LOW TEMPERATURE MODEL FOR PREMIXED METHANE FLAME COMBUSTION

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Abstract

The paper describes the extension of the progress variable combustion model FIRST for methane flames to low temperature regimes. The reaction sources in low temperature regimes (under 1200 K) are computed with a global Arrhenius reaction derived from the ignition delay measurements available in the literature. The model was compared with the combustion model without extension to low temperatures and validated against data from the measurements.

1 Introduction

The demands on modern combustion devices are bringing new challenges to the combustion research. The effect of pollution limits, which are pushed to lower levels, is to force manufactures to use such a combustion conditions, where the problems of stability may arise. Moreover the NOx limits are pushing combustion temperatures down and the models developed on the fast chemistry (still extensively used in the industry) are no longer valid under such operation conditions. The combustion models taking into account the kinetics of the reactions are needed to model the radical concentrations to predict not only pollutant concentrations, but also the temperature and main products concentration. There is a number of approaches to kinetic reaction modelling, each one with its own set of benefits and limits of its applicability. For predictions in industry, the full chemical reaction mechanism is rarely used and various reduction models to lower the number of species are used [1]. Here we use the progress variable model called FIRST, developed at University of Twente by Kok et al. [2]. This model was extended with a semi-empirical correlations to take into account combustion at low temperatures.

2 Model description

2.1 FIRST combustion model description

FIRST combustion model is described in detail in [2] and only brief review is given here. The model is based on 18 reaction methane mechanism. It uses mixture fraction and 3 reaction progress variables (further mentioned as RPV) to model combustion process in the domain. The mapping of the chemical reaction mechanism onto the RPVs is based on the partial equilibrium of fast reactions assumption. Namely the RPVs are $t$, describing the conversion of $CH_4$, $r$ and $s$ showing the departure from the equilibrium for $H_2$ and $CO$ part of the mechanism respectively.
The RPVs are defined as follows:

\[
t = \frac{Y_{CH_4}^* - Y_{CH_4}^u}{Y_{CH_4}^u - Y_{CH_4}^t} = \frac{Y_{CH_4}^* - Y_{CH_4}^t}{Z(i)} \quad (1)
\]

\[
r = \frac{Y_{H_2}^* - Y_{H_2}^u}{Y_{H_2}^u - Y_{H_2}^t} = \frac{Y_{H_2}^* - Y_{H_2}^t}{W(i, t)} \quad (2)
\]

\[
s = \frac{Y_{CO}^* - Y_{CO}^{pb}}{Y_{CO}^{pb} - Y_{CO}^t} = \frac{Y_{CO}^* - Y_{CO}^t}{V(i, t, r)} \quad (3)
\]

where the indexes \(u\) denotes to unburnt, \(b\) for burnt state respectively.

Multidimensional linear database with species concentrations, temperature and density as well as the sources to RPVs is Favre-averaged with presumed shape of pdf to take into account the turbulent fluctuations assuming statistical independence of the scalars. The test case uses premixed mixture with steep variation of burnt and unburnt mixture (progress variable \(t\)), therefore the variance of methane progress variable \(t'\) was introduced. The database is stored separately and the values of density, temperature and sources of RPVs are read every iteration of CFD computation. The CFD code solves averaged momentum and mass equations and also transport equations of RPVs of general form:

\[
\frac{\partial \rho \tilde{u}_k}{\partial x_k} - \frac{\partial}{\partial x_k} \left( \rho \tilde{D} \frac{\partial \tilde{\phi}}{\partial x_k} - \frac{\mu_t}{\sigma_t} \frac{\partial \tilde{\phi}}{\partial x_k} \right) = \overline{S_{\phi}}, \quad (4)
\]

where \(\phi\) stays for reaction progress variables. The source term on the RHS of the equation is zero for conserved mixture fraction \(f\), and have chemical source term part and then turbulent mixing source term parts for RPVs \(t, r, s\). More detailed discussion of the sources can be found in [2, 4].

The FIRST model is very effective, but the assumption of partial equilibrium constrains the model validity to the temperatures above \(1200K\). This results into an overprediction of RPV \(t\) source. Therefore the model was modified to correct the sources in the low temperature region with semi-empirical approach described in the next section.

### 2.2 Ignition model

To model the combustion sources at low temperatures, several approaches could be employed. One method could be to implement the reaction mechanism developed for low temperatures, where different reactions and species need to be addressed [5]. Another method described here is to use the data from ignition delay experiments and derive the global reaction-rate equation. Number of authors published data from ignition delay experiments for methane-air and methane-oxygen mixtures. Lefebvre at al. [6] as well as Petersen [7] and Spadaccini [8] and others formulate the results into the equations for wide range of temperatures, pressures and equivalence ratios. Unfortunately for some measurements authors do not give all important informations and it is therefore hard to use their results. Petersen and Williams & Li used two different correlations for temperatures above and under \(1300K\) as can be seen from Fig.1.

