Test of extended Eddy Break Up model in simulations of turbulent H_2-air combustion

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Abstract

The results of numerical simulation of turbulent hydrogen-air combustion using extended EBU model are presented and compared with experimental data with the aim to define the space of mixture and environment parameters where the simple turbulent combustion models could be used for the calculation of accelerated flames in obstructed areas.

Introduction

Development of simplified models for description of turbulent combustion is of interest when solutions are necessary in practical computing times. Depending on purpose of calculations, type of the flow, and the quantities to be predicted a balance between cost and potential benefit can be achieved by a choice of the model. One of the important practical problems is an estimation of severity of an explosion process under given geometrical configuration, scale, and composition of combustible mixture. Such estimates are required for industrial safety applications ranging from offshore platforms to the containment of a nuclear power plant. The problem is even not to predict details of turbulent flame propagation under given initial conditions, but rather to give estimations for the maximum possible flame speeds and the corresponding level of overpressures which might be generated during explosion.

The most simple and least expensive modeling approach combines k-ϵ model for turbulence and eddy-break-up model for chemistry. This approach has demonstrated its capabilities (e.g., [1, 2]), and it has been shown that further improvement of EBU model are possible and required. Extension of EBU proposed in [4, 3] appeared to be rather promising.

Present work is a continuation of the work cited above on the use of simple and extended EBU models with the aim to study systematically the combustion behavior of lean hydrogen-air mixtures. The results of numerical modeling are compared with experimental data to define the space of mixture and environment parameters where the simple turbulent combustion models could be used for the calculation of accelerated flames in obstructed areas.

Experimental data

Two types of experiments were used for testing the turbulent combustion model. The first type of tests is experiments carried out in a cylindrical combustion tube of 12 m length and an inner diameter equal to 35 cm, closed at both ends. The combustion tube was equipped with pressure transducers spaced 1 m apart along the total length of the tube. The instrumentation included also time-of-arrival diagnostics using infrared photodiodes spaced 1 m apart as well. Annular obstacles with circular openings were located inside the tube. In all tests the distance between obstacles was kept constant and equal to 50 cm. The experiments were performed for BR (blockage ratio) equal to 0.30, 0.45, 0.60 and 0.90, (series with BR equal to 0.75 is underway) while the H_2 concentration was varied from 20% to 10%.

The second type of tests is experiments on hydrogen-air-steam combustion at large scale [5, 6]. The tests were made in RUT 2200 facility: large multi-compartment concrete building. This test series included hydrogen-air-steam combustion experiments with lean and nearly stoichiometric hydrogen concentration and steam content ranging from 6 to 45%. Detailed data on different combustion modes including slow (shock-less) deflagration and fast turbulent deflagration are available.

Data on turbulent flame propagation in a long channel of the facility (2.5×2.3 m in cross-section and ≈ 34.6 m long with obstacles BR equal to 0.3) were simulated in the present work. Two experiments from this series STH 6 and STH 9 were chosen. These two experiments exhibit different modes of flame

Table 1: Experimental conditions

Test	Average concentration H_2%, vol. (dry)	Average concentration H_2O%, vol.	Maximum flame speed, m/s
STH 6	29.6	45.0	780
STH 9	10.1	6.6	250

propagation involving different physical phenomena, appearing to be a good benchmark for numerical model under consideration. In the first test 'sonic' (or 'choking') deflagration regime was identified with the maximum velocity achieved about 800 m/s, and in the second one the slow deflagration was observed with maximum flame speed about 250 m/s. Initial conditions of the tests are listed in Table 1.

Numerical model

Numerical code used for simulation is a 3D unsteady compressible Navier-Stockes solver exploiting standard $k-\epsilon$ model of turbulence and modified Eddy-Break-Up model [4, 3] implemented on a rectangular equidistant grid.

Modified EBU model is an extension taking into account difference between the movement of flamelets and the turbulence itself. Authors of the model showed that the mean reaction rate strongly depends on the ratio of turbulent kinetic energy k to laminar flame velocity U_L (when $k^{1/2}$ is of order of U_L, i.e., when reaction rate is defined not only by turbulence, but also influenced by flamelets properties, which are related to U_L).

Following [3] the modified formula for mean reaction rate of α-component with mass fraction $\widetilde{Y_\alpha}$ reads as

$$\widetilde{w_\alpha} = -\frac{C'_{EBU}}{\tau_t}\left(1 + \frac{4.4}{1+3.2\frac{k^{1/2}}{U_L}}\right)\widetilde{Y_\alpha}\left(1 - \frac{\widetilde{Y_\alpha}}{Y_\alpha^0}\right),$$

here τ_t is characteristic turbulent time (integral turbulence time-scale), which comes from turbulence model, and in our case it is simply k/ϵ. C'_{EBU} is a model constant and require either further modeling or can be fixed using experimental data.

In the limit when $k^{1/2} \gg U_L$ the extended model is reduced exactly to classic Eddy-Break-Up model, i.e., this model can be regarded as an extension of EBU model toward the flames with lower turbulence intensities. The region of parameters where characteristic chemical time τ_c is of order of τ_t is not covered by the model, therefore one can expect that the model will be valid for wrinkled flames only, and not for thickened and thick flames.

Results and discussion

Simulations of medium scale tests (combustion tube) showed that the classic EBU has serious problems to describe the flame propagation at low velocities, which can be related to the assumptions made in EBU formulation. E.g., in the 12 m long tube experiments with BR equal to 30% for the concentrations below 12% H_2 the model does produce wrong flame velocities for the any value of C_{EBU}.

