Numerical Modelling of Emissions of Nitrogen Oxides in Solid Fuel Combustion

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ABSTRACT

Among the combustion products, nitrogen oxides are one of the main contributors to a negative impact on the environment, participating in harmful processes such as tropospheric ozone and acid rains production. The main source of emissions of nitrogen oxides is the human combustion of fossil fuels. Their formation models are investigated and implemented with the goal of obtaining a tool for studying the nitrogen-containing pollutant production. In this work, numerical simulation of solid fuel combustion was carried out on a three-dimensional model of a drop tube furnace by using the commercial software FIRE. It was used for simulating turbulent fluid flow and temperature field, concentrations of the reactants and products, as well as the fluid-particles interaction by numerically solving the integro-differential equations describing these processes. Chemical reactions mechanisms for the formation of nitrogen oxides were implemented by the user functions. To achieve reasonable calculation times for running the simulations, as well as efficient coupling with the turbulent mixing process, the nitrogen scheme is limited to sufficiently few homogeneous reactions and species. Turbulent fluctuations that affect the reaction rates of nitrogen oxides' concentration are modelled by probability density function approach. Results of the implemented model for nitrogen oxides' formation from coal and biomass are compared to the experimental data. Temperature, burnout and nitrogen oxides' concentration profiles are compared, showing satisfactory agreement. The new model allows the simulation of pollutant formation in the real-world applications.

KEYWORDS

Solid fuel combustion, nitrogen oxides, drop tube, CFD.

1 INTRODUCTION

In the eyes of the public, the industry, and the policymakers, renewable energy sources are increasingly being recognised as the favourable energy source. However, despite the significantly more harmful impact on the environment and the human health, the abundance and the low price of fossil fuels assures their position as an important factor in the energy mix for the future electricity production. Among fossil fuels, coal is especially problematic due to its higher CO_2, particle and pollutant emissions. As a part of the tendency towards the cleaner energy production, among new technologies and utilization techniques [1], biomass emerged as one of the important transitional energy sources and technologies for an evolution towards the sustainable society and industry [2]. Its importance lies in the fact that, when used from proper and sustainable sources, it is carbon neutral [3]. Further, when co-fired with coal, it can significantly reduce the CO_2 emissions [4]. However, although biomass has been proved to be a relevant mode of fuel utilisation in the heat and electric power generation [5],

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replacement of coal by it in the existing coal-fired plants may negatively influence the operation and performance of the boilers [6] due to its composition, harmful chemical compounds and behaviour when combusted [7]. Since the experimental implementations of new fuels in existing systems are quite expensive and troublesome, and removal of the already formed pollutants brings additional issues [8], numerical simulations of the thermo-fluid properties are a valuable tool when designing and managing the operation of more sustainable combustion and utilization processes for biomass and coal [9].

Among the variety of the pollutants released during the combustion of solid fuels, nitrogen oxide is among the most harmful ones, participating in the formation of the photochemical smog, acid rain, greenhouse effect and the depletion of stratospheric ozone. Detailed chemical models for describing the pollutant formation from combustion systems include a large number of chemical reactions [10] with a great number of chemical species and, at the present state of computer hardware, require unfeasible computational time for calculation. Therefore, the reduced models sufficiently simplify the chemical mechanisms for describing the formation of the nitrogen oxides and predicting their levels. Work done by Glaborg et al. [11] provides a comprehensive review of the commonly used models for calculation of nitrogen oxides' concentration in solid fuel fired systems, and other work has been focused on various related topics: Molina et al. investigated nitrogen retained in char [12]; functional forms of nitrogen were inspected by Kambara et al. [13]; modelling of coal devolatilization by Jones et al. [14]; its removal from flue gases was investigated by Javed et al. [15] and Fuente-Cuesta et al. [16]; single particle tests performed by Yang et al. [17] showed the validity of the isothermal particle assumption for the pulverised fuel below 200 μm.

In present work, combustion processes from solid fuels, namely coal and biomass, are investigated by numerically simulating the drop tube test – a standard case for evaluating the solid fuel properties and system operation. The commercial software AVL FIRE® is used for simulating the three-dimensional geometry, temperature and turbulent flow fields, concentrations of the reactants, products and pollutants, as well as the two-phase flow of solid fuel particles within the gas phase. Solid fuel reactions such as drying, devolatilization, gaseous species generation and char burnout are considered as well.

A simplified numerical model for nitrogen oxides' formation in solid fuel combustion systems has been used, with thermal and fuel mechanisms and the effect of the temperature fluctuations taken into account.

