Comparative study of different combustion models for turbulent gas flames

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Abstract. Several popular turbulent combustion models have been tested in a computational study of three experimentally well-documented non-swirling and swirling jet flames. Different combinations of turbulence, combustion and reaction mechanisms models were considered. It is shown that the eddy- dissipation concept (EDC) and the probability-density function (PDF) of flamelet combustion models with detailed kinetics mechanisms provide the best results for all flames examined. For some cases, a combination of RANS turbulence models and less costly combustion approaches (Hybrid or EDC with 4 reactions) also gives acceptable results.

Combustion processes are very common in nature and technology. Most of the technological processes that ensure the life necessities of people are based on combustion processes such as energy, transport, metallurgy, petrochemicals, and others. The optimization and development of such systems is impossible without detailed study and modelling of the combustion process. Computational fluid dynamics (CFD) methods are becoming currently increasingly common in industry to solve multi-physical problems. They allow accelerating design and optimization processes of products, thereby reducing the financial costs of the project. At that, CFD allows partial elimination of the need to conduct expensive experiments, as provides an opportunity to optimize the product design based on its virtual model. The gas combustion is a complex process, which is determined by the joint effects of chemical, heat and mass transfer processes in turbulent flows of multicomponent gas mixtures. To calculate gas flames, it is necessary to implement a combination of these processes in computational model. The present paper is dealing with the development and testing of numerical simulation techniques for gas combustion process, as well as its practical use when solving applied problems.

In the calculations we used in-house SigmaFlow software package and Fluent commercial package. The flow parameters and turbulence characteristics were determined on the basis of solutions to both the Reynolds averaged Navier-Stokes equations based on k-ε and MSST models, and using eddy-resolving LES and hybrid RANS/LES turbulence models. To describe the radiation heat transfer we used the discrete ordinates model with the application of the weighted gray gases model to calculate the absorption coefficient.

The calculation of gas combustion was carried out using different approaches and models. In particular, a simple hybrid model, in which the reaction rate is selected as the lower of the rate calculated on the basis of 2-to-4-stage reaction mechanisms ($Ri_{,KIN}$) (Tables 1 and 2) and the turbulent mixing rate of components ($R_{i,EBU}$).

$$R_{i,KIN} = -AM_i X_i^{\nu_i} X_{OX}^{\nu_{OX}} T^{\beta} e^{-E_a/RT}, \quad (1)$$

where X_i, R_i - molar concentration and reaction rate of i-th reagent

A_i,E_i - pre-exponential factor and activation energy

ν_i, ν_{OX}, β - empirical constants

X_{OX} – molar concentration of oxidant

$$R_{i,EBU} = -\frac{\rho\varepsilon}{k} A \cdot MIN(Y_i, \frac{Y_{OX}}{S_{OX}}, B\frac{Y_{pr}}{S_{pr}}) \quad (2)$$

where A и B – coefficients, equals 4.0 and 0.5;

Y_i, Y_{OX}, Y_{PR} - mass concentrations of reagent, oxidant and product of combustion

S_{OX}, S_{PR} - stoichiometric coefficients

$$R_i = -MIN(|R_{i,KIN}|, |R_{i,EBU}|) \quad (3)$$

Table 1. Two-stage methane reaction mechanism [1].

No.	Reaction	E, J/kmol	A, kmol/(м^3·s)	B	Components degree γ
1	$2CH_4+3O_2 \rightarrow 2CO+4H_2O$	$2.03\cdot10^8$	$2.8\cdot10^{12}$	0	γ_{CH4}=-0.3, γ_{O2}=1.3
2	$2CO+O_2 \rightarrow 2CO_2$	$1.67\cdot10^8$	$2.91\cdot10^{12}$	0	γ_{CO}=1, γ_{O2}=0.25

Table 2. Four-stage methane reaction mechanism [2]

