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MODELING HIGH-SPEED REACTING FLOWS WITH VARIABLE TURBULENT PRANDTL AND SCHMIDT NUMBERS

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ABSTRACT

A turbulence model that considers the impact of compressibility effects on turbulence and allows for the calculation of the variable turbulent Prandtl (Pr_T) and Schmidt (Sc_T) numbers as part of the solution is presented. The model is based on modeling the slow part of pressure/scalar-gradient correlation depending on characteristic time of scalar variable fluctuations (the ratio of scalar variable variance to its dissipation rate) and on the assumption that the velocity fluctuations directed normal to the streamlines play a key role in turbulent mixing process. For the validation of the code the described numerical procedures are applied to a series of jet flow problems. These include supersonic turbulent jets of variable composition and high-speed chemically reacting coflows.

INTRODUCTION

The modelling of turbulent heat/mass transfer and turbulence/chemistry interactions are of fundamental importance when simulating turbulent high-speed flows with chemical reactions. Compressibility is another important aspect of supersonic mixing as it limits the spreading rate.

A standard engineering practice in modeling turbulent heat and mass transfer is to employ constant, averaged values for turbulent Prandtl and Schmidt numbers over the domain of interest. These values are considered constant and equal to each other. The assumption implicit in this traditional treatment is that the scalar fluctuations are proportional to the local velocity fluctuations, and a uniform proportionality constant can be applied.

However, the experimental investigation showed that the values of turbulent Prandtl and Schmidt numbers may vary over a very wide range (from ~ 0.2 to ~ 1.5) and vary in various regions of the flow being completely independent from each other. It infers that turbulent heat, mass and impulse transfer are not similar. This phenomenon is very important for turbulent flows with great gradients of temperature, density, pressure, component concentrations, and should be considered in modelling of turbulent flows.

Scientists started to investigate the problems of impact of variable turbulent Prandtl (Pr_T) and Schmidt (Sc_T) numbers on heat and mass transfer in high enthalpy flows only for the last few years. There have been two main lines of research: Hassan 's group [1] and Dash's group [2]. The approaches used in those groups are quite different, and the computation results do not always agree with the experimental data. Achieving an adequate model for turbulent heat and mass exchange that will be able to solve the specified problems requires additional investigation.

In this paper the authors present a model which is based on modelling the slow part of pressure/scalar-gradient correlation depending on characteristic time of scalar variable fluctuations (the ratio of scalar variable variance to its dissipation rate) and on the assumption that the velocity fluctuations directed normal to the streamlines play a key role in turbulent mixing process. Analyzing transport equations for the turbulent fluxes of scalar variable and introducing the equilibrium assumption for the members comprised in these equations resulted in simple equations for turbulent fluxes of enthalpy and species concentrations.

Four equations were added to the compressibility corrected K-ε turbulence model: two equations for thermodynamic enthalpy variance and its dissipation rate to calculate the turbulent thermal conductivity, and two equations for the sum of concentrations variance and its dissipation rate to calculate the turbulent diffusion coefficient. The underlying turbulence model already accounts for compressibility effects.

NOMENCLATURE

a	[m/s]	Speed of sound
f		Scalar value
f''^2		Scalar value variance
h	[m^2/s^2]	Enthalpy
h_I	[m^2/s^2]	Species enthalpy
K	[m^2/s^2]	Turbulent kinetic energy
M_T	[-]	Turbulent Mach Number
N_C	[-]	Number of species
Pr_T	[-]	Turbulent Prandtl number
Sc_T	[-]	Turbulent Schmidt number
T	[K]	Temperature
u_i	[m/s]	Velocity components
V_n''	[m/s]	Velocity fluctuation normal to the streamlines
Y_I	[-]	Species mass fraction

Special characters

ε	[m^2/s^3]	Dissipation rate of turbulent kinetic energy
ε_f		Dissipation rate of f''^2
μ_T	[Pa s]	Turbulent viscosity coefficient
ρ	[kg/m^3]	Density
τ_f	[s]	Time scale of turbulence

Subscripts

a	Nozzle exit
C	Centerline value
e	External flow, ambient

VARIABLE TURBULENT PRANDTL AND SCHMIDT NUMBERS MODEL

Enthalpy, internal energy and species mass fractions are scalar values, so their turbulent fluxes are called *scalar fluxes*. Let's denote all scalar values by f.

