# Performance of Presumed PDF Approach to Model Slow and Fast Flames

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In the frames of PDF approach in turbulent combustion simulations it is necessary to know local chemical kinetics parameters to evaluate mean reaction rate of chemical reaction. In many cases this knowledge appeared to be the most important issue to correctly reproduce characteristic behavior of a combustion process. The problem here is connected with the fact that for an effective use of 'presumed' PDF approach a one-step Arrhenius-like expression for chemical reaction rate is preferable. Therefore the possibility to exploit more accurate methods (such as detailed or multi-step reduced schemes) seems to be hardly useful. From other side the scattering of kinetics data available in the literature raises a question of an adequate choice of appropriate data.

In the present paper we propose an alternative approach of such data generation. Effective Arrhenius reaction rate can be extracted using the Zeldovich description for the planar flame with one-step overall chemical reaction. The reaction rate parameters in Zeldovich model should be chosen to describe the behavior of the real laminar flame with detailed chemical reaction mechanism. The problem of extraction of the basic flame properties including effective reaction rate parameters from data on computed laminar burning velocities was investigated in [1]. It was shown that for the reaction in each particular mixture composition the effective reaction order, activation energy, and pre-exponential factor could be extracted. Introduction of these effective parameters into Zeldovich model for the planar laminar flame would result in the similar behavior of the model and of the real flame with detailed chemical kinetic mechanism. It may be suggested that application of these effective parameters of reaction rate into PDF reaction model in turbulent combustion simulations should be appropriate.

In the present work an attempt is made to incorporate the effective kinetic data from model [1] into turbulent combustion model exploiting presumed β-PDF approach (COM3D code [2]). The code is tested then against experimental data [3]. The tests addressed characteristic features of turbulent flame propagation in hydrogen-air mixtures. The experiments were carried out in a combustion tube (DRIVER facility). The tube was a cylindrical channel with ring-shaped obstacles inside. The tube diameter was 174 mm, its length was 12.2 m. The obstacles' blockage ratio is equal to 0.6 in all the tests; the obstacle spacing is 174 mm (equal to the tube diameter). Uniform premixed hydrogen-air mixtures were tested. Weak electric spark was used for mixtures ignition. One of the important observation obtained in the course of those experiments includes the fact, that the flames can propagate either in subsonic or in supersonic regimes. The threshold between them is extremely sharp and the switch between regimes occurs with small changes in mixture composition (e.g., from 10% to 10.5% vol. of hydrogen in air).

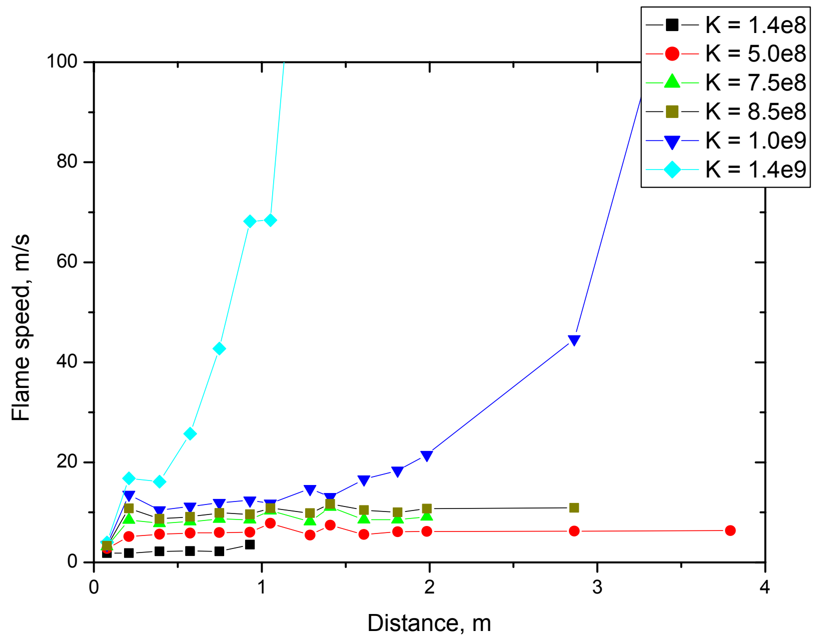


Figure 1. Influence of pre-exponential factor value on flame acceleration distance.

Simulations with COM3D were made using the geometry corresponding to that in the tests. Calculations were made with on a mesh of $10^6$ mesh points. Effective reaction rate parameters were determined for each particular mixture on the basis of the approach of [1]. Effect of reaction rate parameters on behavior of turbulent flames was studied in a series of calculations. It was found that small changes in kinetic parameters lead to sharp changes in flame acceleration behavior (Figure 1), e.g., change of the pre-exponential factor from $1.0 \cdot 10^9$ to $8.5 \cdot 10^8$ suppresses flame acceleration and prohibits the development of the fast (supersonic) combustion regime. Such behavior qualitatively describes the sharp changes in the character of the flame acceleration observed in the experiments with small changes of the mixture compositions.

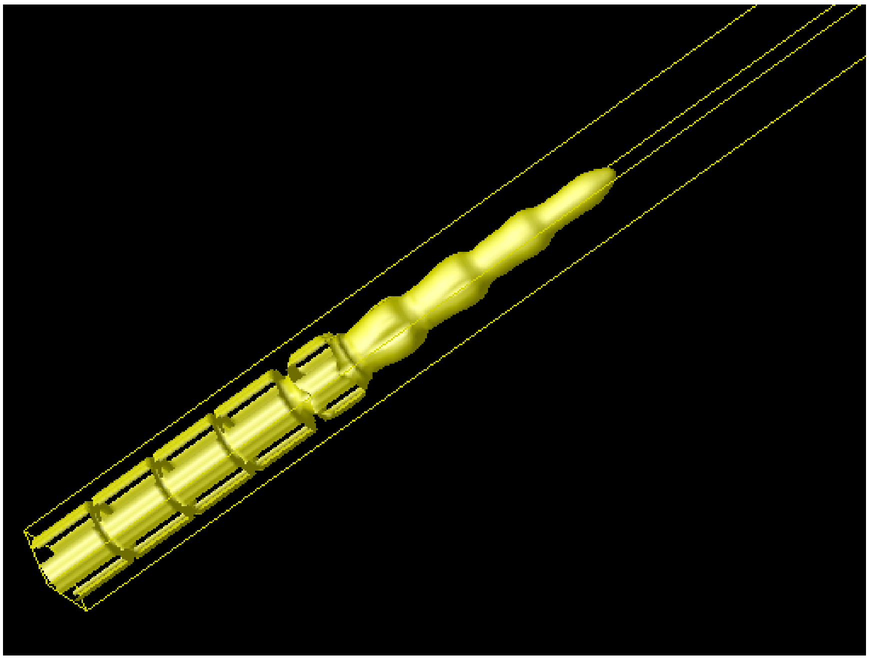

Figure 2. Temperature isosurface (T = 1100 K) of developing flame in hydrogen-air mixture 13% vol. Fragment of about 2 m long of the modeled combustion tube is shown.

The proposed model demonstrated its ability to reproduce main characteristic features of the fast accelerating flames in tubes (Figure 2), including slow acceleration at the initiation stage, elongation of the flame kernel in the stage of acceleration and propagation in ‘choked’ regime at later stage. Comparison of the flame speed and pressure histories with experimental data demonstrated good correspondence. In case of slow flames events of local quenching were detected. The existence of such events is confirmed by experimental observations of the lean mixture combustions and remains an important feature for the adequate combustion description.

An Influence of heat loses on flame acceleration was considered as well. Advantages and limitations of the proposed combustion model are discussed.

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