No.	Reaction	E, J/kmol	A, kmol/(м^3·s)	β	Components degree γ
1	$CH_4+0{,}5O_2 \rightarrow CO+2H_2$	$1.26\cdot10^8$	$4.4\cdot10^{11}$	0	γ_{CH4}=0.5, γ_{O2}=1.25
2	$CH_4+H_2O \rightarrow CO+3H_2$	$1.26\cdot10^8$	$3.1\cdot10^8$	0	γ_{CH4}=1, γ_{H2O}=1
3	$CO+0{,}5O_2+0H_2O \rightarrow CO_2$	$6.69\cdot10^7$	$2.5\cdot10^8$	0	γ_{CO}=1, γ_{O2}=0.3
4	$H_2+0{,}5O_2 \rightarrow H_2O$	$1.46\cdot10^8$	$7.9\cdot10^{10}$	0	γ_{H2}=1, γ_{O2}=0.5

For more complex generalized eddy-dissipation model (EDC) we considered different reduced reaction mechanisms, as well as the PDF technique with the application of laminar flamelets for the detailed GRI 3.0 reaction mechanism.

The verification of the methodology was carried out using experimental data on the direct-flow combustion of methane in a bounded domain [3] and in the open space (Flame D) [4]. When modeling these flames, we used both the k-ε turbulence model and an anisotropic Reynolds stress model (RSM).

The results of the direct-flow combustion simulation in a bounded domain showed that for this problem the use of a 2-stage mechanism for both hybrid model and EDC model gives an overestimation of the temperature. Though, the 4-stage mechanism gives a noticeable improvement. Its application for both models gives a fairly close agreement with the experimental data. The use of more complex reaction schemes with EDC model gives the results for temperature, CH4 and O2 very close to those obtained using the 4-stage scheme. Small differences are observed only in the CO and CO_2 concentration profiles.

