Modeling and Investigation of Dispersed Working Fluids in Application to Catalytic Neutralization of Flue Gas

Ruslan Fedorov, Igor Shepelev, Mariia Maleshina, Daniil Karpov

Laboratory of Interdisciplinary Problems in Energy Production, Ulyanovsk State Technical University, 32 Severny Venetz Street, 432027 Ulyanovsk, Russia

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Abstract

Currently, energy is a key factor in the global economy, and the efficiency of the energy production and consumption processes has significant consequences for society and the environment. Harmful and hazardous substances negatively affect humans, animals, and plants, poison the soil and water bodies, cause diseases, and worsen health. The presence of flue gas-cleaning systems in enterprises is a prerequisite. One of the most effective ways to reduce harmful substances in flue gases is the catalytic cleaning of emissions. The principle of this method is to ensure the chemical conversion of pollutants into harmless or low-harm substances using special catalysts. Catalytic cleaning of gas emissions is applied to a wide range of pollutants, including not only numerous volatile organic compounds formed at metallurgical, chemical, and oil refining plants, but also to flue gases emitted by treatment facilities and installations in the energy sector. This study considered the Computational Fluid Dynamic (CFD) modeling of a device for the catalytic neutralization of flue gas in the Star CCM+ package.

Keywords: Dispersed flows, CFD modeling, Catalytic neutralization

1. Introduction

Currently, energy is a key factor in the global economy, and the efficiency of energy production and consumption processes has significant consequences for society and the environment. According to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change, the world is no longer able to prevent extreme climate change; the International Energy Agency (IEA) effective scenario is not met, and global warming will exceed the planned 2°C unless there is a significant reduction in carbon dioxide and other greenhouse gas emissions in the 2020s [1]. The implementation of this scenario is possible with the improvement of existing technologies and the development of new energy-efficient technologies for the production and conversion of energy into organic and synthetic hydrocarbon fuels. At the same time, increasingly stringent environmental standards have already led to a significant increase and complications in the work processes implemented in modern power plants and complexes, which in most cases are accompanied by a deterioration in their technical and tactical characteristics (including capacity and efficiency) and are in conflict with the requirements of fuel efficiency. Harmful and hazardous substances have a negative impact on humans, animals, and plants, poison soil and water bodies, cause diseases, and worsen health [2].

The presence of flue gas cleaning systems at enterprises is a mandatory requirement, and the amount of Maximum Permissible Emissions (MPE) and the values of Maximum Permissible Concentrations (MPC) are established at the legislative level and are regulated by the Federal Law of January 10, 2002 N 7-FZ "On Environmental Protection" [3]. Exceeding MPC and MPE leads to large fines for the enterprise, and repeated violations may cause temporary or complete shutdown of production.

One of the most effective ways to reduce the content of harmful substances in flue gases is catalytic cleaning. Catalytic cleaning is the chemical conversion of emissions into neutral or low-harm substances using specialized catalysts. Catalytic cleaning of exhaust gases is used for a large number of pollutants, not only numerous volatile organic compounds of the chemical and oil refining industries, but also substances and flue gases emitted by treatment facilities and installations in the energy sector. There are several methods of cleaning industrial exhaust gases using catalysts, which differ in the technological process, the type of catalytic substances used and the chemical composition of the pollutants. The most common catalytic method of gas cleaning is ozone catalysis [4].

Catalysts for cleaning gas emissions are a mixture of a catalytically active substance, a carrier and an activator. A catalyst is an active substance that includes a wide range of chemical compounds. As a result of the catalytic reactions that occur, harmful and hazardous compounds are converted into other substances that do not pose a danger to humans and the environment.

Catalytic methods of industrial exhaust gas purification from harmful emissions have a number of advantages, including high versatility, allowing the removal of a wide range of pollutants from exhaust gases. When purifying exhaust gases using the catalytic method, most of the costs are for the catalyst. The purification process on an industrial scale can be carried out using combined or semi-combined devices.

Research into dispersed flows is actively conducted in major scientific centers in Russia (Joint Institute for High Temperatures of the Russian Academy of Sciences [5], S.S. Kutateladze Institute of Thermophysics of the Siberian Branch of the Russian Academy of Sciences [6]), China [7, 8], etc.

