NUMERICAL SIMULATION OF PROPANE–AIR TURBULENT FLAME ACCELERATION IN STRAIGHT TUBES OF DIFFERENT LENGTH

S. M. Frolov[1], V. S. Ivanov[1], V. A. Smetanyuk[1], B. Basara[2], and M. Suffa[2]

[1]N. N. Semenov Institute of Chemical Physics
 Russian Academy of Sciences
 Moscow, Russia

[2]AVL LIST GmbH
 Graz, Austria

The objective of the study outlined in this paper was to develop the computationally efficient algorithm for multidimensional numerical simulation of initial stages of deflagration-to-detonation transition (DDT) in gaseous explosive mixtures. The new algorithm is based on the Flame Tracking (FT) method implemented into the AVL FIRE code solving the Reynolds Averaged Navier–Stokes equations by the control-volume technique. The FT methodology has been applied to the two-dimensional (2D) numerical simulation of flame acceleration in straight smooth-walled tubes of different length. The predicted flame acceleration dynamics was compared with available experimental data for the stoichiometric propane–air mixture and satisfactory agreement was obtained.

Introduction

Numerical simulation of flame acceleration in long tubes is a complex problem involving flame ignition, various flame instabilities, preflame turbulence generation, turbulence–flame interaction, preflame reactions, etc. There exist many combustion models both for laminar and turbulent flows. If the chemistry is fast as compared to mixing,

the Spalding Eddy-Break-Up model can be used [1]. It is simple but has a limited range of validity. There is a whole class of statistical combustion models (based on the formalism of probability density functions) with probabilistic representation of turbulence and its interaction with chemistry [2]. Despite many attractive features, this approach is still not capable of operating with complex chemistry due to inadequate CPU requirements. Moreover, such approaches do not resolve different scales in the turbulent flow and their energy content. Instead, all scales are treated indifferently whereas their effect on combustion and flame is different. Nevertheless, these approaches look very promising for treating autoignition problems. The other class of models deals with a flamelet approach [3]. In this approach, the instantaneous flame is assumed to consist of localized reactive sheets, which are transported by the flow and wrinkled by turbulent eddies. The flamelet approach is applicable when the characteristic turbulent scales are larger than a typical flame thickness. This condition is satisfied in many practical situations including frontal combustion in piston engines. The flamelet models are usually based on the flame surface density concept or apply probability density functions. One of the most attractive flamelet models is based on the balance equation for the flame surface density. This equation governs the transport of the mean reactive surface by the turbulent flow and includes physical mechanisms responsible for flame surface area production and destruction.

The approach supposed herein for treating the frontal combustion is also based on considering the flame surface area. However, to speed-up calculations, instead of solving the partial differential equation for the flame surface density, it implies tracing of the mean reactive surface and application of the laminar/turbulent flame velocity concepts.

Flame Tracking Method

The approach outlined below will be referred to as the subgrid model of laminar/turbulent combustion. The flame surface shape and area are found based on the Huygens principle: Each elementary portion of the flame surface displaces in time due to burning of the fresh mixture at local velocity u_f (normal to the flame surface) and due to convective motion of the mixture at local velocity V. In case of laminar flame, the

local instantaneous velocity u_f is equal to the local laminar burning velocity u_n, whereas in case of turbulent flame, it is equal to the local turbulent flame velocity u_T. The local instantaneous convective velocity V can be calculated using a standard computational fluid dynamics (CFD) code solving a set of gasdynamic equations.

In the theory of turbulent combustion, there are many correlations between u_T and u_n. One of classical correlations is Shchelkin formula [4]:

$$u_T \approx u_n \sqrt{1 + \frac{u'^2}{u_n^2}} \qquad (1)$$

where u' is the local turbulence intensity, related to the turbulent kinetic energy or to pulsating velocity correlations. Instead of Eq. (1), one can use other available correlations for the turbulent flame velocity. Thus, for laminar/turbulent flame tracking, there is a need in calculating the local instantaneous laminar burning velocity u_n. This task can be solved separately for mixtures of different compositions, including the effects of mixture dilution with combustion products, at different pressures and temperatures with due regard for flame stretching and other relevant phenomena. The values of u_n can be stored in look-up tables.

