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# MATHEMATICAL MODELING OF METHANE COMBUSTION

Milada KOZUBKOVÁ[1], Jaroslav KRUTIL[2], Marian BOJKO[3], Václav NEVRLÝ[4]

**Research article**

**Abstract:** The paper presents the process of the creation of the mathematical model of methane turbulent combustion using ANSYS FLUENT 13.0 software. The decommissioned mathematical model for species transfer with chemical reaction is described, where burning is based on stoichiometric equations of perfect combustion. Work also analyzes the appropriateness of models dealing with the kinetics of burning and describes their mutual comparison.

**Key words:** ANSYS FLUENT, methane, numerical modeling, chemical reactions, combustion.

## Introduction

The basis of the combustion process is a burning fuel. Burning is a physical and chemical process which combines a combustible matter and oxidizer, while chemical reaction occurs, accompanied by heat generation chemically bound in the fuel and lighting effect. This light effect is a result of product temperature which reached the visible spectrum. Therefore we talk about burning. (Kozubková and Krutil, 2012).

Three basic factors of burning process are required:

- combustible material (solid, gaseous, liquid fuel),
- oxidizer (usually oxygen),
- initialization source with sufficient energy and temperature (flame, hot surfaces, sparks).

## Materials and methods

### *Prologue*

The problem definition of mathematical modeling of turbulent combustion is a very complex and lengthy process. Mathematical model of mass, momentum and heat transfer would include the following equation (Shabanian et al., 2012):

- the continuity equation,
- equations of motion,
- energy equation.

Boundary conditions and physical properties of these models can be defined as either constant or temperature dependent. When modeling chemical reactions, the model will be expanded by the following equations:

- equation of heat transfer including member characterizing the heat generated by chemical reactions,
- equation for the mass fractions of species with chemical reactions.

However, only mathematical model dealing with burning of gaseous mixture is analyzed in this paper. This burning is presented by one stoichiometric equation and is called the perfect combustion. The chemical equation describing the perfect methane combustion (oxidation) has the following form (Bebčák et al., 2009):

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad (1)$$

In the ANSYS FLUENT 13.0 program there are several approaches to the modelling of chemical reaction in gases (Richardson and Chen, 2012). To compare the kinetics of combustion, a model based on species transport and chemical reaction was chosen. This model is based on the solution of transport equations for species mass fractions with the reaction mechanism of chemical reactions.

[1] VŠB - Technical University of Ostrava, Faculty of Mechanical Engineering, Department of Hydromechanics and Hydraulic Equipment, Ostrava, Czech Republic, milada.kozubkova@vsb.cz

[2] VŠB - Technical University of Ostrava, Faculty of Mechanical Engineering, Department of Hydromechanics and Hydraulic Equipment, Ostrava, Czech Republic, jaroslav.krutil@vsb.cz

[3] VŠB - Technical University of Ostrava, Faculty of Mechanical Engineering, Department of Hydromechanics and Hydraulic Equipment, Ostrava, Czech Republic, marian.bojko@vsb.cz

[4] VŠB - Technical University of Ostrava, Faculty of Safety Engineering, Department of Fire Protection, Ostrava, Czech Republic, vaclav.nevrly@vsb.cz

## *Mathematical model of species transfer with chemical reaction*

ANSYS FLUENT calculates with "time-averaging values of the species local mass fractions" $\overline{Y}_{i'}$. They are described by similar balancing equation as in the case of energy equation, which have this shape in conservative form (Kozubková, 2003):

$$\frac{\partial}{\partial t}\left(\rho Y_{i'}\right)+\frac{\partial}{\partial x_i}\cdot\left(\rho\overline{u}_i Y_{i'}\right)=-\frac{\partial}{\partial x_i}\vec{J}_{i',i}+R_{i'}+S_{i'} \quad (2)$$

where $\rho$ is density, $\overline{u}_i$ is time-averaging component of flow velocity. On the right side $R_{i'}$ is the rate production of species $i$ through chemical reactions and $S_{i'}$ is the rate of the production increase of distributed phase. The mentioned equation (2) is valid for N-1 species, where N is the total number of species phase in the system. Distribution of species can be carried in different assumptions. Usually the distribution can be distinguished for laminar and turbulent flow (Kozubková, 2003).

