

UNDERSTANDING PROMPT NO_x FORMATION IN SPRAY COMBUSTION WITH OH EXCLUSION

Sarah Falih Kareem^{1*}, Ahmed Abed Al Kadhem Majhool², Faris Alqurashi³

Abstract: This study numerically analyzed NO_x emissions for pentane spray combustion. Thermal and prompt pathways are used to model NO_x formation under the equilibrium oxygen condition and the OH exclusion model. The *k-ε* model analyses the turbulent flow field, and the mixture fraction-probability density function model is used to construct the combustion model. The most important parameters studied are temperature, OH, CO, mass fractions of NO_x, and NO_x generation rates. The results show that prompt NO_x processes produce substantially higher emissions compared to thermal mechanisms. The combined models (prompt and thermal) exhibit a variation of approximately 1% in NO_x mass fractions and their generated rates. The results indicate that the thermal model is better than the prompt model in all the domains studied, especially in reducing nitrogen oxide emissions.

Introduction

Nowadays, about 90% of the energy that we use comes from burning fossil fuels. In light of the rapid depletion of fossil fuel supplies, the increasing global need for energy, and the corresponding environmental concerns, combustion technologies that are both very efficient and minimally polluting have been created. Combustion produces nitrogen oxide (NO), which is rapidly converted to nitrogen dioxide (NO₂) once it reaches the air. NO is created when nitrogen and oxygen in the air are heated to high temperature [32]. Numerous investigations have been conducted in the last several years with the goal of identifying the causes of NO generation and attempting to reduce it. Thermal NO_x generation, prompt, fuel NO_x formation, and intermediate N₂O are the four basic chemical kinetic mechanisms that lead to NO_x creation. Prompt NO_x is generated by a high-speed reaction occurring near the flame front [35]. Fenimore first noted that prompt NO_x production may occur in substantial quantities in some combustion environments, such as those with low temperatures, fuel richness, and short residence durations (e.g. surface burners and gas turbines) [17]. Cooper, et al. [8] studied Variables such as the fuel composition, temperature, and pressure affect the generation of NO_x during combustion, making it a crucial part of chemistry. The research emphasizes the importance of understanding the chemical kinetics associated with the formation of nitrogen oxides (NO_x) under engine conditions. It emphasizes the need for data on hydrocarbon formation (CH) to

¹ Mechanical Engineering Department, College of Engineering, University of Al-Qadisiyah, Iraq.
Email: sarahfalihkareem@qu.edu.iq

² Mechanical Engineering Department, College of Engineering, University of Al-Qadisiyah, Iraq.
Email: ahmed.majhool@qu.edu.iq

³ Mechanical engineering Department, University of Bisha, 67714, Bisha, Kingdom of Saudi Arabia.
Email: fars421@hotmail.com

*Correspondence: sarahfalihkareem@qu.edu.iq

Keywords: Spray combustion, NO_x generation, None OH model, Thermal NO_x model, Prompt NO_x formation, Fluent.

improve the accuracy of prompt-NOx kinetics. Stagni, et al. [30] studied the Flameless combustion technologies to reducing NOx. emissions, particularly when using next-generation fuels. The chemical reactions involving nitrogen in the fuel are of utmost importance in the creation of NOx. Prior studies on thermochemical studies and kinetic modelling demonstrate the importance of NCN radical thermochemistry on NO generation in flames, underscoring the need for precise values to improve NO concentration forecasts. Nehr, et al. [25] investigated the aromatic hydrocarbon reactivity provides valuable information on the formation of HO2 radicals, which contributes to a broader understanding of NOx chemistry in combustion processes. Also, research on the creation of nitrogen oxides (NOx) under high pressure, Prior studies shows that pressure doesn't have a big effect on the immediate formation of NOx. This shows how complicated NOx processes are in different settings. Park [26] discussed heat and fuel nitrogen oxide generation during combustion. They calculate engine nitrogen oxide emissions using Zeldovich, nitrous oxide, Fenimore, and NNH mechanism-based kinetic models. The researchers examine in detail the uncontrolled emission of nitrogen oxide and its causes in internal combustion engines. Amjad, et al. [1] describes nitrogen oxide generation techniques that will help investigate internal combustion engine NO synthesis to understand nitrogen chemistry, apply the processes to modern fuels like biofuels. Additionally, oxygenated biofuels dramatically lower PM emissions. IC engine research focuses on NOx. Low-temperature combustion and pre- and post-treatment technologies may minimize NOx emissions and help create next-generation internal combustion engines. Keller [15] This research presents a numerical simulation that examines a method for reducing thermal NOx emissions by increasing the flame lift-off length to decrease the peak flame temperature PEMS showed that the estimated NOx is similar in magnitude but lower than the NOx detected in field experiments. These findings were anticipated due to the fact that the computation of NOx was only based on the Zeldovich process. However, existing research indicates that the nitrous oxide mechanism actually creates a substantial amount of NOx. The model accurately depicts the correlation between NOx levels and several operational factors, such as equivalency ratio, ambient temperature, humidity, and air pressure. Model enhancements are proposed with the eventual objective of integrating the model. Bo, et al. [4] examined how the diameter and quantity of air nozzles impact the performance of the combustion chamber. The study's results demonstrated that decreasing the diameter of the nozzle led to an increase in the velocity of the air jet, while increasing the quantity of air spraying nozzles resulted in improved combustion efficiency. Perrone, et al. [27] used a novel approach to design an industrial furnace, including five chambers and three outlets for combustion byproducts, while enabling flameless combustion via the use of pure oxygen. Another outcome of his research was a decrease in NOx emissions. Given the most recent research and the industry's significant impact on pollution and environmental damage, there is a growing demand for a comprehensive study of the geometric factors that affect the performance of industrial combustion chambers. Masum, et al. [22] conducted a comprehensive analysis of various fuel composition engine parameters and evaluated the influence of engine adjustments on NOx production. In addition, we investigated a mathematical technique for forecasting NOx levels using ethanol. Hydrous ethanol, in contrast to anhydrous ethanol, has the capacity to provide better results in these engines, namely by decreasing NOx emissions and improving engine performance. Ethanol has a somewhat reduced heating value, which presents a concern. Cerinski, et al. [7] Quantitative methods were used to examine By increasing the number of nozzle apertures and ensuring their precise positioning, it is possible to achieve a

