MODELING DIESEL ENGINE COMBUSTION USING FLAMELET/PROGRESS VARIABLE BASED ON OPENFOAM

QIYAN ZHOU[1], YONG QIAN[2], LIKUN MA[3], JIN XIA[4], XINGCAI LU[5]

[1] *Key Lab. for Power Machinery and Engineering of M. O. E, Shanghai Jiao Tong University, 200240 Shanghai, PR China, Zhou_qy@sjtu.edu.cn*

[2] *Key Lab. for Power Machinery and Engineering of M. O. E, Shanghai Jiao Tong University, 200240 Shanghai, PR China, qiany@sjtu.edu.cn*

[3] *Science and Technology on Scramjet Laboratory, National University of Defense Technology, Changsha 410073, China, malikun@nudt.edu.cn*

[4] *Key Lab. for Power Machinery and Engineering of M. O. E, Shanghai Jiao Tong University, 200240 Shanghai, PR China,* xiajinhb@sjtu.edu.cn

[5] *Key Lab. for Power Machinery and Engineering of M. O. E, Shanghai Jiao Tong University, 200240 Shanghai, PR China, lyuxc@sjtu.edu.cn*

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The flamelet/progress variable (FPV) approach was proposed as a model for non-premixed turbulent combustion and gave encouraging simulation results in several combustion environments [1, 2]. In present study, it was employed to model combustion process inside n-heptane fueling conventional compression ignition engine. The flamelet database was constructed on the basis of counter-flow flame configuration using published n-heptane mechanism [3]. The flame equations were solved by FlameMaster [4] in space of mixture fraction defined by Bilger [5] as follows:

$$Z = \frac{2\frac{Y_C - Y_{C,2}}{M_C} + 0.5\frac{Y_H - Y_{H,2}}{M_H} - \frac{Y_O - Y_{O,2}}{M_O}}{2\frac{Y_{C,1} - Y_{C,2}}{M_C} + 0.5\frac{Y_{H,1} - Y_{H,2}}{M_H} - \frac{Y_{O,1} - Y_{O,2}}{M_O}} \qquad (1)$$

where Y_i and M_i were correspondingly mass fraction and molar mass of elements carbon (C), hydrogen (H) and oxygen (O); and subscripts 1 and 2 respectively referred to mass fraction in fuel stream and oxidizer stream. Figure 1 presents temperature profiles in mixture fraction space obtained from flame solutions. The black lines representing fully burning illustrate that maximum temperature of fully burning flame increases as scalar dissipation rate decreasing, while blue lines describe unstable burning and mixing.

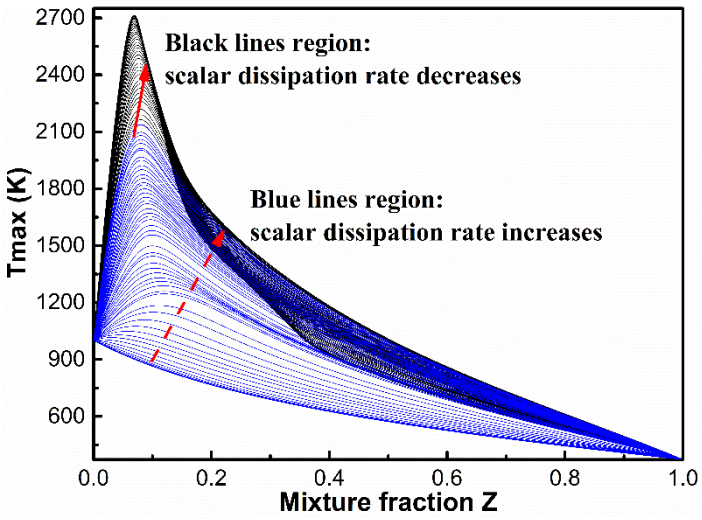

Figure 1: Temperature profile in mixture fraction space

In FPV approach, the flame solutions should be transferred to mixture fraction and progress variable spaces. The following definition of progress variable was used:

$$Y_c = Y_{H_2O} + Y_{CO_2} + Y_{H_2} + Y_{CO} \qquad (2)$$

where Y_i was the mass fraction of species. In order to simplify table look-up procedure, $\mathrm{C} = \frac{Y_c - Y_c^u}{Y_c^b - Y_c^u}$ was introduced as a scaled progress variable to normalize Y_c. The laminar flame solutions were integrated with presumed probability density functions (PDF) to incorporate turbulence-chemistry interaction. For mixture fraction and progress variable, β-PDF and δ-PDF were applied, respectively. The average or filtered quantities were defined as:

$$\tilde{f} = \int_0^1 \int_0^1 f(Z,C)\, \tilde{P}\left(Z;\tilde{Z},\widetilde{Z^{"2}}\right) \tilde{P}\left(C;\tilde{C}\right) dZ\, dC \qquad (3)$$