In the case of laminar flow in equation (2), $J_{i',i}$ represents the diffusion flux of species $i'$ and is defined as:

$$J_{i',i}=-\rho D_{i',m}\frac{\partial Y_{i'}}{\partial x_i} \quad (3)$$

where $D_{i',m}$ is the mass diffusion coefficient for species $i'$ in the mixture.

In turbulent flows, the mass diffusion for species $i'$ is expressed in the following form:

$$J_{i'}=-\left(\frac{\mu_t}{Sc_t}\right)\frac{\partial\overline{Y}_{i'}}{\partial x_j} \quad (4)$$

where $Sc_t$ is the turbulent Schmidt number ( $Sc_t=\frac{\mu_t}{\rho D_t}$ ,where $\mu_t$ is the turbulent viscosity and $D_t$ is the thermal diffusivity, The default $Sc_t$ is 0,7).

It is important to say that the mass diffusion coefficients (for multicomponent mixtures) are calculated using the kinetic theory (Šrůtek, 2009).

## *Models describing the rate of species production*

The reaction rates that appear as source term in equation for species transfer are computed for laminar flow using Arrhenius expression, for turbulent flow they are modeled in accordance to the work of Magnussen and Hjertager and are called the eddy-dissipation model (Ansys, Inc, 2011a).

Constant activation energy and pre-exponential factor have significant effects on the results. In the specialized literature there exist many variants of these constants, for example Zambon Chelliah, Puri-Seshadri, Andersen et al, Bibrzycki-Poinsot etc. In this case, the constants of one-equation model by Zambon Chelliah are used (Kozubková and Krutil, 2012):

- Pre-exponential factor: 1,35.$10^{20}$ [$cm^3.mol^{-2}.s^{-1}$],
- Activation energy: 30000 [$cal.mol^{-1}$].

For the solving of production rate of species $i'$ through chemical reactions, ANSYS FLUENT defines these models (Ansys, Inc, 2011a):

- Laminar finite-rate model - the effects of turbulent fluctuations are ignored and reaction rates are determined by the Arrhenius kinetic expression.
- Eddy-Dissipation model - reaction rates are assumed to be controlled by the turbulence, so expensive Arrhenius chemical kinetic calculations can be avoided. The model is computationally cheap, but for realistic results, only one or two step heat-release mechanisms should be used.
- Finite-rate/Eddy-Dissipation model - combination of the two previous models.
- Eddy-Dissipation-Concept model (EDC model) - this model includes a very detailed kinetics of combustion in the flame.

Because the specific turbulent task was tested, the solving of the first model (laminar model) was no longer considered.

## *Eddy-Dissipation model*

While the chemical reaction proceeds rapidly, the total reaction rate is controlled by turbulent mixing. Basically, there are two basic types of reactions, with the premixed and non-premixed reactants. ANSYS FLUENT provides a turbulence-chemistry interaction model based on the Magnussen and Hjertager work (called the eddy-dissipation model). The average rate of production of species $i'$ in reaction $k$ is given by the smaller of the two expressions below:

$$R_{i'}=M_{i'}\sum_{k=1}^{N_R}\min\left\{\nu'_{i',k}A\rho\frac{\varepsilon}{k}\min_R\left(\frac{Y_R}{\nu'_{R,k}M_{i',R}}\right),\ \nu'_{i',k}AB\rho\frac{\varepsilon}{k}\frac{\sum_P Y_P}{\sum_{j'}^{N}\nu''_{j',k}M_{j'}}\right\} \quad (5)$$

where $Y_P$ is the mass fraction of any product species ($P$), $Y_R$ is the mass fraction of a particular reactant ($R$), $A$ is an empirical constant (equal to 4) and $B$ is

an empirical constant (equal to 0.5), $\rho$ is the density of $i'$ species. The chemical reaction rate is governed by the large-eddy mixing time scale $k/\varepsilon$ as in the eddy-breakup model of Spalding. The process of chemical reaction proceeds when the flow is turbulent ($k/\varepsilon < 0$) (Ansys, Inc, 2011a; Kozubková et al., 2008).

