

DEVELOPMENT OF MATHEMATICAL MODEL FOR CO-FIRING PULVERIZED COAL AND BIOMASS IN EXPERIMENTAL FURNACE

by

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A comprehensive mathematical model for prediction of turbulent transport processes and reactions during co-combustion of pulverized fuels in furnace fired by 150 kW swirl stabilized-burner has been developed. Numerical simulations have been carried out by using an in-house developed computer code, with Euler-Lagrangian approach to the two-phase flow modelling and sub-models for individual phases during complex combustion process: evaporation, devolatilization, combustion of volatiles, and char combustion. For sub-model of coal devolatilization the approach of Merrick is adopted, while for biomass devolatilization the combination models of Merrick, and of Xu and Tomita are selected. Products of devolatilization of both the pulverized coal and biomass are considered to contain the primary gaseous volatiles and tar, which further decomposes to secondary gaseous volatiles and residual soot. The residual soot in tar and carbon in coal and biomass char are oxidized directly, with ash remaining. For volatiles combustion the finite rate/eddy break-up model is chosen, while for char oxidation the combined kinetic-diffusion model is used. The comprehensive combustion model is validated against available experimental data from the case-study cylindrical furnace. The agreement of the simulations with the data for the main species in the furnace is quite good, while some discrepancies from experimental values are found in the core zone. The presented model is a good basis for further research of co-combustion processes and is able to provide analysis of wide range of pulverized fuels, i. e. coal and biomass. At the same time, the model is relatively simple numerical tool for effective and practical use.

Key words: modelling, validation, co-firing, swirl burner, pulverized coal, biomass, experimental furnace, devolatilization, tar, soot

Introduction

Using fossil fuels for energy purposes leads to continuous increase in the concentration of CO₂, CO, SO_x, NO_x, and other harmful oxides in the atmosphere that cause global warming and other negative influences, like acid rains and photochemical smog. The main motivation for co-firing coal with biomass is to reduce CO₂ emissions as the so-called greenhouse gas (because the greatest impact on global warming), but may also contribute to reduction of nitrogen and sulphur oxides [1], depends on composition of the fuel. This procedure contributes to increased use of biomass as a renewable energy source [2].

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The complexity of the flow and installation, lack of measurement equipment and costs of experiments, often make it impossible, or difficult to perform experimental tests in furnaces. Because of that, mathematical models are developed based on theoretical considerations of physical processes and chemical reactions as well as empirical values from the literature and experimental tests [2]. The CFD may offer an effective and low cost toll for analysis and optimization of the processes under a wide range of operating conditions [3-7].

Review articles can be found, which describe modelling approaches to predict biomass co-firing with pulverized coal [8-10]. Since the sub-models of pulverized biomass combustion are based on pulverized coal combustion sub-models, it is necessary to have good knowledge in modelling combustion of coal. These sub-models contain mathematical and numerical representations of the fundamental principles that characterize the physicochemical phenomena of interest.

In this paper a new comprehensive mathematical model for prediction of pulverized coal and biomass co-firing with special focus on chemical reactions is proposed and validated against available measurements. The model includes the individual phases during complex combustion process: evaporation, devolatilization, combustion of volatiles, and char combustion.

Devolatilization process plays a significant role in co-combustion pulverized coal with biomass and two main approaches are used for devolatilization modelling: network devolatilization models and empirical devolatilization models [11]. The network models are able to accurately predict the rates, yield and composition of volatile using as input experimental data. On the other hand, the network models are quite-complex and require significantly larger computational resources in compare with empirical devolatilization models. In this work, the single kinetic rate model (SRM) is chosen for process of devolatilization. The empirical approaches, like this one, do not predict the composition of volatiles. Therefore, it is necessary to define the sub-model for determination of the composition of volatiles, as well. A considerable difference between coals and biomass required selecting different approaches to describe devolatilization process.

The swirl burners used in pulverized coal are designed to ensure flame stability and to make short, intense flames in an effort to reduce furnace size and increase fuel burnout. Both objectives are met by swirling the secondary air prior to entering the furnace [12, 13]. The circulation of hot combustion gases ensure flame stability, while swirled secondary air also increases fuel and air mixing, producing short, intense flames. Task of the swirl burner is to minimize concentration of NO_x with maintaining flame stability and overall burnout.

