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CHEMISTRY-TURBULENCE COUPLING IN A MODEL OF INHOMOGENOUSLY PREMIXED COMBUSTION

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Abstract: Results of work on an extension of the turbulent flame speed model used for a mathematical description of partially premixed combustion are presented. The approach is based on the concept of internal coupling between the turbulence of the mixed fuel and oxidizer stream with the reaction progress variable. The model after implementation has been calibrated and tested on a BERL benchmark experiment.

Keywords: premixed combustion, turbulence, progress variable, BERL combustion chamber

1. Introduction

An enhancement of results of the numerical investigation of the BERL combustion chamber, which have recently been shown in an internal report [1], have informed us precisely about some discrepancies in the foundations of the turbulence-flame-speed model, for a detailed description of a premixed turbulent flame. These discrepancies are seen especially when the field distribution of the basic unknowns is qualitatively compared with the experiment. Differences have also been observed in the distribution of particular reactions components. It has also been found in [1], that the primary sources of these imperfectios of the contemporary CCD (Computational Combustion Dynamics) models is due to the lack of proper coupling of the reaction process with the turbulence evolution. Even if there is a weak turbulence-chemistry coupling, the chemistry-turbulence coupling is usually omitted or treated indirectly. Apart from this, sometimes [2, 3], the chemistry-turbulence coupling is understood to be completely indirect, based on the *turbulent temperature* and energy equation only. It has already been proposed by Ochrymiuk [4] that a full coupling of the chemistry turbulence type, should include the influence of the reaction progress variable on the change of the effective viscosity of the mixture. Unfortunately, there is no confirmation of the Ochrymiuk type of coupling.

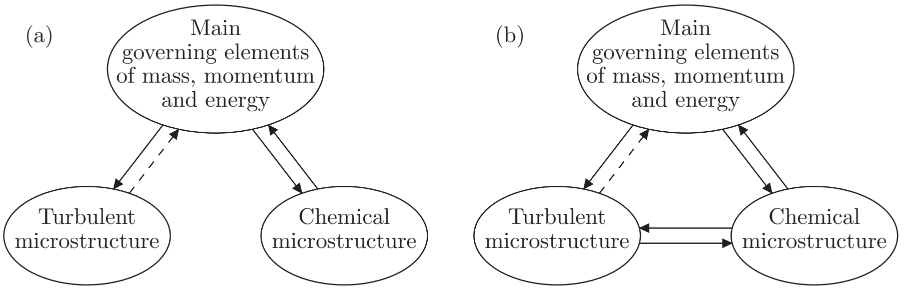

Figure 1. Scheme of the classic (a) and proposed (b) modes of chemistry-turbulence coupling

In this respect, the paper presents an original type of coupling of the chemical process with the mixture flow. The basic assumption of the present work is that the combustion process should be modeled in terms of a single (transport-like) evolution equation for a reaction progress variable, c. This model is significantly more efficient in technical applications than a multistep reaction mechanism with the turbulent and global-kinetic rate coefficients [5]. The reaction process variable, defined as the normalized mass fraction of products ($c=0$ in the unburnt mixture, $c=1$ in the products), may influence the turbulent momentum transport also by its spatial gradients. In other words, the spatial gradients of c may be a factor that strongly determines the evolution of turbulent kinetic energy through the change of its sources. This coupling allows for a direct influence of the combustion process on turbulent energy and momentum transport, not only via temperature, as it is classically stated. In order to check and calibrate the model, numerical results should be compared with benchmark experimental data. In our case, detailed data of a BERL experiment have been used for the comparison [1] of our model with the inhomogeneously premixed combustion process.