Scalar turbulent fluxes are most often closed by a classical Boussinesq-like formulation:

$$\bar{\rho} u_j'' f'' = -\frac{\mu_T}{\sigma_f} \frac{\partial f}{\partial x_j}, \tag{1}$$

where σ_f - a numerical coefficient.

For enthalpy: $\sigma_f = \mathrm{Pr}_T$ - turbulent Prandtl number; for species mass fractions: $\sigma_f = \mathrm{Sc}_T$ - turbulent Schmidt number. Usually it is assumed that: $\mathrm{Pr}_T = \mathrm{Sc}_T = 0.7$ for free shear layers and $\mathrm{Pr}_T = \mathrm{Sc}_T = 0.9$ for near-wall flows.

The turbulent Prandtl and Schmidt numbers have a significant influence on heat flux and turbulent diffusion in supersonic reacting flows. The typical assumption that they are constant and equal to each other is often inaccurate.

Numerous experimental data [3] showed that turbulent Prandtl and Schmidt numbers may vary within quite a big range: from 0.1 to 2.

Analyzing the transport equation for scalar value f turbulent flux and assuming that diffusion and convection are balanced in this equation, we can obtain the following formula for turbulent flux of scalar value in normal direction:

$$V_n'' f'' = -\frac{V_n''^2}{K} \frac{\tau_f}{C_{1\varphi}} K \frac{\partial f}{\partial n}, \tag{2}$$

where τ_f - time scale of turbulence. Usually the ratio K/ε is used for this time scale, which actually characterizes only velocity fluctuations. It would be more accurate to consider the time scale of scalar value fluctuations - ratio f''^2/ε_f. Here ε_f - the dissipation rate of scalar value f''^2.

This paper proposes using the geometric average between these two time scales:

$$\tau_f = \sqrt{\frac{K}{\varepsilon} \frac{f''^2}{\varepsilon_f}} \tag{3}$$

In formula (2) constant $C_{1\varphi} = 3.0$

This paper uses the modification of K-ε turbulence model from [4]. The following formula for turbulent viscosity is used

$$\mu_T = \frac{(1-C_2)}{C_1} \frac{V_n''^2}{K} \cdot \bar{\rho} \frac{K^2}{\varepsilon}, \tag{4}$$

where

V_n'' - velocity fluctuation normal to the streamlines, for which it is true:

$$\frac{V_n''^2}{K} = \frac{2}{3}\left[1 - \frac{(1-C_2)}{C_1}(1 + C_M M_T)\right], \tag{5}$$

M_T - Mach turbulent number

$$M_T = \frac{\sqrt{2K}}{a} \tag{6}$$

The following numerical constants are used:

$$C_1 = 1.8; \quad C_2 = 0.6; \quad C_M = 0.4 \tag{7}$$

The transport equations for f''^2 and ε_f are as follows[2]:

$$\frac{\partial}{\partial t}\left(\bar{\rho} f''^2\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j f''^2\right) = \frac{\partial}{\partial x_j}\left[\frac{\mu_T}{\sigma_{K,f}} \frac{\partial f''^2}{\partial x_j}\right] + 2\frac{\mu_T}{\sigma_f}\left(\frac{\partial \tilde{f}}{\partial x_j}\right)^2 - 2\bar{\rho}\varepsilon_f, \tag{8}$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\varepsilon_f\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j \varepsilon_f\right) = \frac{\partial}{\partial x_j}\left[\frac{\mu_T}{\sigma_{\varepsilon,f}} \frac{\partial \varepsilon_f}{\partial x_j}\right] + \frac{\mu_T}{\sigma_f}\left(C_{d1}\frac{\varepsilon_f}{f''^2} + C_{d2}\frac{\varepsilon}{K}\right)\left(\frac{\partial \tilde{f}}{\partial x_j}\right)^2 + C_{d3}\frac{\varepsilon_f}{K}\mathrm{P}_K - \bar{\rho}\varepsilon_f\left(C_{d4}\frac{\varepsilon_f}{f''^2} + C_{d5}\frac{\varepsilon}{K}\right) \tag{9}$$

where constants are equal to [2]:

$$C_{d1}=2.0;\ C_{d2}=0.0;\ C_{d3}=0.72;$$
$$C_{d4}=2.2;\ C_{d5}=0.8;\ \sigma_{\varepsilon,f}=1;\ \sigma_{K,f}=1 \qquad (10)$$

Equation (9) is used as proposed in Ref. 3 but slightly altered because a compressibility effect in this paper is considered in a different way.