The main fundamental difficulties arising in modeling two-phase turbulent flows are associated, firstly, with the turbulent nature of the motion, and secondly, with specific physical processes: interaction of particles (droplets, bubbles) with turbulent vortices of the continuous phase; interaction of particles of a dispersed cluster with each other as a result of collisions; evolution of the particle size spectrum of a dispersed cluster due to phase transitions, coagulation or fragmentation; the effect of turbulent fluctuations on the rates of phase transitions; interaction of particles with the flow-limiting surface of the flow path and sedimentation; the inverse effect of particles on turbulence; dispersion, accumulation and fluctuations of particle concentration.

When analyzing possible tools in the field of providing accurate results for problems of aerodynamics and thermochemistry of power plants, taking into account the calculations of turbulence and heat fluxes in various operating modes, it should be noted that many scientists use software packages based on CFD when studying processes and optimizing operating modes. According to scientists, the use of CFD allows us to avoid the need for expensive full-scale experiments before making changes to the system and, in some cases, gives us information that is quite difficult to obtain experimentally. However, to obtain satisfactory modeling results using CFD, significant resources must be expended.

In this paper, we considered the modeling of a water-air scrubber using CFD for catalytic neutralization of flue gases in the Star CCM+ package.

2. Digital model

The paper considers a two-stage ozone catalytic gas cleaning process in a water-air scrubber. The method of cleaning nitrogen oxides with ozone consists of oxidizing the oxides with ozone and then binding them with ammonia. Flue gases are sent to a unit into which ozone and spray liquid are supplied, as a result of which lower nitrogen oxides NO and NO_2 (equations 1 - 9) are converted into higher ones. The CFD modeling of the NO_x absorption process in this study is based on chemical reactions inside liquid droplets in combination with NO_x mass transfer and dispersed flow hydrodynamics. When in contact with water, nitric acid is formed. Some of the reactions are presented below:

$$NO + O_3 \rightarrow NO_2 + O_2 \quad (1)$$

$$NO_2 + O_3 \rightarrow NO_3 + O_2 \quad (2)$$

$$NO + NO_2 \rightarrow N_2O_3 \quad (3)$$

$$NO_2 + NO_2 \rightarrow N_2O_4 \quad (4)$$

$$NO_2 + NO_3 \leftrightarrow N_2O_5 \quad (5)$$

$$N_2O_3 + O_3 \rightarrow N_2O_4 + O_2 \quad (6)$$

$$N_2O_4 + O_3 \rightarrow N_2O_5 + O_2 \quad (7)$$

$$NO_2 + H_2O \rightarrow HNO_2 + HNO_3 \quad (8)$$

$$N_2O_5 + H_2O \rightarrow HNO_3 \quad (9)$$

In the following, ammonia-based reducing agents are most commonly used, and the reaction processes are reflected in the following equations:

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \quad (10)$$

$$4NH_3 + 2NO_2 + O_2 \rightarrow 3N_2 + 6H_2O \quad (11)$$

$$2\,NH_3 + NO + NO_2 \rightarrow 2N_2 + 3H_2O \quad (12)$$

Since the flue gas temperature is high and contains water vapor, if the oxidation temperature is too low, the water vapor will condense and react with the oxidation product to form nitrous acid and nitric acid, which will seriously corrode the equipment. However, if the oxidation temperature is too high, it will cause thermal decomposition of O_3 and reduce the oxidation efficiency [9]. Therefore, in order to prevent the condensation of water vapor in the flue gas and achieve a higher oxidation effect, the scrubber is installed after the regenerative air heater. To increase efficiency, a catalyst packing containing TiO_2, V_2O_5 and MnO as the main components was used.