2. A combustion model coupled with the turbulence kinetic energy equation

In the presented model, only one differential equation is directly stated to determine the progress of the combustion process:

$$\frac{\partial}{\partial t}(\rho c)+\frac{\partial}{\partial x_j}(\rho v_j c)=\frac{\partial}{\partial x_j}\left(J_j^c\right)+\rho S_c, \tag{1}$$

where c is the reaction progress variable defined as follows:

$$c=\frac{\sum_{i=1}^{n} Y_i}{\sum_{i=1}^{n} Y_{i,ad}} \tag{2}$$

with n denoting the number of products, Y_i – the mass fraction of i – components, Y_{ad} – the mass fraction of the component i after adiabatic, stechiometric combustion. Further, J_j^c – denotes the progress flux, usually defined as:

$$J_j^c=\frac{\mu_t}{\mathrm{Sc}_t}\frac{\partial c}{\partial x_j}, \tag{3}$$

where μ_t is the so-called turbulence viscosity of the mixture, Sc_t – the turbulent Schmidt number, which denotes a dimensionless coefficient of the *progress diffusity.*

The most important element of the evolution equation (1) is a source term, ρS_c, which directly depends on the gradient of the reaction progress variable [2]:

$$\rho S_c = \rho_u V_t |\bigtriangledown c|. \tag{4}$$

In Equation (4), V_t is the turbulent flame speed which describes the average velocity with which the flame brush moves in the normal direction of the flame surface, towards the reactants.

Numerous closures for flame speed, V_t, are to be found in the literature. Therefore, in the work [1], a comprehensive analysis of most of the verified closures has been done. In particular, three closures have been included:

- the Zimont closure (present in the FLUENT code [6]),
- the Liu-Ziegler-Len closure (implemented to the solver by subroutines),
- the Peters closure (implemented to the solver by subroutines).

The results of this analysis, according to [1], indicates slight discrepancies between the above closures, although with substantial differences in comparison with the experiment. It is in agreement with Dinhelacker *et al.* [2] and Karcz [1] that the Lin-Zieler-Len closure gives the least divergent results. Therefore, the Zimont closure has been chosen for the present analysis, in the following form:

- turbulent flame speed

$$\frac{V_t}{V_l} = 0.52 \cdot \mathrm{Pr}^{0.25} \cdot \mathrm{Re}_t{}^{0.25} \cdot \left(\frac{u'}{V_l}\right)^{0.5}, \tag{5}$$

- molecular Prandtl number

$$\mathrm{Pr} = \frac{\mu \cdot c_p}{\lambda}, \tag{6}$$

- turbulent Reynolds number

$$\mathrm{Re}_t = \frac{\rho u' l_t}{\mu}, \tag{7}$$

- turbulent lenght scale

$$l_t = C_D \frac{u'^3}{\epsilon}, \tag{8}$$

- root mean square of velocity fluctuation u',
- laminar flame speed V_l.

According to the basic model assumption, the direct chemistry-turbulence coupling can be properly modeled if the gradient of the progress variable is added to the sources, thus leading to more intensive evolution of the turbulent kinetic energy, k. Thus, the evolution equation for k has the following extended form:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho v_j k) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + \rho S_k. \tag{9}$$

The source of the turbulent kinetic energy rate is proposed to be:

$$\rho S_k = C_c \rho |\bigtriangledown c|. \tag{10}$$

The free parameters C_c need calibration in a benchmark experiment. Therefore, in the present paper, we will focus on the prediction of a universal value of the C_c coefficient and its interpretation.

3. Numerical calculation

In a BERL combustion chamber, natural gas with the following chemical compositions:

- $X_{CH_4} = 0.966$
- $X_{C_2H_6} = 0.017$
- $X_{C_3H_8} = 0.001$
- $X_{CO_2} = 0.001$
- $X_{N_2} = 0.013$

has been burnt with oxides containing two components:

- $X_{O_2} = 0.21$
- $X_{N_2} = 0.79$

In Figure 2, a detail the FVM discretization grid is shown. The burner contains 24 radial holes for fuel supply at an inlet temperature of $T = 312$K and atmospheric pressure. The computation domain is descretized with a total of 130830 non-equidistant finite volumes. The computations are carried out three-dimensionally for a 15 degree *slice* of the burner.