When modeling turbulent diffusion fluxes, the species mass fractions Y_m are used as scalar value f :

$$f=Y_m \qquad (11)$$

It is more convenient not to use equations(8), (9) for each species mass fraction separately but to solve equations governing the sum of the mass fraction variances and its dissipation rates:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\varphi\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\varphi\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_T}{\sigma_{K,f}}\frac{\partial\varphi}{\partial x_j}\right)+2\mathrm{P}_{\varphi}-2\bar{\rho}\varepsilon_{\varphi}, \qquad (12)$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\varepsilon_{\varphi}\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\varepsilon_{\varphi}\right)=\frac{\partial}{\partial x_j}\left[\frac{\mu_T}{\sigma_{\varepsilon,f}}\frac{\partial\varepsilon_{\varphi}}{\partial x_j}\right]$$
$$+\left(C_{d1}\frac{\varepsilon_{\varphi}}{f''^2}+C_{d2}\frac{\varepsilon}{K}\right)\mathrm{P}_{\varphi}+C_{d3}\frac{\varepsilon_{\varphi}}{K}\mathrm{P}_K \qquad (13)$$
$$-\bar{\rho}\varepsilon_{\varphi}\left(C_{d4}\frac{\varepsilon_{\varphi}}{\varphi}+C_{d5}\frac{\varepsilon}{K}\right),$$

where

$$\mathrm{P}_{\varphi}=\frac{\mu_T}{Sc_T}\sum_{I=1}^{Nc}\frac{\partial Y_I}{\partial x_j}\frac{\partial Y_I}{\partial x_j},\quad \varphi=\sum_{I=1}^{Nc}Y_I''^2,\quad \varepsilon_{\varphi}=\sum_{I=1}^{Nc}\varepsilon_{C,I} \qquad (14)$$

When modelling turbulent fluxes of enthalpy, only its thermodynamic part h_T is used as scalar value f .

The species enthalpy h_k consists of two quite different parts

$$h_I=h_{0,I}+\int_{T_0}^{T}C_{P,I}\,dT=h_{0,I}+h_{T,I} \qquad (15)$$

The first part is species enthalpy of formation at a standard temperature T_0 and is essential for flows with chemical reactions. The second part for each species only depends on temperature; it is called species thermodynamic enthalpy.

The thermodynamic enthalpy of gas mixture is estimated as

$$h_T=\sum_{I=1}^{N_C}h_{T,I}Y_I \qquad (16)$$

Such approach allows for distinguishing the effect of temperature fields on turbulence.

Thus, equations(8),(9) are used for the enthalpy variance $h_T''^2$ and its dissipation rate ε_h.

From equations (4), (1), (2) and (3) one can derive the formula for σ_f :

$$\sigma_f=\frac{\left(1-C_2\right)C_{1\varphi}}{C_1}\sqrt{\frac{K}{\varepsilon}\frac{\varepsilon_f}{f''^2}} \qquad (17)$$

Particularly for turbulent Prandtl and Schmidt numbers we have:

$$\mathrm{Pr}_T=\frac{\left(1-C_2\right)C_{1\varphi}}{C_1}\sqrt{\frac{K}{\varepsilon}\frac{\varepsilon_h}{h_T''^2}}, \qquad (18)$$

$$\mathrm{Sc}_T=\frac{\left(1-C_2\right)C_{1\varphi}}{C_1}\sqrt{\frac{K}{\varepsilon}\frac{\varepsilon_{\varphi}}{\varphi}} \qquad (19)$$

As mentioned, the constants in the model are as follows:

$$C_1=1.8;\quad C_2=0.6;\quad C_M=0.4;\quad C_{1\varphi}=3.0;$$
$$C_{d1}=2.0;\quad C_{d2}=0.0;\quad C_{d3}=0.72; \qquad (20)$$
$$C_{d4}=2.2;\quad C_{d5}=0.8;\quad \sigma_{\varepsilon,f}=1;\quad \sigma_{K,f}=1$$

COMPUTATIONAL RESULTS

For the validation of proposed turbulence model and numerical scheme seven tests were performed.

