HCCI combustion modeling using detailed chemistry coupled to LEM-based advection

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1 Introduction

Homogeneous-Charge Compression Ignition (HCCI) engines have potentially higher thermal efficiencies and lower NO_x and soot emissions compared to conventional Spark Ignition and Diesel engines, respectively. One major problem in the design of such engines is the control of the very large heat release rates which may cause excessively rapid pressure rise under perfectly homogeneous conditions. One method to reduce the maximum heat release rate is the introduction of thermal or mixture inhomogeneities which leads to a spreading of the heat release over several crank angles.

In recent Direct Numerical Simulation (DNS) studies [1, 3] it has been demonstrated that both ignition fronts and deflagration-like fronts may be present under thermal stratification under HCCI-like conditions. With increasing stratification the subtle interaction between turbulent mixing and chemistry becomes increasingly important and needs to be taken into account in computational models of HCCI engines. Cook et al. [2] presented a one-dimensional flamelet-type model in enthalpy space capable of capturing HCCI combustion in both relevant regimes identified in the DNS simulation. The model offers the potential to be used as a combustion model for CFD calculations of HCCI engines. However, for closure the enthalpy-based flamelet model needs a probability density function (PDF) for enthalpy and a model for the enthalpy dissipation rate. Using those data directly from the DNS [2], the enthalpy flamelet model was able to achieve good agreement with the DNS results.

In this work we use the Linear-Eddy Model (LEM) [5] to investigate the influence of thermal stratification on auto-ignition under HCCI conditions. The (one-dimensional) LEM model is capable of representing the turbulence-chemistry interaction at all scales. In comparison to the flamelet-based modeling [2] the LEM approach after calibration does not need additional input for closure. We compare some first results obtained with LEM with DNS data of Hawkes et al. [3]. The predicted heat release rates agree reasonably well with the DNS results. The simple one-dimensional model is capable of capturing the key combustion characteristics for the combustion regime of spontaneous ignition fronts, for the deflagration dominated case, and lastly for the mixed one. The 1D strategy enables parametric studies including modification of mixture inhomogeneity in a reasonable computational time. Furthermore, LEM has been used successfully in the past as a subgrid combustion model for Large Eddy Simulations. The results presented in this work suggest that LEM is a potential candidate as a combustion model for CFD calculations of HCCI engines.

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2 Model formulation

The Linear-Eddy Model was proposed by Kerstein in [5] for non-reacting flow and extended to reactive flow in [6]. It has been discussed in detail in the literature and, therefore, is only briefly summarised here. The overall LEM concept for turbulent reactive flow consists of two concurrent processes representing the respective influences of dilatation-induced advection, molecular diffusion, chemical reactions and turbulent transport. The first process is time advancement of the reactive zero-Mach-number equations on a one-dimensional domain resolving all spatial and temporal scales. The second process, turbulent transport, is implemented using a stochastic sequence of statistically independent stirring events.

The zero-Mach-number equations for reactive flow
We solve the variable density zero-Mach-number equations in one spatial dimension on a fixed grid. The balance equations for species mass fractions and temperature are

$$\rho\frac{\partial Y_s}{\partial t}+\rho u\,\frac{\partial Y_s}{\partial x} = -\frac{\partial j_s}{\partial x}+M_s\,\dot\omega_s,\quad s=1,\,\ldots,\,n_s \tag{1}$$

$$\rho c_p\frac{\partial T}{\partial t}+\rho u c_p\,\frac{\partial T}{\partial x} = \frac{\mathrm{d}p}{\mathrm{d}t}-\frac{\partial q}{\partial x}-\sum_s j_s\,\frac{\partial h_s}{\partial x}-\sum_s h_s\,M_s\,\dot\omega_s, \tag{2}$$

where ρ is the density, u the velocity, j_s the species diffusive flux, M_s the molecular weight of species s, $\dot\omega_s$ the chemical source term of species s, c_p the heat capacity at constant pressure, p the pressure, q the heat flux, and h_s the enthalpy of species s including the heats of formation. In the Zero-Mach number limit the pressure is spatially cosntant and we have a divergence constraint on the velocity

