Testing of a Model for Multi-Dimensional Computations of Turbulent Combustion in Spark Ignition Engines

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ABSTRACT

A turbulent flame speed closure model for multidimensional computations of premixed turbulent combustion is tested against an extensive set of experimental data obtained by various teams employing different methods in combustion bombs. The model correctly predicts the development of the turbulent flame speed, the effects of the initial pressure, temperature, mixture composition, and turbulent length scale on the growth of the flame kernel radius, and the effects of r.m.s. turbulent velocity and burning mixture composition on the rate of the pressure rise; the same value of the only relevant model constant being used for various mixtures. The model is modified and implemented into the FIRE code to compute 3D combustion in an SI-engine. The results agree well with experimental data.

INTRODUCTION

The modeling of combustion is a critical area of multi-dimensional computations of SI engines and this issue has received much attention, recently. Various approaches mentioned elsewhere\(^{(1)}\) have been developed over the past years. The main goal of this work is testing the so-called Turbulent Flame Speed Closure Model (TFSCM) put forward by Zimont\(^{(2)}\). The model is briefly discussed in the first section. In order to clearly assess advantages and drawbacks of the model and to reliably validate it, the focus of testing is placed on turbulent flame development in well-defined simple cases. These tests are summarized in the second section. The third section is devoted to further modifications of this model and 3D simulations of an SI-engine by using the TFSCM.

THE MODEL

Since the TFSCM is discussed elsewhere\(^{(1)-(8)}\), we restrict ourselves to a brief summary of the model. It is based on the widely used assumptions that 1) the state of the gas in premixed flames is completely defined by a single progress variable, \(\tilde{c} = 0\) in the unburned gas and \(\tilde{c} = 1\) in the equilibrium products, and 2) the combustion chemistry can be reduced to a single global reaction. The model gives the following balance equation

\[
\frac{\partial \tilde{c}}{\partial t} + \frac{\partial (\tilde{c} \bar{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \tilde{c} (D_L + D_t) \frac{\partial \tilde{c}}{\partial x_j} \right] + (1)
\]

\[
\frac{\tilde{c} (1 - \tilde{c})}{t_e (1 + D_t / \kappa_b)} \exp \left( -\frac{\Theta}{T} \right) + \rho_u U_t \left\{ \sum_{j=1}^{3} \left( \frac{\partial \tilde{c}}{\partial x_j} \right)^2 \right\}^{1/2}.
\]

Here, \(t\) is time, \(x_j\) and \(u_j\) are the coordinates and flow velocity components, respectively, \(\tilde{c}\) is the gas density, subscripts \(u\) and \(b\) label the unburned and burnt gas, respectively, and both the Reynolds averages denoted by overbars and the Favre averages, such as \(\tilde{\rho} \tilde{c} = \bar{\rho} \bar{c}\), are used. The turbulent diffusivity \(D_t\) and flame speed \(U_t\) are closed as

\[
D_t = D_{t,0} \left[ 1 - \exp \left( -\frac{t}{\tau'} \right) \right], \quad (2)
\]

\[
U_t = A u' \left[ \frac{L}{u' \tau_c} \right]^{1/4} \left( 1 + \frac{\tau'}{\tau} \left[ \exp \left( -\frac{t}{\tau} \right) - 1 \right] \right)^{1/2}. \quad (3)
\]

The time scale \(\tau' = D_{t,0} / u'^3\) controls the development of the turbulent diffusivity. The r.m.s. turbulent velocity \(u' = \sqrt{2k/3}\), integral turbulent length scale \(L = C_D u'^3 / \tilde{c}\), and the steady turbulent diffusivity \(D_{t,0} = C_u k^2 / (\tilde{c} \sigma_c)\) are evaluated using, for example, the standard \(k-\epsilon\) turbulence model\(^{(6)}\). Time-dependent Eq. 3 is based on Eq. 2 which is often used to approximate the development of turbulent diffusivity \(D_t\) in inert flows\(^{(7)}\). The time-behavior of \(D_t\) and \(U_t\) is discussed, in detail, elsewhere\(^{(1)}\). It is associated with the fact that only turbulence scales smaller than the admixture cloud may wrinkle the cloud surface. Then, the effective turbulent diffusivity increases with time as the cloud is spread by diffusion.

