|_\xi}$. The scalar dissipation rate, N, is defined as $D\frac{\partial\theta}{\partial x_j}\frac{\partial\theta}{\partial x_j}$ where D is the molecular diffusivity, considered 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 S_θ results from the source term of the normalised enthalpy. It is also assumed that the cylinder charge is statistically homogeneous and hence the spatial terms in the physical space are ignored.

NUMERICAL METHOD AND TEST CASES STUDIES

The CMC model is implemented into the open source C++ computational fluid dynamic (CFD) code known as OpenFOAM. The CFD solver is modified to represent compression heating and expansion cooling effects. In each time step, the inert mass source term is first calculated using Eq. (6) and Eq. (7) and then Eq. (1), Eq. (2) and Eq. (4) are solved on the CFD grid. Using flow variables obtained from the CFD solver, the conditional scalar dissipation rate, $\langle N|_\xi \rangle$, and convective velocity in conditional space, v_ξ, are calculated at each CMC bin and passed to the CMC solver. In order to update conditional temperature, which is required to calculate conditional reaction rate, and conditional density, $\overline{\rho|_\xi}$, in the CMC domain, conditional pressure, h_{min} and h_{max} are also passed to the CMC solver. Then, CMC equations, Eq. (10), are solved in ξ-space. In this study, a Dirac-delta PDF for the enthalpy is assumed to obtain Favre-averaged species mass fractions on the CFD grid from conditional species mass fractions. More details about CFD-CMC solver can be found in Refs. (Salehi *et al.*, 2015*b*,*a*).

Five two-dimensional DNS cases were used to evaluate the performance of the CFD-CMC solver. The DNS cases feature ignition of a lean ethanol/air mixture with temperature inhomogeneities (Bhagatwala *et al.*, 2014). The physical domain in the DNS study was 3.6 mm square with a periodic boundary conditions were applied in both directions. As shown in Table 1, the effect of compression heating and expansion cooling was considered in the first three cases with $T' = 15$, 25 and 40 K whereas the other two cases with $T' = 15$ and 40 K were simulated with the same initial conditions but do not consider this effect. The initial mean temperature, pressure and equivalence ratio are 924 K, 45 bar and 0.4 respectively. In all cases, a dilution level of 33% mole fraction of simulated exhaust gas recirculation (EGR) was employed. These simulated EGR composition included products of complete combustion of a stoichiometric ethanol/air mixture, i.e. 12% CO_2, 18% H_2O and 70% N_2. The simulated engine speed is 1200 revolutions per minutes (RPM) while the compression ratio is 18. The initial crank angle is 11 degree before TDC. As discussed previously, in DNS study the piston compression and expansion in cases 1-H, 2-H and 3-H were emulated through the inert mass source term which was presented here (Eq. (6)). A 29-species reduced ethanol/air chemistry mechanism (Bhagatwala *et al.*, 2014) was employed in both DNS and CMC.

A uniform grid spacing of 20 μm was employed for all cases, compared with the DNS grid spacing of 5 μm. Note that the DNS needed to resolve species that fluctuate on smaller length scales while in the CFD-CMC solver only the length scales of enthalpy and velocity fluctuations need to be resolved. Then, a coarser mesh can be used for the CMC-based model. The CMC conditioning variable domain included 101 equally spaced grid points. The initial and boundary conditions for the CFD-CMC were the same as those in the DNS cases.

Table 1. Physical parameters of the DNS and CMC cases.

Case	$T'(K)$	Compression Heating
1-H	15	Yes
2-H	25	Yes
3-H	40	Yes
4-NC	15	No
5-NC	40	No

RESULTS

Figure 1 presents the temporal evolution of mean pressure and heat release rate for all cases. As can be seen, the CMC model can reasonably capture the overall behaviour in all cases. The agreement between the CMC model and the DNS for cases featuring compression heating and expansion cooling (Fig. 1a and b) is excellent which has not been previously demonstrated. The prediction of the CMC-CFD solver for case 4-NC with $T' = 15$ K and without compression heating and expansion cooling (Figs. 1c and d) is also satisfactory whereas for case 5-NC with $T' = 40$ K, the agreement is not as good as the other cases. For this case, the CFD-CMC solver predicts a longer ignition delay time (τ_{ig}) and a higher peak heat release in comparison with the DNS. As discussed in our previous works (Salehi *et al.*, 2015*b*,*a*), the reason for discrepancy between the CMC results and DNS in case 5-NC is possibly due to the importance of deflagration mode in this case. Further investigation using the DNS data will be presented in the forthcoming sections to shed light on the effect of compression heating and expansion cooling on the performance of the CMC model.