$$\begin{aligned}\frac{\partial u}{\partial x} &= -\frac{1}{\gamma\,p}\frac{\mathrm{d}p}{\mathrm{d}t}-\frac{1}{\rho c_pT}\left\{\frac{\partial q}{\partial x}+\sum_s j_s\,\frac{\partial h_s}{\partial x}\right\}-\frac{1}{\rho}\sum_s\left\{\frac{M}{M_s}\frac{\partial j_s}{\partial x}\right\}+\frac{1}{\rho}\sum_s\left\{\frac{M}{M_s}-\frac{h_s}{c_pT}\right\}\dot\sigma_s\\ &= -\frac{1}{\gamma\,p}\frac{\mathrm{d}p}{\mathrm{d}t}+\mathcal{U}.\end{aligned} \tag{3}$$

Integrating (3) over the whole domain results in an equation for the global pressure change

$$\frac{\mathrm{d}p}{\mathrm{d}t}=\frac{\gamma\,p}{L}\left\{\int_{x=x_1}^{x_1+L}\mathcal{U}\;\mathrm{d}x-(u_2-u_1)\right\}. \tag{4}$$

For periodic or zero-velocity boundary conditions we have $u_1=u_2$ and the last term in (4) vanishes. The density is calculated from the equation of state for an ideal gas $p=\rho\,T\,\sum_s Y_s\,R_s$. It is important to note that similar to a DNS, in the LEM concept equations (1) and (2) need to resolve all spatial scales of a turbulent reacting flow. The velocity u in eq. (1) and (2) represents the flow velocity induced by dilatational effects due to compression, conduction, and chemical reactions as given by (3).

Linear eddy mixing / turbulent transport
In the LEM concept, turbulent advection is implemented explicitly by stochastic eddy events. Each eddy event involves a rearrangement of all scalar quantities using so-called 'triplet maps.' The effect of a triplet map is a three-fold compression of the scalar fields in a selected spatial interval whose size is denoted l. This map increases the scalar gradients within the selected interval, analogous to the effect of compressive strain in turbulent flow, without creating discontinuities. Three parameters are needed to implement the eddy events: eddy size l, eddy location within the domain, and the eddy event frequency. The eddy location is randomly sampled from a uniform distribution, and the eddy size is usually randomly sampled from a given size distribution (e. g., a distributioon based on the Kolmogorov inertial-range scaling). However, due to the low Reynolds number in the calculations reported here, we used a single eddy size equal to the integral length scale l_t. The event frequency per unit length is chosen so that eddy events induce a random walk of fluid parcels whose diffusivity is equal to the turbulent

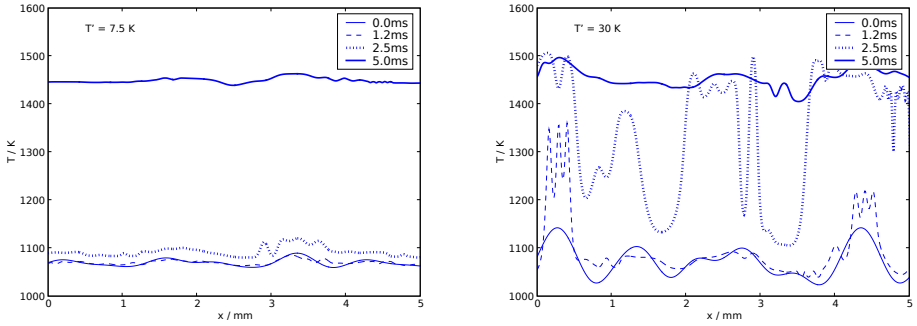

Figure 1: Temperature profiles at different times for $T' = 7.5$ K and 30 K.

diffusivity D_t. l_t and D_t are the required inputs to the single-eddy-size LEM formulation used here. D_t is determined from $D_t = C_D\, l_t u'$ with $C_D = 1/15$.