The model includes a single unknown input parameter, a constant \(A\) which needs adjustment, and a set of
physico-chemical characteristics, such as molecular heat diffusivity $\kappa$ of the mixture and the mass diffusivity $D_L$ of the deficient reactant, activation temperature $\Theta$ and time scale $t_*$ of a single global combustion reaction. An advanced submodel for evaluating chemical time scale $\tau_c$, affected substantially by the Lewis number $Le = \kappa / D_L$, is discussed, in detail, elsewhere\(^{(5),(6)}\). For lean and stoichiometric mixtures of heavy hydrocarbons, when $Le \geq 1$, the chemical time scale can be evaluated as

$$\tau_c = \frac{\kappa u'}{U_L^2}. \quad (4)$$

The laminar burning velocity $U_L$ is assumed to be known from measurements. The reaction time scale $t_r$ must be calculated so that it yields the known value of $U_L$ when $u' = 0$. It is worth noting that joint variations in $\Theta$ and $t_r$ affect weakly the turbulent combustion rate predicted by the TFSCM, provided that this set of values of $\Theta$ and $t_r$ yield the correct value of $U_L$ when $u' = 0$.

VALIDATION OF THE MODEL

In order to test the TFSCM in well-defined simple cases, we have used the experimental data obtained by four different teams\(^{(9)-(14)}\) in fan-stirred bombs, by the Rouen team\(^{(16)}\) in a bomb with a moving grid, and by Hainsworth in an uniform flow behind a grid (this data was taken from Ref. 16). All these measurements were performed for expanding statistically-spherical flames during a period characterized by a slight or zero pressure rise. Flame kernels were ignited by a spark in homogeneous, isotropic, stationary\(^{(9)-(14)}\) or decaying\(^{(15)}\) turbulence. Groff\(^{(10)}\), Bradley et al.\(^{(12)-(14)}\), Moukalled et al.\(^{(15)}\), and Hainsworth determined flame radii using high-speed Schlieren movies. Karpov and Severin\(^{(9)}\) and Kido et al.\(^{(11)}\) evaluated turbulent combustion velocities by processing the pressure diagrams using the different methods.

All these experiments were modeled by numerically solving the above equations of the TFSCM, written for the spherically symmetry case and supplemented by mass conservation equation, enthalpy balance equation, the standard $k-\epsilon$ turbulence model, the standard thermochemistry for a single reaction, and the ideal gas state equation. The full set of governing equations, boundary and initial conditions, and input parameters are reported, in detail, elsewhere\(^{(1)}\). It is worth emphasizing that we computed all these tests by using the same governing equations and the same value $A = 0.40$ for the only constant of the TFSCM. Since the Schlieren images are commonly associated with the leading edge of turbulent flames, the computed flame radius $\bar{r}_f$ was equal to the radius of the surface where $\bar{c} = 0.1$. The flame speed was calculated as $s_t = d\bar{r}_f / dt$. The methods of processing the computed pressure histories corresponded to the methods employed by Karpov and Severin\(^{(9)}\) and by Kido et al.\(^{(11)}\).

Figure 1 summarizes the results of testing the TFSCM in well-defined simple cases. Here and below, symbols show experimental data with the vertical bars indicating the mean scatter obtained for a set of equivalent runs; whereas curves have been computed. The initial values of r.m.s. turbulent velocity $u'$ and length scale $L$, pressure $P$, temperature $T$, and mixture composition characterized by a fuel and equivalence ratio $F$ are presented in the figure legends and headings. These values, as well as $U_L$, have been taken from the corresponding experimental works.

It is worth noting that the model was developed for computations of turbulent flames; whereas the treatment of spark ignition is not a feature of the TFSCM and a study of this process is outside the objectives of the paper. For this reason, the development of a small initial kernel is not discussed here and certain results presented in Fig. 1 are restricted to relatively large flame radii. In the computations, the spark ignition was simulated by inserting a source term $Q_{ig}$, strongly localized in space and time, into the enthalpy balance equation, this submodel is discussed, in detail, elsewhere\(^{(1)}\). Figure 1b shows that variations in the ignition energy $E_{ig}$ = $\int \int \Delta H_{ig} dx dt$ shift the computed $\bar{r}_f(t)$ along the time axis but the slopes of three-dotted-dashed curves, computed with $E_{ig} = 0.2, 1, \text{and } 10 \text{ mJ}$, are roughly equal for the developed flames. This result implies a weak effect of $E_{ig}$ on the computed flame speed. Similarly, predicted $s_t(\bar{r}_f)$, presented in Fig. 1c, is weakly affected\(^{(1)}\) by the value of $E_{ig}$ The experiments of Bradley et al. show similar trends\(^{(12)}\): $s_t(\bar{r}_f)$, obtained for a set of runs, is roughly the same despite the substantial scatter of the corresponding measured $\bar{r}_f(t)$.

The burning velocities, presented in Figs. 1a-1h, have been computed without any adjustment of $E_{ig}$ and these predictions are controlled by the only model parameter, a constant $A$. However, when using the measured values of $\bar{r}_f(t)$ (see Figs. 1a-1d), we had to adjust $E_{ig}$ in order to match the computed and measured $\bar{r}_f(t)$ curves at a small $\bar{r}_f$ for each set of initial conditions. This method does not hinder a quantitative test of the TFSCM relevant to the flame propagation, rather than a spark ignition. In fact, this method gives more or less reasonable initial conditions for testing the model. This adjustment was necessary due to both 1) the simplifications of the ignition model and 2) the lack of reliable data on the values of $E_{ig}$ in the measurements.

