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Numerical Modelling of Combustion in 1.5 MW Low-NO_x Burner

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Results from CFD simulations of swirling non-premixed gas flame using a low-NOx gas burner are presented and compared to experimental data measured during a testing campaign in a semi-industrial water-cooled combustion chamber. The burner is both fuel- and air-staged with maximum capacity of 1.5 MW. Numerical simulations are performed with Ansys Fluent software using Reynolds-averaged Navier-Stokes (RANS) turbulence model coupled with eddy-dissipation chemistry model (EDM) and discrete ordinates radiative heat transfer model. This modelling approach is preferable for large-scale combustion applications such as process fired heaters, where employing advanced models (e.g. Large Eddy Simulation) is still computationally demanding.
It is shown, how results are sensitive to the mixing rate constant of EDM, which is employed in a simulation of swirling turbulent diffusion flame. Specifically, temperatures are overestimated with the constant being set to 4 (the default value in Ansys Fluent), which leads to false prediction of NOx formation. Temperature peaks are reduced by lowering the mixing rate constant. An acceptable agreement with measured outlet and peak flame temperatures is achieved, when the constant is set to 0.6. With this value, however, highly increased concentrations of unburned species are reported at the outlet. Predicted values deviate from the measurements about three orders of magnitude. Based on the concentrations of unburned species and oxygen in the flue gas at the outlet, the best results are obtained with the constant 1.2.

1. Introduction

Computational Fluid Dynamics (CFD) has become a standard supporting tool used for design, optimization and troubleshooting of various engineering applications. Present-day CFD codes offer a large variety of physical and chemical models, from which a CFD analyst can select the most appropriate one for a particular application. For large-scale combustion applications such as process fired heaters, however, the choice is usually limited to less demanding ones due to limited computational resources. Increased demands in terms of CPU costs is not only due to model specifications, but also a large span of scales in the geometry (Jegla et al., 2015). Nevertheless, even for complex swirling turbulent flows encountered in engineering practice, it was shown in (Wegner et al. 2004) that unsteady RANS (URANS) turbulence models are adequate to capture main turbulent flow features and instabilities both qualitatively and in parts quantitatively. The modelling approach was validated by comparison both with experiments and Large Eddy Simulation (LES).
Combustion applications require in addition coupling of flow and turbulence equations with equations of energy and species transport, radiation heat transfer and chemical reactions. Among all chemical models, EDM is very often used in large-scale applications due its simplicity and reasonable computational demand. It is based on the assumption “what is mixed is burned” (Magnussen and Hjertager, 1977). The underlying principle of the model restricts a number of reactions, so that no more than a global two-step mechanism should be used. This inevitably leads to over-predicted peak flame temperatures. The rate of a reaction can be controlled by a so-called Magnussen constant or mixing rate constant, which is used in simulations as a tuning parameter to match numerical results with measurements.

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Unfortunately, there seems to be no universal value valid for a wide range of applications. Reported values vary mostly in the range from 0.3 to 4 and depend mainly on the aim of the adjustment (e.g. matching peak flame temperature or CO concentrations). For instance, a value of 0.6 was used in (Yin et al., 2008) to reduce peak flame temperature in simulation of combustion in a biomass grate-fired boiler. For a straw-fired vibrating grate furnace, a value of 2 was used in (Yang et al., 2007) to match concentrations of CO.
There is also a number of works related to adjustment of the constant in prediction of swirling turbulent flames. (Vondál, 2012) systematically analysed effects of various physical models settings including the mixing rate constant on flame temperatures and distribution of local heat fluxes to walls of a combustion chamber. The change of the value from 4 down to 0.6 caused a decrease of temperature peaks by 26 %. The effect of the value on concentrations of CO emissions was not reported. (Li et al., 2015) proposed a modified model for calculation of the constant based on a local Reynolds number. However, the effect of the constant on species concentrations was not investigated.
This work is motivated by results from preliminary CFD simulations performed during development of a new 1.5 MW low-NO_x burner. During the past three years, several design variants of the burner have been developed and experimentally tested at the burners testing facility located at Brno University of Technology. For results from the extensive testing campaign, please refer to (Bělohradský, 2015). Results from a testing campaign of an earlier design variant of the burner are available in (Skryja et al., 2015).
The article reports and summarizes CFD modelling approach that has been adopted during development of the burner. Measured data are compared to predicted values. It is shown, how results are sensitive to settings of the Eddy Dissipation Model (EDM). In this regard, it also extends the work of (Vondál, 2012).

