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Optimisation of flue gas purification systems at thermal power plants for increasing operational efficiency and reducing harmful emissions

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ABSTRACT

The article deals with the current problem of optimising flue gas cleaning systems at thermal power plants (TPPs) to increase the efficiency of power plants and reduce harmful emissions into the atmosphere. It was established that the main pollutants generated during the combustion of solid fuel at a TPP are nitrogen oxides, sulphur oxides, and particulate matter (PM). The Primary and secondary methods of reducing emissions were reviewed, among which special attention was paid to technologies of selective catalytic reduction (SCR) of nitrogen oxides. Flue gas cleaning processes were simulated in the COMSOL Multiphysics environment to evaluate the kinetics of NO reduction reactions with the participation of ammonia under reciprocating flow. A numerical experiment established that the NH_3:NO ratio within 1.3–1.4 is required for the effective course of the NO reduction reaction. It was found that temperature is a key factor affecting the conversion rate and catalyst efficiency, which requires detailed control under practical conditions. The influence of fuel type on emissions was also analysed. The obtained results can be used to develop new strategies for the modernisation of combined heat and power plants (CHPP), justify the choice of fuel and combustion modes, and implement effective emission control methods.

Keywords: thermal power industry, thermal power plants, steam boilers, boiler rooms, heating stations, heat exchangers.

INTRODUCTION

Issues of environmental safety and energy efficiency are of particular importance in the current operating conditions of TPPs (Park et al., 2019). The problem of removing harmful impurities from flue gases is becoming increasingly urgent in the context of increasing requirements for environmental protection and public health. Flue gases are one of the main sources of atmospheric pollution. They contain a large number of harmful substances, in particular sulphur dioxide (SO_2), nitrogen oxides (NO_x), PM, heavy metals, and other toxic compounds (Rakgetse and Maseeng, 2025; Gharrafi and Nacer, 2025). The increasing air pollution rates caused by the activities of industrial enterprises, power plants, and the transport sector are a serious environmental problem. It requires the introduction of effective technologies to reduce emissions of hazardous components, in particular sulphur dioxide (SO_2), nitrogen oxides (NO_x), and PM. In this study, NO_x refers to the total concentration of nitrogen oxides, while NO is considered the key component in the SCR reaction mechanism.

The energy sector remains one of the main sources of such pollution, in particular thermal power plants that operate on fossil fuels, primarily coal (Rakuta et al., 2025). According to the statistics, more than 60% of the world's electricity in 2021 was generated by burning fossil fuels. In particular, coal provided 34%, and gas – 27% of global electricity production (EXPRO, 2021). Coal combustion, in particular, is accompanied by significant harmful emissions. PM, sulphur dioxide, and nitrogen oxides pose the greatest danger among them. These are the main components that determine the level of man-made load on the atmosphere. In recent decades, there has been a positive trend in reducing global SO_2 and NO_x emissions in the electricity generation sector (EXPRO, 2021; Mishra et al., 2024). This has become possible due to the active development and implementation of modern flue gas cleaning technologies. At the same time, many TPPs continue to operate outdated or insufficiently efficient cleaning systems, which do not enable achieving current emission standards (Dennis et al., 2024).

In this context, optimisation of flue gas cleaning systems is a key factor in the sustainable development of the domestic energy sector. Traditional flue gas cleaning systems used at most TPPs are often insufficiently efficient, outdated, or not adapted to current environmental standards (Ahmed et al., 2022; Apon et al., 2025). In addition to environmental consequences, insufficient efficiency of flue gas cleaning systems negatively affects the overall productivity and economic feasibility of TPP operation. Increasing energy efficiency while reducing harmful emissions requires the implementation of new technical solutions, improving existing purification technologies, as well as an integrated approach to optimising the operation of gas purification systems. So, there is a need for scientific justification of effective methods for optimising flue gas purification systems. This will reduce the man-made load on the environment and increase the environmental and economic efficiency of TPPs (Bagheri et al., 2015; Sabadash and Lopushansky, 2024).

The academic novelty of the research is the proposed integrated approach to optimising flue gas cleaning systems, which combines mathematical modelling, assessment of the effectiveness of various cleaning technologies, and environmental criteria. A feature of the research is the considered dependence of the efficiency of emission reduction on the geometric parameters of the catalyst, combustion modes, and fuel composition. The research is also the first to propose an adaptive approach to selecting a cleaning system taking into account local conditions of TPP and its operational characteristics.

The hypothesis of the study is that optimisation of design parameters and operating modes of flue gas cleaning systems significantly increase the overall environmental efficiency of TPPs. This, in turn, enables reducing harmful emissions without a significant increase in energy costs for cleaning.

The aim of the research was to substantiate and develop scientifically based approaches to optimising flue gas cleaning systems at TPPs. This should contribute to increasing the efficiency of the installations and reducing the amount of emissions of harmful substances into the atmosphere. The aim involves the fulfilment of the following research objectives:

- analyse modern flue gas cleaning technologies at TPPs, determine their advantages and limitations, and develop a mathematical model that describes the flue gas cleaning process;
- conduct numerical modelling of the influence of design and technological parameters on the cleaning efficiency;
- assess the effectiveness of alternative approaches to optimisation taking into account technical, economic, and environmental indicators.

The problem of reducing harmful emissions during electricity generation is extremely relevant in the context of modern challenges of climate policy and the transition to sustainable development (Rakgetse and Maseeng, 2025). Emissions of nitrogen oxides (NO_x), sulphur (SO_2), PM, and carbon dioxide (CO_2) from TPPs are one of the key threats to the environment and human health (Ahmed et al., 2022; Sabadash and Lopushansky, 2024). A number of studies prove that the efficiency of denitrification systems can be increased by improving the chemical processes of ammonia-NO_x interaction in catalysts. The denitrification process is based on the catalytic reduction of NO to N_2, which contributes to overall NO_x removal efficiency. The modelling of reaction kinetics in environments such as COMSOL Multiphysics is of particular importance in this context (EXPRO, 2021; Mishra et al., 2024). For example, Dennis et al. (2024) analysed the kinetics of NO_x reactions in the context of ammonia-hydrogen gas turbines, which allows extrapolating these approaches to CHPP systems. However, it should be noted that most such models are based on simplified assumptions regarding flow homogeneity and ideal reaction conditions, which limits their applicability to real operational situations.