The main aim of this work is development of mathematical model and computer code representing complex tool for analysis of processes during combustion and co-combustion, which would include pulverized solid fuels in a wider range of characteristics. The developed model has to be efficient for practical application and to enable the complex parametric analysis in real conditions.

The swirl burner and the furnace configuration and co-firing conditions

Numerical simulations are used to validate model with experimental available data in a 150 kW swirl-stabilized down-fired dual-feed burner flow reactor, which were performed by Brigham Young University, Provo, Ut., USA, [12]. The down-scaled dual-feed swirl burner is placed on the top of the furnace and fires the coal and biomass downward into the reac-

tor. The straw is fed into the burner through the center tube with central air, while the coal is fed through annulus with annular air.

The schematic drawing of the dual-feed burner and furnace interior is presented graphically in fig. 1. The fuels used for co-firing are coal (Blind Canyon, a high volatile bituminous coal) and wheat straw. This combination of coal and biomass enables us to analyse the combustion of pulverized solid fuels in a wider range of characteristics. The main properties of fuels and firing conditions are given in tab. 1.

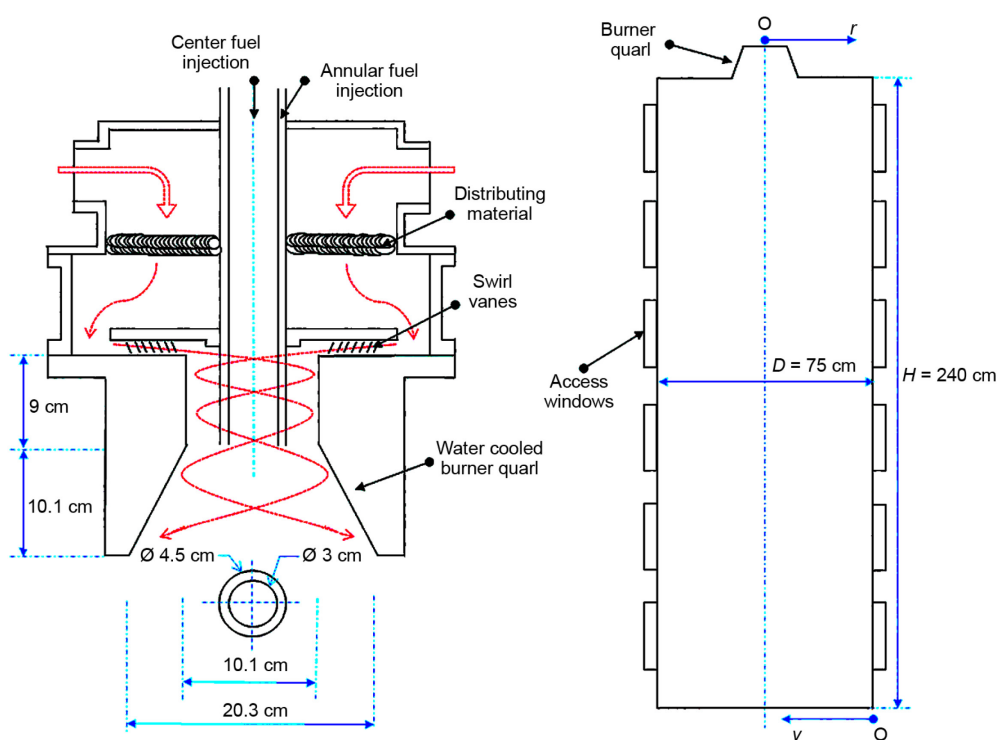


Figure 1. Dual-feed burner cross-section and scaled view furnace interior

The mathematical model for co-firing pulverized coal and biomass and the numerical code