Within this approach, local instantaneous energy release rate due to frontal combustion $\dot{Q}_f$ can be calculated based on the estimated instantaneous flame surface area S_f and local flame propagation velocity u_f:

$$\dot{Q}_f = Q \sum S_{f_i} u_{f_i}$$

where Q is the combustion heat; S_{f_i} is the ith flame segment surface area which is calculated directly from geometrical considerations; and summation is made over all flame segments in a computational cell.

Thus, the subgrid model of turbulent premixed combustion does not differ much from that of the laminar premixed combustion, except for using u_T instead of u_n. Moreover, the formulae like Eq. (1) are asymptotically valid for the subgrid model of laminar combustion (when $u' \to 0$, $u_T \to u_n$). It stands to reason that the turbulent combustion model will be also valid for laminar combustion as a limiting case. This is one of model advantages. This feature will allow using the same model to calculate the initial laminar flame kernel growth from the spark ignition with continuous transition to turbulent combustion. The

subgrid combustion model under consideration does not contain tuning parameters (some parameters can be introduced with the equations replacing Eq. (1)). This is the other important model advantage.

It is expected that the accuracy of the computational results will be mainly affected by the turbulence model used. The main problem in implementing such a combustion model into a CFD code is the development of an efficient algorithm for "mean" flame-shape tracking inside computational cells. This algorithm should meet the constraints on the flame-front continuity, connectivity, etc., and the constraints on the CPU time consumption.

The 2D FT method has been developed and implemented into AVL FIRE code [5]. Within the FIRE, Reynolds averaged Navier–Stokes equations are solved in a general curvilinear nonorthogonal coordinate system by the finite-volume method.

Look-up Tables of Laminar Burning Velocity

As mentioned above, the FT algorithm should be supplemented with the database of tabulated laminar burning velocities u_n. Such a database was developed for air mixtures of methane, ethanol, propane, n-heptane, iso-octane, and n-decane in the wide ranges of initial temperatures, pressures, equivalence ratios, and the degree of exhaust gas recirculation (for automotive applications). The look-up tables contain information on flammability limits to identify the conditions of flame quenching. For obtaining the value of laminar burning velocity a one-dimensional (1D) problem of steady-state laminar premixed flame propagation has been solved using code [6]. In the code, the following set of equations is solved numerically:

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right) - c\rho_0 u_n\frac{\partial T}{\partial x} + \Phi = 0\,;$$

$$\frac{\partial}{\partial x}\left(\rho D_j\frac{\partial Y_j}{\partial x}\right) - \rho_0 u_n\frac{\partial Y_j}{\partial x} + w_j = 0\,,\quad j = 1, 2, \ldots, N\,,$$

(2)

where $-\infty < x < +\infty$ is the coordinate; T is the temperature; Y_j is the mass fraction of the jth species in the mixture; N is the total number of reactive species; ρ is the density; c is the specific heat at constant

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Table 1 Overall reaction mechanism of hydrocarbon fuel oxidation

No.	Reaction
1	$C_nH_mO_l + [0.5(n-1) + 0.25m]O_2 \rightarrow nCO + 0.5mH_2$
2	$H_2 + H_2 + O_2 \rightarrow H_2O + H_2O$
3	$CO + CO + O_2 \rightarrow CO_2 + CO_2$
4	$CO + H_2O \leftrightarrow CO_2 + H_2$
5	$H_2O + M^a \leftrightarrow R^b + R + M$
6	$R + H_2 + H_2 + O_2 \leftrightarrow R + R + R + H_2O$

[a] M is any third species.
[b] R is the generalized radical.

pressure; λ is the thermal conductivity; D_j is the molecular diffusion coefficient; Φ is the rate of chemical energy release; and w_j is the rate of change of the jth species mass fraction in the ith reaction:

$$w_j = G_j \sum_{i=1}^{M} (\nu'_{ij} - \nu_{ij}) A_i T^{n_i} \exp\left(\frac{E_i}{R^0 T}\right) \prod_{k=1}^{N} \left(\frac{\rho Y_k}{G_k}\right)^{\nu_{ik}}$$
$$(j = 1, 2, \ldots, N) \quad (3)$$

In Eq. (3), M is the total number of chemical reactions; R^0 is the universal gas constant; G_j is the molecular mass of the jth species; A_i, E_i, and n_i are the preexponential factor, activation energy, and temperature exponent, respectively; and ν_{ij} and ν'_{ij} are the stoichiometric coefficients for reactants and products, respectively.