2 NUMERICAL MODEL

Simulations of solid fuel combustion and pollutant formation require comprehensive modelling – to correctly predict the concentrations of nitrogen oxides from coal and biomass, all relevant physicochemical phenomena must be taken into account. Solid fuel particles are introduced into the domain and the Euler-Lagrangian method is used for solving the multi-phase flow. In this approach, the gas is described by the Eulerian formulation of conservation equations, while the discrete phase is treated by the Lagrangian approach. Lagrangian formulation groups the particles of identical properties and size into the samples called parcels. They are then tracked together in the domain, which saves computational time when compared to calculating the trajectories of individual particles. The expression below is used tracking the parcels:

$$\rho_P \frac{du_P}{dt} = \sum F \tag{1}$$

Here, on the left-hand side ρ_P and u_P are the density and the velocity, while F represents the forces acting on the parcel – drag, pressure, buoyancy, gravity and other external forces [18]. The coupling between the phases is achieved by using the source terms for the mass, momentum, energy and chemical species.

2.1 Solid fuel combustion

Thermal decomposition and combustion of solid fuel are treated within the Lagrangian module as homogeneous and heterogeneous thermochemical reactions, providing additional sinks and sources for enthalpy and species equations in the gas phase. This way, all calculations are made on the parcel level, representing the processes occurring in the identical group of solid fuel particles. Further, the particle radiation model is integrated into the used CFD software as well.

The solid fuel particle introduced into the computational domain passes through four stages [19]: the particle is drying (Eq. 2), followed by the pyrolytic decomposition during which the significant mass loss occurs due to the volatiles being emitted into the gas phase (Eq. 3). The amount and the composition of volatiles depend on biomass or coal particle size, temperature and chemical composition, given by the fuel's proximate and ultimate analysis [20,21]. Particle mass loss is modelled by the reaction rates of the chemical reactions, connecting the phases via sources and sinks. Heterogeneous particle combustion is modelled as the char oxidation of the isothermal particle, which is a simplified approach compared to some models that account for the particle ignition [22]. Following pyrolysis, only char and ash remain in the solid particle. Former is being oxidised to CO_2 parallel to the pyrolysis (as in Eq. 4), while latter is the residue. Following equations are the chemical reactions occurring in the coal particle, but analogous is valid for the biomass as well:

$$\textit{wet}\ \mathrm{Coal(s)} \xrightarrow{H_2O\ \textit{evaporation}} \textit{dry}\ \mathrm{Coal(s)}, \tag{2}$$

$$\textit{dry}\ \mathrm{Coal(s)} \rightarrow C_{48}H_{18}O_4N_2\mathrm{(s)}, \tag{3}$$

$$\begin{aligned} C_{48}H_{18}O_4N_2\mathrm{(s)} &\xrightarrow{\textit{pyrolysis}} 3CO\mathrm{(g)} + H_2O\mathrm{(g)} \\ &+ CH_4\mathrm{(g)} + H_2\mathrm{(g)} + HCN\mathrm{(g)} + C_6H_6\mathrm{(g)} \\ &+ NH_3\mathrm{(g)} + 37C\mathrm{(s)}, \end{aligned} \tag{4}$$

$$C\mathrm{(s)} + O_2(g) \rightarrow CO_2(g), \tag{5}$$

$$HCN / NH_3(g) + O_2(g) \rightarrow NO(g) + ..., \tag{6}$$

$$HCN / NH_3(g) + NO(g) \rightarrow N_2(g) + ..., \tag{7}$$

$$Volatiles(g) + O_2(g) \rightarrow H_2O(g) + CO_2(g). \tag{8}$$

Equations 2, 3 and 4 are responsible for coupling the mass between solid particles and gas phase via the sources and sinks. The rest of the homogeneous reactions, including the Eq. 8 – oxidation of the volatiles – are treated within the FIRE general gas phase reactions module, where volatile species taken into account are CO, CH_4, H_2, C_6H_6, NH_3 and HCN. Here the HCN and NH_3 are the part of the general species transport model already present in FIRE, but in the model presented below calculates them differently, and as a part of a post-processing step, without the influence on the general species model.

2.2 Nitrogen Oxides' Formation Model

The detailed chemical models for nitrogen-containing pollutant formation account for hundreds of elementary reactions and species– a computationally demanding task and not a viable solution at the present time. Thus, the current model is based on coupling the combustion process with the reduced chemical reaction mechanism [10], and takes nitric oxide (NO) as the most significant species, since it represents most (up to 90-95%) of the total emissions [23]. The rest of the compounds have a minor effect and are neglected during the combustion process. The following transport equation treats the formation and the transport of nitric oxide, with $\tilde{Y}_{NO}$ being the mean mass fraction of NO, and $\overline{S}_{\mathrm{NO}}$ denoting the source of nitric oxide integrated with respect to the turbulent fluctuations:

$$\frac{\partial(\bar{\rho}\tilde{Y}_{\mathrm{NO}})}{\partial t}+\frac{\partial(\tilde{u}_i\bar{\rho}\tilde{Y}_{\mathrm{NO}})}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\Gamma\frac{\partial\tilde{Y}_{\mathrm{NO}}}{\partial x_i}\right)+\overline{S}_{\mathrm{NO}} \tag{9}$$

Since the NO concentrations are very small and do not affect the flame structure or the fluid flow significantly, they can be decoupled from the combustion and flow field calculations. Furthermore, the timescales of the fast combustion reactions and the slower NO formation are different, further justifying this assumption. This way, NO can be calculated as the passive scalar that is computed after the combustion and mass transfer are finished at the end of a time step, saving computational time without significant sacrifice of the result accuracy. When calculated in a post-processing approach, NO concentrations prediction highly depends on the quality of the converged solution for the combustion flow field and the flame structure.