Figure 2 presents isocontours of heat release rate obtained using the DNS and the CFD-CMC solver at the time

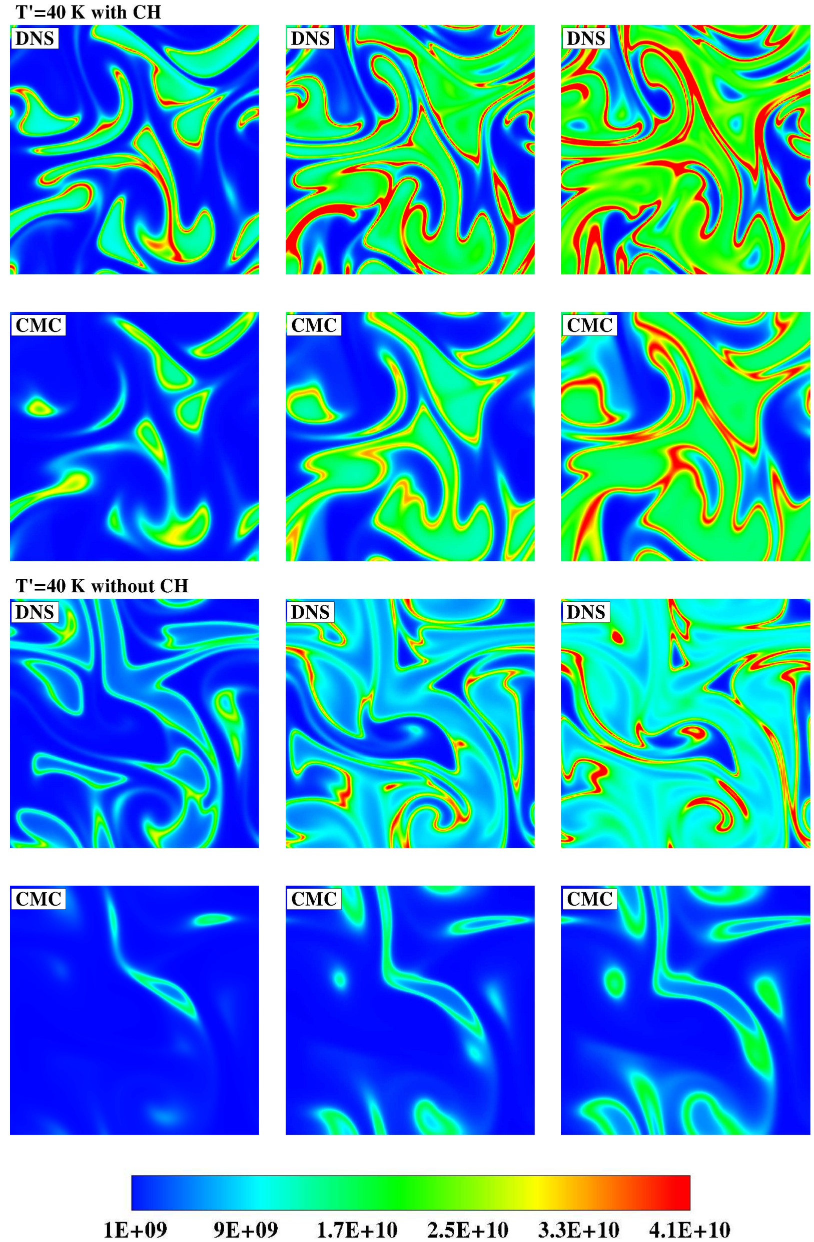

Figure 2. Isocontours of heat release rate obtained using the DNS and the CFD-CMC solver at t_1, t_2 and t_3 for cases 3-H and 5-NC with $T' = 40$ K.

instants t_1, t_2 and t_3. These instants are defined as the time when the mean heat release rate is a quarter (t_1), half (t_2) and three quarters (t_3) of the peak mean heat release rate, respectively. The first two rows show the results for cases 3-H ($T' = 40$ K) with compression heating and expansion cooling, whereas the second and third rows show the results for case 5-NC ($T' = 40$ K) with no compression heating and expansion cooling. In case 3-H, the agreement between the CMC and DNS at an early stage ($t = t_1$) is not very good while at a later stage ($t = t_3$) a better agreement is observed. This can be due to the increasing importance of the spontaneous mode of combustion over the deflagration mode since the pressure increases more significantly in cases featuring compression heating and expansion cooling. This is investigated further in the followings.