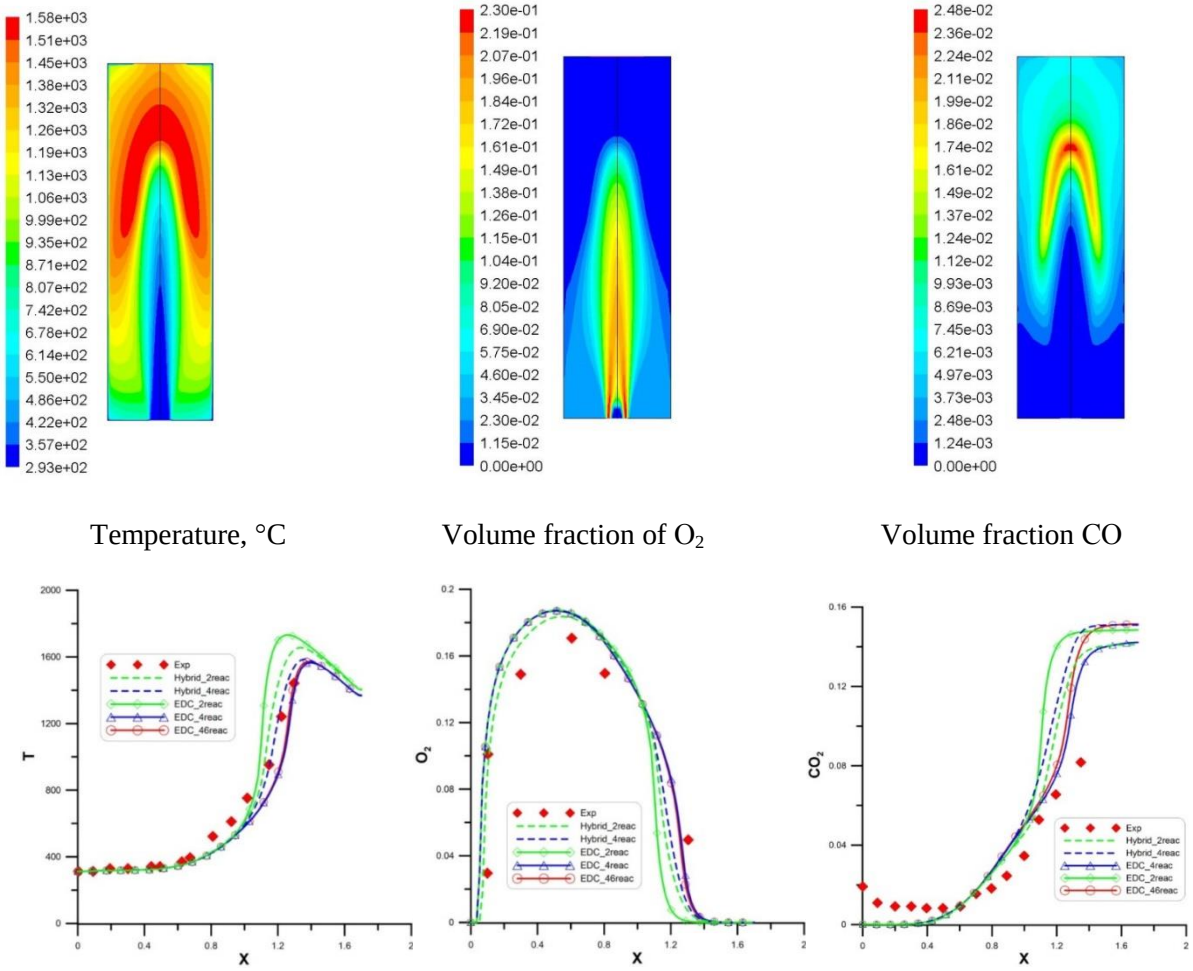


Figure 1. Direct-flow flame in a bounded domain. Temperature, O_2 and CO concentration fields. Temperature, O_2 and CO_2 concentration profiles along the axis of the burner.

The Flame D simulation results showed that the EDC model with 4-stage mechanism gives the result, which is far from the experimental data in terms of all the evaluation criteria. However, the transition to the use of more detailed chemistry (46 reactions) drastically changes the outcome. We have obtained close agreement between calculated and experimental data. The PDF Flamelet model with detailed GRI 3.0 reaction mechanism showed good results as well. It is worth noting that for the considered direct-flow flames the influence of the used turbulence model on the simulation result is less pronounced than the effect of the chosen reaction mechanism.