2. Simulated unit

The simulated unit consists of two parts, a burner and two-shell horizontal water-cooled combustion chamber with a stack. The chamber is located at the burners testing facility at Brno University of Technology, where all combustion experiments were carried out. The construction allows to simulate conditions similar to those in process fired heaters. The shell of the chamber is divided lengthwise into seven sections with independent supply of cooling water. It allows to measure local wall heat fluxes extracted from the flame into each of the section. Furthermore, pressure, temperature and flue gas species concentrations can be measured both in the chamber and in the stack. Such configuration provides experimental data for validation of a CFD model not only by a finite set of point values (e.g. temperature), but also area-integrated values (heat fluxes).
The burner is both fuel- and air-staged with a flame holder placed just before the primary head (Figure 1).

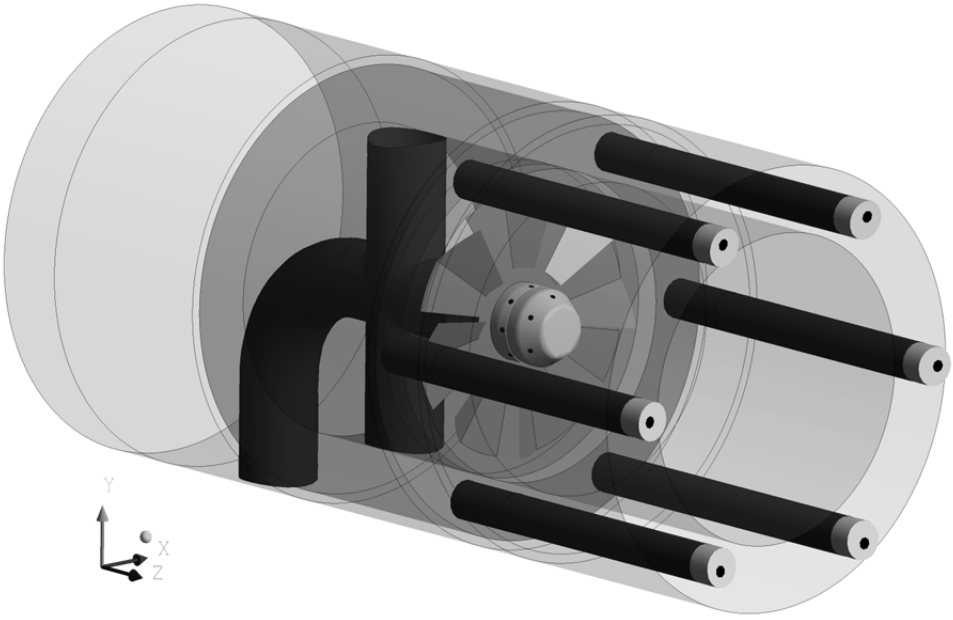

Figure 1: Simulated burner. The combustion air is introduced to the burner from the left side

There are two sets of nozzles of different diameter on the primary head. Axial guide vanes on the flame holder generate swirling motion to stabilize flame and enhance mixing of combustion air with the gas fuel. The pitch angle of vanes is 30°. The combustion air is split into two streams (primary and secondary stages) by a

special cylindrical fitting. Outside the fitting, there are six equal-sized uniformly distributed secondary nozzles. The pitch angle of each secondary head's tip is 5°.
The characteristic dimensions of the computational domain span three orders of magnitude. While the length and diameter of the chamber are 3.8 m and 1 m, respectively, the smallest diameter of nozzles on the primary head is 2.9 mm. The total length of the domain is 5.9 m.

3. Computational model setup

3.1 Operational and boundary conditions

Operational and boundary conditions are set according to the experimental conditions and are summarized in Table 1. While front and rear faces of the chamber are adiabatic, temperature boundary condition is prescribed at the outer wall of the shell, which is modelled as a thin wall with a thickness of 10 mm for the calculation of thermal resistance. The temperature is estimated using a stand-alone simulation of cooling water flow in the shell, for which heat fluxes from the flame to each section are known and evaluated from the experiment. Calculated area-weighted temperatures are within the range from 77 °C to 127 °C with the peak value located in the fourth section.