The use of plug flow models, as well as three-dimensional numerical simulations, enables a more accurate determining the influence of temperature, the NH_3:NO reagents ratio, and the geometric parameters of the reactors on the gas purification level (EXPRO, 2021; Mishra et al., 2024). However, the literature does not pay enough attention to the influence of changes in the load of CHPP on the dynamics of purification processes, as well as interaction with other processes in the heat and electricity generation system. The issue of fuel selection also occupies a significant place in recent studies. In particular, Rakuta et al. (2025) indicate that a significant amount of harmful compounds is formed during the fluidised bed combustion (FBC), which requires an integrated approach to purification. However, there is a limited number of studies that combine modelling of combustion processes with the prediction of the volume and composition of emissions, which complicates the assessment of the environmental efficiency of certain types of fuel under different conditions.

In parallel, other researchers emphasise the appropriateness of integrating renewable energy sources into the power system to reduce the load on thermal plants and reduce total emissions (Ahmed et al., 2022, Apon et al., 2025; Bagheri et al., 2015). Apon et al. (2025) considered in detail the issue of integrated planning and effective energy dispatching management in systems where traditional and renewable energy sources are combined. These studies substantiate the potential for reducing greenhouse gas emissions by optimally distributing the load between sources. At the same time, the available literature lacks models that would integrate these strategies with data on the real technical limitations of CHPPs and their inertia.

Sabadash and Lopushansky (2024) and Sabadash et al. (2023) made an important contribution to the study of dust pollution reduction methods. They emphasised the use of adsorption technologies and statistical estimation of PM_{10} and $PM_{2.5}$ particle levels in urban areas, which has a direct relationship with the CHPP emission levels. However, most studies focus on post-treatment technologies, leaving out the possibility of real-time integration with emission sources.

Hakimuddin et al. (2020) studied automatic generation control in power systems with hydro, thermal, gas, and wind plants. This has direct implications for reducing overloads and increasing generation efficiency from an ecological perspective. Although their study outlines important aspects of load balancing, it does not pay enough attention to the issues of flue gas cleaning as a separate ecosystem problem.

Li et al. (2023) considered stochastic optimal control of integrated electricity, gas, and heat supply systems, taking into account the corresponding consumer responses. This approach reduces the overall energy load and the emission levels under increased load variability. However, the research focused primarily on control optimisation, rather than on the technical aspects of cleaning systems. Zhang et al. (2022) proposed the concept of cooperative optimisation for multi-energy systems that take into account carbon capture technologies. However, the model is mainly conceptual and does not cover the specifics of emissions of different pollutant classes, such as NO_x, SO_2, or dust.

The study by Protsko et al. (2021) deals with the complex treatment of flue gases, describing modern methods of filtration, desulphurisation, denitrification, and dust collection. Such technologies include selective catalytic reduction (SCR) systems, which are actively studied as a method of multi-pollutant treatment. However, most of the existing studies focus on individual aspects of such systems, without considering their integration into energy processes taking into account economic efficiency. Wang et al. (2021) critically reviewed the capabilities of SCR in the context of flue gas treatment of NOx and SO_2, which is of great practical importance for the optimisation of treatment systems at CHPPs.

The classic study by HasIbeck et al. (1990) demonstrated that alternative technologies, such as the NOxSO process, provide for the simultaneous removal of NOx and SO_2 from flue gases. However, their study also lacks data on their adaptation to the conditions characteristic of Ukrainian CHPPs, in particular solid fuel-fired ones. Regarding the evaluation of the efficiency of the treatment systems themselves, Mohammadi et al. (2021) compared the efficiency evaluation models using the analytic hierachy process (AHP) and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) methods. This study may be useful in selecting technologies for CHPP modernisation based on multi-criteria analysis, but it requires further verification under specific technical constraints and real industrial loads.

Ahmed et al. (2022), as well as Masoomi et al. (2020) considered the issue of reducing greenhouse gas emissions in electricity generation using effective dispatching control. The latter used the long-range energy alternatives planning (LEAP) model to assess various emission reduction scenarios in Iran, which can be adapted to Ukrainian realities. However, extrapolation of the results without taking into account local regulatory requirements and fuel composition raises doubts about the accuracy of the estimates. The study of Yang et al. (2024) is worth mentioning, which analysed decision-making on load distribution taking into account energy storage and distributed generation. This approach can also serve as a means of regulating peak emissions and increasing the overall efficiency of the system, but the issue of their interaction with cleaning systems is not fully covered.

In recent studies, considerable attention has been paid to the implementation of ultra-low emission technologies, especially in the plants that burn solid fuel waste. However, most of the studies demonstrate fragmented approaches, focusing on individual technological solutions without a proper comprehensive assessment of the systemic impact on the environmental efficiency of power units. The literature review indicates high scientific interest in the field of reducing emissions of harmful substances from flue gases, but also reveals certain limitations and contradictions. Xiao et al. (2022) demonstrated the effectiveness of post-combustion technology for reducing NOx when using coal sludge in circulating fluidised beds. It is difficult to disagree with this position, because such conditions ensure improved mixing of reagents and longer contact with the catalyst. At the same time, this technology has limited application in old CHPPs operating through a traditional combustion scheme.

In the context of alternative fuels, Yuan and Abu Saleh (2024) emphasise the importance of switching from traditional fossil fuels to biofuels or other environmentally friendly options. Such a replacement significantly reduces emissions of harmful substances, in particular CO, NOx, and PM. This approach seems reasonable, but, in authors' opinion, the technological and economic adaptation of CHPPs to such changes in fuel composition is insufficiently considered. Primary emission reduction – changes introduced at the combustion stage – is also particularly relevant. In their review, Jafarsalehi et al. (2025) analyse a set of measures for cleaner biomass combustion. These include improving fuel quality, airflow management, boiler design, and the role of auxiliary equipment. There is a reason to agree with the authors about the need for a systemic approach, although their review does not sufficiently consider the impact of these parameters on long-term operation of the equipment.

