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Ignition and Combustion Model for Explicit Flame Tracking

S. Frolov[1,2], V. Ivanov[1,2], B. Basara[3], P. Priesching[3], M. Suffa[3]

[1] *N.N. Semenov Institute of Chemical Physics, 4, Kosygin Street, 119991 Moscow, Russia*

[2] *Center for Pulse Detonation Combustion, 4, Kosygin Street, 119991 Moscow, Russia*

smfrol@chph.ras.ru

[3]*AVL LIST GmbH, 1, Hans-List Platz, A-8020 Graz, Austria, branislav.basara@avl.com*

Abstract – A new ignition/combustion model for explicit flame tracking has been developed and tested against various internal combustion (IC) engines and operation conditions. The model is physically grounded and contains only one fitting constant with a default value of unity. The model is based on the understanding that turbulent flame evolution involves two major stages: initial and regular. Combustion at the initial stage is mostly governed by local physicochemical properties of the reactive mixture and by small-scale turbulence, whereas combustion at the regular stage is largely governed by large-scale turbulence.

1. Introduction

When simulating combustion in IC engines and confined/vented vessels numerically, pressure evolution in an enclosure appears to depend on an adopted ignition and combustion models and various model parameters like ignition kernel size, ignition duration, flame surface density, characteristic time and length scales, etc. Since such parameters are not known *a priory*, there is usually a need in tuning the ignition and combustion models against available measurements. The situation is complicated by the necessity of considering turbulence–chemistry interaction, which is a problem itself. In view of it, the predictive capabilities of numerical simulations of ignition and combustion in enclosures are currently based largely on the available experimental data. Hence, well-grounded attempts of reducing the dependence of computational models on empirical information could be considered as steps forward in the combustion theory.

The objective of this work is to develop the ignition/combustion model for explicit flame tracking (FT) in the turbulent flow field of premixed fuel and air (Frolov et al., 2013) and to validate the models against available experimental data.

2. Ignition/combustion model

The new ignition/combustion model is based on differences in physics of flame propagation immediately after ignition and at a finite time after ignition. At the ignition stage, the flame is known to develop from the small-size discharge channel through the phase of mixture ignition and flame formation. Combustion at this stage (from now on called initial stage) is mostly governed by local physicochemical properties of the reactive mixture and by small-scale turbulence. In the fully developed turbulent flame (regular stage properly treated in the FT model, see below), combustion is largely governed by large-scale turbulence. Of course, there is a need in proper tailoring the initial and regular stages of flame propagation. Physically, the turbulent flame in enclosures like IC engine is the highly wrinkled laminar flame. Therefore, one can use the classical expression for the turbulent flame velocity u_t at such conditions:

$$u_t = u_n \sqrt{1 + \frac{\nu_t}{\nu_m}} \tag{1}$$

where u_n is the local instantaneous laminar flame velocity, ν_t is the turbulent (eddy) viscosity, and ν_m is the molecular viscosity. The turbulent (eddy) viscosity entering Eq. (1) is by the order of magnitude a product of the pulsating velocity u' and the characteristic turbulence length scale l,

$$\nu_t \sim u' l \tag{2}$$

At the initial stage of flame propagation, including ignition stage, when the flame kernel is small (the initial size of flame kernel is d_{ign}), the flame front can be wrinkled only by the low-energy flow velocity pulsations u'_u with the length scale l_u less than the characteristic size (diameter) of flame kernel $d_f \geq d_{ign}$. In this case, all velocity pulsations of the larger scale play the role of the mean convective flow displacing the flame kernel as a whole. Since at the initial stage the flame size in URANS simulations is about grid spacing, it appears that u'_u and l_u are in general the unresolved pulsating velocity and length scale (this is the reason for the subscript *u*, which means "unresolved"). Thus at the initial stage of flame propagation (at time $t>t_{ign}$, t_{ign} is the time of ignition triggering), the turbulent (eddy) viscosity in Eq. (2) should be estimated based on the time dependent unresolved pulsating velocity $u'_u(t)$ of scale $l_u(t)$ lower than the instantaneous equivalent flame kernel diameter d_f, i.e.,