Comprehensive axisymmetric 2-D mathematical model in cylindrical co-ordinates is used for numerical prediction of processes in two-phase flow under stationary conditions. The model for co-combustion includes sub-models of dispersed (particle) phase and gas phase. Gas phase is modelled using Reynolds averaged Navier-Stokes equations approach with standard $k-\varepsilon$ turbulence model [14, 15]. Heat exchange by radiation in reactor is simulated by discrete ordinates (flux) model. Interaction between fluid and particles is modelled using particle source in cell method, and particle collisions are neglected. The motion of dispersed phase is modelled using Basset equation in a Lagrangian frame, taking into account that only drag and gravity forces acting on the particles [15]. All particles are assumed to have a spherical shape in this proposed model. Unlike coal particles, biomass particles are relatively large in size and non-spherical in shape, that considerably affect the motion and conversion of

Table 1. Main properties and firing conditions of the two fuels [12]

Proximate analysis data (the base: AR = as received; D = dry; DAF = dry ash-free; % on mass)					
	Moisture [%, AR]	Volatiles [%, D]	Fixed carbon [%, D]	Ash [%, D]	
Coal	2.1	40.6	51.5	7.89	
Straw	7.7	79.5	15.6	4.91	
Ultimate analysis data (% on mass)					
	C [%, DAF]	H [%, DAF]	O [%, DAF]	N [%, DAF]	S [%, DAF]
Coal	81.22	5.52	10.97	1.66	0.63
Straw	49.73	5.97	43.73	0.57	<0.01
Operational parameters of coal/straw co-firing					
Central fuel (straw) [kg ^h ⁻¹]	Annular fuel (coal) [kg ^h ⁻¹]	Central air [kg ^h ⁻¹]	Annular air [kg ^h ⁻¹]	Secondary air [kg ^h ⁻¹]	Swirl number
15.1	7.5	9	12	160	1
Particle size and fuel particle density					
	Mean diameter, d_p , [μm]		Density, ρ_p , [kgm ⁻³]		
Coal	110.4		1400		
Straw	451.0		600		

fuel particles in furnace. For this reason, drag coefficient of biomass particle is calculated as a function of spherical particle Reynolds number and shape factor [16, 17]. Initial and boundary conditions are applied, and the corresponding *wall functions* are implemented for conditions near the walls, which also have significant impact on the accuracy of numerical results [15, 18].

Moisture present in the coal and biomass is released during heating of the particles to about 100 °C and the rate of moisture evaporation is calculated by the kinetic rate expression:

$$\frac{dm_p}{dt} = -A \exp\left(-\frac{E}{RT}\right) m_p \quad (1)$$

Further heating over 400-500 °C, the volatiles are released (combustible volatile matter). For process of devolatilization empirically SRM is selected, supported by the sub-model for determination of the composition and the amount of volatile. The SRM assumes that the rate of devolatilization is first-order dependent on the amount of volatiles remaining in the particle:

$$\frac{dm_p}{dt} = k_{vol} [m_p - (1 - f_{v,0})(1 - f_{w,0})m_{p,0}] \quad (2)$$

The SRM does not predict the composition of the volatiles, and therefore the sub-models for determining the composition of volatiles of coal and biomass are defined, as well.

A sub-model for the determination of the composition and amount of the coal volatiles is selected by using a matrix defined by Merrick in [19]. The sub-model determines the

composition and amount of the volatiles, based on the known proximate and ultimate analysis of the fuel. For the prediction of effective volatile matter in function of the volatile matter proximate analysis, the expression (3) is used:

$$V = p - 0.36p^2 \quad (3)$$

The matrix proposed by Merrick makes a system of ten equations with ten unknowns, which is solved simultaneously. By introducing mathematical correction matrix, the five unknowns can be solved explicitly: $\text{CHAR} = 1 - V$, $\text{CH}_4 = 1.31 \cdot \text{H}$, $\text{C}_2\text{H}_6 = 0.22 \cdot \text{H}$, $\text{CO} = 0.32 \cdot \text{O}$, and $\text{CO}_2 = 0.15 \cdot \text{O}$. The remaining components of the coal volatiles: TAR, H_2 , H_2O , NH_3 , and H_2S , can be simultaneously solved by an implicit system of five equations with five unknowns:

$$\begin{bmatrix} 0.85 & 0 & 0 & 0 & 0 \\ 0.082 & 1 & 0.1111 & 0.1765 & 0.0588 \\ 0.049 & 0 & 0.8889 & 0 & 0 \\ 0.009 & 0 & 0 & 0.8235 & 0 \\ 0.01 & 0 & 0 & 0 & 0.9412 \end{bmatrix} \begin{bmatrix} \text{TAR} \\ \text{H}_2 \\ \text{H}_2\text{O} \\ \text{NH}_3 \\ \text{H}_2\text{S} \end{bmatrix} = \begin{bmatrix} \text{C} - 0.98 \cdot \text{CHAR} - 0.75 \cdot \text{CH}_4 - 0.8 \cdot \text{C}_2\text{H}_6 - 0.4286 \cdot \text{CO} - 0.2727 \cdot \text{CO}_2 \\ \text{H} - 0.002 \cdot \text{CHAR} - 0.25 \cdot \text{CH}_4 - 0.2 \cdot \text{C}_2\text{H}_6 \\ \text{O} - 0.002 \cdot \text{CHAR} - 0.5714 \cdot \text{CO} - 0.7273 \cdot \text{CO}_2 \\ \text{N} - 0.01 \cdot \text{CHAR} \\ \text{S} - 0.006 \cdot \text{CHAR} \end{bmatrix} \quad (4)$$

With Merrick's matrix a bad solutions for some species of the fuel volatiles with large contain of volatile is obtained, as it is the case with biomass. For sub-model of biomass devolatilization the combination models of Merrick, and Xu and Tomita [20] are adopted. In sub-model which proposed Xu and Tomita, the yields of CO and H_2O (DAF) varied linearly with the mass fraction of each element in the ultimate analysis [21], as can be seen in eqs. (5) and (6):

$$\frac{16}{28}[\text{CO}] = 0.1657 \cdot \text{O} \quad (5)$$

$$\frac{16}{28}[\text{H}_2\text{O}] = 0.2933 \cdot \text{O} \quad (6)$$

They also obtained a correlation (7) between the mass fractions of tar (DAF) and proximate volatile matter as follows [21]:

$$[\text{tar}] = 0.48p \quad (7)$$

The rest of biomass volatiles are determined by using Merrick's matrix.

Discretizations of PDE are done by control volume method and hybrid differencing scheme, and discretized equations are solved by SIPSOL method. Numerical simulation is carried out by using the in-house developed CFD code, in which sub-models for particle phase during complex combustion process (evaporation, devolatilization, combustion of volatile, and char combustion) are implemented.

Results and discussion

For numerical simulations three structured numerical meshes are used, which consist of 5080, 19656, and 77308 cells (coarse, medium, and fine grid, respectively). Stability and convergence of the model are tested, as shown in fig. 3, and computational grid of 19656 nodes is adopted, which is sufficient in order to obtain a grid independent solution.

The well-converged results obtained by numerical simulations are compared with the available experimental data in the furnace. Regarding the behaviour of the flame, an internal and an external re-circulation zone are formed in the top section of the furnace, just as expected for a confined swirl burner, as shown in fig. 4. The internal re-circulation zone forces gas-flow toward the burner along a portion of the centerline and thereby slowing the entering fuel particles. An external re-circulation zone is formed in the upper corners where the furnace wall meets the top, transporting hot combustion products to the top wall of the furnace.