In the present work, thermal NO reaction mechanism is applied for modelling the pollution concentration. The source term can be defined as follows, with *M* being the molar mass, and *c* being the concentration:

$$S_{\mathrm{NO}}=M_{\mathrm{NO}}\frac{dc_{\mathrm{NOthermal}}}{dt} \tag{10}$$

Thermal NO forms at high temperatures by dissociation of the molecular nitrogen from the air and subsequent reactions of atomic nitrogen with oxygen. Due to the high energy needed for breaking the strong intermolecular nitrogen bonds, thermal NO is highly dependent on the temperature, nitrogen and oxygen concentrations, as well as the residence times. Following equations describe this process, commonly known as the extended Zeldovich mechanism.

$$\mathrm{N}_2+O\overset{k_1}{\leftrightarrow}\mathrm{NO{+}N} \tag{11}$$

$$\mathrm{N}+\mathrm{O}_2\overset{k_2}{\leftrightarrow}\mathrm{NO{+}O} \tag{12}$$

$$\mathrm{N}+\mathrm{OH}\overset{k_3}{\leftrightarrow}\mathrm{NO}+\mathrm{H} \tag{13}$$

Using the quasi-steady-state assumption for the rate of production and depletion of the nitrogen radicals, the net rate of NO formation needed for the source calculation can be formulated as in Eq. 14, with *k* being the forward or backwards rate coefficients taken from the literature [24]. The necessary concentrations and temperature are taken from the flow field results.

$$\frac{dc_{\mathrm{NO}}}{dt} = 2k_{1f}c_{\mathrm{O}}c_{\mathrm{N_2}} \frac{\left(1 - \frac{k_{1b}k_{2b}c_{\mathrm{NO}}^2}{k_{1f}c_{\mathrm{N_2}}k_{2f}c_{\mathrm{O_2}}}\right)}{\left(1 + \frac{k_{1b}c_{\mathrm{NO}}}{k_{2f}c_{\mathrm{O_2}} + k_{3f}c_{\mathrm{OH}}}\right)} \tag{14}$$

2.3 Fuel NO Model

Unlike the importance of the thermal mechanism in the internal combustion engines [25] or the gas-powered boilers, in solid fuel combustion systems, the dominant mode of production of nitrogen oxides is the fuel mechanism [26]. This is especially true for the combustion temperatures below approximately 1500 K, at which the thermal mechanism is very weak. In solid fuels, nitrogen is usually contained as one of the functional groups – pyridinic, pyrrolic and quaternary in coal [13], and as amino acids and proteins (amine-N and protein-N) in biomass, with a small share as pyroll-N and pyridine-N [27]. They break apart and react at different temperatures and conditions, and the general conclusions about their behaviour and pollutant formation are hard to make. Chemical mechanisms and pathways from solid fuel nitrogen to nitrogen oxides are not precisely known and depend on combustion conditions such as temperature, flow, air-fuel ratio, fuel type, particle sizes, residence times and type of combustion. During pyrolysis, tar and volatiles are emitted and subsequently form the intermediate species – hydrogen cyanide or ammonia – and nitrogen oxides are produced by their oxidation. Small quantities of nitrogen gas forming directly from pyrolysis are neglected. Parallel to the production path from volatiles is the heterogeneous reaction of nitrogen retained in char that produces either intermediate species or nitrogen oxide directly. General approximations valid for all fuel types and combustion conditions are hard to make, and for this model, it is assumed that all the char nitrogen forms the intermediate species.

Usually, the solid fuel description is given as the ultimate and the proximate analysis, providing only the elemental composition and the division according to the fuel’s behaviour under thermogravimetric analysis [28]. This is not enough to describe functional groups that nitrogen is contained in, and thus for the purposes of this work, detailed pathway choice depending on them is omitted. Further, the only intermediate species taken into account is the hydrogen cyanide, which is an assumption commonly made in modelling the emissions from solid fuel.