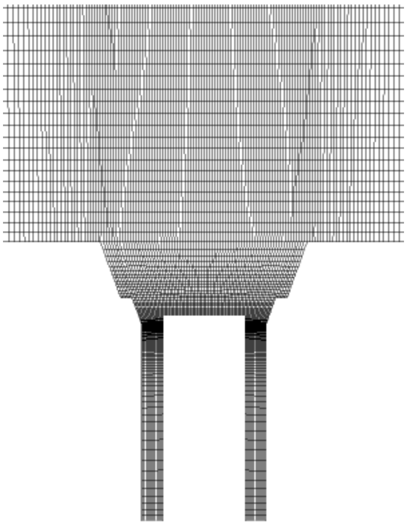

Figure 2. The FVM grid details of BERL burner

Results of numerical calculations obtained for the Zimont closure and the additional term of the chemistry-turbulence coupling in Equation (9) are presented below. The free parameter C_c has been defined as a multiplication of the A constant and the specific heat of the mixture, c_p. To achieve a correct calibration procedure, four series of calculations have been made with the value A equal to 0.01, 0.1, 0.5 and 2.0. The results with a value of $A = 0.1$ are presented in Figures 3–7 below. These show the axial velocity, circumferential velocity and mass fraction of CO_2 and oxygen, O_2. These results have been compared with experimental data for three different cross-sections of a BERL chamber, $x = -0.027$, 0.109 and 0.343m.