Table 1: Summary of operational and boundary conditions.

Parameter	Settings			
Pressure at the outlet (in the stack)	101,225 Pa			
Total mass flow rate of methane	0.02 kg/s			
Mass flow rate of methane through primary nozzles	0.0036 kg/s			
Excess of combustion air	1.15			
Mass flow rate of combustion air	0.598 kg/s			
Composition of air (vol. %)	O_2	N_2	H_2O	CO_2
	20.7668	78.536	0.6673	0.0299
Inlet temperature of methane and air	13 °C			

3.2 Physical and chemical models

The choice and setup of physical models is based on settings described in (Vondál, 2012). The study included effects of several RANS turbulence models, radiation heat transfer parameters (namely absorption coefficient and emissivity of the chamber wall) and chemical models. Results suggest that, for investigated thermal duties of 745 kW and 1,120 kW, *k*-ω SST turbulence model coupled with EDM provided reasonably accurate predictions. Predictions were improved also by modification of standard absorption coefficient calculation in Weighted Sum of Grey Gases Model (WSGGM) as described in (Yin et al., 2010). Therefore, the same modelling approach has been adopted in the present work.
The setting of a chemical model requires further explanation. EDM is a computationally affordable model applicable to turbulent diffusion flames. The value of the constant originally proposed by (Magnussen and Hjertager, 1977) is 4. In correspondence with aforementioned research works, it has been observed during the development of the computational model, that the value lead to over-predicted temperature peaks, which was undesirable for NO_x prediction. It has been decided to decrease the value to 0.6 as recommended by (Yin et al., 2008). However, highly increased concentrations of unburned species have been reported at the outlet. In order to examine effects of the constant on prediction of heat fluxes, temperatures and concentrations of combustibles at the outlet, two other values have been tested, i.e. 1.2 (twice as many the value of 0.6) and 2 (twice as less the value of 4). Physical and chemical models setup is summarized in Table 2.

Table 2: Settings of physical and chemical models.

Model or modelling parameter	Settings
Turbulence model	*k*-ω SST
Radiation model	Discrete ordinates with modified absorption coefficient (Yin et al., 2010)
Emissivity of walls	0.9 (Vondál, 2012)
Chemistry	EDM with global two-step mechanism (Westbrook and Dryer, 1981)
Mixing rate constant of EDM	0.6, 1.2, 2, 4

3.3 Discretization

The computational domain is discretized into approximately 1.7 million control volumes, 1.5 million of which are hexahedral and the rest are polyhedral cells. Although turbulent fluctuations are usually severe in swirling

turbulent flows, so that a steady simulation does not converge, steady simulation is performed and presented within this work, too. It provides a rough estimate of combustion parameters including local wall heat fluxes, temperature, species concentrations and length of the flame. However, due to the fluctuations, unsteady simulation is carried out in order to correctly capture the fluctuations. The discretization setup is summarized in Table 3.

Table 3: Discretization schemes and settings

Variable/Parameter	Scheme/settings
Solver	SIMPLE
Pressure	PRESTO!
Density	Second order upwind
Momentum	Third order MUSCL
k-ω SST turbulence equations	Third order MUSCL
Species	First order upwind
Energy	First order upwind
Discrete ordinates	Second order upwind
Transient formulation	Second order implicit
Time step	0.002 s

4. Results and discussion

Results from simulations and experiment are summarized in Table 4. It includes area-weighted heat fluxes to individual sections denoted as S1 through S7, the total extracted heat denoted as Total, mass-weighted flue gas temperature at the outlet T_{out}, maximum gas temperature in the domain T_{max} and mass-weighted concentrations of carbon monoxide (CO), methane (CH_4) and oxygen (O_2) in dry flue gas. Lines of the Table 4 are organized in pairs according to the value of the constant A. For each pair, results from steady and transient formulation are presented, denoted as (s) and (t), respectively.