The article by An et al. (2021) is interesting from the perspective of hybridisation of technologies, which considers combined De-NOx systems that combine catalytic and non-catalytic reduction methods in a combined cycle. Selective catalytic reduction (SCR) involves the use of a catalyst to enhance NO reduction at lower temperatures, whereas selective non-catalytic reduction (SNCR) occurs without a catalyst and requires higher temperatures (850–1100 °C). This approach deserves attention in terms of flexibility; however, as the authors themselves rightly note, it causes difficulties in precise control of parameters and requires significant capital investments in infrastructure modernisation. The study of Sigal et al. (2022) is also worth noting, which considers methods of primary NOx reduction during gas combustion. They demonstrate that a significant effect can be achieved by multi-stage air supply, reducing the combustion temperature and controlling the duration of fuel residence in the reaction zone. This eliminates the need for modernisation using expensive filtration systems (Lysiak, 2023). This approach seems especially valuable in the context of a phased transition of CHPP to gas fuel, although it requires precise control over the combustion dynamics, which is not always possible under real production conditions (Nielsen et al., 2021; Rušeljuk et al., 2021).

Despite the significant number of studies in the field of flue gas cleaning, there are a number of gaps that require further study. In particular, a comprehensive assessment of the effectiveness of cleaning systems when using mixed or alternative fuels in real-life operation of TPPs has been poorly covered. Besides, the analysis of the integration of primary and secondary emission reduction methods into a single optimised system needs to be expanded. There has also been limited research on the long-term impact of changes in design parameters on the energy efficiency and environmental sustainability of the plants.

MATERIALS AND METHODS

The process of cleaning flue gases from nitrogen oxides (NO) by their reduction with ammonia (NH_3) was simulated in this study. Visualisation of catalytic oxidation used in this process is a key element in emission control systems. This approach is widely used to reduce the concentration of NO in gases, in particular in the automotive industry, as well as in TPPs operating on solid fuels. Calculations and visualisation of the model were performed in the Comsol Multiphysics environment (Mayboudi, 2022; Luo et al., 2025; Chaurasia, 2021).

The reaction of NO reduction with ammonia usually occurs in the channels of a monolithic catalyst located in the flue gas flow. The efficiency of this process depends on the balance between the amount of ammonia and nitrogen oxides. An excess of NH_3 at the reactor outlet is undesirable in terms of environmental and economic factors, while its deficiency can limit the nitrogen reduction reaction. The process is further complicated by the possibility of ammonia oxidation, entering into a side reaction that competes with the main reduction reaction. Both processes are temperature-dependent and depend on the concentrations of the components.

The Reaction Engineering interface in the COMSOL Multiphysics environment was used to model the process, with an idealised Plug Flow Reactor scheme (EXPRO, 2021; Mishra et al., 2024). This approach is used to analyse the reaction kinetics in the flow direction without taking into account back mixing along the reactor's length. The main goal of the simulation is to investigate the selectivity of the reactions, i.e. the ratio between the desired NO reduction reaction and the side reaction of NH_3 oxidation under different conditions (temperature and mixture composition) (Mishra et al., 2024). A system of material and energy balance equations was solved based on the built model, in particular:

- equation of change of molar velocity of components along the reactor;
- equation of heat balance taking into account thermal effect of reactions;
- dependence of reaction rates on temperature (for example, according to Arrhenius law).

The model allowed to visualise the change in NO, NH_3 concentrations, as well as the temperature profile along the reactor's length. Special attention was paid to the parameters that affect the cleaning efficiency, in particular the initial concentrations of reagents and the temperature regime. The modelling results can be used to optimise the process of selective catalytic reduction of NO (SCR) in CHPPs in order to reduce harmful gas emissions and increase the efficiency of gas cleaning systems. The reduction of nitrogen oxides (NO) with ammonia (NH_3) can be summarised by the general reaction:

$$4NO + 4NH_3 + O_2 \rightarrow 4N_2 + 6H_2O \quad (1)$$

This reaction underlies the Selective Catalytic Reduction (SCR) process, which is widely used to clean flue gases from NO_x in industry and the energy sector. However, ammonia can enter into a side oxidation reaction, which reduces its effectiveness as a reducing agent:

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

This process is undesirable, as it leads to excessive ammonia consumption and increased temperature of the medium because of the exothermic nature of the reaction. Heterogeneous catalytic conversion of NO to N_2 occurs according to the *Eley-Rideal mechanism*. In this mechanism, the key step is the interaction of NO in the gas phase with NH_3, which is adsorbed on the catalyst surface. This approach takes into account the complex surface phenomena characteristic of monolithic reactors. The main reduction reaction rate is described by the following kinetic equation (dimensionality: mol/(m^3·s)):

$$r_1 = \frac{k_1 C_{NO}}{1 + aC_{NH_3}} \quad (3)$$

where: r_1 – NO reduction reaction rate; C_{NO} – NO concentration in the gas phase; C_{NH3} – NH_3 concentration; k_1 – reaction rate constant, which is described by the Arrhenius dependence: $k_1 = A_1 \exp\left(-\frac{E_1}{RT}\right)$; α – NH_3 sorption coefficient, which also depends on temperature: $a = a_0 \exp\left(\frac{E_a}{RT}\right)$; where: A_1 – pre-exponential factor; E_1 – reaction activation energy; α_0 – coefficient related to the initial NH_3 sorption capacity; E_a – NH_3 sorption energy on the catalyst surface; R – gas constant; T – absolute temperature, K.

The rate for the side reaction of ammonia oxidation is given by the following equation:

$$r_2 = k_2 C_{NH_3} \quad (4)$$

where: $k_2 = A_2 \exp\left(-\frac{E_2}{RT}\right)$ – NH_3 oxidation rate constant, A_2; E_2 – kinetic parameters of the adverse reaction.

Taking into account two competing reactions – the desired (reduction of NO) and the undesired (oxidation of NH_3) – is key to realistic modelling of processes in a monolithic catalyst. Their ratio determines the selectivity of the system, which should be maximally shifted towards the formation of nitrogen (N_2) without loss of NH_3. The model analyses the influence of temperature, initial concentrations of reagents, and design characteristics of the reactor on the final efficiency of the flue gas cleaning from NO_x.

