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MODELLING OF DIESEL SPRAY FLAME UNDER ENGINE-LIKE CONDITIONS USING AN ACCELERATED EULERIAN STOCHASTIC FIELDS METHOD: A CONVERGENCE STUDY OF THE NUMBER OF STOCHASTIC FIELDS

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Introduction

The use of transported Probability Density Function (PDF) methods allows a single model to compute the auto-ignition, premixed mode and diffusion flame of diesel combustion under engine-like conditions [1,2]. The Lagrangian particle based transported PDF models have been validated across a wide range of conditions [2,3]. Alternatively, the transported PDF model can also be formulated in the Eulerian framework [4]. The Eulerian PDF is commonly known as the Eulerian Stochastic Fields (ESF) model. When the same chemical mechanism and micro-mixing model were used, both ESF model and its Lagrangian counterpart generated similar results. The principal motivation for ESF compared to Lagrangian particle based PDF is the relative ease of implementation of the former into Eulerian computational fluid dynamics (CFD) codes [5]. Several works have attempted to implement the ESF model for the simulations of diesel spray combustion under engine-like conditions. The current work aims to further evaluate the performance of the ESF model in this application, with an emphasis on examining the convergence of the number of stochastic fields, n_{sf}. Five test conditions, covering both the conventional diesel combustion and low temperature combustion regimes, are used. The associated ambient conditions and injection characteristics are provided in Table 1.

Table 1: Test cases used in the convergence study.

Case	ρ (kg/m^3)	T (K)	[O_2]	P_{inj} (bar)	D_{inj} (μm)
1	22.8	900	15%	1500	90
2	14.8	800	15%	1400	108
3	14.8	1100	15%	1400	108
4	14.8	800	21%	1400	108
5	14.8	1100	21%	1400	108

Note: ρ, T and [O_2] represent the ambient density temperature and oxygen concentration (by mole fraction). P_{inj} denotes the injection pressure while D_{inj} is the injector hole diameter.

Numerical model formulation

The multi-dimensional CFD spray combustion simulations are carried out using the open-source code, OpenFOAM version 3.0.1. The fuel spray, flow and combustion processes are modelled using the Eulerian-Lagrangian approach. The liquid phase of the diesel fuel is modelled with discrete parcels whose motion is described using the Lagrangian particle tracking approach. The gas phase is described in the Eulerian framework using the unsteady Reynolds-averaged Navier–Stokes equations where the standard k–ε model is implemented for turbulence modelling. The skeletal n-heptane mechanism developed by Liu et al. [5] is used as the diesel surrogate model. The interaction between the turbulence and chemistry is simulated using the ESF method [1]. The turbulent reactive flows are represented by n_{sf} stochastic fields. The governing equation for the n-th stochastic field is

$$\begin{aligned}\bar{\rho} d\phi_\alpha^{(n)} = &-\bar{\rho} u_i \frac{\partial \phi_\alpha^{(n)}}{\partial x_i} dt + \bar{\rho} S_\alpha^{\,r}(\phi^{(n)}) dt + \bar{\rho} S_\alpha^{\,S}(\phi^{(n)}) dt \\ &+ \frac{\partial}{\partial x_i}\left(\Gamma_t \frac{\partial \phi_\alpha^{(n)}}{\partial x_i}\right) dt - \frac{1}{2}\bar{\rho} C_\phi (\phi_\alpha^{(n)} - \phi_\alpha)\omega_t dt \\ &+ \bar{\rho}\sqrt{\frac{\Gamma_t}{\bar{\rho}}}\left(\frac{\partial \phi_\alpha^{(n)}}{\partial x_i}\right) dW_i^{(n)} \end{aligned} \quad (1)$$

where ϕ_α denotes the mass fraction of species (Y_i) or the enthalpy of the mixture (h), and $\phi^{(n)}$ = [$Y_1^{(n)}$, …, $Y_i^{(n)}$, $h^{(n)}$]. $\Gamma_t = \mu_t/\sigma_t$ is the turbulent diffusivity, where μ_t is the turbulent viscosity and σ_t is the turbulent Schmidt number in the transport equations for chemical species or the Prandtl number in the enthalpy equation. $\bar{\rho} S_\alpha^{\,r}(\phi^{(n)})dt$ and $\bar{\rho} S_\alpha^{\,S}(\phi^{(n)})dt$ are the source term increments due to the chemical reactions and the spray evaporation, respectively. The term involving C_ϕ in Equation (1) represents the molecular mixing, which is modelled using the Interaction with Exchange to the Mean model. The mixing constant, C_ϕ value is fixed to two. ω_t is the turbulence frequency obtained from $\omega_t = \varepsilon/k$. $dW^{(n)}$ represents a vector Wiener process that is spatially uniform but different for each field. The Chemistry Coordinate Mapping (CCM) method is coupled with the ESF solver to integrate the source terms due to chemical reactions efficiently. Details about the ESF-CCM method can be found in [1].