$$\nu_t(t) \sim u'_u(t) l_u(t) \text{ at } l_u(t) \leq d_f(t) \tag{3}$$

From now on, for the sake of simplicity, we will skip time dependence in the formulae, however keeping it always in mind. Without loss of generality, one can assume that $l_u \approx d_f$ and rewrite Eq. (3) as

$$\nu_t \sim u'_u d_f \tag{4}$$

To estimate u'_u, one can use the approach suggested by Girimaji (2006) who introduced the ratio of unresolved-to-total turbulent kinetic energies $f_k = k_u / k$, where $k_u \approx (3/2)u'^2_u$ is the unresolved turbulent kinetic energy and $k = (3/2)u'^2$ is the resolved turbulent kinetic energy, whereas u'_u and u' are the unresolved and resolved pulsating velocities, respectively. According to Girimaji and Hamid (2005), the ratio of unresolved-to-total turbulent kinetic energies depends upon the characteristic grid spacing Δ as

$$f_k \sim \frac{1}{\sqrt{C_\mu}} \left(\frac{\Delta}{\Lambda} \right)^{2/3} \tag{5}$$

where

$$\Lambda = k^{3/2} / \varepsilon \tag{6}$$

is the integral length scale of turbulence (ε is the turbulence dissipation rate), and $C_\mu = 0.09$ is the constant in the $k-\varepsilon$ model of turbulence. According to Basara et al. (2011), relationship (5) can be applied to time dependent conditions once f_k is larger than the ratio between unresolved and total kinetic energy. Because we are interested in the unresolved turbulence on

scale d_f rather than of scale Δ one can rewrite Eq. (5) as

$$f_k \sim \frac{1}{\sqrt{C_\mu}}\left(\frac{d_f}{\Lambda}\right)^{2/3} \tag{7}$$

Now, taking into account that $C_\mu = 0.09$ and using Eqs. (4) and (6), one finally obtains for the turbulent flame velocity at the initial stage $u_{t,ini}$ of Eq. (1) the following relationship:

$$u_{t,ini} = u_n\sqrt{1+\frac{\nu_{t,ini}}{\nu_m}} \sim u_n\sqrt{1+1.5\frac{\varepsilon^{1/3}d_f^{4/3}}{\nu_m}} \tag{8}$$

where index *ini* denotes the properties at the initial stage of flame propagation. Note that all quantities entering Eq. (8) are treated as local instantaneous values directly ahead of the flame. To make this relationship quantitative, it is instructive to introduce the empirical parameter p^2 under the square root of Eq. (8):

$$u_{t,ini} = u_n\sqrt{1+1.5p^2\frac{\varepsilon^{1/3}d_f^{4/3}}{\nu_m}} \tag{9}$$

It can be expected that in general parameter p^2 is a function of fuel type and local instantaneous conditions in the vicinity to the ignition site (e.g., equivalence ratio, temperature and pressure). This function can be found by fitting computational and experimental data for different conditions (see below).

Note that Eq. (9) has been derived using Eqs. (4) and (7) determining the properties of unresolved turbulence. Physically, when the initial stage of turbulent flame propagation ends, the flame velocity can be determined based on the resolved velocity pulsations and integral turbulence length scale, e.g., by one of the correlations available in the literature for turbulent flame propagation. One of such correlations is the expression of Guelder (1990):

$$u_t = u_n\left[1+0.62\left(\frac{u'}{u_n}\right)^{1/2}\left(\frac{u_n l}{\nu}\right)^{1/4}\right] \tag{10}$$