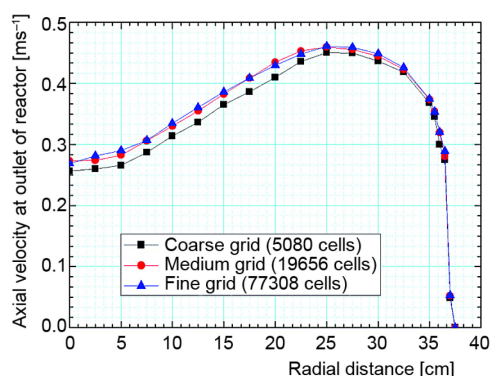


Figure 3. Grid independency test results

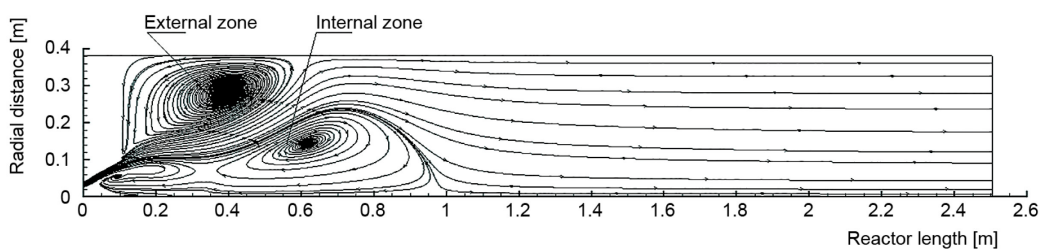


Figure 4. Sketch of external and internal zone of co-firing flame

In the co-firing flame, most of the coal particles which are smaller in compare with particles of biomass, are rapidly dry, begin devolatilization upon injection into the burner quarl and affected by the secondary air jet with increased residence time. Unlike them, particles of biomass are less influenced by the secondary air, mainly pass through internal re-circulation zone and thus reduce residence time in the reactor. Trajectories of pulverized fuel particles follow the gas-flow field as expected, as can be seen in fig. 5.

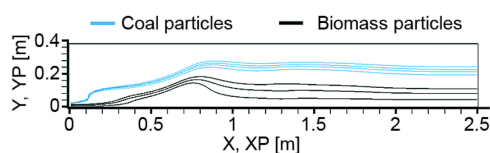


Figure 5. Trajectories of pulverized coal and biomass

After they enter the reactor, due to the intensive heat exchange, pulverized coal and biomass particles undergo a series of transformations. Pulverized fuels fed into the furnace,

when heated to 100-105 °C are dried at first, *i. e.* the moisture from the fuels evaporates. Further heating, in addition to moisture release, starts the devolatilization process – the release of combustible volatile compounds (CH_4 , CO , H_2 ...). The volatiles released during the devolatilization mix with oxygen from the air, ignite, and combust. In fig. 6 the CFD results of methane molar concentration field in the furnace are shown. After the devolatilization process is finished, the solid particles – char residues (containing carbon and mineral matter) remain, which further combust through the heterogeneous reactions.

Gas sampling system was used in investigation [12] for producing quantitative maps of gas species in co-firing flames, which was serve as a benchmark for CFD validation. The

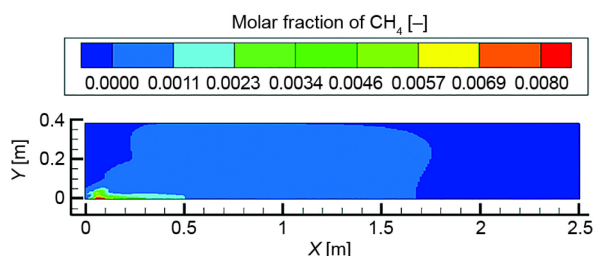


Figure 6. The CFD results for molar fraction of methane (for color image see journal web site)

most important components of the gas sampling system in discussing co-firing flame issues are the gas sampling probe with FTIR-based long-pass gas cell analyser and a Horiba gas analyser. A FTIR gas analyser works on the principle of absorbance of infrared light and quantifies species concentrations from gases sampled in the flame. A Horiba gas analyser was also used to measure gas species and requires a dry measurement, so a desiccant dried the sample gases after the FTIR. Also, the thesis [12] explained difficulties of measuring gas species and why the obtained experimental data did not exhibit perfect symmetry about the geometric centerline.

The CFD results of CO_2 and O_2 are compared with the experimental data from [12] along the radial direction at different axial distances downstream of the burner for the co-combustion (coal and straw) flame, as shown in figs. 7 and 8. Given concentrations of combustion products reflect the complex turbulent transport processes and reactions in the furnace. Results are shown in the entire cross-section of the reactor because the measured profiles are somewhat different due to the influence of the measuring device.

The comparison between the predicted values of CO_2 and O_2 are found to show a quite satisfactory agreement with the measured data, which also agree with expectations on the profiles of the species, while the somewhat noticeable deviation from experimental values is found in the core zone. The reliability of numerical modelling for complex swirling flows with co-firing is highly determined by the accuracy of the turbulence model in the core region, so that with other models of turbulence better agreements might be obtained. Towards the furnace outlet, the flow develops; the deviations become smaller and near the outlet of the reactor average discrepancies do not exceed 4%.