The set of Eqs. (2) is supplemented with the validated overall reaction mechanism [7] of hydrocarbon fuel oxidation (Table 1) and with the equation of state:

$$p = \rho R^0 T \sum_{j=1}^{M} \frac{Y_j}{G_j}$$

where p is the pressure. The boundary conditions used in [6] are:

$$x \rightarrow -\infty; \qquad T = T_0, \qquad Y_j = Y_{j0} \qquad (j = 1, 2, \ldots, N);$$
$$x \rightarrow \infty; \qquad \frac{dT}{dx} = 0, \qquad \frac{dY_j}{dx} = 0 \qquad (j = 1, 2, \ldots, N).$$

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Table 2 Example of look-up table for laminar burning velocity u_n (in cm/s) in the stoichiometric propane–air mixture

p, MPa	T, K				
	300	450	600	750	900
0.1	39	78	143	247	451
0.3	28	55	102	178	306
1.0	19	35	64	112	191

Table 2 shows the example of look-up tables for the laminar burning velocity in the stoichiometric propane–air mixture for the initial temperatures and pressures ranging from 300 to 900 K and from 1 to 10 bar, respectively. When using such a look-up table in the FT method, one needs to interpolate u_n.

Results of Calculations

The 2D FT method has been used for calculating flame propagation in straight rectangular 40×40 mm smooth-walled channels 2.6, 3.5, 5.1, and 6.1 m long with one closed and one open end filled with the stoichiometric propane–air mixture at normal initial conditions as used in experiments [8].

Figure 1 compares the results of calculations with the experiments in terms of the time histories of the distance traveled by the flame. Solid curves correspond to the predicted results whereas the dashed curves correspond to the measurements. The walls of the channel were assumed isothermal ($T_w = 293$ K). At the open end, a constant-pressure ($p_0 = 0.1$ MPa) boundary condition was applied. The stoichiometric propane–air mixture was assumed initially quiescent at $T_0 = 293$ K and $p_0 = 0.1$ MPa. The initial flame kernel was taken as a circle 1 mm in radius with the center located 1 cm from the closed end-wall at the symmetry plane (similar to experimental ignition conditions). The turbulent flame velocity was modeled by the Shchelkin formula (Eq. (1)). The laminar burning velocity u_n was linearly interpolated using the data of Table 2. Turbulence was modeled by the standard k–ε
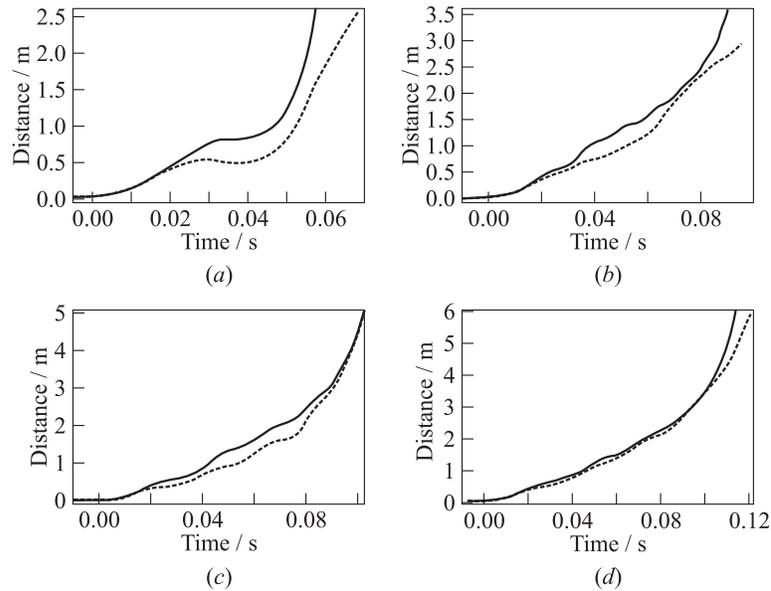
Figure 1 Comparison between predicted (solid curves) and measured [8] (dashed curves) distances traveled by the flame vs. time in 40×40 mm straight channels of different lengths filled with the stoichiometric propane–air mixture: channel length 2.6 m (a), 3.6 (b), 5.1 (c), and 6.1 m (d)