As it has already been mentioned, steady simulations have not fully converged due to turbulent fluctuations. However, residuals of governing equations decreased to and kept around low values for hundreds of iterations. Such an estimate of the solution is valuable in preliminary design of a burner. Especially in large-scale applications, where rigorous time-averaging is impossible due to high computational demands, it provides an estimate for main combustion parameters of interest, such as heat transfer rates, outlet temperatures and concentrations of species.

More realistic results are expected to be obtained with transient formulation. However, rigorous time averaging (i.e. over many residence times) is time-consuming even with the time step being 0.002 s and residence time around 3 s. Therefore, calculated time averages over one residence time presented in the study represent only estimates of the true averages.

The last line of Table 4 contains measured values averaged over 40 min with two-minute sampling interval.

Table 4: Calculated and measured values of heat flux, flue gas temperature and concentration

	Heat Flux to sections								Temperature		Concentration		
	S1	S2	S3	S4	S5	S6	S7	Total	T_{out}	T_{max}	CO	CH_4	O_2
Unit				kW/m^2				kW	°C	°C	ppm	ppm	vol. %
A0.6(s)	23.6	27.2	44.4	61.5	65.0	60.0	43.3	557.6	862.7	1,237	1,363	394	3.16
A0.6(t)	20.9	27.0	42.8	59.0	63.9	60.2	44.6	549.6	873.8	1,152	1,568	475	3.21
A1.2(s)	24.2	32.2	48.4	63.6	65.5	59.6	43.2	575.7	847.4	1,632	25.4	3.7	3.00
A1.2(t)	21.5	29.5	46.8	61.4	63.7	58.0	44.9	561.2	877.9	1,558	29.6	4.9	2.99
A2.0(s)	23.8	32.6	48.5	61.3	63.3	59.3	44.3	571.4	858.6	1,820	0.4	0.04	2.92
A2.0(t)	21.4	30.7	47.5	60.0	62.5	58.3	45.8	563.2	869.7	1,778	0.5	0.05	2.88
A4.0(s)	20.6	28.7	48.7	61.2	63.4	60.2	45.6	566.7	866.5	1,920	10^{-4}	10^{-5}	2.88
A4.0(t)	21.4	29.4	45.8	60.1	63.8	58.9	45.8	561.7	871.8	1,919	10^{-4}	10^{-5}	2.84
Meas.	29.9	39.4	57.3	63.8	59.8	50.1	37.4	567.9	846.9	NA	0.9	NA	3

It can be seen that settings of EDM with A set to 0.6 lead to over-predicted both outlet and peak flame temperature. The peak flame temperature is not available in the measurement. However, based on the results from the testing campaign of the same type of the burner with a pitch angle of the blades 20° as published in one of the authors' previous works (Bělohradský et al., 2015), temperature maxima should be around

1,300 °C. Concentrations of flue gas species at the outlet indicate that the reaction is too fast with this value of the constant A. This results not only in high temperatures, but also in too low concentration of all flue gas species at the outlet. The concentration of oxygen indicates that too much of O_2 has been depleted in reactions, hence very low levels of combustibles are reported, too (for sake of readability, only the order of the values are given). Note that a portion of oxygen reported at the outlet would be consumed by NO_x formation reactions, which are not considered in the study.

On the other hand, the value of 0.6 of the mixing constant under-predicts temperature maxima. Highly increased concentrations of CO and CH_4 are reported at the outlet, as well as higher volume of O_2 compared to the measurement. The reason is that the rate of reactions is rapidly slowed down with the value. Doubling that causes CO and CH_4 concentrations to decrease about two orders of magnitude. Further increase of the value to 2 decreases concentrations again about two orders of magnitude close to the measured values, but it also leads to too high peak flame temperature . Therefore, based on concentrations of combustible species at the outlet and peak flame temperature, the best results are obtained with the mixing constant of 1.2.