To investigate the importance of the deflagration mode in cases studied here, three different DNS-CMC tests are introduced as follows. In the first test the conditional dissipation rate, $\langle N|_\xi \rangle$, and convective velocity in conditional space, v_ξ, are evaluated directly using the DNS data. The CMC equations (Eq. 10) are then solved using the terms obtained from the DNS. In the second test, it is assumed that the effect of convection term in the normalised enthalpy domain is small and therefore the CMC equations can be rewritten as follows:

$$\frac{\partial Q_\alpha}{\partial t} = \langle N|_\xi \rangle \frac{\partial^2 Q_\alpha}{\partial \xi^2} + \frac{\overline{\dot{\omega}_\alpha|_\xi}}{\overline{\rho|_\xi}}, \tag{11}$$

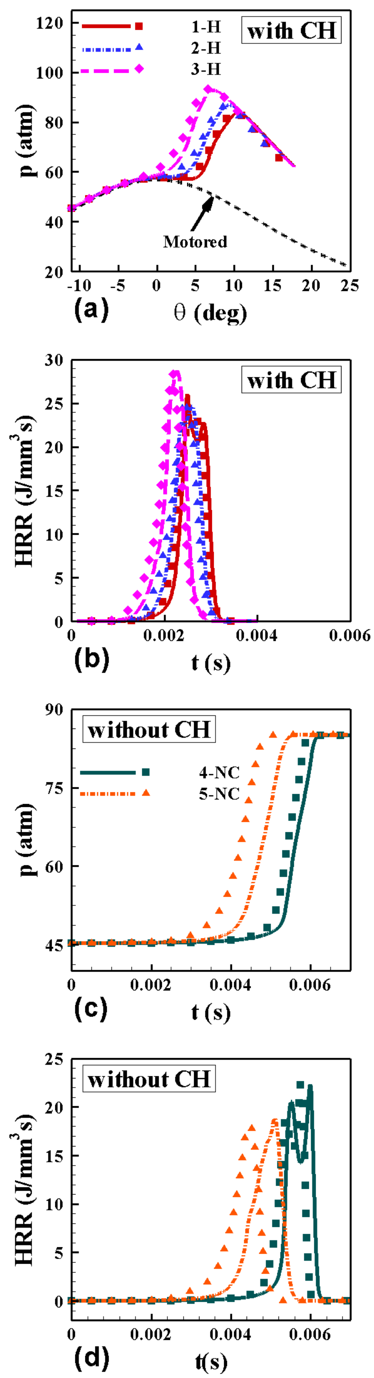

Figure 1. Temporal evolution of the pressure and the mean heat release rate obtained using the CFD-CMC solver (lines) in comparison with the DNS (symbols) for cases a-b) with and c-d) without compression heating and expansion cooling.

and hence the conditional dissipation rate, $\langle N|_\xi \rangle$, alone, is evaluated directly from the DNS. In the third test, both convective and diffusion terms are assumed to be negligible and therefore the CMC equations are simplified as:

$$\frac{\partial Q_\alpha}{\partial t} = \frac{\overline{\dot{\omega}_\alpha|_\xi}}{\overline{\rho|_\xi}}. \tag{12}$$