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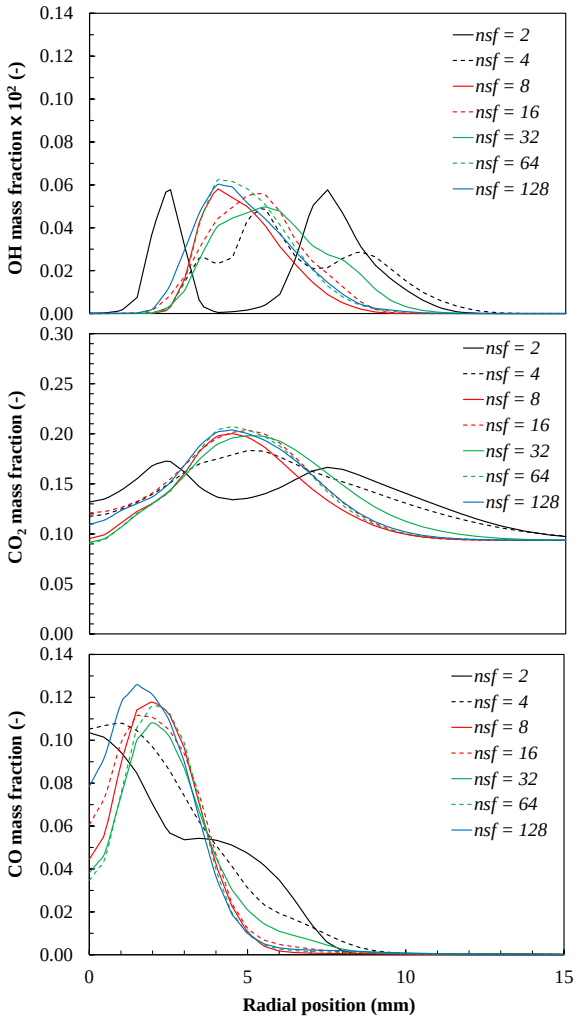

Figure 1: Comparisons of OH mass fraction, CO_2 mass fraction and CO mass fraction using different number of stochastic fields across the diffusion flame.

Results and conclusions

Effects of n_{sf} are evaluated based on combustion characteristics such as ignition delay time and lift-off length. Apart from those, radial profiles of OH, CO and CO_2 mass fractions near the lift-off position and across the diffusion flame are also used to evaluate the effects of n_{sf}. The convergence study is first carried out using Case 1, which is also known as the Spray A case of the Engine Combustion Network. The convergence performance of 2, 4, 8, 16, 32, 64 and 128 stochastic fields is assessed. The use of 2 and 4 stochastic fields unexpectedly predicts reasonable ignition delay time and lift-off length. However, the associated flame structures are consistently wider than those generated using larger n_{sf}. Also, the associated OH and CO_2 profiles from the 2 and 4 stochastic fields show several distinct peaks, indicating that the results are spatially unsmooth. Relative differences (*R.D.*) of peak temperature as well as peak mass fractions of OH, CO_2 and CO are evaluated based on the results generated using 128 stochastic fields. The *R.D.* are computed using *R.D.* = $|\alpha_{nsf,i}-\alpha_{nsf=128}|/\alpha_{nsf=128}$ x 100%, where α represents different combustion properties and i is results calculated using different n_{sf}. It is found that with 8 and more stochastics fields, the *R.D.* remains below 25%.

The convergence study is extended to 800 K and 1100 K at the ambient density of 14.8 kg/m^3. These are used to represent low and high ambient temperature conditions, respectively. The convergence study is carried out for both 15% and 21% O_2 with 8, 16 and 32 stochastic fields. These configurations are selected as they reach a balance between computational efficiency and accuracy. Here, 32 stochastic field results serve as the new base for comparison purposes. In all these configurations, the ignition delay time and lift-off length are identical. Near the lift-off position, the temperature and species concentration fields predicted by 16 stochastics fields are found to converge reasonably well, apart from the CO results in Case 2. Across the diffusion flame, results are generated by all three configurations are close in most of the conditions but those generated by 16 stochastic fields converge better. The associated *R.D.* remains within 25% and 14% for the ambient O_2 of 15% and 21%, respectively. On the other hand, those of 8 stochastic fields have a maximum value of 71% and 21%, respectively.

Results produced by the 16 stochastic fields are next validated using experimental data. It is shown that the ESF-CCM model with 16 stochastic fields reproduces reasonably well the ignition delays and lift-off lengths. The transient development of the spray flame in Case 1 is also predicted. Although further model validation may have to be carried out for a wider range of operating conditions, the current results show that the ESF-CCM model is a promising alternative to modelling turbulence chemistry interaction in diesel engines where multiple combustion modes are observed.

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