### Finite-rate/Eddy-Dissipation model

Another turbulent model is a combined finite-rate/eddy-dissipation model. In this model, the rate of reaction is determined by the Arrhenius and by eddy-dissipation equation. Local reaction rate is given as the minimum value from these two equations. Although ANSYS FLUENT allows multi-step reaction mechanisms for the eddy-dissipation model and finite-rate/eddy-dissipation model, these will likely produce incorrect solutions. The reason is that multi-step chemical mechanisms are based on Arrhenius rates and these chemical mechanisms are differing for each reaction. In the eddy-dissipation model, every reactions have the same rate and therefore the model will be used only for one-step (reactant → product), or two-step (reactant → intermediate product, intermediate product → product) global reactions (Ansys, Inc, 2011a; Kozubková et al., 2008).

### Eddy-Dissipation-Concept (EDC model)

In this model, the multi-step chemical kinetics mechanism is included. This model assumes that reaction occurs in small turbulent structures, called the fine scales (Ansys, Inc, 2011a; Kozubková et al., 2011). Due to chemical reaction for species $i'$, the source term $R_{i'}$ included in the equations of energy is calculated using the relation (6), where $Y_{i'}$ is the mass fraction of species $i'$, $Y^*_{i'}$ is the mass fraction of species $i'$ for the fine scaled, $C_\xi$ is a volume fraction constant (equal 2,1377), $C_r$ is a time scale constant (equal 0,4082), $\nu$ is kinematic viscosity (Ansys, Inc, 2011a; Kozubková et al., 2008).

$$R_{i'} = \left(Y_{i'}^{*} - Y_{i'}\right)\left(\frac{\rho C_\xi^{\,2}\left(\frac{\nu\varepsilon}{k^2}\right)^{1,5}}{C_r\sqrt{\frac{\nu}{\varepsilon}}\left[1-\left(C_\xi^{\,3}\left(\frac{\nu\varepsilon}{k^2}\right)^{2.25}\right)\right]}\right) \qquad (6)$$

If the chemical reaction is too fast, then this model uses the STIFF mechanism. It is the auxiliary mechanism that includes a constant activation energy and pre-exponential factor.

## Results

### Numerical model of non-premixed methane combustion in the tube

To solve this case, the finite element method is used. The geometry and grid are shown in Fig. 1, where the characteristic dimensions are indicated. It can be seen very well that the grid model is made up exclusively of rectangular cells and is composed from 4800 cells. For the simplification, this model is solved in 2D space as an axially symmetrical model. The axis of symmetry is identical to the axis of the tube.

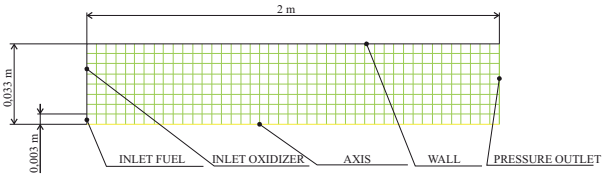


Fig. 1 Geometry and grid of the mathematical model

Boundary conditions of the model are shown in Fig. 1. Fuel enters to area through the narrow slit (see Fig. 1) by the velocity $v_{CH4}$ = 10 m.s$^{-1}$. The fuel temperature at input is 300 K. Oxidizer enters to tested area separately from the fuel. Composition of oxidizer is defined by $N_2$ = 77 %, $O_2$ = 23 %. The oxidizer temperature is 300 K and the velocity is $v_{N2,O2}$ = 0,5 m.s$^{-1}$.

### Graphical evaluation of results

The aim of the work was to create mathematical models of gaseous fuel combustion and then to compare the results of three basic turbulent models contained in the numerical software ANSYS FLUENT. The temperature fields and detection of flame behavior during combustion were of interest. Fig. 2 shows the comparison of temperature fields in all three models.