The selection of each test case was based on two principles: 1) each test had to introduce an additional unique feature to be investigated; 2) the test data should be fully understandable and reproducible.

Test 1. Supersonic oxygen jet in high-temperature ambient.

This test aimed at investigating the effect of high ambient temperature field on the supersonic oxygen jet behaviour. This kind of a flow has great gradients of density and temperature.

For this purpose, simulation was performed for a jet with the following parameters:

$u_a=451\,m/s;\quad T_a=190K;\quad p_a=10^5\,Pa$,

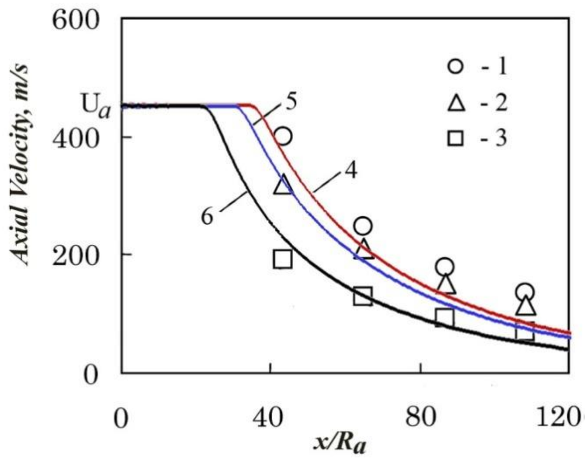
jet fluid – O_2

Nozzle exit radius: $R_a=9.2mm$

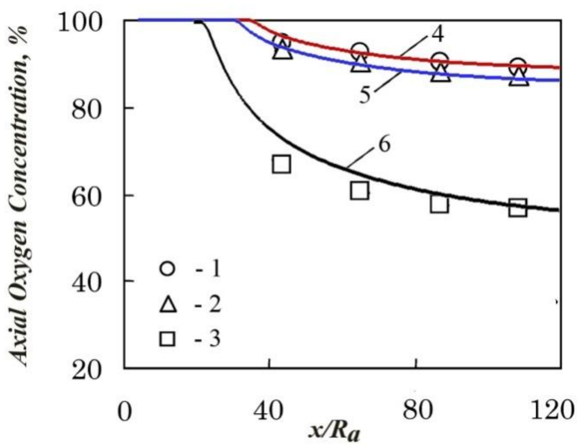
Three variants of ambient parameters were considered:

$T_e\,[K]$	$\%O_2$	$\%N_2$	$\%CO_2$
285	54	46	0
772	85	9	6
1002	88	3	9

The simulation results were compared with the experimental data of Sumi et al. [5]. In Ref. [5] supersonic oxygen jet behaviour in a high-temperature field was investigated by measuring the velocity, O_2 concentration and temperature of the oxygen jet in a heated furnace.



(1a)



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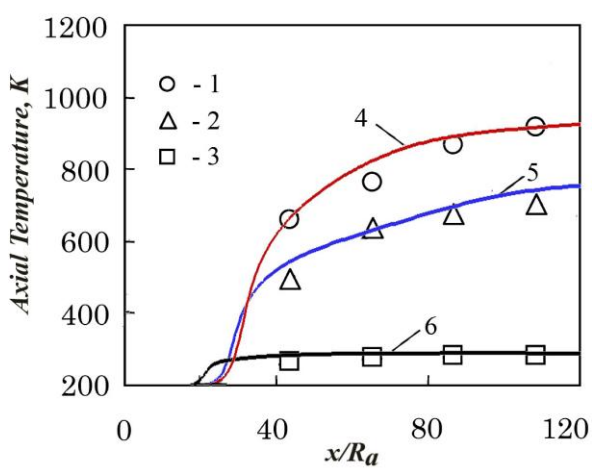


(1c)

Figure 1 Centreline (1a) velocity, (1b) oxygen concentration and (1c) temperature profiles.

1,2,3 – Sumi et al.[5] experiment: 1 - $T_e = 1002\ K$, 2 - $T_e = 772\ K$, 3 - $T_e = 285\ K$;

4,5,6 – simulations using present turbulence model: 4 - $T_e = 1002\ K$, 5 - $T_e = 772\ K$, 6 - $T_e = 285\ K$

Figures 1a,1b,1c present the distribution of velocity, the concentration of oxygen and temperature on the jet axis at different ambient temperatures. The comparison of the simulation results using the presented method with the experimental data of Sumi et al. [5] shows a good agreement and also demonstrates the fact that the attenuation of the jet is restrained as the ambient temperature increases.