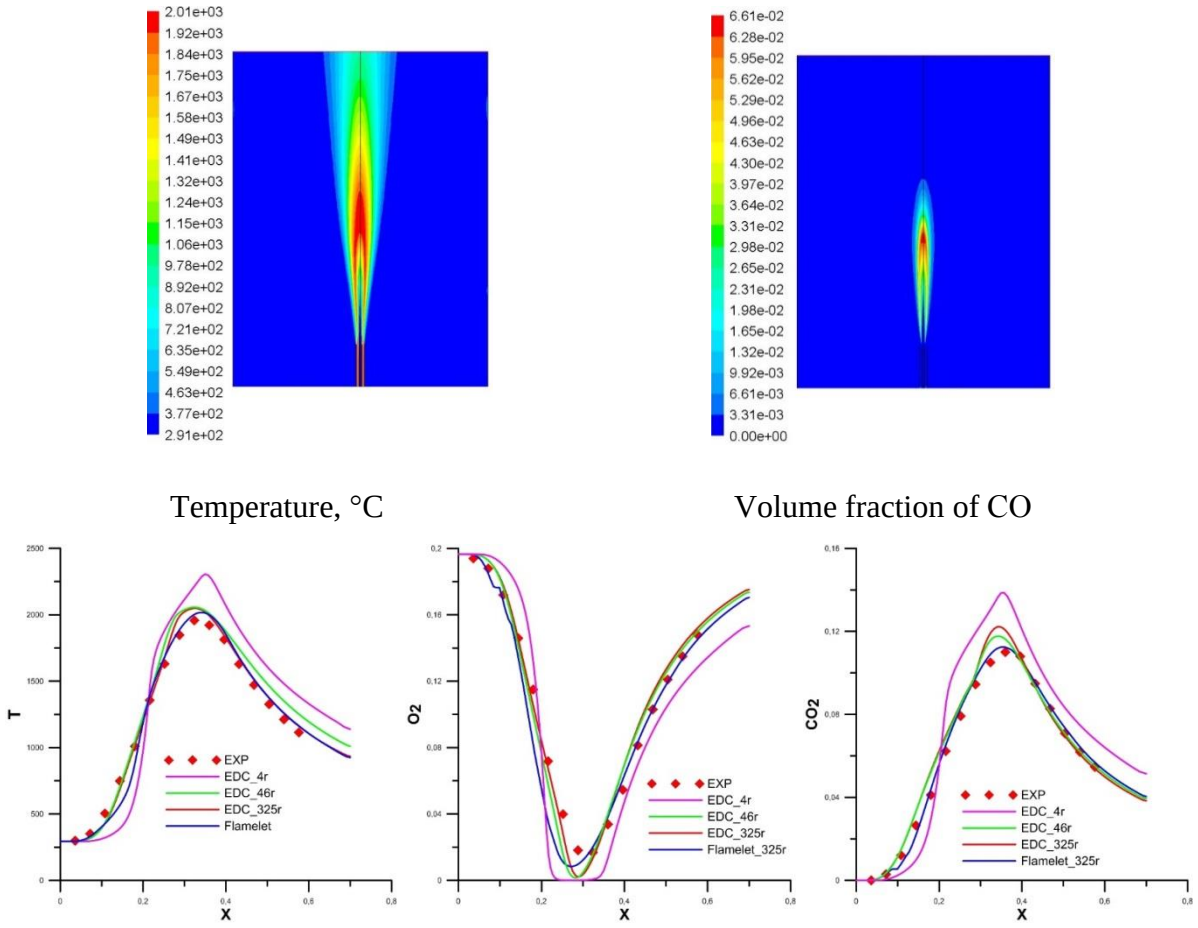


Figure2. Direct-flow flame in an open space (Flame D). Temperature and CO concentration fields. Temperature, O_2 and CO_2 concentration fields along the axis of the burner.

To test the swirling flame models we used the data obtained from the laboratory-scale burner at University of Sydney [5]. Various modes were studied in terms of the mixture composition and twist parameter. For simulation of unsteady flow, we used the URANS and LES approaches, while the EDC model and flamelet technique with different reaction mechanisms were used as combustion models. The close agreement with experimental data was obtained in terms of the temperatures and the gas mixture components (Figure 3,4).

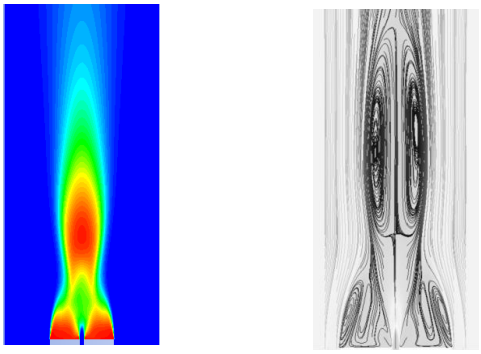


Figure 3. A swirling flame in the burner of the University of Sydney (SM1 regime). The temperature field and the streamlines.