The reactions of nitrogen-containing volatiles and char are modelled with the finite reaction rates, with sources and sinks of the intermediate HCN contributing to the additional transport equation for HCN concentration (Eq. 15). This means that the calculation of the HCN and NO is decoupled from the general gas phase reactions. Figure 1 shows the reaction mechanism scheme used in the model.

$$\frac{\partial(\bar{\rho}\tilde{Y}_{HCN})}{\partial t} + \frac{\partial(\tilde{u}_i\bar{\rho}\tilde{Y}_{HCN})}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\Gamma\frac{\partial\tilde{Y}_{HCN}}{\partial x_i}\right) + \bar{S}_{HCN} \tag{15}$$

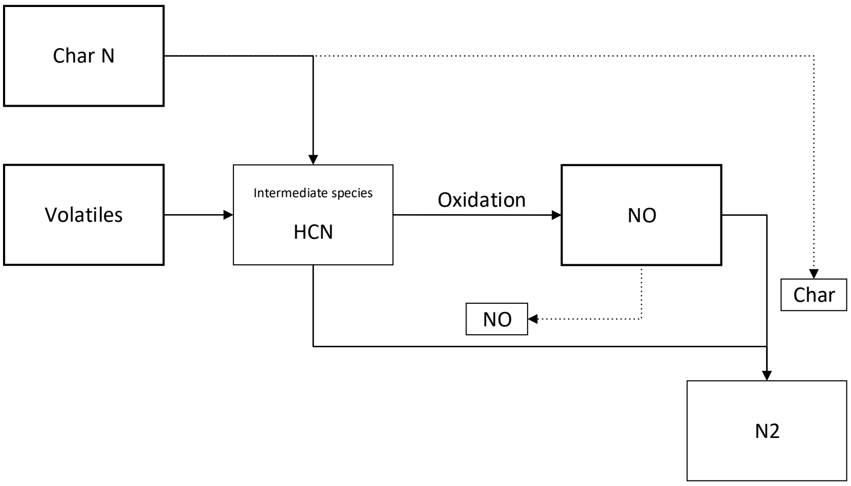

Figure 1 Reaction mechanism scheme

In addition to thermal NO source (Eq. 10), due to the reaction from HCN, an additional NO source is added to the transport equation source. Heterogeneous reactions of nitrogen oxides with char are modelled according to [29], and in Eq. 16 c_{part} is the particles concentration, A_{part} is the surface area, M is the molar mass and $r_{NO,char}$ is the reaction rate.

$$S_{char,NO} = c_{part} A_{part} M_{NO} r_{NO,char} \tag{16}$$

HCN has two production sources: it forms from the volatiles emitted from particles and by the char reactions. These reactions are described by Eq. 17, where all of the char nitrogen is assumed to be converted to the HCN [30], and with Eq. 18. In them, S_c is the char burnout rate and S_{vol} represents the source of volatiles from the particle.

$$S_{HCN,char} = \frac{S_c Y_{N,char} M_{HCN}}{M_N V} \tag{17}$$

$$S_{HCN,volatiles} = \frac{S_{vol} Y_{N,vol} M_{HCN}}{M_N V} \tag{18}$$

Depletion of the intermediate HCN occurs due to forming NO and N_2, Eq. 19. Again, r represents reaction rates obtained from literature [31].

$$S_{HCN,NO/N_2} = r_{HCN,NO/N_2} \frac{M_{HCN}\, p}{R_M T} \tag{19}$$

In the fuel NO production model there are several simplifications made. The chemical mechanism used is reduced and consists of only one intermediate species. Usually, HCN and NH_3 are the most important species, but in this work, only HCN has been taken into consideration. Heterogeneous reactions with char are also simplified and modelled as a rate reaction on a surface of the particle, while the surface area is defined as a specific area of solid fuel per unit mass. As stated above, post-processing approach has been used and justified by the slower timescales and small pollutant concentrations and the isothermal particle assumption impacts the combustion behaviour.

2.4 The Effect of Turbulence

Combustion process occurs under highly turbulent conditions, which have a great impact on the NO production. Using the averaged temperature field does not provide correct results since the influence of the temperature on the reaction rates is highly nonlinear. The presumed probability density function (PDF) is used to model the effect of turbulent fluctuations on the NO kinetic rates, integrating the rates with respect to the temperature:

$$\overline{S}_{\mathrm{NO}} = \int_0^1 P(T) S_{\mathrm{NO}}(T)\,dT \tag{20}$$

P(T) is the probability density function of the normalised temperature field, and the S_{NO} is the instant NO source. The beta function for the temperature PDF is given as:

$$P(T) = \frac{T^{\alpha-1}(1-T)^{\beta-1}\,dT}{\int_0^1 T^{\alpha-1}(1-T)^{\beta-1}\,dT} = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} T^{\alpha-1}(1-T)^{\beta-1} . \tag{21}$$

The parameters α and β depend on the mean temperature and the variance of the main combustion calculation, and Γ represents the gamma function [32]. The additional transport equation is needed for the temperature variance ($\tilde{T}''^2$), which can again be solved as active scalar coupled with the rest of the calculation, or in a post-processing step as a passive scalar.