Figure 2 demonstrates the effect of using variable $\Pr_T$ model on the simulation results.

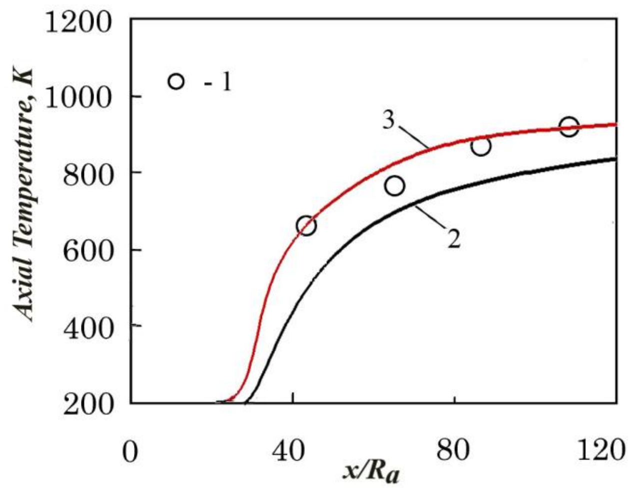


Figure 2 Centreline temperature vs. normalized distance from nozzle exit x/R_a, calculation results for various $\Pr_T$ models (constant and variable), $T_e = 1002\ K$

1 – Sumi et al.[5] experiment; 2,3 – simulations: 2 – constant $\Pr_T = 0.7$, 3 – variable $\Pr_T$ model.

The variable $\Pr_T$ model result is improvement compared with the constant $\Pr_T = 0.7$ model.

Figure 3 presents predicted $\Pr_T$ distribution. The noticeable decrease of $\Pr_T$ number in the mixing layer causes the oxygen temperature approach faster to the ambient temperature. This effect only appears at high values of T_e and actually does not influence on velocity distribution.

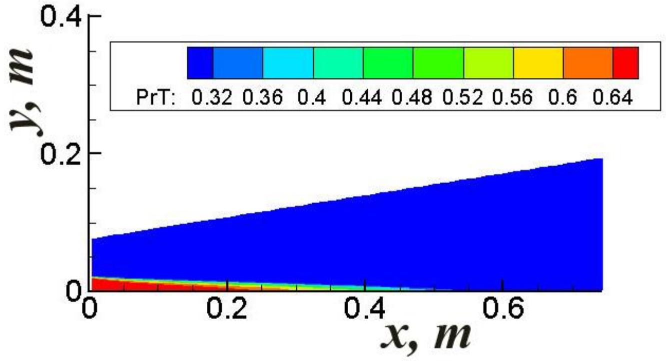


Figure 3 Predicted turbulent Prandtl number distribution for – Sumi et al. [5] experiment, $T_e = 1002\ K$

Test 2. Supersonic hydrogen jet in supersonic vitiated air coflow.

The presented method was applied to the high speed jet flame of Evans et al. [6]. In this experiment, a Mach 2 hydrogen jet was exhausted into a co-axial stream of vitiated air at Mach 1.9. The jet issued from a nozzle with inner diameter $d_j = 0.009525m$ and outer diameter $D = 0.0653m$. A schematic of the experimental apparatus is shown in Figure 4.

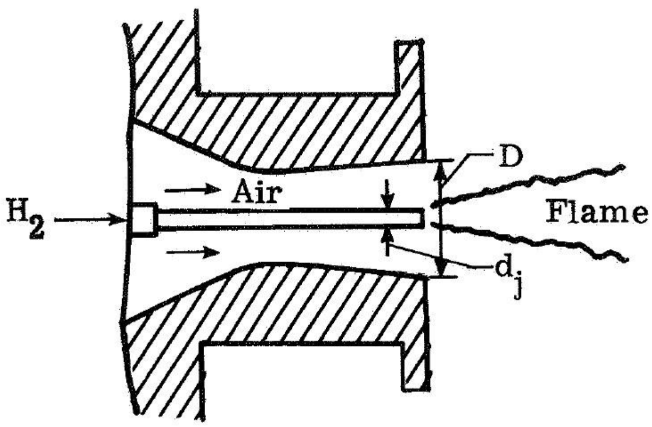
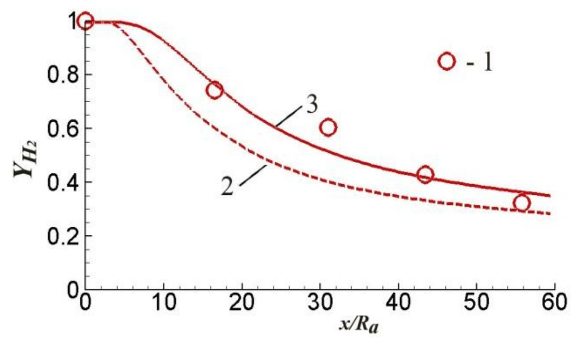