Besides, the table solution of FPV approach was set to $\tilde{Z} \times \widetilde{Z^{"2}} \times \tilde{C} = 101 \times 41 \times 101$.

The simulations in present work were carried out on basis of open source CFD package-OpenFOAM [6]. Reynolds Averaged Navier-Strokes (RANS) based k-ε model was used for three-dimensional (3-D) turbulent simulation and the Reitz-Diwakar model was chosen to mimic spray atomization and droplet break up. New libraries were created for FPV tabulated approach in framework of OpenFOAM. New solver referred as "sprayEngineFPVFoam" was developed to model diesel engine. The following additional transport equations were added:

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t} + \frac{\partial\left(\bar{\rho}\widetilde{u_j}\tilde{Z}\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\bar{\rho}\left(\widetilde{D} + D_t\right)\frac{\partial \tilde{Z}}{\partial x_j}\right] + \tilde{S}_Z \qquad (4)$$

$$\frac{\partial \bar{\rho}\tilde{Y}_c}{\partial t} + \frac{\partial\left(\bar{\rho}\widetilde{u_j}\tilde{Y}_c\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\bar{\rho}\left(\widetilde{D} + D_t\right)\frac{\partial \tilde{Y}_c}{\partial x_j}\right] + \bar{\omega}_{Y_c} \qquad (5)$$

$$\frac{\partial \bar{\rho}\widetilde{Z^{"2}}}{\partial t} + \frac{\partial\left(\bar{\rho}\widetilde{u_j}\widetilde{Z^{"2}}\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\bar{\rho}\left(\widetilde{D} + D_t\right)\frac{\partial \widetilde{Z^{"2}}}{\partial x_j}\right] + 2\bar{\rho}D_t\left(\frac{\partial \tilde{Z}}{\partial x_j}\right)^2 - C_{d,Z_v}\bar{\rho}\frac{\varepsilon}{k}\widetilde{Z^{"2}} \qquad (6)$$

$$\tilde{\chi} = C_{d,\chi}\bar{\rho}(\varepsilon/k)\widetilde{Z^{"2}} \qquad (7)$$

where mean progress variable source term due to reaction was tabulated and mixture fraction source term ($(\tilde{S}_Z = -\frac{1}{V_c}\sum_p \dot{m}_p N_p)$ introduced by liquid fuel evaporation was modeled referred to Baba et al. [7].

To investigate the capability of FPV approach, general computed combustion characteristics were compared and validated with experiments conducted by authors on a single-cylinder direct-injection and naturally aspirated diesel engine. Figure 2 presents comparison between experimental and calculated in-cylinder pressure trace. It demonstrates that FPV approach can well reproduce the pressure history of engine operating under different conditions. Besides, influence of injection pressure on in-cylinder pressure trend is also precisely predicted. Specifically, peak pressure goes higher as injection pressure increasing.

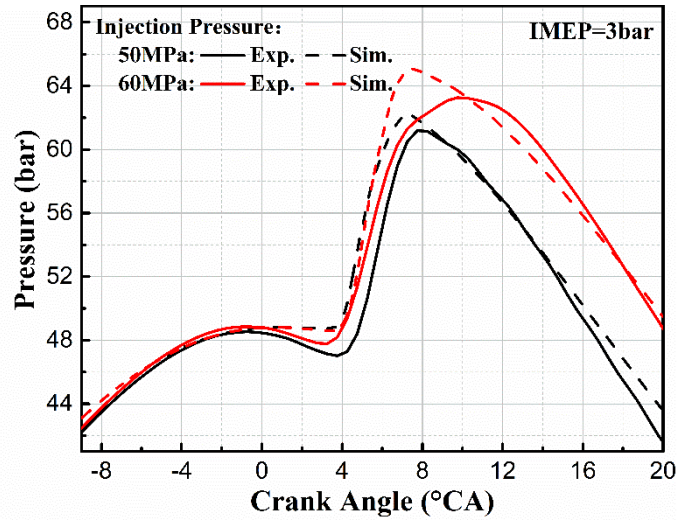

Figure 2: In-cylinder pressure trace

In Figure 3, comparisons of engine ignition delay are shown for all operation loads with injection pressure maintained at 50MPa and 60MPa, respectively. Although negligible ignition delay variations resulted from fixed injection timing, agreement between simulated and measured results is good, which proves the capability of FPV approach to predict the onset of combustion.