For strong turbulence, the TFSCM cannot predict the constancy or even decrease of the combustion velocity when increasing $u'$ (see crosses in Fig. 1f, or triangles in Fig. 1g, or squares and triangles in Fig. 1h). These phenomena are commonly associated with the stretching of flamelets by turbulent eddies and a method of treating these effects is discussed elsewhere\(^{(4),(5)}\). However, this method involves a second input parameter which should be adjusted for each burning mixture. For this reason, we restrict, here, our discussion to the range of moderate turbulence, that is, the range where combustion velocities increase with $u'$.

Figure 1 shows that, for this moderate turbulence, the TFSCM predicts the experimental data reasonably well. The worst agreement has been obtained for the data of Groff\(^{(10)}\) at $u' = 0.5 \text{ m/s}$ (cf. the dotted-dashed curve
Fig. 1: Testing of the TFSCM for spherically expanding turbulent flames.
and circles in Fig. 1c). However, this disagreement is associated with the modeling of the ignition stage, rather than with the TFSCM. Indeed, for the developed flame, the slope of the measured data approximated by the long-dashed curve is roughly equal to the slope of the computed dotted-dashed curve. This fact implies that the TFSCM predicts a correct flame speed even in this case. For the data of Kido et al.\(^{(11)}\), the predictions are not well enough (see Fig. 1h). This result is associated with the aforementioned stretching effects because, for these very lean mixtures, the existence of the domain of moderate turbulence is unclear. For the very lean methane mixture (cf. the dashed curve and squares in Fig. 1h), the model underestimates combustion velocity but this is associated with the Lewis number effects discussed elsewhere\(^{(8)}\). Finally, the model slightly overestimates combustion velocity for small u'\(^2\)/U\(_L\) (cf. the solid curve and circles in Fig. 1f or the dashed curve and squares in Fig. 1g).

As a whole, bearing in mind the substantial variations in u', L, mixture composition, initial temperature and pressure, experimental setup and methods; Fig. 1 appears to indicate the reasonable accuracy and predictive potential of the TFSCM. These features make the TFSCM particularly interesting for applications to SI-engines. The goal of the following Section is to check the fitness of the model for 3D computations of engines.

**USE OF TFSCM IN SI-ENGINE SIMULATIONS**

**Modifications of the Model**

In order to predict combustion processes in SI-engines, the TFSCM should be modified in order to account for 1) the combustion acceleration due to mixture compression in the cylinder and 2) the inhomogeneity of the burning mixture. To account for these effects, the dependence of the chemical time scale \(\tau_c\) on the mixture composition, pressure \(P\) and unburned gas temperature \(T_u\) must be implemented into the TFSCM. Here, this dependence is modeled through functions of \(\kappa_u(T_u, P)\) and \(U_L(F, T_u, P)\), approximated as

\[
\kappa_u = \kappa_{u,0} \left( \frac{T_u}{T_0} \right)^{1.6} \left( \frac{P_0}{P} \right),
\]

\[
U_L = [B_m + B_2(F - F_m)^2] \left( \frac{T_u}{T_0} \right)^\alpha \left( \frac{P_0}{P} \right)^\beta,
\]

where \(\alpha = 2.18 - 0.8(F - 1), \beta = -0.16 + 0.22(F - 1), B_m = 0.2632 \text{ m/s}, B_2 = -0.8473 \text{ m/s}, T_0 = 298 \text{ K}, \) and \(P_0 = 1 \text{ atm} \). Equation 6 and the above parameters, suggested by Metghalchi and Keck\(^{(17)}\), are widely used to model SI-engines. The equivalence ratio \(F\) can be calculated by solving the standard balance equation for an inert mixture fraction. Then, the chemical time scale is determined from Eqs. 4-6 with \(\kappa_u\) being roughly independent of the equivalence ratio. This method involves neither new unknown input parameters nor new model constants but the laminar burning velocity is the key input parameter of the model.

Second, Eq. 2 gives zero \(D_1\) at the ignition moment. This simplification is consistent with the effect of the turbulent diffusion on the inhomogeneities created by the combustion but ignores the effect of the turbulent diffusion on the inhomogeneities in the unburned mixture. The simplest way to reduce this inconsistency is to use Eq. 2 only inside the flame (where \(\hat{c} > 0\)), whereas \(D_1 = D_{1,0}\) if \(\hat{c} = 0\), as was done in this work.