For CFD modeling, the Star CCM+ software package was used. Flue gas is considered as a continuous single-phase medium, including NO_x (qualitative and quantitative data are taken from the E-500-13.8-560GMN boiler unit passport). Flue gases enter the spray scrubber at the inlet at a uniform speed of 10 m/s. The condition of adiabatic walls is imposed on the internal walls and surfaces of pipelines. Gas phase conservation equations are described based on Lagrangian Multiphase. Turbulent gas flow is solved using Reynolds-averaged Navier-Stokes equations based on the Realizable k-ε (Two-Layer y+ Wall Treatment) turbulence model.

$$\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho k \bar{v}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho(\varepsilon - \varepsilon_0) + S_k \quad (13)$$

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¿

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \varepsilon \bar{v}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \frac{1}{T_e} C_{\varepsilon 1} P_\varepsilon - C_{\varepsilon 2} f_2 \rho \left(\frac{\varepsilon}{T_e} - \frac{\varepsilon_0}{T_0} \right) + S_\varepsilon \quad (14)$$

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where S_k and $S_\varepsilon$are the user-specified source terms.

A three-dimensional polyhedral cell mesh was created for the calculations. The computational domain is represented by several zones: the densest mesh in the area of mixing of flue gas and liquid flows (3% of the basic grid size); the next less dense zone along the axis of the spray devices (10% of the basic grid size); in the rest of the scrubber, a grid with the basic size. The total number of cells was 3,865,450.

To validate computational fluid dynamics models describing chemical reactions in combination with gas transport behavior, they are compared with corresponding experimental data. The simulation continues until 1000 iterations are completed or the continuity residual criterion of 1.0E-4 is met.

3. Results

The flue gas removal conditions of thermal power plants and industrial boilers are different due to the complex operating conditions. The main studies were related to the factors influencing the reduction of NO_x emissions – oxidation temperatures and the O_3/NO molar ratio (MR). The results are presented in Figures 1–4.

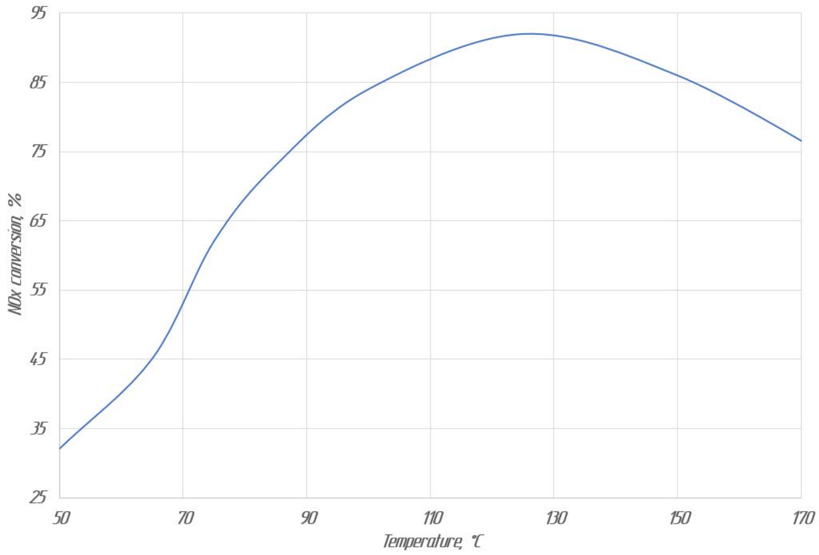

Figure 1: Efficiency of catalytic conversion of NO_x depending on temperature

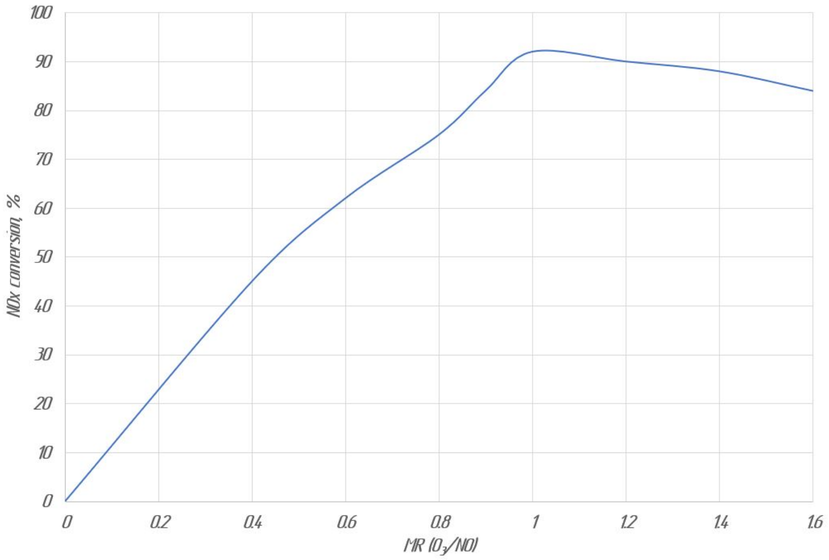

Figure 2: Efficiency of catalytic NO_x conversion as a function of the MR (O_3/NO)