model. The computational grid was uniform with square cells 2×2 mm. The flame front in a computational cell was normally represented by no less than 15 segments. As seen from Fig. 1, the predicted flame front trajectories agree satisfactory with the measurements despite the 2D representation of essentially three-dimensional (3D) phenomena in the experiments. It is worth noting that the numerical simulation is capable of adequate predicting the effect of various pressure waves on flame motion which is obvious from simultaneous appearance of crests on the curves.

Differentiation of solid curves shown in Fig. 1 allows obtaining the local instantaneous visible velocities of flame propagation. As an example, Fig. 2 shows the variation of visible flame velocity with distance in the tube 6.1 m long. Towards the end of the tube, the visible

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flame velocity is seen to increase above 400 m/s. Flame acceleration is not monotonous. The periodic drops and humps in the visible flame velocity are caused by flame interactions with compression/rarefaction waves reflected from the open and closed ends of the channel. Such interactions result not only in flame deceleration/acceleration, but also in the variation of flame shape. Figure 3 shows the shapes of the flame at different stages of its propagation in the 6.1-meter tube. Clearly, flame–pressure wave interactions result in drastic changes of the mean flame shape. Very similar qualitative and quantitative findings are reported in [8].
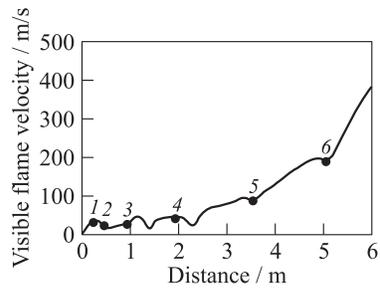
Figure 2 Predicted flame propagation velocity in the 6.1-meter tube. Black dots denote locations with different flame shapes shown in Fig. 3
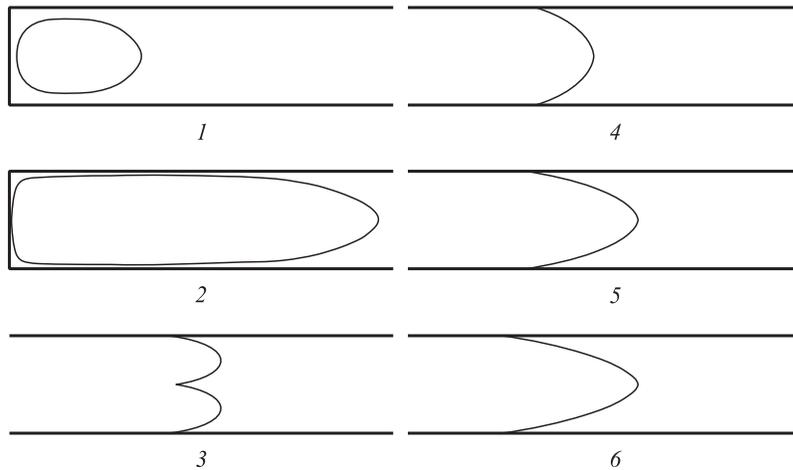
Figure 3 Snapshots of mean flame shapes at different locations in the 6.1-meter tube shown by black dots in Fig. 2

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It is worth noting that the FT method avoids numerical smearing of the flame front: the combustion products are separated from the fresh mixture by a single computational cell in which flame segments are located.

Concluding Remarks

An FT method for simulating laminar/turbulent combustion in channels and enclosures has been developed and tested at 2D computational examples with propane–air flame acceleration in straight rectangular channels of different length. The calculations showed that the method is capable of quantitatively describing the temporal dynamics of accelerating flames including local instantaneous flame propagation velocity, flame–pressure wave interactions, and flame shape variation. The developed methodology can be readily applied for studies of flame propagation in internal combustion engines and various industrial burners as well as for studies of explosion safety issues.

Acknowledgments

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