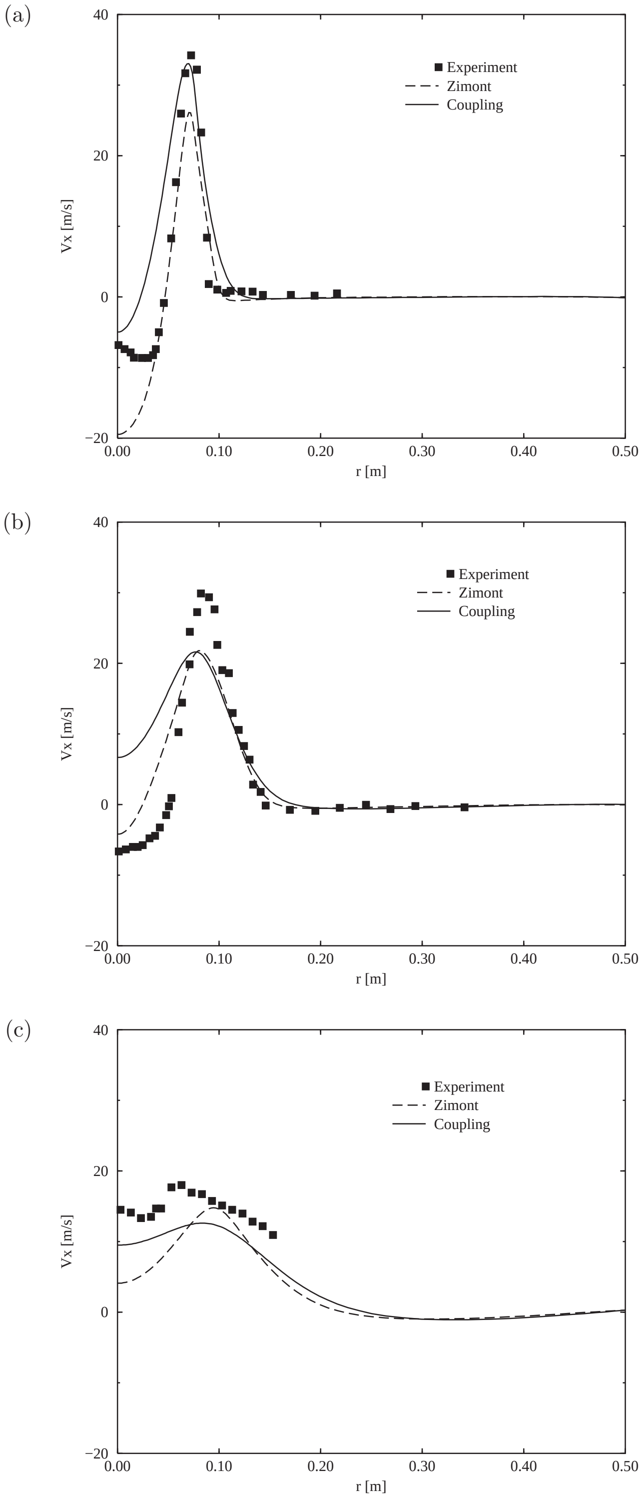

Figure 3. Profiles of the axial velocity component: (a) $x = -0.027$, (b) $x = 0.109$, (c) $x = 0.343$

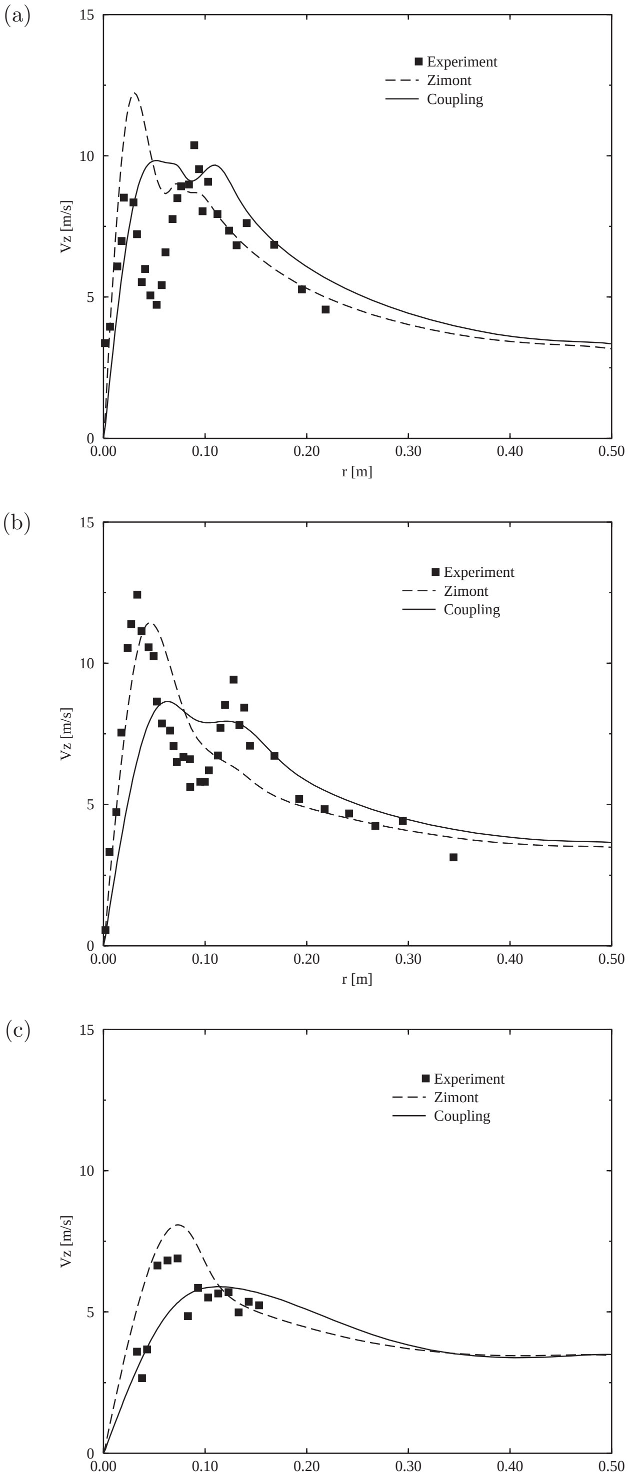

Figure 4. Profiles of the circumferential velocity component: (a) $x = -0.027$, (b) $x = 0.109$, (c) $x = 0.343$