Numerical implementation
The zero-Mach-number equations are solved numerically using standard second-order finite-difference discretization. No-flux boundary conditions are applied. (Periodic boundary conditions, consistent with the DNS comparison case, will be applied in the future. Results thus far indicate that this change will have negligible effect.) The time integration of the stiff set of equations is performed using the DAE solver IDA of the SUNDIALS package [4]. Thermodynamic and transport properties as well as reaction rates are calculated using the C++ interface of the CANTERA software package [9]. Diffusion velocities are calculated using a mixture-based formulation with variable Lewis numbers for all species.

3 Results and Discussion

We test LEM against some DNS results presented in [3]. Integral turbulent length and velocity scales for the LEM runs are taken from the DNS and are $l_t = 0.34$ m/s and $u' = 0.5$ m/s. A random temperature field with a Passot-Pouquet spectrum is superimposed on the mean temperature field to specify initial temperature inhomogeneities with different R.M.S. values T'. The equivalence ratio of the initially homogeneous H_2-air mixture was 0.1 in all cases. In order to get meaningful statistics comparable to the DNS it is necessary to either perform many different realizations on a small domain or to run a calculation on a domain much larger than the DNS. All the LEM simulations presented here have been run on a domain which size is 50 times the domain size of the DNS (4.1 mm). Detailed investigations on the influence of the domain size on the statistics will be presented in forthcoming studies.

Figure 1 shows temperature profiles at different times for $T' = 7.5$ K and 30 K. The low fluctuations in the first case lead to an almost homogeneous autoignition. From the $T' = 30$ K case it becomes obvious that the large initial temperature fluctuations induce locally different ignition delays between initial minimum and maximum values resulting in large temperature gradients. These temperature gradients are subject to intense turbulent mixing during the 'delay time window.'

Figure 2 shows the time history of heat release rates for four different T' values. Time and heat release rates have been made non-dimensional by the ignition delay time and the peak heat release rate of the homogeneous reactor, respectively. With increasing T', the heat release is spread over a longer time period. Reasonable agreement is obtained between the DNS results of Hawkes et al. [3] and the LEM model for temperature fluctuations $T' = 3.75$ K, 7.5 K, and 15 K, but LEM has a longer ignition delays for the case with the strongest fluctuation, $T' = 30$ K. Note there are some important differences between the DNS and the LEM simulations here. Whereas the DNS represents decaying turbulence, the LEM model mimics a constant turbulence level. Stronger turbulence enhances turbulent mixing resulting

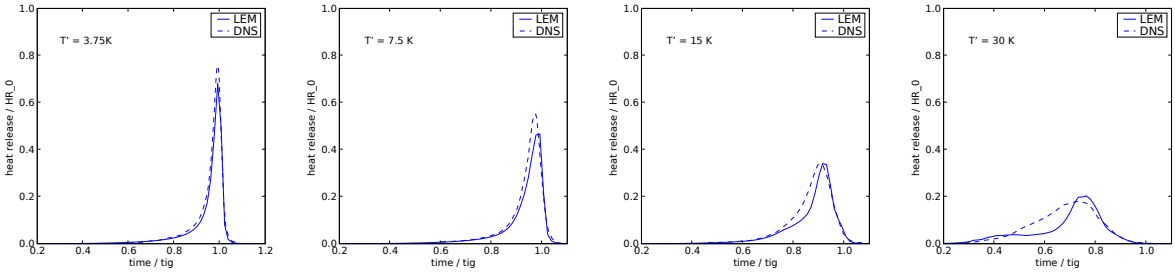

Figure 2: Normalised heat release rates versus non-dimensional time for temperature fluctuations $T' =$ 3.75 K, 7.5 K, 15 K, and 30 K. DNS data are taken from [3].

in an ignition behaviour closer to the homogeneous reactor case. The influence of this difference between the two models will be investigated in further studies. In addition, the reaction scheme taken from Li et al. [8] for the LEM model has a slightly longer ignition delay time of 3.2 ms compared to the 2.9 ms of the reaction scheme used for the DNS. From Figure 2 one can also observe that the total heat release in the LEM model is slightly lower than in the DNS.

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