After detailed study and comparison of these results the equation of Petersen [7], as a first approach was chosen as it is in accord with other authors and reports good match to the experimental data:

\[
\tau_{ig} = 4.99 \times 10^{-14} [CH_4]^{-0.38} [O_2]^{-1.31} \exp\left(\frac{19000}{RT}\right) \quad (5)
\]

This equation is used to derive effective reaction rate for temperatures under \(1200K\) adopting approach of Kok [9] successfully used for syngas \((CO - H_2)\) flames. For the lack of space only the resulting reaction rate equation is presented here:

\[
\frac{d[CH_4]}{dt} = 1.4073 \times 10^{-4} [O_2]^{1.05} [CH_4]^{0.38} \frac{T^2 \exp \left(-\frac{9651}{T}\right)}{T} \quad (6)
\]

This equation is used to 1400 \(K\) to calculate the chemical source of equation \(t\) to its transport equation.
3 Setup of simulation

3.1 Moreau Experiment

New combustion model described shortly above was validated against the experimental data of P. Moreau and A. Boutier [10] who measured velocity and fuel concentration profile in a premixed flame with recirculation. The setup is depicted in Fig.2 where the modelled part consists of the channel with cross section of $100 \times 100 \text{ mm}^2$ and length $1.3 \text{ m}$. There is inlet of hot recirculated flue-gases with velocity of $130 \text{ m/s}$ and temperature $2000 \text{ K}$ in the region of $y = 0 - 20 \text{ mm}$ and parallel inlet of the fresh mixture of $CH_4$ and air with the velocity of $65 \text{ m/s}$ and temperature $600 \text{ K}$ in the region of $y = 20 - 100 \text{ mm}$. The measurements were performed in 30 second intervals to prevent overheating of the walls. No wall temperatures are provided from the measurements, therefore the temperature of $600 \text{ K}$ was assumed. The maximum adiabatic temperature for the mixture with the inlet temperature of $600 \text{ K}$ is $2300 \text{ K}$ which is for $300 \text{ K}$ different from the experiment, possibly due to heat loss of the inlet pipe or incorrect temperature measurements. It is not trivial to run a computations with lower temperature at the hot inlet for given mixture as the temperature in the model is calculated property of the mixture. Therefore the temperature difference is neglected, in spite its influence on the results. The inlet velocity in the simulation is corrected to take into account different density.

3.2 Simulation setup

Simulations were done using CFX 5.7 commercial CFD package of ANSYS using CFX coupled solved with second order differencing schema. The flow was considered incompressible with the density dependent only on temperature. The coupled solver of CFX was used to compute mean velocities and mass equation using $k - \epsilon$ model of turbulence and transport equations for mixture fraction and RPVs plus variance of $t$ variable with their corresponding source terms. Every iteration the values for density and RPVs sources were read from the thermochemical database computed beforehand. The combustion was considered to be adiabatic according to the experimental conditions. The computational grid consist of 1500 elements in stream-wise direction and 95 elements in cross-flow direction giving maximum element size of $1 \text{ mm}$. The velocity, turbulent kinetic energy and turb. kinetic energy dissipation profiles are taken form the experiments. At the hot - burnt inlet values of scalars are given as $f = 1, t = 1, r = 1$ while for fresh mixture inlet the values are $f = 0, t = 0, r = 1$; where $r = 1$ designates equilibrium in hydrogen combustion.

4 Results

The results from the CFD computations are compared with the experimental data of Moreau [10]. In Fig.3 the velocity profiles in 4 different cross-sections are shown. The FIRST label is referring to the original FIRST model, igFIRST label to new model presented and Moreau to experiments respectively. It can be seen, that the velocity is lower from new model, fitting experiments at first, but is lower at further downstream. Still overprediction at the low y is evident. This is obviously the effect of the incorrect temperature (therefore density) setting for the calculations as described in the previous section.

In the next figure, Fig.4 the concentration profiles are shown in three cross sections different to velocity profiles following the profiles available from the experiments. The computed profiles by new model igFIRST are not in a good match with the experiments. On the other hand they represent well the average value of methane concentrations in the cross-section. The profiles from the previous model are not shown for sake of clarity of the picture, but the concentrations with old model were overpredicted to much greater extend. The different slope of methane concentration change may be given by two different factors. One is probably the different level of turbulent mixing, which would spread the concen-
tration line to fit the experiments. Therefore indicating incorrectly predicted turbulent mixing of the \( t \) variable source, or its variance. The other issue is the concentration itself. Measuring the fuel concentrations in the combusting flow may introduce quite large errors. It follows that the model must be verified on the different set of measurements, where the products or intermediates were measured. This will allow to choose appropriate ignition closure to model the source of \( t \) correctly.

5 Conclusions

The new kinetic model of methane–air partially premixed mixture was developed using semi-empirical approach. New model is based on the reaction progress variable model FIRST developed by Kok at al.[2] using kinetic correlations from Ignition time delay experiments. The model was tested on simple tube co-flow experimental burner designed by Moreau. New model gives better results, however the problems the model as well as the experimental data available were found concluding necessity of other validation against different experiment data.

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References


Appendix – Figures

Figure 1: Different Ignition time delay correlations at 1 bar

Figure 2: The experimental setup

Figure 3: Velocity profiles at different cross-sections

Figure 4: Concentration profiles at different cross-sections