It is worth noting that in all the tests defined above, the CMC solver was run in a stand-alone mode using the DNS input. The PDF of the normalised enthalpy, $P(\xi)$, is also obtained from the DNS data whereas the conditional reaction rates are computed using the first order assumption in the CMC code. The temporal evolution of mean heat release rate obtained using these tests is shown in Fig. 3 for cases 1-H ($T' = 15$ K) and 3-H ($T' = 40$ K) with compression heating and expansion cooling and cases 4-NC ($T' = 15$ K) and 5-NC ($T' = 40$ K) with no compression heating and expansion cooling. The comparison between the results obtained using the first test (green dashed line) and the second test (long-dashed pink line) shows that the effects of the convective term is negligible in all cases. The results obtained using the second and the third tests reveal that considering the diffusion term in the CMC equations has an insignificant effect in both cases 1-H ($T' = 15$ K) and 3-H ($T' = 40$ K) with compression heating and expansion cooling. On the other hand, in cases without compression heating and expansion cooling, the effect of the diffusion term on the results is only negligible in the case with a low level of thermal stratification (case 4-NC). As the diffusion term is considered in the CMC equations, the heat release rate is spread out in case 5-NC resulting an advanced ignition. It is worth noting that, even though both cases 3-H and 5-NC have the same level of thermal stratification, the effect of diffusion term in the former is insignificant. As discussed in Ref. (Salehi *et al.*, 2015*b*), the diffusion term in the CMC equations represents the importance of the deflagration mode, hence, it can be concluded that deflagration is only dominant in case 5-NC. Increasing the pressure before TDC in the compression heated mixture in case 3-H leads to the decreasing the importance of the deflagration mode even though the temperature inhomogeneities are still large.

CONCLUSION

The CMC model was used to simulate ignition in thermally stratified lean ethanol/air mixtures under HCCI-like conditions. To evaluate the performance of the CMC model, a set of DNS data featuring compression heating and expansion cooling effects with temperature inhomogeneities of 15-40 K were considered. Two more DNS cases with $T' = 15$ and 40 K with no compression heating and expansion cooling were also studied. The effects of compression heating and expansion cooling were emulated using an inert mass source term added to the governing equations. The CMC model predicted the ignition process with a good accuracy in all cases featuring compression heating and expansion cooling whereas the largest disagreement between the CFD-CMC and DNS results was observed in the case with the largest temperature inhomogeneities featuring no compression heating and expansion cooling.

To investigate the conditional closure in the CMC equations, a set of DNS-CMC tests were introduced. It was found that in spite of the same level of temperature fluctuations in both cases 3-H (with compression heating and expansion cooling) and 5-NC (without compression heating and expansion cooling), the contribution of the diffusion

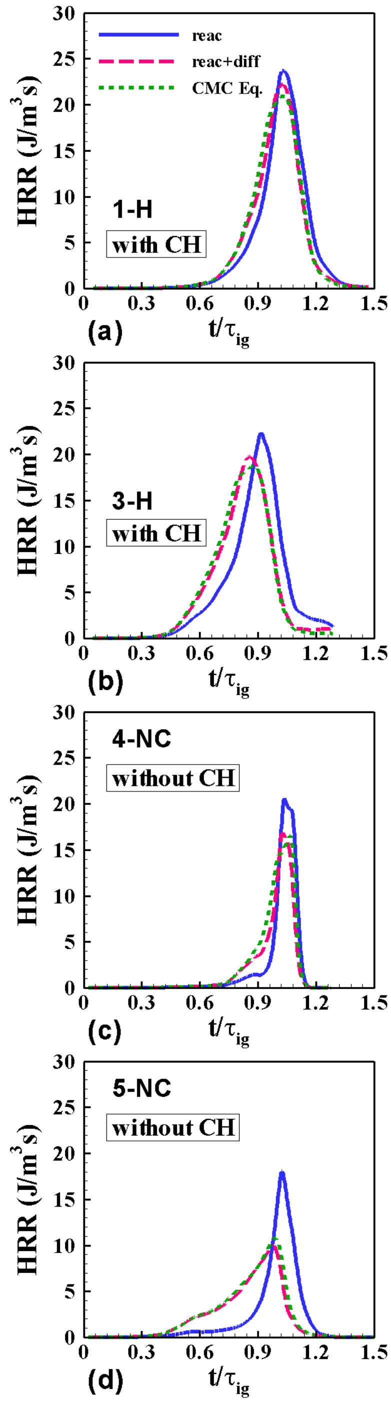

Figure 3. Temporal evolution of the mean heat release rate obtained using three different DNS-CMC tests for cases a) 1-H, b) 3-H, c) 4-NC and d) 5-NC.

term in the CMC equations, representing the dominance of the deflagration mode, was most significant in case 5-NC.

Overall, increasing pressure in the heated mixture before TDC serves to decrease the effect of diffusion in cases featuring compression heating and expansion cooling. As a result, the deflagration mode was suppressed in this condition and the CMC model was able to predict the ignition process more accurately (even for the case with a large level of thermal stratification) compared with cases with no compression heating and expansion cooling.

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