Results are also compared in terms of predicted heat fluxes into the sections of the water-cooled chamber and the total extracted heat. Comparison of heat fluxes as obtained by the measurement and steady simulations is shown in Figure 2. Results from transient simulations compared to the measurement are depicted in Figure 3. It can be seen that while calculated heat fluxes are under-predicted in the first half of the chamber, higher values are predicted in the second half as compared to the measurement. The simulated trends seem to be shifted from the measured ones by one section. According to (Vondál, 2012), for high flow rates through a swirl generator (corresponding to thermal duty of 1 MW), this can be attributed to low capabilities of the turbulence model to properly predict all features of swirling flows, which affect mixing of the fuel with air and, hence, the heat release. The total extracted heat is best predicted with the mixing constant of 4. However, longer time-averaging is needed to improve the statistics of predicted quantities for all cases due to the thermal inertia of the chamber.

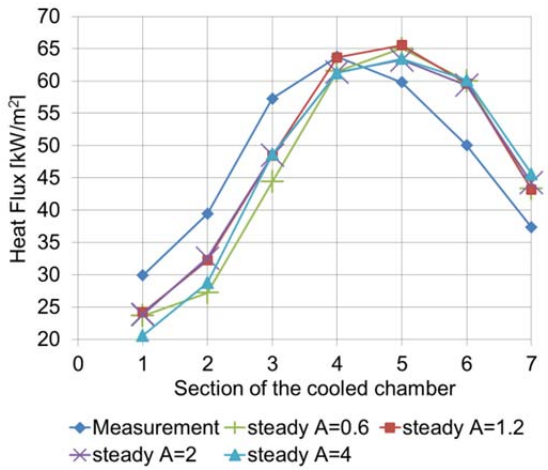

Figure 2: Comparison of heat fluxes into sections of the cooled chamber as obtained by measurement and steady simulation

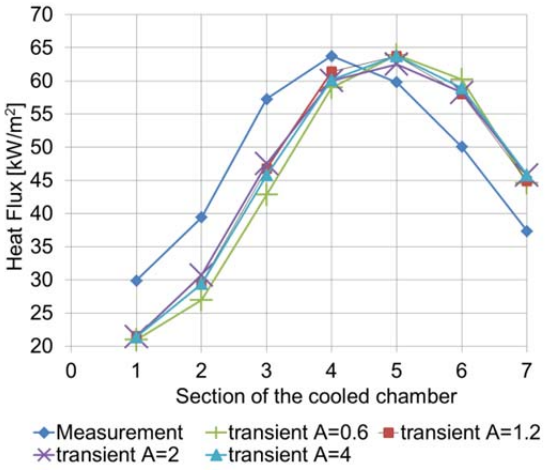

Figure 3: Comparison of heat fluxes into sections of the cooled chamber as obtained by measurement and transient simulation

5. Conclusions

Effects of the Magnussen constant of EDM on CFD predictions of swirling diffusion methane flame of an industrial low-NOx burner are studied. Investigated parameters include wall heat fluxes, temperatures and concentrations of species in the flue gas. Both steady and unsteady simulations are performed for values of the constant of 0.6 (as used in (Vondál, 2012) in order to decrease peak flame temperature), 1.2, 2 and 4 (originally proposed by (Magnussen and Hjertager, 1977)).

While the value of 0.6 has a potential for better predictions of NO_x formation as it predicts the peak flame temperature close to the measured one, it leads to high concentrations of unburned CO and CH_4 as well as oxygen at the outlet. This is due to too low mixing rate of reactions.

The total extracted heat by the chamber walls is best predicted with the value of 4. This, however, over-predicts both outlet and the peak flame temperature. Since reactions proceed fast due to the value,

combustible species burn almost completely. This, however, does not correspond with the measurement. The rate of the reaction is also reflected in the predicted concentration of oxygen at the outlet, which is lower compared to the measured value of 3 % by volume.
Simulations show that increasing the value of 0.6 to 1.2 decreases concentration of unburned species about two orders of magnitude. The same trend is observed with further increase of the value to 2, for which the concentration of CO matches the measured value fairly well. However, both outlet and peak flame temperature are over-predicted.
The best results in terms of reported and measured concentrations of gas species and temperature maxima in the simulated domain are obtained with the value 1.2. Based on the results, an optimal value, however, is not found, yet. Results also need to be improved by longer time-averaging corresponding to several residence times.
While peak values of local wall heat fluxes are predicted reasonably well, the location of maxima is shifted about 0.5 m towards the outlet. The behaviour can be attributed to the use of RANS turbulence model.

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