



Research article

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.

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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 CO₂, particle and pollutant emissions. As a part of the tendency towards the cleaner energy production, among new technologies and utilization techniques (Nyashina et al., 2018), biomass emerged as one of the important transitional energy sources and technologies for an evolution towards the sustainable society and industry (Mikulčić et al., 2017). Its importance lies in the fact that, when used from proper and sustainable sources, it is

carbon neutral (Johnson, 2009). Further, when co-fired with coal, it can significantly reduce the CO₂ emissions (Pereira et al., 2016). However, although biomass has been proved to be a relevant mode of fuel utilization in the heat and electric power generation (Ko and Chang, 2008), replacement of coal by it in the existing coal-fired plants may negatively influence the operation and performance of the boilers (Mikulčić et al., 2014) due to its composition, harmful chemical compounds and behaviour when combusted (Vanreppelen et al., 2013). 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 (Baleta et al., 2017), 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 (Mikulčić et al., 2016).

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

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ozone. Detailed chemical models for describing the pollutant formation from combustion systems include a large number of chemical reactions (Hill and Smoot, 2000) 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 Glarborg et al. (Glarborg et al., 2003a) 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 (Molina et al., 2000); functional forms of nitrogen were inspected by Kambara et al. (1995); modelling of coal devolatilization by Jones et al. (1999); its removal from flue gases was investigated by Javed et al. (Tayyeb Javed et al., 2007) and Fuente-Cuesta et al. (2012); single particle tests performed by Yang et al. (2008) showed the validity of the isothermal particle assumption for the pulverized 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:

$$\rho_p \frac{du_p}{dt} = \sum F \quad (1)$$

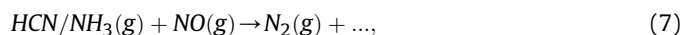
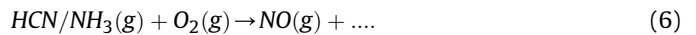
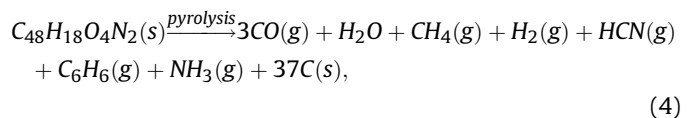
Here, on the left-hand side ρ_p and u_p are the density and the velocity, while F represents the forces acting on the parcel – drag, pressure, buoyancy, gravity and other external forces (Wang et al., 2017). The coupling between the phases is achieved by using the source terms for the mass, momentum, 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 (Williams et al., 2012): 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 (Wang et al., 2014a, 2014b). 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 (Glushkov et al., 2015). 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:



Equations (2)–(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 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 (Hill and Smoot, 2000), and takes nitric oxide (NO) as the most significant species, since it represents most (up to 90–95%) of the total emissions (Mehmood et al., 2015). The rest of the compounds have a minor effect and are neglected during the

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