$$\frac{\partial}{\partial t}\left(\overline{\rho}\tilde{T}''^2\right) + \frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\tilde{T}''^2\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\frac{\nu_t}{\sigma_t}\frac{\partial \tilde{T}''^2}{\partial x_i}\right) + 2\overline{\rho}\frac{\nu_t}{\sigma_t}\left(\frac{\partial \tilde{T}''}{\partial x_i}\right)^2 - 2\overline{\rho}\frac{\varepsilon}{\tilde{k}}\tilde{T}''^2 \tag{22}$$

2.5 Calculation Settings and Numerical Setup

With the aim of numerically studying the solid fuel combustion, the formation of nitrogen oxides and other flow characteristics, a three-dimensional geometry of a drop tube has been used. In order to minimize the influence of more complex geometries on the flow and the turbulence, a simple cylindrical domain has been utilized.

The simulation parameters for the combustion experiment conducted in an electrically heated drop tube are taken from the literature for coal [20] and biomass [21]. Figure 2 shows the boundary sections for the drop tube, which is a model of a 1200 millimetres long reaction tube, with the diameters of coal and biomass being 38 and 50 millimetres, respectively. Wall temperatures are set to 1100°C for the first 800 millimetres, and 900°C and 300°C for the subsequent 200-millimetre sections. Milled pine branches were taken as the representation of the biomass, and their proximate and ultimate analysis and the size distribution can be found in the aforementioned literature.

The coal mesh consists out of 9600 cells, while 12900 cells were employed for the biomass mesh. The mesh dependency tests have already been obtained in the work by the authors [33].

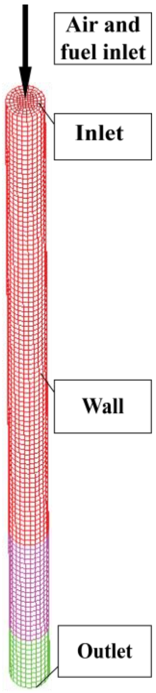

Figure 2 Computational mesh with the selections

The transient simulation mode has been employed, with the timestep of 2.5×10^{-4} seconds. The MINMOD Relaxed differencing scheme was used for momentum, energy equations, and for turbulence and scalar equations, the Upwind scheme was employed [34].

The inlet parameters for the solid fuel and air are given in Table 1, the turbulence modelling is done by the standard k-ε model, and the radiative heat transfer and the influence of the particle radiation are taken into account by applying the P-1 radiation model.

Table 1 Simulation inlet parameters

	Tube diameter [mm]	Temperature [°C]	Velocity [m/s]	Mass flow [g/h]
Coal	38	80	0.19	25
Biomass	50	25	0.1235	22
Air		25	Same as the fuel used	

3 RESULT AND DISCUSSION

The simulation results of temperature and particles burnout profiles were compared to the experimental results for coal [20] and biomass [21]. It can be seen in Figure 3 and Figure 4 that the temperature profiles along the reaction tube axis match the experimental data for both the biomass and the coal combustion. There is an overprediction of the temperature present towards the end of the tube for both the coal and biomass cases, and a slight overprediction in the middle part of the tube for the biomass case.

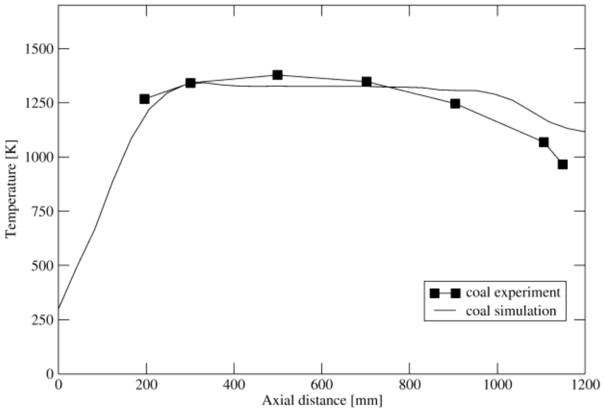

Figure 3 Axial temperature profile for coal

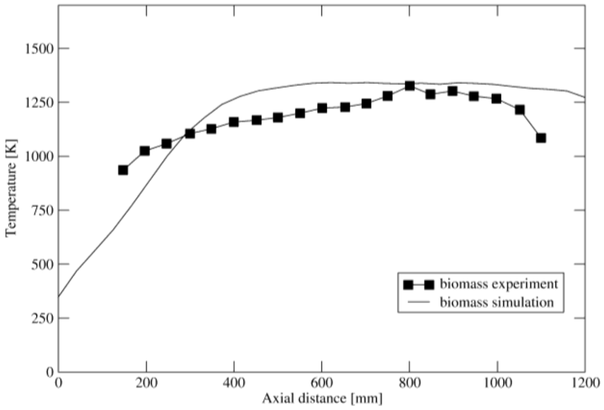

Figure 4 Axial temperature profile for biomass

Burnout rates along the furnace axis, showing the combustion of solid particles and defined with the experiment [20], are shown in Figure 5 and 6 for coal and biomass combustion. When compared to the experimental data, both the coal [20] and the biomass [21] burnout rates show good agreement. Together with the presented temperature profiles, these results indicate that the used mechanism correctly predicts the combustion processes, which is one of the goals behind this work, as well as a prerequisite for the correct nitrogen oxides' calculation.