Qualitatively, all profiles correspond to the reference measurements. According to the results of the comparisons it can be concluded that the proposed mathematical model has been successfully validated.

Conclusions

Co-firing of pulverized coal and biomass is a potentially valuable method used to help decreasing greenhouse gas and other emissions in coal-fired boilers.

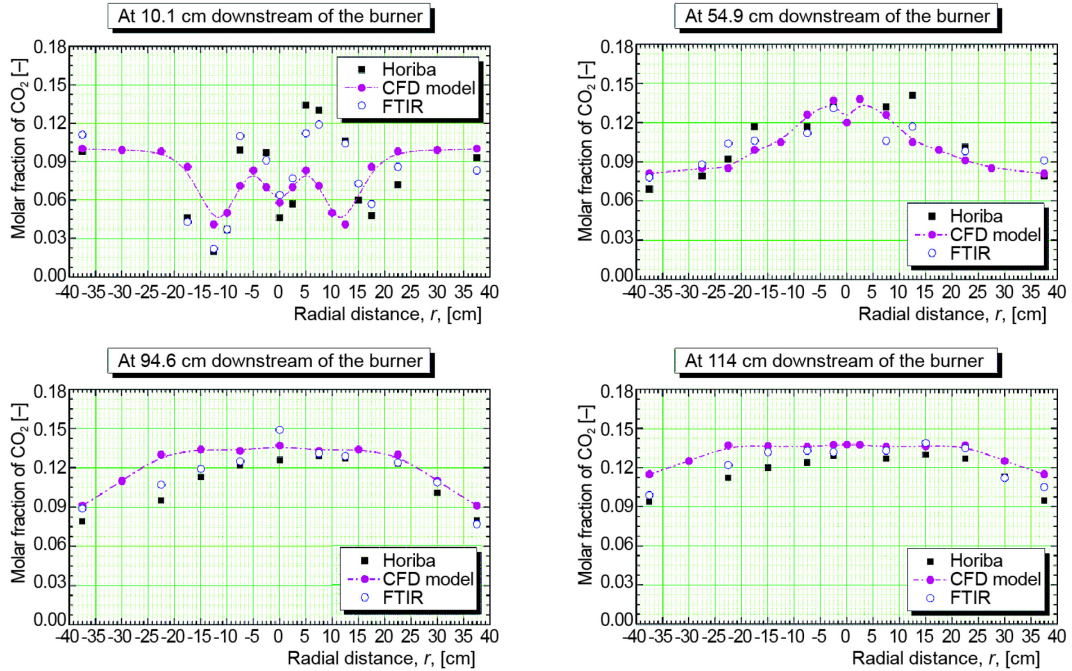


Figure 7. Comparison of experimental data and CFD model results for molar fraction of CO₂