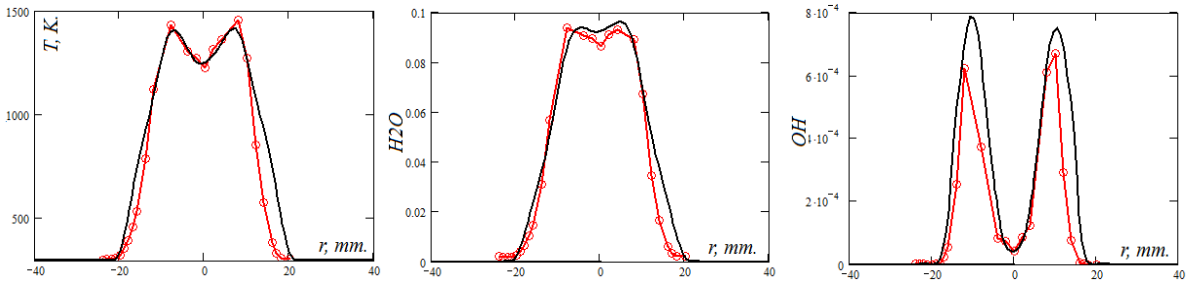
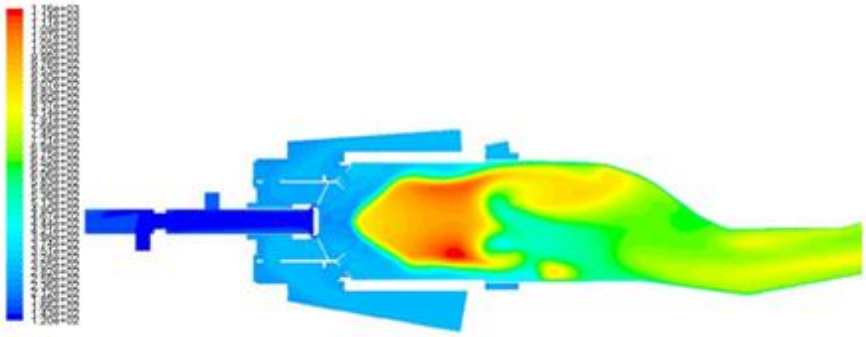


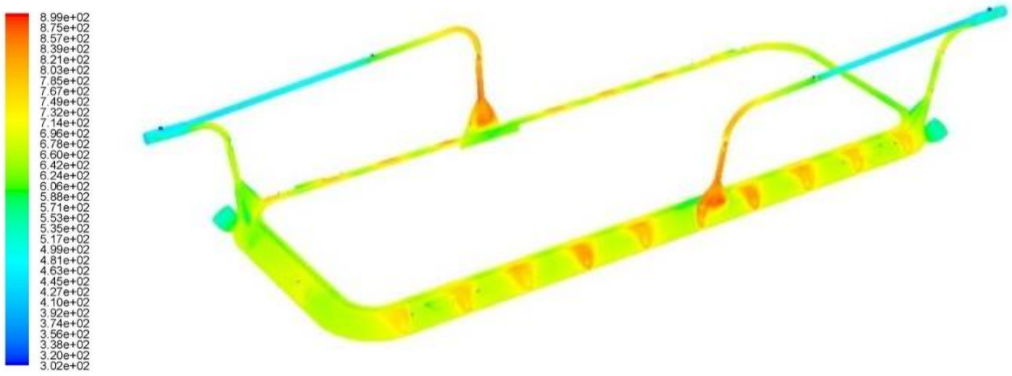
Figure 4. A swirling flame in the burner of the University of Sydney (SM1 regime). Comparison of temperature, H_2O and OH concentration profiles with the experimental data in section x=40 mm. Red line – experiment, black one – calculation

The fine-tuned calculation technique was applied successfully in calculations of burners for the combustion of wet oil-associated gas in oil and gas production, in modelling of operation modes of the gas turbine combustion chamber, optimization of the afterburning process of anode gases from electrolytic cells, and for the evaluation of heat fluxes to the ground in the event of spontaneously igniting oil and gas torches under natural conditions (Figure.5).

The oil-associated gas combustion system. Temperature isosurface of 1200°C.



The temperature field in the combustion chamber of a gas turbine, °C.



The temperature field in the gas-collecting dome of the electrolysis unit

Figure 5. Examples of calculations used for various combustion applications.

Overall, the research results have shown that the use of the EDC and PDF combustion models with flamelets, when using detailed kinetic mechanisms in combination with the eddy-resolving turbulence models provides the best results for all flames. However, such simulations require large computer resources. In some cases, more simple combustion models can be applied in combination with RANS/URANS turbulence models to obtain acceptable results with a much lower computational cost.

To obtain the correct simulation results, when performing applied calculations, it is necessary to carry out the preliminary analysis of possible correct use of the RANS turbulence models and simple reaction mechanisms.

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