Figure 4 Schematic of the Evans et al. [6] experimental set-up. $D = 0.0653m$, $d_j = 0.009525m$, injector lip thickness – $0.0015m$

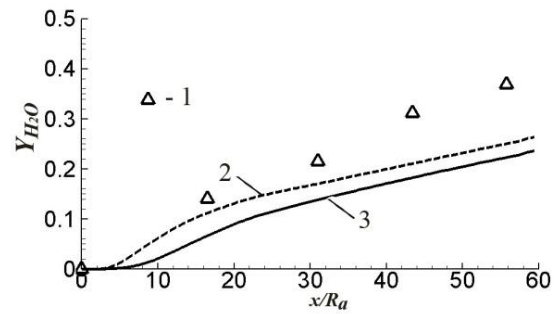
The test conditions for this case are:

	Hydrogen jet	Free stream
Mach number, M	2.00	1.90
Temperature, T, K	251	1495
Velocity, u, m/s	2432	1510
Pressure, p, MPa	0.1	0.1
Y_{H_2}	1.0	0.0
Y_{O_2}	0.0	0.241
Y_{N_2}	0.0	0.478
Y_{H_2O}	0.0	0.281

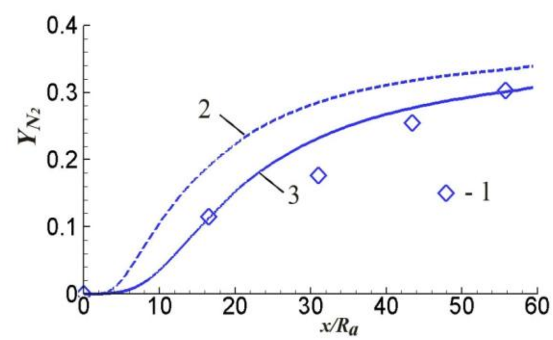
Figures 5, 6 present the axial distributions and radial profiles of species mass fractions obtained though simulation using constant and variable $\Pr_T, Sc_T$ models and compared with the Evans et al. [6] data.



(5a)



(5b)

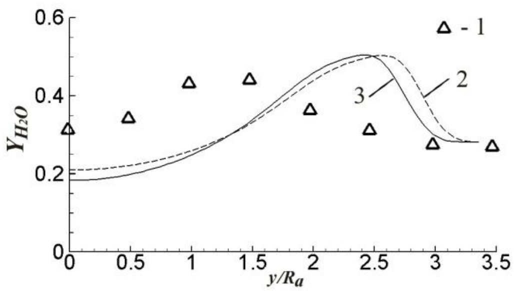


(5c)

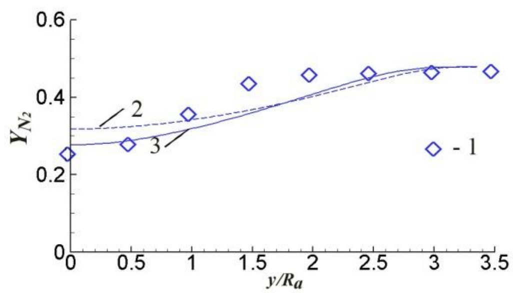
Figure 5 Centreline profiles of (5a) H_2, (5b) H_2O and (5c) N_2 mass fractions.

Calculation results (lines) for various $\Pr_T, Sc_T$ models (constant and variable) are compared to the experimental data (points). 1 – Evans et al. [6] experiment; 2 – simulation using constant $\Pr_T = Sc_T = 0.7$; 3 – simulation using variable $\Pr_T, Sc_T$ model.