Assuming a stationary regime, the material balance equation for an ideal plug-flow reactor (PFR) has the following form (Marzouk, 2025):

$$\frac{dF_i}{dV} = R_i \tag{5}$$

where: F_i – molar flow rate of component i (dimensions: mol/s); V – reactor volume (м³); R_i – chemical reaction rate for component i (mol/m³·s).

The molar flow rate F_i is related to the concentration of the component c_i and the volumetric flow rate v by the following relationship:

$$F_i = vC_i \tag{6}$$

where: v – volumetric flow velocity, defined as $v = uA$; u – average linear flow velocity (m/s); A – cross-sectional area of the reactor (m²).

The energy balance equation is used to analyse thermal effects in a reactor:

$$\sum_i C_{P,i} F_i \frac{dT}{dV} = Q_{ext} + Q \tag{7}$$

where: $C_{P,i}$ – molar heat capacity of component i (J/(mol·K)); Q_{ext} – the amount of heat supplied from outside to the system per unit volume of the reactor (W/m³); Q – the amount of heat generated or absorbed as a result of the chemical reaction (W/m³), which can be calculated through the thermal effect of the reactions: $Q = -\Sigma j H_j r_j$; where: H_j – the thermal effect of reaction j (J/mol), r_j – the rate of reaction j (mol/m³·s).

The model is solved based on Equations 4, 5, 6 taking into account different ratios of reactant concentrations (NH_3 to NO) and at a temperature regime that varies along the reactor. During the simulation, the molar rates of NH_3 and NO are considered constant to investigate the effect of temperature on the reaction. Equation 5 is included to take into account the thermal effects accompanying the reaction, as temperature significantly affects the rate of NOx formation.

Uncertainty quantification procedure

To evaluate the robustness of the numerical model and identify the dominant parameters affecting reactor thermal behaviour, an uncertainty quantification analysis was performed using a variance-based global sensitivity approach. Since the kinetics of the selective catalytic reduction (SCR) process are strongly temperature-dependent through Arrhenius-type reaction rate expressions, the reactor temperature was selected as the principal response variable for the uncertainty analysis. The model output was represented by the COMSOL variable root.comp1.re.Tode, which corresponds to the calculated temperature field in the reaction engineering domain. This variable was used as an indicator of the thermal state of the reactor, directly influencing reaction rates, NO conversion efficiency, and the probability of undesired side reactions such as ammonia oxidation.

The uncertain input parameters considered in the analysis included the channel length L, inlet gas temperature T_{in}, ambient temperature T_{amb}, channel radius r, average gas velocity v_{av}, channel cross-sectional area A, and volumetric flow rate v_{rate}. These parameters were selected because they characterise the main geometric, thermal, and hydrodynamic features of the SCR reactor. Each variable was varied within realistic engineering ranges around its nominal operating value.

Global sensitivity analysis was carried out using Sobol variance decomposition, where the total variance of the model response (the model response Y was partitioned into contributions of individual parameters and their interactions:

$$\mathrm{Var}(Y) = \sum_i V_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \cdots \tag{8}$$

where: Y – root.comp1.re. Tode, V_i is the variance contribution of parameter x_i, and V_{ij} denotes interaction effects between parameters.

The first-order Sobol index (S_i) was calculated as:

$$S_i = \frac{V_i}{\mathrm{Var}(Y)} \tag{9}$$

which quantifies the direct influence of parameter x_i on the reactor temperature. The total Sobol index was determined by:

$$S_{Ti} = 1 - \frac{\mathrm{Var}(Y|X_{\sim i})}{\mathrm{Var}(Y)} \quad (10)$$

where: S_{Ti} – total Sobol index; $X_{\sim i}$ – the set of all parameters except x_i.

This index includes both direct and interaction effects.

RESULTS AND DISCUSSION

Analysis of the kinetics of chemical reactions determines the optimal ratio between ammonia (NH_3) and nitrogen oxides (NO) for effective flue gas cleaning. At the first stage of the study, the rates of the main reaction – NO reduction were analysed. The side reaction – NH_3 oxidation – was also studied at fixed molar rates of NH_3 and NO depending on the temperature and the ratio of reactants.

Figure 1 shows the dependence of the rate of the NO reduction reaction (reaction 1) on the temperature for different values of the initial NH_3:NO ratio (denoted as X0), which varies from 1 to 2. The NO concentration in the flue gas inlet stream entering the catalyst was 0.0411 mol/m³. The molar rates of NH_3 and NO remained constant throughout the reactor volume.

Analysis of the obtained curves (Figure 1) showed that the NO reduction rate passes through a maximum and decreases with further increase in temperature. Moreover, with an increase in the NH_3:NO ratio, the maximum of the reaction rate shifts towards higher temperatures. The observed non-monotonic dependence of the NO reduction rate on temperature is governed by the interplay of three competing mechanisms. At lower temperatures, the reaction rate is limited by the intrinsic kinetics, as described by the Arrhenius dependence of the rate constant k_1, resulting in a gradual increase in the NO conversion rate with temperature.

As the temperature increases, the reaction reaches an optimal regime, where the balance between kinetic acceleration and surface availability of ammonia provides maximum efficiency. However, further temperature increase leads to a decline in the reaction rate due to two simultaneous effects. First, the desorption of NH_3 from the catalyst surface reduces the surface coverage required for the Eley–Rideal mechanism. Second, the rate of the side reaction of ammonia oxidation increases significantly due to the higher activation energy E_2, leading to additional consumption of the reducing agent. As a result, the availability of NH_3 for the main reduction reaction decreases, causing a reduction in the overall NO conversion rate at elevated temperatures. As shown in Figure 1, this transition occurs in the temperature range of approximately 680–710 K, depending on the NH_3:NO ratio. The decrease in the reaction rate at elevated temperatures is attributed to the desorption of NH_3 from the catalyst surface, which limits its availability for the Eley-Rideal mechanism (Mishra et al., 2024). This nature of the dependence is explained by the fact that at elevated temperatures, the rate of ammonia desorption from the catalyst surface becomes higher than the rate of its interaction with NO in the gas phase. As a result, the amount of adsorbed NH_3 available for the reduction reaction decreases, thereby reducing the overall efficiency of the process in case of excessive heating. However, the analysis does not account for potential parallel side reactions