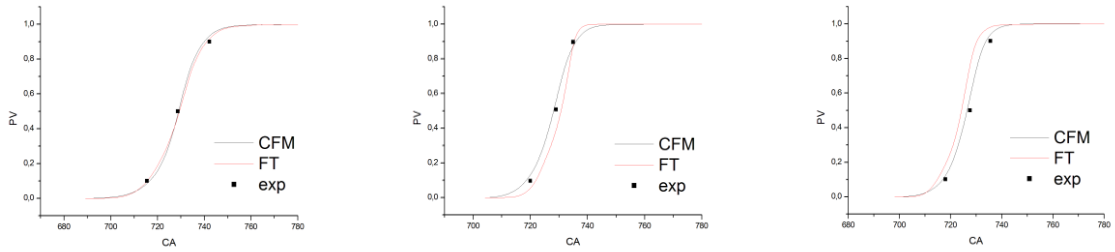
This constraint can be used as tailoring condition between the initial and regular stages of flame propagation. By other words, the turbulent flame velocity in the turbulent combustion model can be calculated as:

$$u_t = \begin{cases} u_n\sqrt{1+1.5p^2\dfrac{\varepsilon^{1/3}d_f^{4/3}}{\nu_m}} & at \quad u_{t,ini} < u_t \\ u_n\left[1+0.62\left(\dfrac{u'}{u_n}\right)^{1/2}\left(\dfrac{u_n l}{\nu}\right)^{1/4}\right] & at \quad u_{t,ini} \geq u_t \end{cases} \tag{11}$$

To find parameter p^2 entering Eq. (9), we have made a number of calculations for different IC engines at different loading conditions. The resultant relationship is:

$$p(u_n) = \alpha\left[-0.2 + 4.04\exp\left(-4.405u_n\right) + 0.47\exp\left(-0.465u_n\right)\right] \tag{12}$$

where α is the fitting constant with the default value $\alpha = 1$. Thus, the new ignition/combustion model for explicit flame tracking contains only one fitting constant (α) at a given ignition kernel diameter d_{ign}.



1500rpm_2bar 1500rpm_WOT 3000rpm_WOT

Figure 1: Comparative performances of the new ignition/combustion model (black curves) and standard CFM model (red curves) in terms of the Progress Variable vs. Crank Angle dependences against experimental points for a particular IC engine at different loading conditions.

Results and Discussion

Figure 1 shows the performance of the model in terms of the Progress Variable vs. Crank Angle curves (predictions) and points (measurements) for a particular IC engine at different load conditions. The red curves correspond to the new ignition/combustion model with the default value of $\alpha = 1$ and $d_{ign} = 3$ mm. The black curves correspond to the standard CFM model and are obtained as the best fit to the experimental points using the flame surface density varying within an unphysically large range of values. Clearly, the new model provides satisfactory predictions.

Concluding Remarks

A new ignition/combustion model for explicit flame tracking has been developed and tested against various IC engines and operation conditions. The model is physically grounded and contains only one fitting constant with a default value of unity. The model is based on the understanding that turbulent flame evolution involves two major stages: initial and regular. Combustion at the initial stage is mostly governed by local physicochemical properties of the reactive mixture and by small-scale turbulence, whereas combustion at the regular stage is largely governed by large-scale turbulence.

References

1. S.M. Frolov, V.S. Ivanov, B. Basara, M. Suffa. Numerical simulation of flame propagation and localized preflame autoignition in enclosures. *Journal of Loss Prevention in the Process Industries*, 26: 302-309, 2013.
2. S. Girimaji, and K.S. Abdul-Hamid. Partially–Averaged Navier–Stokes Model for Turbulence: Implementation and Validation, AIAA Paper 2005-0502, Reno, NV, 2005.
3. S. Girimaji. Partially-Averaged Navier-Stokes Model for Turbulence: A Reynolds-Averaged Navier-Stokes to Direct Numerical Simulation Bridging Method. *Journal of Applied Mechanics*, Vol. 73: 413-421, 2006.
4. Basara, B., Krajnovic, S., Girimaji, S. and Pavlovic, Z.: Near-Wall Formulation of the Partially Averaged Navier–Stokes Turbulence Model. *AIAA Journal*, Vol. 49(12), pp. 2627-2636, 2011.
5. Ö.L. Guelder. Turbulent premixed flame propagation models for different combustion engines. *Proc. Comb. Inst.* 23: 743-750, 1990.