**3D Computations of an SI-Engine**

To test the TFSCM, the experimental data\(^{(18)}\) obtained in a 4-valve SI-engine have been used. Before, this engine was extensively computed by one of the authors\(^{(19)}\) using the FIRE code\(^{(20)}\). Since the only change made in this work was the replacement of the Magnussen model by the TFSCM, whereas all other parameters (the engine geometry, the computational mesh, the numerical method, the boundary and initial conditions, the input parameters, the ignition submodel, the time step, etc.) were exactly the same, we restrict ourselves to a brief discussion of the computations.

The main characteristics of the engine are presented in Table 1. The calculations were performed for a single cylinder and were started at 133 crank angle degrees (CAD) after top dead center (TDC), which corresponded to the open exhaust valve. The geometry and the computational mesh containing 75000 cells are shown in Fig. 2. The computations of the exhaust, the intake and compression stroke were performed using the original FIRE code\(^{(20)}\) that solved the averaged Navier-Stokes equations, the balance equations for the thermal energy, inert and fuel mass fractions (the fuel was initially deposited at a very rich pre-vaporized mixture behind the intake valves), and the \(k - \epsilon\) balance equations with a dilatation term.

The ignition submodel employed in the original code\(^{(20)}\) was used without modifications. The input parameters of this submodel corresponded exactly to the computations of Grantner et al.\(^{(19)}\) The combustion was modeled by Eqs. 1-6; but the time-dependent turbulent diffusivity controlled by Eq. 2 was used only inside the flame, whereas \(D_1 = D_{1,0}\) in the domain where \(\hat{c} = 0\). The mean progress variable was defined through the fuel mass fraction \(Y_f\) as follows \(\hat{c} = 1 - Y_f/Y_{f,u}\).

The equations of the TFSCM were implemented straightforwardly into the subroutines computing the mean reaction rate and heat and mass diffusivities. On the one hand, this method results in an increase in the computational time because certain calculations duplicate each other. On the other hand, it is more reliable and its use appears to be a reasonable first stage of the code modifications. When employing the TFSCM in the SI-engine computations, we faced no numerical problems.

Figures 3-5 show spatial distributions of the gas flow velocity, turbulent kinetic energy, and equivalence ratio, computed for the non-reacting flow at the ignition moment. The spatial distributions of the mean temperature, computed at 20, 10 and 0 CAD before TDC, are shown in
Fig. 6. These results indicate that the TFSCM predicts a thick turbulent flame brush. The model predictions are compared with the available experimental data\(^{(18)}\) in Fig. 7. It is worth emphasizing that the value of the only TFSCM constant \(A = 0.40\) is the same as that used in the bomb simulations discussed above and no other input parameters have been adjusted. For the flame propagation phase, the agreement between the measurements and computations is quite reasonable. For the end phase of the combustion process, the computations slightly underestimate the burnt fuel mass fractions. This disagreement does not appear to be a drawback of the TFSCM, because the end phase of the combustion process is substantially influenced by near-wall phenomena, whereas the model does not account for near-wall effects.

CONCLUSIONS

For a set of experiments performed by various teams at different well-defined conditions, the TFSCM reasonably well predicts the growth of the flame radius and the development of the flame speed at various initial pressures, temperatures, mixture compositions, r.m.s. turbulent velocities \(u'\) and length scales \(L\), as well as the rate of the pressure rise in bombs at various \(u'\), \(L\), and mixture compositions. All these predictions were made with the same value of the only relevant model constant.

The TFSCM was implemented into the FIRE code. The modified code was employed to compute 3D turbulent combustion in an SI-engine and the results agree reasonably well with the available experimental data.

ACKNOWLEDGMENTS

This work has been supported by the Chalmers Combustion Engine Research Center (CERC) and Volvo.

REFERENCES

Table 1: Engine characteristics

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<th>Characteristic</th>
<th>Value</th>
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<tr>
<td>Bore</td>
<td>83 mm</td>
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<tr>
<td>Stroke</td>
<td>90 mm</td>
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<tr>
<td>Connecting rod length</td>
<td>139.5 mm</td>
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<tr>
<td>TDC clearance height</td>
<td>1.0 mm</td>
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<tr>
<td>Engine speed</td>
<td>1800 r.p.m.</td>
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<td>Mean piston speed</td>
<td>5.4 m/s</td>
</tr>
<tr>
<td>Injected fuel mass</td>
<td>4.4 mg/cyl./cycle</td>
</tr>
<tr>
<td>Fuel type</td>
<td>octane</td>
</tr>
<tr>
<td>Lower calorific value, $q_f$</td>
<td>44000 kJ</td>
</tr>
<tr>
<td>Ignition duration</td>
<td>4 CAD BTDC</td>
</tr>
</tbody>
</table>

Fig. 2: Engine geometry and computational mesh

Fig. 3: Mean gas flow velocity at the ignition time

Fig. 4: Turbulent kinetic energy at the ignition time

Fig. 5: Equivalence ratio at the ignition time

Fig. 6: Evolution of the temperature field.

Fig. 7: Fuel consumption history.