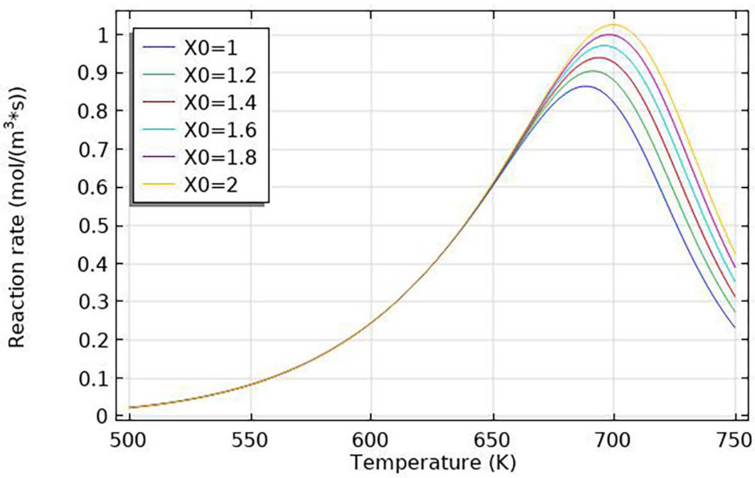

Figure 1. Dependence of the NO reduction reaction rate r_1 on temperature at different NH_3:N ratios

(e.g., NH_3 oxidation), which may also contribute to the observed decline in NO reduction efficiency at higher temperatures. In addition, the absence of experimental validation of surface coverage limits the robustness of the proposed mechanistic interpretation.

The obtained results indicate the existence of an optimal temperature regime and the ratio of reagents for achieving maximum purification efficiency. This conclusion is important for further optimisation of the operation of selective catalytic reduction systems at TPPs. Figure 2 shows the spatial distribution of the nitrogen oxide (NO) conversion rate in the channels of the monolithic catalyst. The isosurfaces depicted in the graph demonstrate how the efficiency of NO conversion depends on the spatial arrangement of an individual channel within the reactor, which clearly illustrates the three-dimensional nature of the process.

The isosurfaces that reflect the NO conversion rate in the reactor volume (Figure 2) show the gas flow from left to right. According to the simulation, the average conversion at the reactor outlet is 97%, which is slightly lower than the 99% predicted by the single-channel model. This difference indicates non-uniform reaction conditions in the three-dimensional reactor volume. In particular, local variations in temperature and reactant concentrations between channels reduce the overall efficiency. The result suggests that simplified one-dimensional models tend to overestimate conversion due to the neglect of inter-channel interactions and spatial gradients. Therefore, accurate prediction of reactor performance requires full three-dimensional modelling, especially for the systems with strong coupling between heat transfer and reaction kinetics. The minimum amount of ammonia participating in the catalytic reaction was found by using visualisation according to the reaction Equation 2 of the mathematical model (Figure 3).

The ideal flow displacement model was used for the purification of flue gases containing 41.1 mmol/m³ of nitrogen oxide (NO) at a temperature of 523 K, passing through a monolithic catalyst with a flow velocity of 0.3 m/s. According to the simulation results, it is necessary that the NH_3:NO ratio exceeds 1.2 to ensure the effective course of the nitrogen oxide reduction reaction with ammonia over the entire of the channel length. This ensures that a sufficient amount of ammonia as a reducing agent remains throughout the catalyst volume. Under the given conditions (Figure 3), the reactor length is 0.36 m, and its internal volume is 4.5×10^{-5} m³. Therefore, maintaining the optimal ratio of reactants is a key condition for achieving a high NO conversion rate, avoiding ammonia losses, and ensuring stable operation of the purification system.

At the same time, this result is obtained under the assumption of ideal plug flow, which neglects axial mixing and radial gradients. In real reactors, incomplete mixing and channel-to-channel variations can lead to local NH_3 deficiency or excess. This may reduce conversion efficiency and increase the risk of ammonia slip at the outlet. Therefore, the threshold value NH_3:NO>1.2 should be considered as an optimistic estimate, and additional correction may be required for practical applications.

The final stage of the simulation (Figure 4) involved the analysis of the temperature distribution and the NO conversion rate along one channel of the monolithic reactor. For two values of the initial ratio of NH_3:NO reagents (X_0 = 1.3 and X_0 = 1.5), the maximum temperature in the reactor

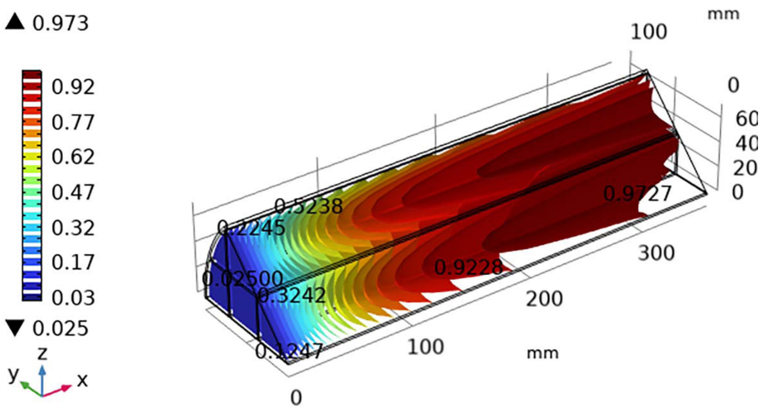

Figure 2. 3D visualisation of the distribution of nitrogen oxide conversion rate in the reactor zone

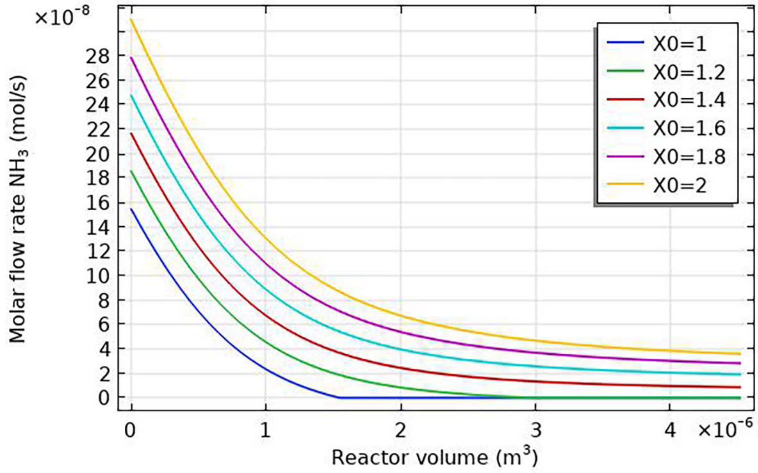

Figure 3. Molar flow rate of ammonia (F_{NH3}) depending on the catalyst channels volume (V)