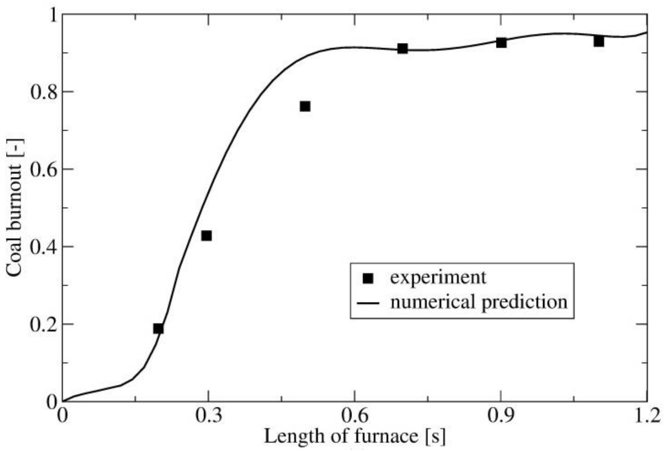

Figure 5 Axial profile for coal burnout

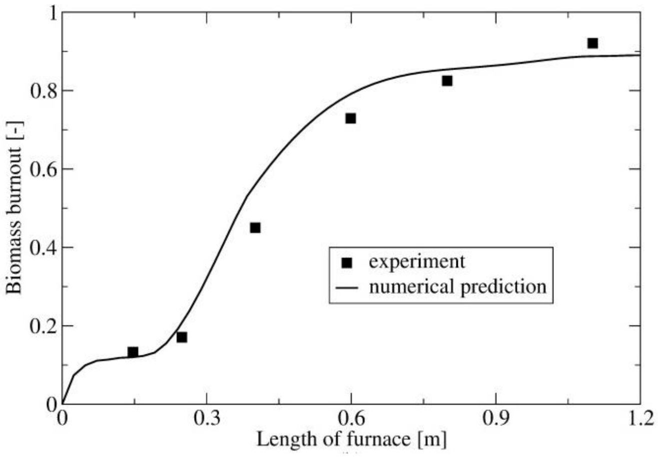

Figure 6 Axial profile for biomass burnout

Firstly, nitrogen oxide concentration predictions were simulated only with the thermal NO mechanism, which on its own provides poor results due to the influence of the turbulent flow field inside the combustion chamber. However, even when the significant influence of the turbulence-chemistry interactions on the NO formation rates was taken into account by the temperature fluctuations mechanism, concentrations were orders of magnitude lower than those reported in the experiments. For solid fuel combustion, nitrogen oxides originating from the nitrogen contained in the fuel make up for the major share of the overall NO production. Due to this, the appropriate results were obtained only with the newly implemented model for fuel NO included in the calculations as well.

Figure 7 compares the results of NO concentrations for coal when calculated by the general gas phase reactions, the approach by the newly implemented model, and the experimentally obtained data. It can be seen that the general gas phase reactions model underpredicts the concentrations by several orders of magnitude and that the current model approaches levels reported in the literature [20].

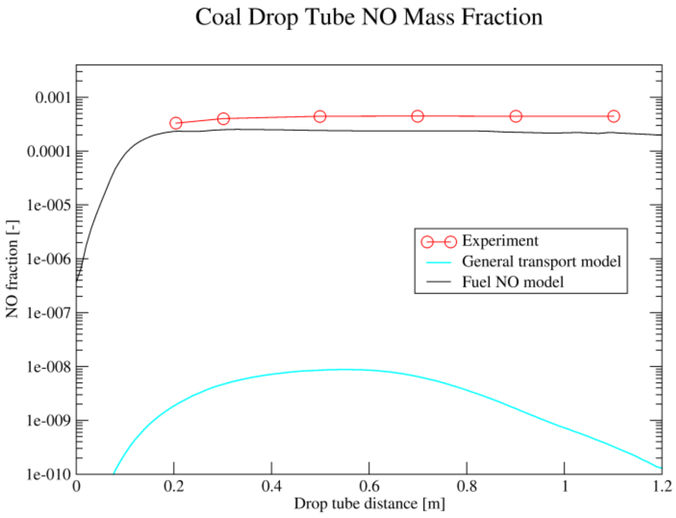

Figure 7 Comparison of experiment, general gas phase reaction and the implemented model