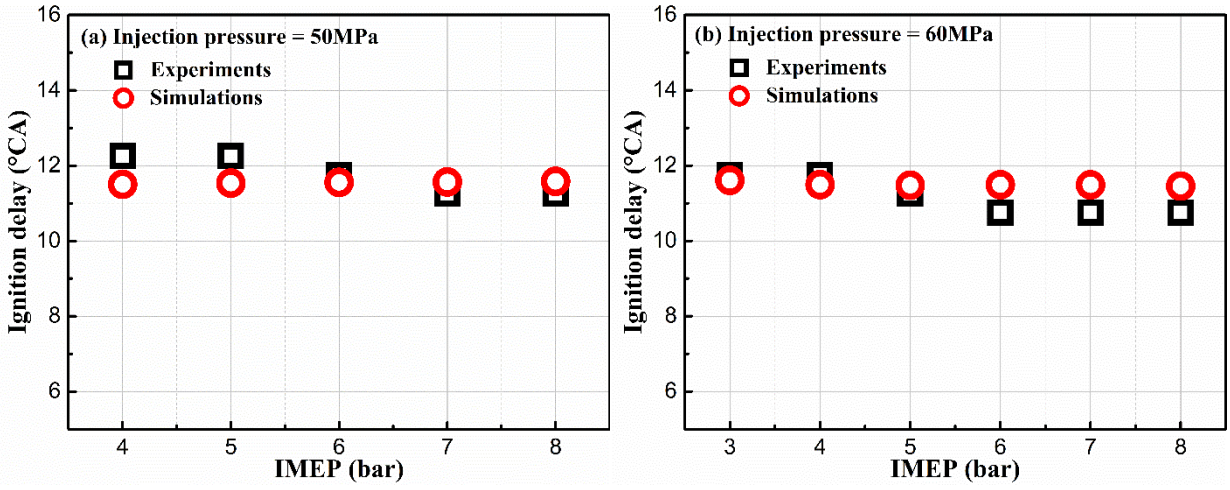

Figure 3: Ignition delay versus IMEP with injection pressure fixed at (a) 50MPa and (b) 60MPa

Figure 4 displays the distribution of progress variable reaction rates in space of scalar dissipation rate approaching ignition.

As time propagating towards ignition, progress variable reaction rate is intensified. In addition, it can also be observed from blue scatters on behalf of the onset of combustion, the ignition occurs in the region with extremely low scalar dissipation rate.

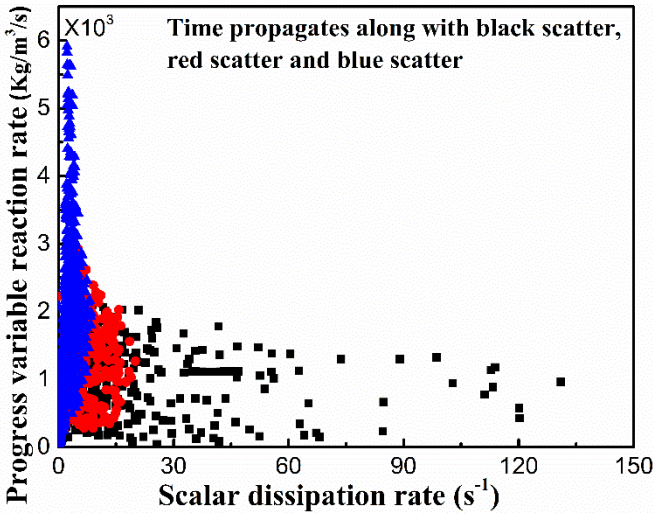

Figure 4: Distribution of progress variable reaction rates with scalar dissipation rates before ignition

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