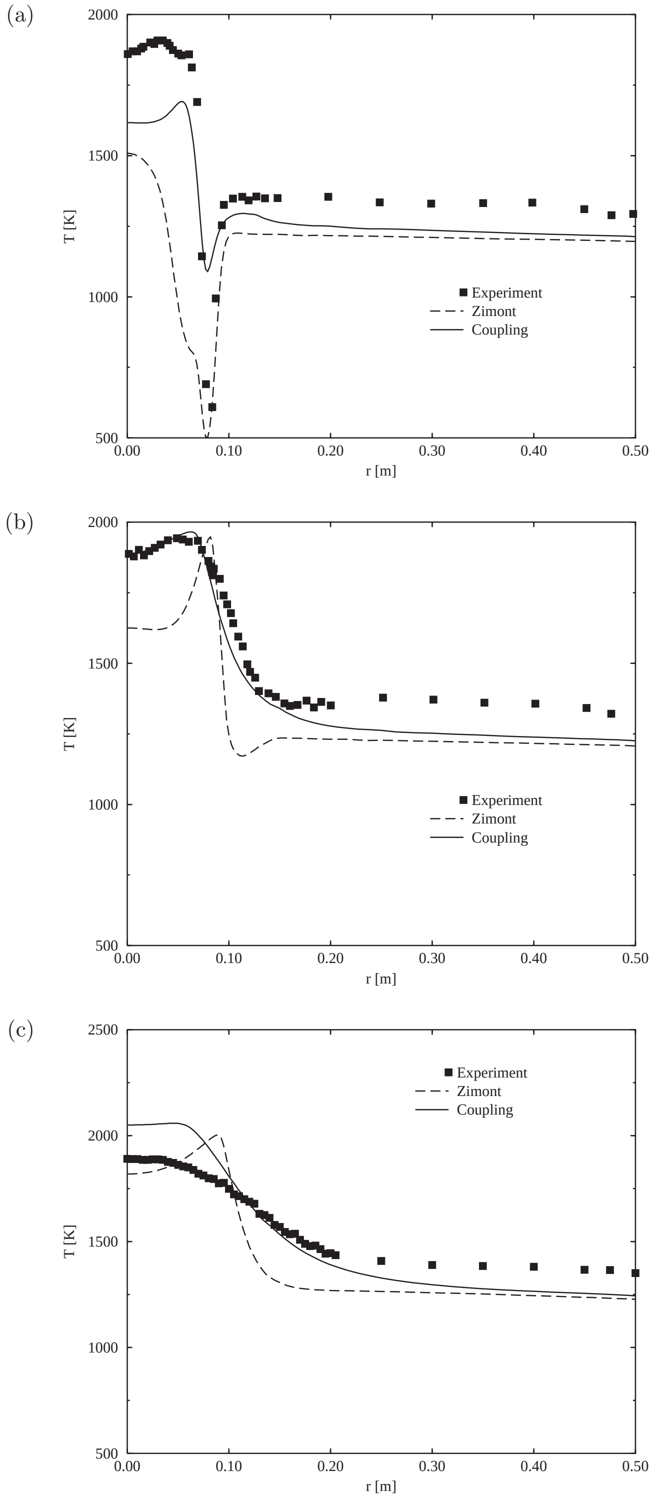

Figure 5. Profiles of static temperature: (a) $x = -0.027$, (b) $x = 0.109$, (c) $x = 0.343$