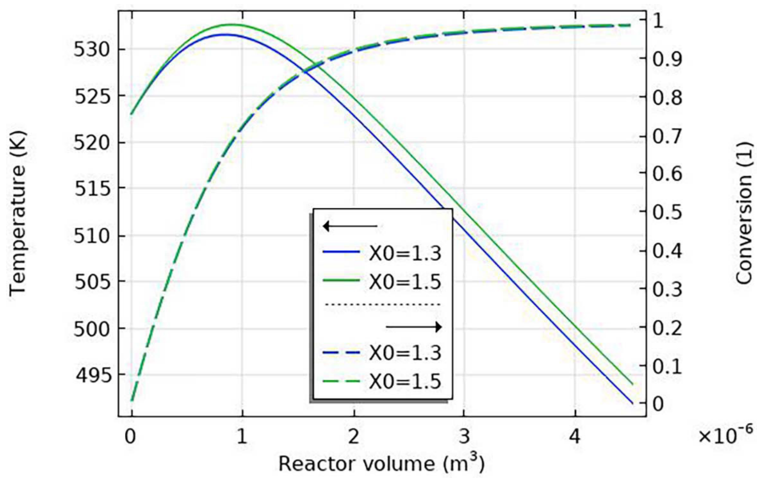

Figure 4. Dependence of temperature in the reaction zone on the reactor volume at different nitrogen oxide conversion rates, where __ - X_0 = 1.3; __ X_0 = 1.5; - - conversion when X_0 = 1.3; - - conversion when X_0 = 1.5

was 532 K and 533 K, respectively. At the same time, the NO conversion rate approached unity – about 99%, which indicates almost complete removal of nitrogen oxides from the gas stream. The results of the calculation of the dependence of the conversion on the reactor volume (Figure 4) showed very close values , and the lines almost overlap. These results confirm that temperature is a critical factor for efficient ammonia dosing. Even minor temperature fluctuations along the length or between channels can significantly affect the reaction and purification efficiency. It is necessary to create a full-fledged three-dimensional model of the reactor for more accurate optimisation, as the temperature is distributed unevenly between individual channels under real conditions of a monolithic catalyst. However, the conclusions are based on a simplified single-channel model, which may underestimate the influence of flow maldistribution and inter-channel interactions under real operating conditions. In addition, the recommended NH_3:NO ratio range requires validation under transient regimes, where temperature and concentration fields are not steady. Based on the calculations using the single-channel model, it was established that to ensure high efficiency of flue gas purification at an CHPP, it is appropriate to maintain the NH_3:NO ratio in the range of 1.3 to 1.4. This ensures almost complete conversion of NO, while minimising excessive use of the reagent and secondary pollution with ammonia. The obtained data can be used to improve dosing systems and temperature control in selective catalytic systems at operating TPPs. The obtained temperature range (523–533 K) corresponds to typical operating conditions of SCR units installed downstream of economisers

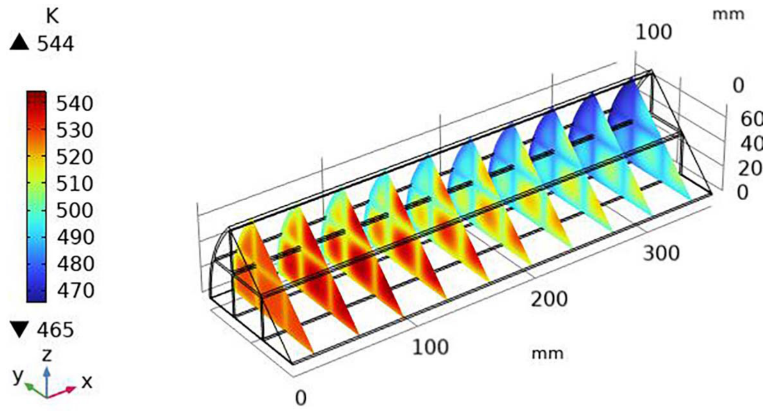

Figure 5. 3D visualisation of temperature distribution in the reactor zone

in TPPs, which confirms the practical relevance of the model (Park et al., 2019).

Figure 5 shows the temperature and flow rate distribution inside a tubular reactor. This reactor was used to model the flue gas cleaning process using the example of the NO_x reduction reaction in three-dimensional format.

Figure 5 shows the temperature profile along the reactor (from ~470K to 540K). There is a gradual increase in temperature from the inlet to the outlet section, which corresponds to the active chemical reaction zone. However, the analysis does not quantify temperature gradients across the reactor cross-section, which may mask local hot spots or inactive zones. In addition, the absence of validation against experimental data limits confidence in the predicted temperature field. Figure 6 presents the temperature distribution depending on the reactor volume.

The chart gives grounds to evaluate the efficiency of heat transfer along the reactor and the spatial temperature change, which is critical for temperature-sensitive reactions (for example, selective catalytic reduction of NO_x). It also helps determine the conditions to ensure reaction uniformity and avoid local overheating or insufficient heating. Simulation data in the COMSOL environment can be used to improve the flue gas cleaning process at TPPs.