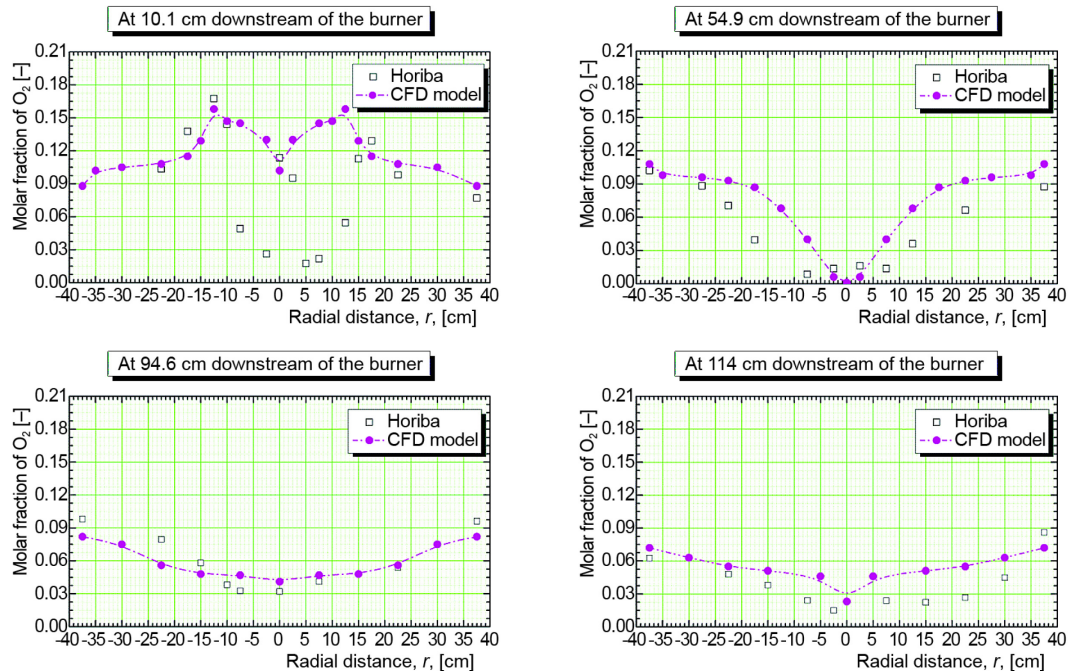


Figure 8. Comparison of experimental data and CFD model results for molar fraction of O₂

A new comprehensive differential mathematical model and computer code are developed, validated, and applied for investigation of co-firing processes in a 150 kW swirl-stabilized down-fired dual-feed burner flow furnace.

Numerical simulations are carried out by an in-house developed computer program, which has incorporated solid particles tracking and combustion reactions sub-models for complex in-furnace process. Comparisons of the simulations results with the available measurements for the main species in the case-study experimental furnace are quite satisfactory, especially with respect to the complexity of the problem considered.

The presented model is a good basis for further research of co-firing processes and is able to provide analysis of wide range of pulverized fuels, *i. e.* coal and biomass, and at the same time, is relatively simple tool for effective and practical use.

For further improvements of the comprehensive mathematical model non-isothermal particle heating could be taken into account, which can be important especially for some cases of combustion of large biomass particles. In order to optimize the processes during co-firing and improve the industrial furnaces exploitation in real conditions, regarding both the emission and the efficiency, a complex numerical analysis must be conducted, with numerous parameters varied, such as fuel and air distribution, fuels particles shape and size, *etc.*

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Nomenclature

A, A_h – frequency factors in Arrhenius relations, [s^{-1}]	x_{fu}, x_{ox} – mass concentrations of combustible gas and oxidant, [$kgkg^{-1}$]
A_{hi} – coefficient for homogeneous reaction, [–]	x_{mol}^{ox} – oxidant molar concentration, [$molm^{-3}$]
A_p – particle cross-section area, [m^2]	<i>Greek symbols</i>
E – activation energy, [$Jmol^{-1}$]	ε – turbulent kinetic energy dissipation, [m^2s^{-3}]
$f_{v,0}$ – mass fraction of volatiles initially present in the particle, [–]	ρ – fluid density, [kgm^{-3}]
$f_{w,0}$ – mass fraction of moisture, [–]	Ω_{ch}, Ω_{ct} – kinetic and turbulent mixing reaction rates of homogeneous reaction, [$kgm^{-3}s^{-1}$]
k – turbulence kinetic energy, [m^2s^{-2}]	<i>Subscripts and superscripts</i>
k_r – reaction rate parameter in kinetic regime, [s^{-1}]	a, b, c – coefficients of homogeneous reaction
k_d – diffusion parameter of mass transfer, [s^{-1}]	fu – fuel
k_{vol} – kinetic rate of devolatilization, [s^{-1}]	mol – molar
M_p – molar mass of particle, [$kgmol^{-1}$]	ox – oxidant
m_p – particle mass, [kg]	p – particle
$m_{p,0}$ – initial particle mass, [kg]	v, vol – volatile
p – proximate analysis of volatile matter, [–]	w – wet
R – universal gas constant, [$Jmol^{-1}K^{-1}$]	<i>Acronym</i>
R_c – heterogeneous reaction rate, [$kg s^{-1}$]	FTIR – Fourier transform infrared
s – stoichiometric coefficient, [–]	
T – temperature, [K]	
t – time, [s]	
V – effective volatile matter, [–]	

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