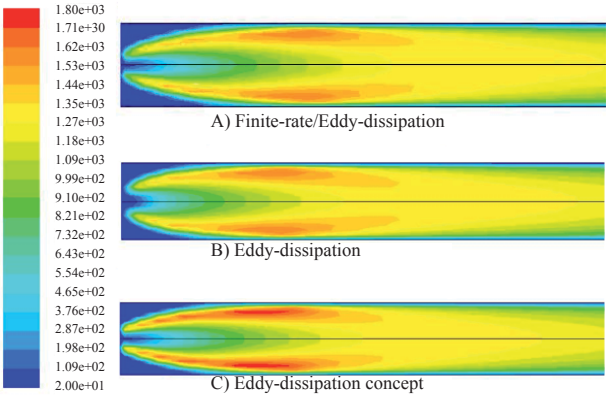


Fig. 2 Temperature fields in solved models [K]

Fig. 3 shows a place where methane burns with oxygen (an envelope of flame). The comparison of three models is introduced again.

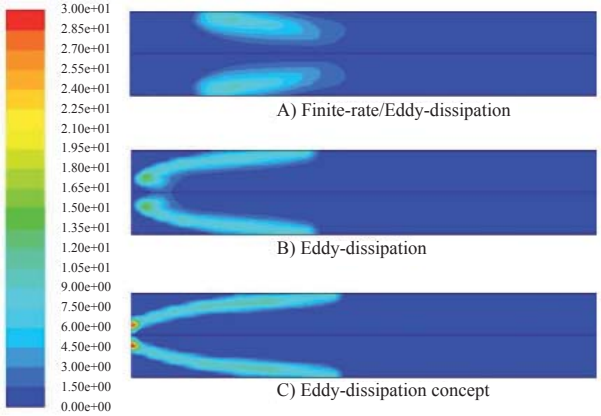


Fig. 3 Heat of reaction of gas mixture [W]

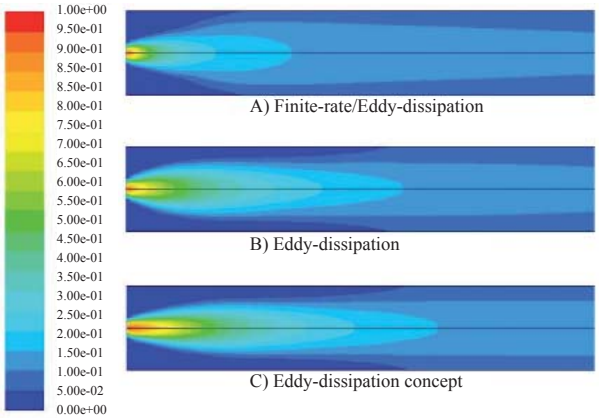


Fig. 4 Decrease of a methane mass fraction influence by combustion gas mixture

Process of decreasing the methane mass fraction by combustion of gaseous mixtures is shown on Fig. 4.

Temperature profile is compared in conclusion. Comparison is made in the axis of tube. We observe in Fig. 5, that the temperatures in all three models are almost identical.

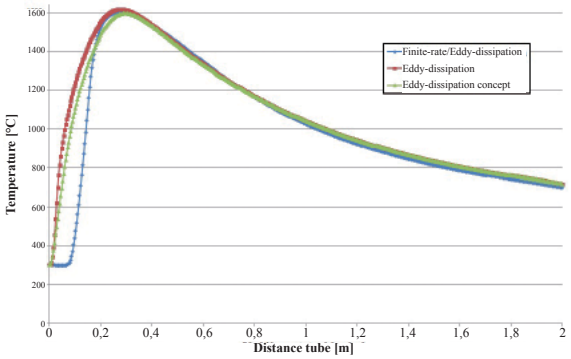


Fig. 5 Temperature profiles depending on the distance (in axis of tube)

## Conclusion

The article is devoted to the possibilities of the mathematical modeling of turbulent methane combustion. Introduction of modeling is focused on the solving of equations for species transport with chemical reactions. The work also compares the possibility of using a mathematical model of turbulence with respect to the three different expression rates of the production of species through chemical reaction. From comparison of the results, it is evident, that all three of these models achieved very similar results (temperature field), see Fig. 5. Models Finite-Rate/Eddy-Dissipation and Eddy-Dissipation Concept did not acquire maximum values as high as that of Eddy-Dissipation model. This means that it does not burn so intensely. Finally, we can say that much accuracy in model results has the value of activation energy and pre-exponential factor in Arrhenius expression.

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