Uncertainty quantification was performed to evaluate the robustness of the numerical predictions and the influence of uncertain input parameters on the model response. The analysis considered realistic variations in reactor geometry, inlet temperature, flow conditions, and selected kinetic parameters within prescribed operating ranges. A variance-based global sensitivity method using Sobol indices was applied to quantify the contribution of each parameter to the output variance. The results indicate that the predicted NO conversion remains stable over the investigated parameter space, with the overall uncertainty estimated to be within approximately ±3% under nominal operating conditions. The largest contribution to output uncertainty

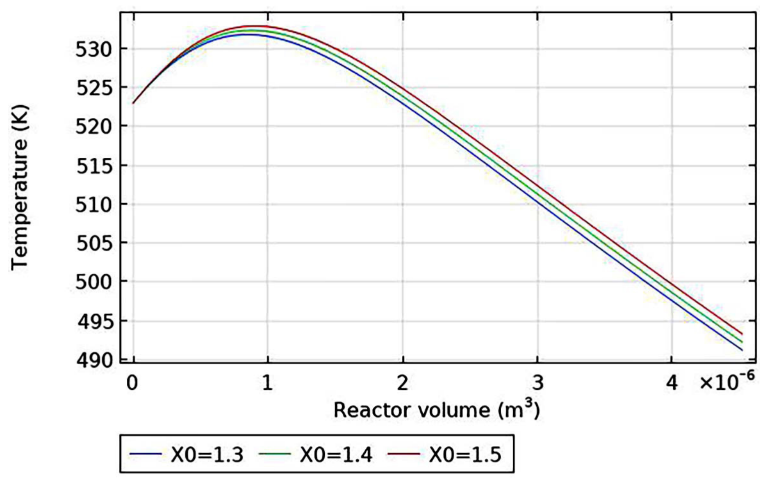

Figure 6. Temperature distribution depending on the reactor volume

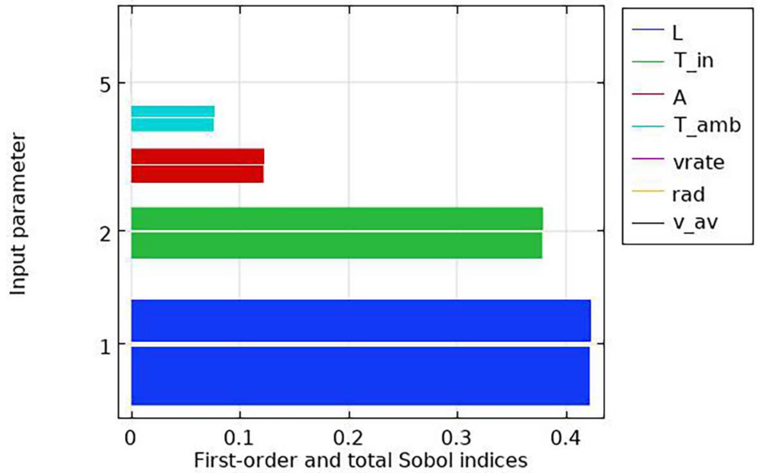

Figure 7. Sobol sensitivity analysis of the flue gas purification model parameters

was associated with channel length and inlet gas temperature, whereas flow-related parameters exhibited comparatively small effects. These findings confirm the reliability of the proposed model for engineering analysis and optimisation of SCR systems at thermal power plants. The Sobol sensitivity analysis results are presented in Figure 7, illustrating the relative contribution of the input parameters to the variance of the model output.

The horizontal bars represent the first-order and total Sobol sensitivity indices for the selected input variables: channel length (L), inlet temperature (T_{in}), channel cross-sectional area (A), ambient temperature (T_{amb}), volumetric flow rate (v_{rate}), channel radius (r), and average gas velocity (v_{av}). The results indicate that the channel length (L=0.3±0.1 m) has the greatest influence on the model response, with a sensitivity index of approximately 0.42. The inlet temperature (T_{in} = 523±10 K) is the second most significant parameter, with an index close to 0.38. These two variables dominate the system behaviour and largely determine the pollutant removal efficiency and reactor thermal performance. A moderate contribution is observed for the channel cross-sectional area (A = πrad²), while the ambient temperature (T_{amb}=350 ± 10 K) has only a minor effect. The influence of volumetric flow rate (vrate = v_av·A), channel radius (rad = 2 mm), and average gas velocity (v_av =0.3±0.1m/s) is negligible within the investigated operating range.

Overall, the analysis demonstrates that optimisation of the flue gas purification system should primarily focus on reactor geometry (channel length) and thermal operating conditions (inlet gas temperature), as these parameters provide the highest potential for increasing operational efficiency and reducing harmful emissions.

Table 1 shows the generalised emission indicators for individual components (NO_x, SO_2, CO, CO_2, N_2O). These data were obtained as a result of the analysis for different types of coal used at power plants of different capacities, taking into account the features of the combustion process.

The analysis of tabular data established that the most environmentally appropriate fuel is Donetsk coal, Deposit 1. According to Table 1:

- the Donetsk coal, Deposit 1 has the lowest emission rates of nitrogen oxides (NO_x) and nitrogen dioxide (NO_2);
- carbon dioxide (CO_2) emissions are also at a fairly moderate level, compared to other types of fuel;

Table 1. Results of calculations of NO_x, SO_2, CO, CO_2, N_2O emissions for different types of fuel

Coal type	(g/m³)	K_{SO2} (g/m³)	K_{CO} (g/m³)	K_{CO2} (g/m³)	K_{N2O} (g/m³)
Donetsk coal, Deposit 1	22.099	61.868	3.948	91.343	1.4
Donetsk coal, Deposit 2	12.663	77.335	19.694	94.274	1.4
Donetsk coal, Deposit 3	59.947	77.335	4.973	91.995	1.4
Olexandriia brown coal (B1R)	46.611	77.335	7.525	111.473	1.4
Mukachiv coal	90.207	77.335	1.273	113.488	1.4
Lviv-Volyn coal (LV-GR)	24.695	77.335	0.965	95.300	1.4

- all considered types coal have the same generalised emission rate of nitrogen oxide (I) (N_2O), which indicates a similar mechanism of its formation when combusted;
- the indicators of other coal brands demonstrate either significantly higher emissions of SO_2 and CO, or lower efficiency in the context of the total load on atmospheric air.

Further research in the field of analysis of emissions during the combustion of solid fuels is aimed at creating mathematical models for predicting emissions under different combustion conditions. Such models will become the basis for the development of effective combustion management strategies, as well as provide scientifically grounded recommendations for fuel selection depending on the boiler plant type. The implementation of such approaches will contribute to reducing the environmental burden on the environment without disrupting the stability of energy supply.

The study extends existing SCR modelling approaches by integrating: temperature-dependent adsorption kinetics, spatial (3D) distribution of temperature and concentrations, analysis of competing reactions within a unified framework. This enables more accurate prediction of NO conversion under non-uniform reactor conditions and provides a basis for optimising denitrification processes in real TPP systems.