Nitrogen oxide levels follow the same trend as the experimental results and remain at the approximately constant level after the influence of the colder air from the inlet diminishes and

the pyrolysis and combustion initiate. Although still lower than the experimental results, the NO levels are good enough for determining general trends and the location of the phenomena in the combustion system. By introducing the assumptions in the model, a more general tool is developed, able to perform faster calculations of complex phenomena on a wider range of conditions and fuel types, but at the same time sacrificing the accuracy of the results. When compared to the similar literature results and technologies, it can be seen that the nitrogen oxides levels are comparable, and around 1000°C rise to approximately 300-500 ppm [35].
Figure 88 shows the NO concentrations and the temperature field on the axial cut of the reaction chamber for coal fuel. It appears as if the influence of temperature fluctuations does not induce large asymmetries in the flow field and that the two-dimensional calculations could be used, but the impact of turbulence is larger on the NO formation rates is much larger than on the flow field.

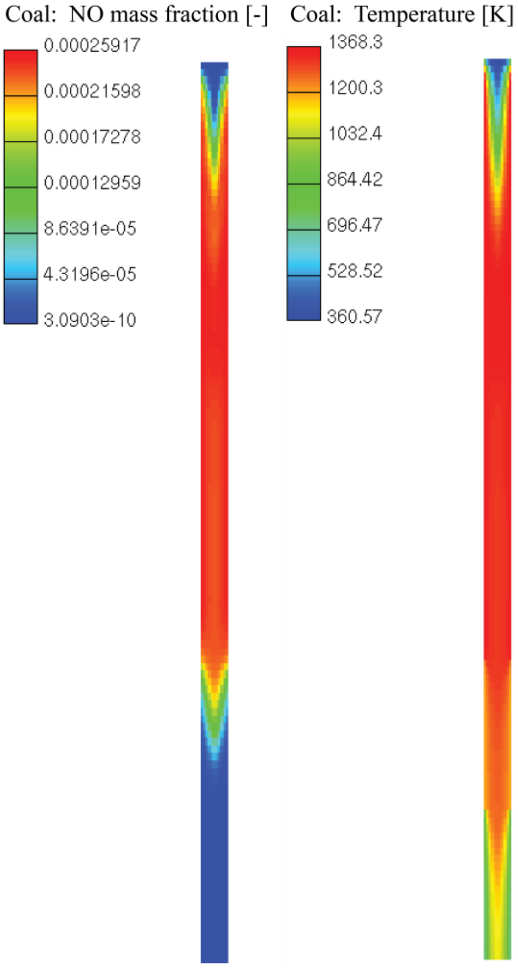

Figure 8 Coal NO and temperature fields

It can be seen that the influence of fuel in a stream of ambient temperature air at the inlet of the tube lowers temperatures and, consequently, NO concentrations. As the fuel dries, heats up and emits the volatiles under the influence of heated walls of the chamber, devolatilization initiates, combustion starts and the temperature rises. Sources of thermal NO production develop near the walls, where the influences of heaters and combustion combine and result in higher temperatures. Although the Zeldovich mechanism for NO formation is present, its influence is too low when compared to the fuel nitrogen. Volatiles are emitted from the injected particles and form HCN, along with the reaction from char nitrogen. Nitrogen oxide forms from HCN and is transported towards the bottom of the drop tube under the influence of the flow field. Lower temperature at the end of the tube is due to the decreased temperature of the electric heaters, and prevents the conversion of nitrogen atoms into nitrogen oxide, decreases devolatilization of the particles that already have reduced char nitrogen level, and they are recombined back into their molecular form.

Simulation for pine biomass provides the similar results as the coal case, but with a slightly elevated NO concentration. Figure 9 shows the similar profile as the coal case, with somewhat lower concentrations at the inlet of the geometry. This can also be seen in the axial cuts in Figure 10, and could be attributed to the lower temperatures at the beginning of the tube and consequently lower influence of the thermal NO.