The simulated distributions of H_2 and N_2 mass fractions are in a good agreement with the experimental data. The predicted distributions of Prandtl and Schmidt turbulent numbers presented in Figure 7 demonstrate the fact that the values of these parameters increase in the vicinity of flame front, which slightly slows the process of species mixing, shown in fig 5, 6.



(6a)



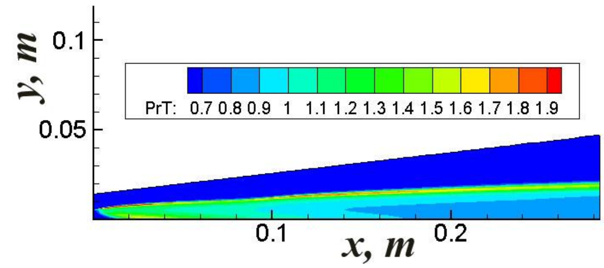
(6b)

Figure 6 Radial profiles of (6a) H_2O and (6b) N_2 mass fractions.

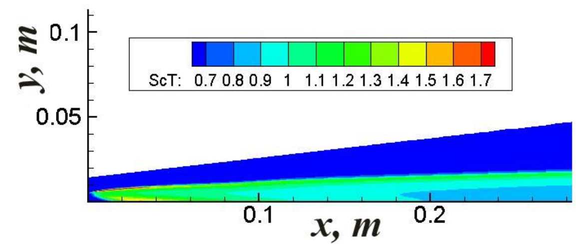
Calculation results (lines) for various $\Pr_T, Sc_T$ models (constant and variable) are compared to the experimental data (points).

1 – Evans et al. [6] experiment; 2 – simulation using constant $\Pr_T = \mathrm{Sc}_T = 0.7$; 3 – simulation using variable $\Pr_T, \mathrm{Sc}_T$ model.

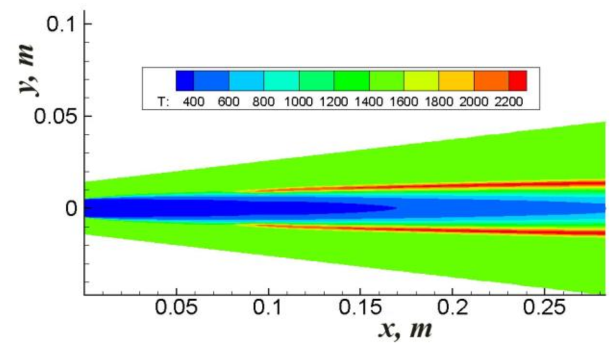
The situation with water mass fraction is worse. This may be accounted for the fact that low-temperature reaction chains including such species as H_2O_2, HO_2 were not considered in the kinetic process of hydrogen burning in the present paper. It is assumed that these species are essential for hydrogen ignition.



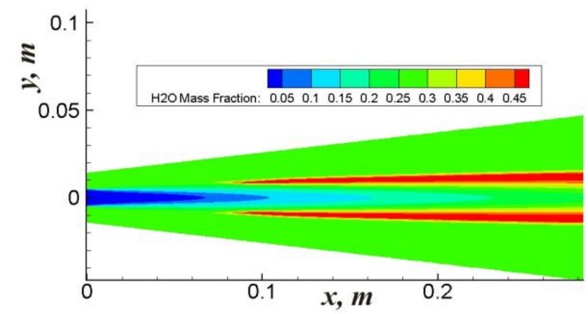
(7a)



(7b)



(7c)



(7d)

Figure 7 Predicted (7a) turbulent Prandtl number, (7b) turbulent Schmidt number, (7c) temperature, (7d) H_2O mass fraction distributions for – Evans et al. [6] experiment.

CONCLUSION

A turbulence model that considers the impact of compressibility effects on turbulence and allows for the calculation of the variable turbulent Prandtl (Pr_T) and Schmidt (Sc_T) numbers as part of the solution is presented.

The simulation results were compared with the available experimental data, which led to the following conclusions:

1) The simulations performed with considering variable turbulent Prandtl and Schmidt numbers had a better agreement with the experiment than the simulations based on the assumption that these values were constant. The variable Prandtl and Schmidt number formulation works well for both reacting and non-reacting flows.

2) Turbulent scalar transport (as characterized by the turbulent Prandtl and Schmidt numbers) was found to vary strongly, both spatially and with the level of compressibility.

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