The obtained results of the study indicate the appropriateness of an integrated approach to the optimisation of flue gas cleaning systems at TPPs. The simulation conducted in the COMSOL Multiphysics environment identified the influence of temperature, stoichiometric ratio NH_3:NO and geometric parameters of the catalyst channels on the efficiency of selective reduction of nitrogen oxides. The model was validated qualitatively by comparing the obtained kinetic trends and optimal operating conditions with published data on SCR systems (Mishra et al., 2024; Wang et al., 2021), demonstrating good agreement in terms of temperature dependence and NH_3:NO ratios. It is shown that almost complete (≈99%) conversion of NO is achieved at a temperature of 523–533 K and a ratio of NH_3:NO within 1.3–1.5, which is consistent with the literature data (Mishra et al., 2024; Protsko et al., 2021). The obtained values exceed the results presented in EXPRO (2021) by 10%. However, it should be taken into account that the distribution of temperature and reagent concentrations under real conditions of a multi-channel monolithic reactor is uneven.

This is confirmed by the results of three-dimensional simulation, according to which the cleaning efficiency depends on the spatial position of the channels (Figure 3). This feature necessitates precise control of reagent dosing and ensuring uniform temperature distribution in the reactor. This is consistent with the data of the study EXPRO (2021), which indicates that the temperature distribution and concentration profile inside the reactor are related to the yield of the reaction product. It was found that lowering the temperature below the optimal range leads to ammonia "breakthrough", and too high a temperature causes oxidation of the reducing agent, which complicates the control of secondary pollutant emissions. This effect is consistent with the studies (Mishra et al., 2024; Ahmed.et al., 2022)

In the situations where boiler replacement is not possible and the installation of additional flue gas cleaning systems is limited for financial or technical reasons, the selection of the optimal type of coal becomes key to reducing the level of emissions of harmful substances. Different brands of coal differ significantly in the content of sulphur, volatile substances, and ash content, which directly affects the amount of emissions of sulphur oxides (SO_x), nitrogen (NO_x), and particulate matter during combustion (Bagheri et al., 2015; Sabadash and Lopushansky, 2024). The use of fuel with a low sulphur and ash content significantly reduces the negative impact on the environment, even without the use of additional gas cleaning systems. This is especially relevant for low-power boilers or enterprises with limited funding for modernisation.

In addition to fuel selection, an important factor is the optimisation of the combustion process, in particular, control of the temperature in the reaction zone and air supply parameters. The strategy for minimising fuel costs and emissions also formed the basis of the study by Apon et al. (2025). It is known that high temperatures contribute to the formation of NO_x, and an excess of oxygen in the air increases the concentration of solid particles in flue gases (Dennis et al., 2024; Sabadash and Lopushansky, 2024). Therefore, the setting of the combustion mode in layer (stationary) boilers can significantly affect the level of harmful emissions. The use of methods for regulating the air supply (for example, stepped or reverse supply) allows reducing the concentration of pollutants and achieve more environmentally friendly fuel combustion (Sekhavati and Yengejeh, 2021; Vakkada Ramachandran et al., 2022). The proposed approach to optimising flue gas cleaning systems can be practically implemented at operating thermal power plants and boiler houses using solid fuel or mixed fuels.

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The results of numerical modelling and analysis of various configurations of flue gas cleaning systems confirm the hypothesis advanced in the introduction. In particular, it was found that optimisation of the geometric parameters of the catalyst, rational regulation of the temperature regime and reagent consumption allow reducing the concentrations of NO_x, SO_2, and PM in the exhaust gases by 12–35% without a significant increase in energy or financial costs for the cleaning system operation. Therefore, the hypothesis of the possibility of increasing the environmental efficiency of TPPs through technical and technological optimisation was fully confirmed. This is consistent with the results of leading scientific research (Li et al., 2023; Protsko et al., 2021). The obtained results can be used for:

- modernisation of existing gas purification plants in order to reduce costs and emissions;
- development of technical regulations for the design of new power plants with increased requirements for environmental safety;
- preparation of feasibility studies for investment projects in the field of energy efficiency;
- creation of software that enables selecting the optimal parameters of purification systems in the simulation mode, depending on the fuel composition, combustion temperature, and other technological factors.

The main contribution of this study is the integration of kinetic modelling with spatial temperature distribution in a multi-channel reactor, enabling more accurate prediction of NO conversion under non-uniform operating conditions.

CONCLUSIONS

The obtained results confirm the importance of an integrated approach to optimising flue gas cleaning systems. This is extremely relevant in the context of current challenges of energy security, environmental sustainability, and harmonisation with European environmental standards. In view of the increasing requirements for reducing the man-made load on the environment, the results of the study can become a practical basis for increasing the environmental efficiency of TPPs without a significant increase in energy consumption. The study proves that an effective flue gas cleaning system at TPPs should be based on a combination of primary and secondary technological methods. In this case, it is necessary to take into account the fuel type, design restrictions, and environmental standards. Special attention is paid to studying the influence of regime and technological parameters and the choice of fuel type.

Furthermore, the purification processes were simulated using the methods of selective reduction of nitrogen oxides in the COMSOL Multiphysics environment to find the optimal operating conditions of gas purification systems. The results showed that the purification efficiency depends on the position of the channels in the catalyst. Numerical simulation in COMSOL Multiphysics established that the optimal ratio of NH_3:NO within 1.3–1.4 at a temperature of 523–533 K provides up to 99% NO conversion. Such a result is a high efficiency indicator for SCR.

Analysis of the spatial distribution of temperature and concentrations in a monolithic reactor confirms the need to use three-dimensional models for accurate assessment of purification processes and optimal placement of catalyst channels. Calculations of emissions of harmful substances when using coal of different grades showed that coal from the Donbas Basin (grade 1) is the least environmentally hazardous. It provides lower NO_x, SO_2, and N_2O emissions without the use of additional purification equipment. The obtained results can be used for the feasibility study of the modernisation of existing flue gas cleaning systems, as well as for the development of regional environmental strategies in the energy sector. The prospects for further research are the development of adaptive control systems for cleaning processes, taking into account changes in the composition of flue gases and operating conditions of TPPs.

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