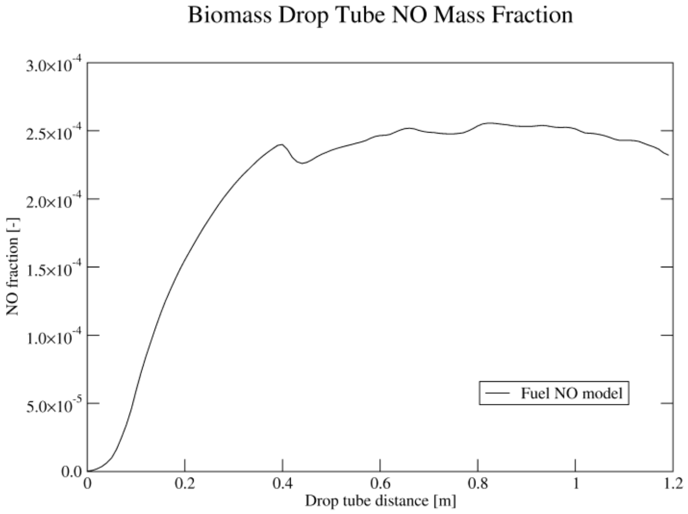

Figure 9 Nitrogen oxides concentration along the axial profile for biomass fuel

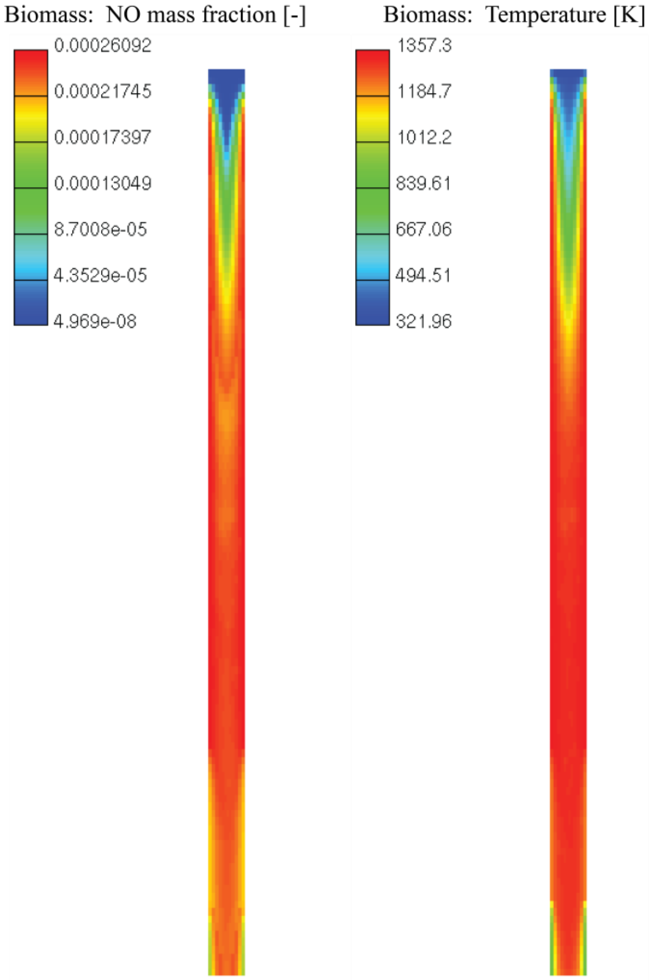

Figure 10 Biomass temperature and NO concentration

4 CONCLUSION

Numerical simulations of solid fuel combustion can provide valuable information about the complex processes occurring in the combustion systems, whether the focus is on particle kinetics, temperature distribution, pollutant emissions or various other phenomena. The presented numerical model for predicting the solid fuel combustion can give deeper insight into the new geometry or the fuel whose application is being investigated.

The combustion model in the commercial CFD software FIRE accounts for the effects of drying, degradation and devolatilization of solid fuel, along with the homogeneous gas reactions and the heterogeneous reactions in char. Although the model considers only isothermal particles with somewhat simplified chemical reactions and mass loss, it can predict the relevant physical and chemical processes while being simple enough for usage in the CFD simulations of the real industrial applications, such as boilers and furnaces.

Simulations were performed on three-dimensional geometries of the simplified drop tube furnaces, and results were compared to the available experimental data. Good agreement of temperature and particles' burnout profiles along the tube axis with the experimental measurements indicates that the presented model accurately predicts the combustion process.

For pollutant emission predictions, when thermal NO mechanism was used along with the temperature fluctuations model that included the effect of turbulence-chemistry interactions, the results showed significant underprediction when compared to the experimental data. In solid fuel combustion systems, the chemical kinetic process of fuel NO formation has a major influence on the overall pollutant concentration. Implemented model for prediction of nitrogen oxides from solid fuels on the same test cases provides the more realistic results that are in better agreement with the experimental data. However, due to the significant approximations made in order to make the model as robust and as universal as possible, experimental results cannot be exactly matched. Currently, the limitations of the model are the inability to choose different pathways and intermediate species and simplified chemical reaction scheme.

This model can thus be used for the pollution trend prediction and investigation of combustion systems with satisfactory accuracy. It is applicable for the pulverized biomass or coal as fuels under the real operating conditions in boilers, furnaces and drop tubes. In the presented work, it is shown that the model is applicable for investigating different fuel combustion characteristics on three-dimensional geometries, and it can be used for evaluating the pollutant formation in real industrial applications.

5 ACKNOWLEDGEMENTS

This work has been supported by the Croatian Science Foundation.

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