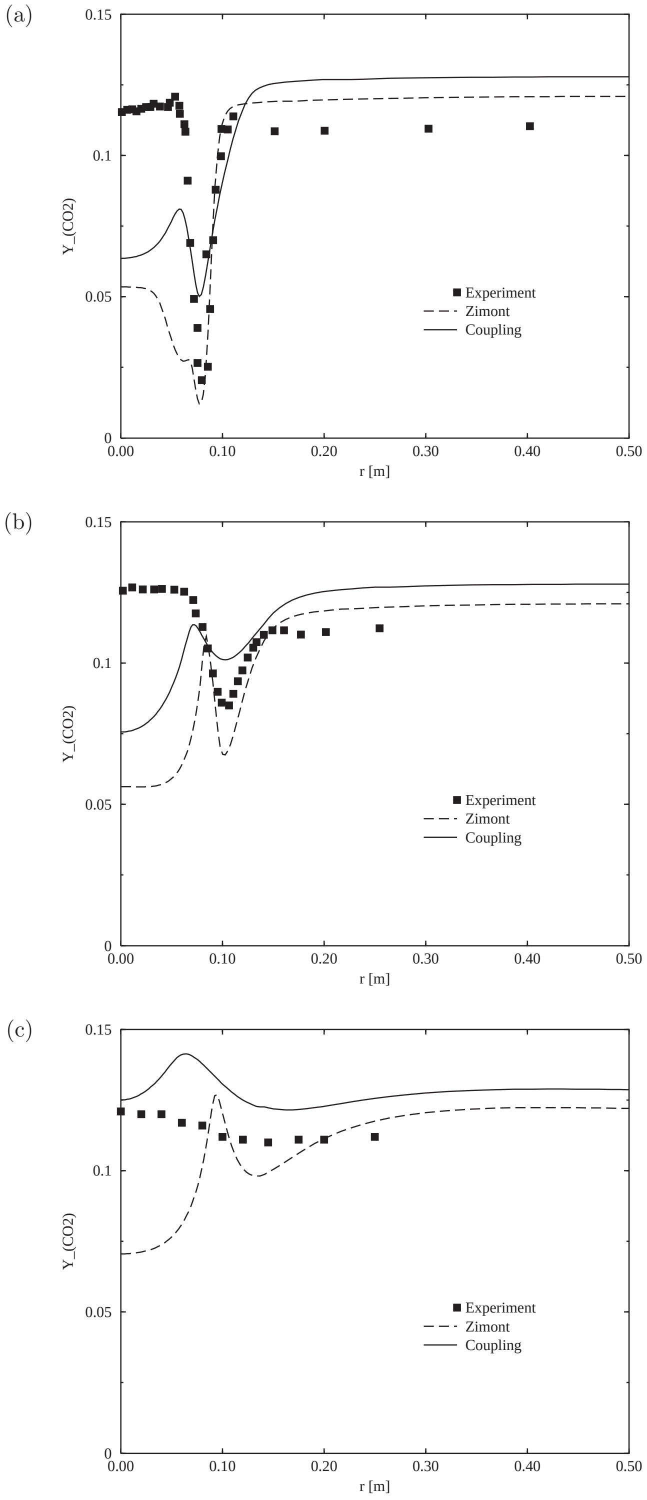

Figure 6. Profiles of the mass fraction of CO_2: (a) $x = -0.027$, (b) $x = 0.109$, (c) $x = 0.343$