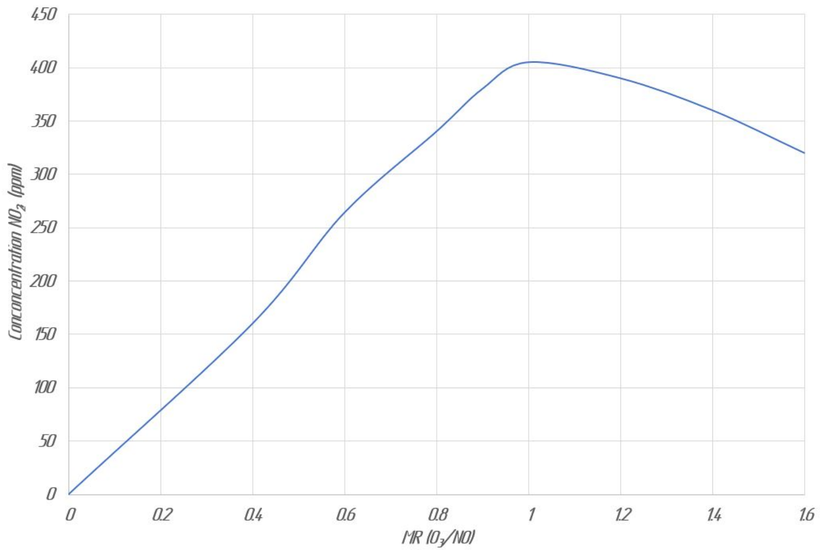

Figure 3: NO_2 concentration as a function of the molar ratio (MR) (O_3/NO)

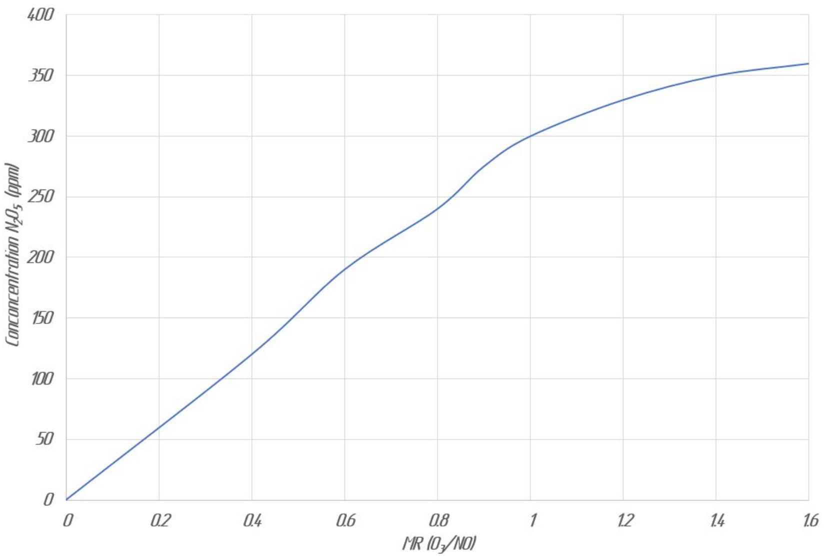

Figure 4: N_2O_5 concentration as a function of the molar ratio (MR) (O_3/NO)

As we can see from Figure 1, the conversion process is most effective at a temperature of 125 °C. Also, from the analysis of Figures 3 and 4, we see that for maximum cleaning efficiency, it is necessary to maintain a molar ratio of O_3/NO of about 1. At such molar ratios of O_3/NO, the main oxidation product will be NO_2.

4. Conclusions

The article discusses mathematical modeling of the catalytic cleaning process in a scrubber using computational fluid dynamics in the Star CCM+ package. It was found that the process is most effective at a temperature of 125 °C and maintaining a molar ratio of O_3/NO of about 1.

5. Acknowledgement

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