Simulations of the tube experiments with modified EBU model gave remarkable results: all of the experiments (where data were available) were reproduced with good accuracy using close values of $C'_{EBU} = 5-8$. Table 2 presents the adjusted values of C'_{EBU} constant found in attempts to obtain the best coincidence between recordings of photo-diodes and pressure transducers and their numerical analogs. Full experimental test matrix includes also combustion tests with hydrogen concentration equal to 10% H_2. However, all the attempts to simulate these experiments were not successful.

If one would try to classify all these experiments depending on phenomena watched, the following regimes can be outlined:

fast acceleration with following deflagration-to-detonation (DDT) transition (typical flame velocities before DDT 1200 m/s, e.g., test 20% H_2 - BR 0.30);

Table 2: Values of C'_{EBU} constant in simulation of combustion tube experiments

Blockage	Hydrogen concentration, vol. %			
ratio	20%	15%	12%	11%
0.30	6.0	6.0	4.9	5.5
0.45	6.0	6.0	5.0	5.5
0.60	6.0	6.0	no data	no data
0.90	no data	8.0	7.0	7.0

fast acceleration and then propagation in 'sonic' regime (typical velocities 600 m/s - 700 m/s, e.g., test 15% H_2 - BR 0.60);

acceleration with moderate rate up to the end of the tube (typical velocities 400 m/s - 500 m/s, e.g., test 12% H_2 - BR 0.60);

unstable regime, characterized by short initial acceleration phase followed by local quenching with a series of possible reignitions (typical velocities < 200 m/s, e.g., test 10% H_2 - BR 0.30).

In the result of simulation it was found that only experiments referring to one of first three types can be simulated successively, while the experiments with local quenching appeared to be not reproducible with the adopted combustion model. It can be easily explained taking into account that the model does not have any mechanism for quenching. Remaining in the frames of this classification the following remarks can be made from this consideration: for all experiments with characteristic velocities above 200 m/s the combustion model appeared to be valid, and hence the assumption that $Da = \tau_c/\tau_t < 1$ for these types should be valid as well. For the cases of lean mixtures with hydrogen concentrations less than 10% the model loses its validity either due to violation of $Da < 1$ condition or due to another reasons.

On the basis of the results obtained in calculations it is possible quantitatively to outline the region of parameters where combustion model remains valid. In addition, the common statement concerning the EBU model as a model which is valid only in a very small domain of parameters requires definitive understanding what does it mean 'very small' from the point of view of practical calculations.

Usually accepted (e.g., [7]) that the region of interest for spark ignition engines can be limited by the turbulence Reynolds numbers between 10 and 10^4 and Damköhler numbers between 10^{-4} and 1. For industrial application in large scales this region can be expanded toward higher turbulence Reynolds numbers up to values of the order of 10^6.

In the calculations turbulence Reynolds number $Re_t = u'l_t/\nu$ can be estimated as $\tau_t k/\nu$ (here ν is molecular viscosity), and Damköhler number Da as τ_c/τ_t, here τ_c is characteristic chemical time. Definition of τ_c implies the knowledge of the chemical properties of the mixture and therefore brings some uncertainties in its estimation. Assuming the following approximation of laminar flame velocity $U_L = (\sigma^2\nu(T_{max})/\tau_c)^{1/2}$, where σ denotes expansion ratio and $\nu(T_{max})$ is molecular viscosity taken at maximal temperature, τ_c can be estimated if laminar flame velocities are known. Burning velocities of hydrogen-air mixtures were intensively studied (e.g., [8]) and different approximate formulas are available.

Estimation of the domain limits where modified EBU produces satisfactory results give the following values: $10^2 < Re_t < 10^6$ and $0.08 < Da < 8 \cdot 10^{-4}$. This domain covers almost whole region of interest in industrial applications, excluding relatively narrow part of thickened flames where $1 < Da < 0.1$, and provide therefore a good basis for numerical simulations of the processes involving all types of wrinkled flames.

The validity of the model and the adjusted value of C'_{EBU} was proved in simulations of large-scale tests. In this set of calculations the geometry of the facility was approximated by cubic numerical grid with relatively high degree of detailization (cell size 12.5 cm; grid $44 \times 50 \times 501 \approx 1,100,000$ cells). In the calculations conditions were supposed to be uniform with the values equal to their average meanings.

Comparison of the simulation results and corresponding measured values demonstrates good agreement in the details of the process development: flame acceleration in the obstructed channel, and the following propagation with the varying flame speed in other parts of the facility.

Summary

Comparison of experimental and calculated results demonstrated that the extended model can be used for the channel-like combustion simulations for fast deflagrations before DDT, in the 'choking' regime and for medium-slow flames (above 100 m/s) for a range of mixture compositions and details of obstruction. The validity domain of extended EBU model covers the all kinds of wrinkled flames in the reacting flows with $Re_t = 10^2 - 10^6$ and $Da = 0.08 - 8 \cdot 10^{-4}$. Compared to standard EBU, the extended one gives a possibility to use fixed C'_{EBU} constant for modeling of combustion processes in a wide range of propagation speeds and mixture reactivities. This allows safety related calculations to be made and estimates of severity of explosion processes to be obtained. Such a calculations are able to describe dominant effects of scale, geometrical configuration, and mixture composition on the resulting explosion mode. Improvement of eddy-break-up model broadens the frames of its applicability and makes it possible to use extended model for the description of relatively wide class of processes having practical interest.

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