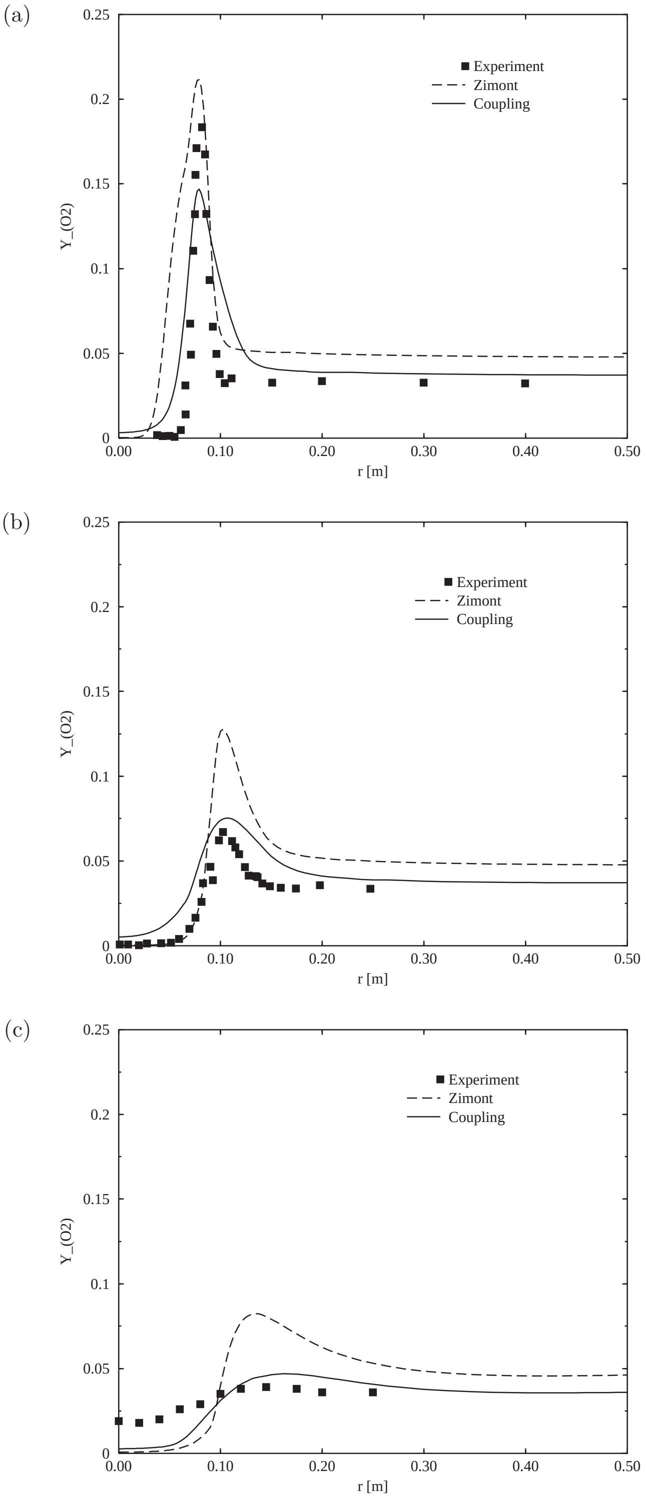

Figure 7. Profiles of the mass fraction of oxygen, O_2: (a) $x = -0.027$, (b) $x = 0.109$, (c) $x = 0.343$

4. Summary and conclusion

Local unsteadiness and stormy chemical reactions, especially in the combustion process, are the sources of flow turbulence. This kind of coupling has not always been reflected in mathematical and numerical modelling. It has been shown practically in the present paper that even a simple chemistry-turbulence coupling improves the accuracy of simulations. The model proposed here assumes an extension of the source term in the evolution equation for turbulent kinetic energy, Equation (9). Serious corrections of the results are visible especially at the cross-sections further than $x > 0.2\,\mathrm{m}$. It may be added that the model is computationally robust and very efficient, especially when compared with other combustion models [1, 4].

References

[1] Karcz M 2002 *Internal Report of Institute of Fluid-Flow Machinery PAS-ci*, Gdansk, Poland **2653/02** 1 (in Polish)

[2] Dinkelacker F, Hozlzler S and Leipertz A 1999 *Proc. ICEDERS'99*, http://www.iwr.uni-heidelberg.de/ iceders99/program.htm

[3] Polifke W, Flohr P and Brandt M 2002 *J. Engng. Gas Turbines and Power* **124** 58

[4] Ochrymiuk T 2001 *Numerical Modelling of Turbulent Gas Combustion with Reduced and Full Kinetic of Chemical Reaction*, PhD Thesis, Institute of Fluid-Flow Machinery PAS-ci, Gdansk, Poland (in Polish)

[5] Badur J and Ochrymiuk T 1998 *Scientific Biulletin of Institute of Fluid-Flow Machinery PAS-ci* Gdansk, Poland **491/1456/98** (in Polish)

[6] *FLUENT User's Guide* 1997–2002 Fluent Inc., Lebanon, USA