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Numerical simulation of urea based selective non-catalytic reduction deNOx process for industrial applications

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ABSTRACT

Industrial processes emit large amounts of diverse pollutants into the atmosphere, among which NOx takes a significant portion. Selective non-catalytic reduction (SNCR) is a relatively simple method for the NOx reduction in large industrial facilities such as power plants, cement plants and waste incinerator plants. It consists of injecting the urea-water solution in the hot flue gas stream and its reaction with the NOx. During this process flue gas enthalpy is used for the urea-water droplet heating and for the evaporation of water content. After water evaporates, thermolysis of urea occurs, during which ammonia, a known NO_x reductant, and isocyanic acid are generated. In order to cope with the ever stringent environmental norms, equipment manufacturers need to develop energy efficient products that are at the same time benign to environment. This is becoming increasingly complicated and costly, and one way to reduce production costs together with the maintaining the same competitiveness level is to employ computational fluid dynamics (CFD) as a tool, in a process today commonly known under the term "virtual prototyping".

The aim of this paper is to show capabilities of the developed mathematical framework implemented in the commercial CFD code AVL FIRE®, to simulate physical processes of all relevant phenomena occurring during the SNCR process. First, mathematical models for description of SNCR process are presented and afterwards, models are used on the 3D geometry of an industrial reactor and a real industrial case to predict SNCR efficiency, temperature and velocity field. Influence of the main operational parameters on NOx reduction efficiency was performed on the same case. Finally, conclusions about validity of current framework are given together with recommendations for further work.

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1. Introduction

The latest report from the scientific panel on anthropogenic global warming indicates that remarkable and joint global action is required to reduce greenhouse gas emission and harmful emissions in generally, and the longer we wait to address this issue, the more difficult, technologically challenging and expensive it will become [1].

Fossil fuel burning in industry, fertilisers containing nitrogen and transport produce the majority of NO_x emissions. Nitrogen-oxides (NO_x) contribute to acid deposition and eutrophication of soil and water. The subsequent impacts of acid deposition can be significant, including adverse effects on aquatic ecosystems in rivers and lakes and damage to forests, crops and other vegetation. Eutrophication can lead to severe reductions in water quality with subsequent impacts including decreased biodiversity, changes in species composition and dominance, and toxicity effects. NO_2 is associated with adverse effects on human health and also contributes to the formation of secondary particulate aerosols and tropospheric ozone in the atmosphere, both of which are important air pollutants due to their adverse impacts on human health and other climate effects [2].

Despite the fact that the European Environment Agency (EEA)-33 emissions of nitrogen oxides (NOx) decreased by 44% between 1990 and 2011 [2], they are still subject to the current and upcoming emission standards [3] in order to minimise their harmful environmental impact. In 2011, the most significant sources of NOx emissions were road transport (41%), energy production and distribution (23%) and the commercial, institutional and households (13%) sectors [2].

Amount of formed NOx is influenced by several factors such as combustion temperature, flow velocity field in combustion chamber, design of the combustion chamber and burner, fuel composition, and ratio of fuel and air dosage. There are three kinds of NOx production mechanisms taking place during combustion

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processes: fuel NOx, thermal NOx and prompt NOx [4]. Fuel NOx is produced from the oxidation of fuel bonded nitrogen, whilst thermal and prompt NOx require atmospheric nitrogen for reaction. Production of the fuel NOx is especially pronounced in the cases of coal and biomass combustion due to the relatively high content of fuel contained nitrogen [5]. Triple bonds in the nitrogen molecules could be broken only by introducing large amount of energy in the reaction system. Therefore, thermal NOx is only formed in significant quantities at temperatures above 1500 °C.

Methods of NOx control may be categorised into primary methods, which prevent formation of NOx and secondary NOx control methods, which are focused on the reduction of already formed NOx [6]. Selection of individual method or combination of methods is always conditioned by economic balances and legislation.

First option of primary NOx control methods consists of regulation of the excess air, keeping at the same time in mind the fact that it directly affects unburned carbon emissions. Combustion air staging creates fuel-rich primary zone and fuel-lean secondary zone, suppressing that way creation of fuel and thermal NOx. Similarly like combustion air, fuel can also be staggered through creating a fuel-rich secondary combustion zone, where NOx formed in the primary combustion zone is decomposed. Exhaust gas recirculation, a technique frequently employed in modern internal combustion engines [7], as well represents one of the primary NOx reduction measures which can significantly reduce thermal NOx generation by lowering combustion temperatures and excess air. Tightened NOx emission standards [8,9] on industrial emissions from combustion plants cannot be met using described primary NOx reduction techniques anymore. Also, it is difficult to implement those techniques into existing facilities. Taking stated into account, it can be clearly seen that the answer to those challenges should be found in utilising exhaust gas aftertreatment. Although some new technologies emerged during the last few years, such as pulsed corona discharge and electron beam flue gas treatment [4], selective non-catalytic reduction (SNCR) as well as selective catalytic reduction (SCR) have proven to be optimal from both the cost and NOx reduction efficiency view point.

