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

Pang, Kar Mun; Jangi, Mehdi; Bai, X.-S.; Schramm, Jesper; Walther, Jens Honore

Publication date: 2016

Document Version
Peer reviewed version

Link back to DTU Orbit

Citation (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.
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

K.M. Pang\(^1\), M. Jangi\(^2\), X.-S. Bai\(^3\), J. Schramm\(^1\), J.H. Walther\(^1,4\)

\(^1\)DTU Mechanical Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark
\(^2\)School of Engineering & Information Technology, Murdoch University, 6150 Perth, Australia
\(^3\)Department of Energy Sciences, Lund University, 22100 Lund, Sweden
\(^4\)Computational Science and Engineering Laboratory, ETH Zürich, CH-8092 Zürich, Switzerland

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, \(n_s\). 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>
<thead>
<tr>
<th>Case</th>
<th>(\rho) (kg/m(^3))</th>
<th>(T) (K)</th>
<th>([O_2])</th>
<th>(P_{inj}) (bar)</th>
<th>(D_{inj}) (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>22.8</td>
<td>900</td>
<td>15%</td>
<td>1500</td>
<td>90</td>
</tr>
<tr>
<td>2</td>
<td>14.8</td>
<td>800</td>
<td>15%</td>
<td>1400</td>
<td>108</td>
</tr>
<tr>
<td>3</td>
<td>14.8</td>
<td>1100</td>
<td>15%</td>
<td>1400</td>
<td>108</td>
</tr>
<tr>
<td>4</td>
<td>14.8</td>
<td>800</td>
<td>21%</td>
<td>1400</td>
<td>108</td>
</tr>
<tr>
<td>5</td>
<td>14.8</td>
<td>1100</td>
<td>21%</td>
<td>1400</td>
<td>108</td>
</tr>
</tbody>
</table>

Note: \(\rho\), \(T\) 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 simulation 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 \(k\)-\(e\) 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 \(n_D\) stochastic fields. The governing equation for the \(n\)-th stochastic field is

\[
\overline{\rho} d\phi_n = -\overline{\rho} u_i \frac{\partial \phi_n}{\partial x_i} dt + \overline{\rho} S_e^{(n)} dt + \overline{\rho} S_a^{(n)} dt
\]

where \(\phi_n\) denotes the mass fraction of species \((Y_i)\) or the enthalpy of the mixture \((h)\), and \(\phi^{(n)} = [Y_i^{(n)}, \ldots, Y_i^{(n)}, h^{(n)}]\). \(I_i = \mu_i / \sigma_i\) is the turbulent diffusivity, where \(\mu_i\) is the turbulent viscosity and \(\sigma_i\) is the turbulent Schmidt number in the transport equations for chemical species or the Prandtl number in the enthalpy equation. \(\overline{\rho} S_e^{(n)}\) and \(\overline{\rho} S_a^{(n)}\) are the source term increments due to the chemical reactions and the spray evaporation, respectively. The term involving \(C_k\) in Equation (1) represents the molecular mixing, which is modelled using the Interaction with Exchange to the Mean model. The mixing constant, \(C_d\) value is fixed to two. \(\omega_t\) is the turbulence frequency obtained from \(\omega_t = \epsilon / k\). \(dW^{(n)}\) 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].

\(^c\)Corresponding author: kmpan@mek.dtu.dk
The convergence study is first carried out using 8 stochastic fields. 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 stochastic 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.

**Results and conclusions**

Effects of $n_f$ 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 $n_f$. 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 $n_f$. 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 un-smooth. 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 $R.D. = \frac{|\alpha_{n_f=2} - \alpha_{n_f=128}|}{\alpha_{n_f=128}} \times 100\%$, where $\alpha$ represents different combustion properties and $i$ is results calculated using different $n_f$. It is found that with 8 and more stochastic 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 stochastic 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.

**Acknowledgements**

The authors gratefully acknowledge funding from the Innovation Fund Denmark and MAN Diesel & Turbo A/S through the SULCOR project. The computation was performed using Abisko cluster at High performance Computing Center North (HPC2N).

**References**