SCR offers higher denitrification efficiencies with respect to SNCR, although investment cost is much higher [10] and it is not suitable for retrofitting due to clogging problems and loose of catalytic efficiency in such cases. On the other side, SNCR is a proven cost-effective secondary method of NOx control from big stationary sources such as power plants, incinerators, boilers and cement calciners. The process is operated by the controlled injection of reducing agents such as ammonia or urea [11]. The performance of SNCR process has been shown to be influenced by reducing agent residence time, temperature profile in reaction zone, quality of mixing of reagent with flue gases, concentration of NOx in flue gases, ammonia slip and normalised stoichiometric ratio [12]. Residence time is a factor whose increase enables longer contact between reducing agent and NOx. Its value is highly dependent on flow geometry and velocities inside the region where SNCR is taking place. Most researchers agree that optimum SNCR process is taking place within relatively narrow temperature range between 800 and 1100 °C [10]. Above this temperature ammonia tends to oxidise and below the 800 °C reduction rate is too slow. Mixing quality of reagent and exhaust gases is dependent upon velocities and swirl in reaction zone, and also upon the injecting conditions, whilst the concentration of NOx in flue gases could be affected using primary NOx reduction measurements, and also differs between various applications such as power plants, utility boilers, and incinerators. Normalised stoichiometric ratio (NSR) refers to the ratio between reducing agent and NOx. It is preferable to have it high but one must take into account also toxic ammonia slip which is limited by various legislations and norms. Previous research showed that optimum NSR value in terms of NO reduction efficiency is between 1.5 and 2 [13].

All operating conditions are interdependent and show that, although SNCR process is principally very simple, design of optimum process or retrofitting existing facility is far beyond trivial. There are several arguments for using computational fluid dynamics in SNCR applications. Firstly, in view of shortening development cycles and reducing development costs, early stage assessment of the performances of different setups as well as various design parameters becomes very important [14,15]. Also, in reality, it is very difficult to study SNCR processes at large utility boilers directly through measurement because of the limited experimental access. Large space and strong turbulence cause a very poor accuracy and hinder the essential operational characteristics. Finally, improved computational design tools are needed for design and optimisation of SNCR performance due to tightened emission regulations and requests for decreasing price of NOx emission controlling system [16]. By incorporating suitable mathematical representation of relevant physical phenomena taking place in SNCR system, CFD can give detailed insight into all flow variables and replace expensive and intrusive experimental tests [17–19].

Taking all of the above mentioned into account, the aim of this work is the incorporation of the reduced kinetic mechanism of deNOx processes taking place inside the SNCR facility. First step was testing of all relevant models preceding the incorporated mechanism on well-established experimental case of Kim [20]. Parametrization of urea thermolysis model was performed on one case, yielding good agreement on all other cases. Furthermore, implemented mechanism was validated on the real industrial reactor for which experimental results can be found in the literature as well as on the case of municipal waste incinerator. Simulated results show satisfactory agreement of simulation results with measured data and encourage commercial application of developed framework.

2. Mathematical model

In order to accurately represent all relevant physical phenomena occurring during the injection of urea-water solution (UWS) into hot flue gases mathematical description of processes is needed as follows:

- solution of gas phase;
- description of spray droplets motion inside the domain;
- evaporation of urea-water solution droplets;
- thermal decomposition of urea;
- chemical reactions taking place in the gas phase;
- accurate and computationally economical representation of turbulence.

Equations of continuum mechanics are based on the conservation laws for mass, momentum and energy. The general form of the time averaged conservation equation for any dependent variable φ of the continuous phase in the differential form is:

$$\frac{\partial}{\partial t}(\rho\varphi) + \frac{\partial}{\partial x_j}(\rho\varphi u_j) = \frac{\partial}{\partial x_j}\left(\Gamma_\varphi \frac{\partial \varphi}{\partial x_j}\right) + S_\varphi \quad (1)$$

where ρ is the density, u_j Cartesian velocity, Γ_φ diffusion coefficient, and S_φ is the source term of the dependent variable φ. The source term S_φ is used for the coupling of the liquid phase of spray droplets to the gaseous phase.

Experimental observations as well as the knowledge obtained from the instability analyses form the basis for numerical modelling of liquid spray. The most commonly used method for spray calculation today is Discrete Droplet Method (DDM) [21] although in some special cases, such as dense spray regions near the nozzle, Euler–Eulerian multiphase approach is gaining increasing

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