significant 60% reduction in emissions. They may attribute the behavior noted earlier to the specific arrangement of spray clouds and smaller regions with elevated temperatures. Prior literature discovered that using coarser sprays in flameless combustion mode resulted in a notable increase in acoustic emissions. Additionally, it generated a slightly uneven temperature distribution and led to higher CO and NO_x emissions. Bohon and Roberts [5] studied how burning fuel with a high oxygen mass percentage releases nitrogen oxides (NO_x) at very low concentrations. The researchers deliberately chose glycerol as the fuel and conducted a comparison with diesel combustion, using the same circumstances of a high swirl turbulent spray flame. The research findings suggest that the combustion of glycerol leads to NO_x emissions that are much lower, by up to ten times, compared to those seen in diesel fuel. Xu, et al. [33] This article provides a concise overview of the progress made in comprehending nitrogen chemistry in flames over a span of twenty years after the influential studies. They also explore different pathways that form NO_x, such as the recently proposed NNH route, and stimulate NO through NCN and other precursor molecules. Zhong, et al. [37] Demonstrate that increased mixing is the main factor responsible for the decrease in soot in the 900 and 950 K scenarios. On the other hand, the 1000 K case releases more soot due to the self-ignition of the methanol/air mixture. This shortens the n-heptane spray flame's lift-off length and lowers the oxygen level in the air. The present dual-fuel setups show that the impact of oxygen concentration and heat capacity on ignition delay time and maximum flame temperature due to methanol dilution is negligible. During dual-fuel combustion, the surrounding temperatures influence the impact of methanol on NO_x generation. At a temperature of 900 K, the rate of NO_x production is lower in the dual-fuel scenario compared to the single-fuel scenario. However, when the temperature reaches 1000 K, a contrasting pattern of NO_x generation rate is revealed. The primary cause of the heightened NO_x emission is the expansion of the high temperature zone resulting from the interaction between the spray flame and the burning of the surrounding mixture. Golchert, et al. [11] showed Molecular nitrogen is one of the elements found in natural gas. This proportion varies between about one and seven percent of the overall mass fraction. Furthermore, the aluminum industry is actively investigating methods to reduce NO_x emissions. An approach involves substituting a portion of the combustion air with pure oxygen. This decreases the nitrogen input into the boiler but simultaneously increases the combustion temperature, potentially leading to an increase in NO_x output. The study employs extensive computer simulations to investigate the effects of varying nitrogen levels in the air and the replacement of pure oxygen with air in an aluminum furnace. The study examines the impact of changes in nitrogen concentration on the production of pollutants. The discussion will cover trends and the optimal oxygen content for a certain nitrogen mass fraction. Löffler, et al. [19] introduce a newly developed, streamlined model that integrates thermal NO production, N₂O/NO, and the NNH pathway. The steady-state approximation is used for the intermediate species, namely N, N₂O, NNH, and NH. By using four algebraic equations, the concentrations of the substances can be determined. Furthermore, they compute the NO generation rate solely using reaction kinetics, eliminating the need for any model parameter. Furthermore, combustion calculations must determine the levels of O₂, N₂, H₂, and H₂O, as well as the reactive species O, H, OH, and HO₂. They assessed the model by comparing it to the predictions of a comprehensive response mechanism, which demonstrated favorable concurrence over a broad spectrum of situations. Only when the fuel conditions are extremely rich does disregarding the creation of quick NO have an impact on the expected NO emissions. Regardless of these conditions, the overall production of NO is low. As a

result, the absence of fast NO generation does not affect the model's performance. Prior studies show that the small hydrocarbon combustion reaction mechanism, potentially incorporating kinetic data from the prompt NO route via NCN. NO formation correlations with calculated C₂O radical concentrations strongly suggest including the C₂O-N₂ reaction and reducing the CH-N₂ reaction rate constant. Tajik, et al. [31] The objective of the present study is to create a precise numerical framework for forecasting the combustion and emission properties of an anode baking furnace. Circulating a portion of the exhaust gases through the ABF crossovers results in a decrease in the concentration of oxygen. This leads to improved fuel efficiency, reduced emissions of pollutants, and a more uniform flow and temperature distribution. Sirignano [29] provides a thorough evaluation of recent theoretical advances in droplet vaporization in a high temperature setting and spray combustion. The theory emphasizes analytical and computational contributions, with some reference to empirical evidence. The researcher provides a detailed discussion of four fundamental phenomena: (i) the movement and internal flow of droplets; (ii) the temporary heating of droplets; (iii) the evaporation of fuel with multiple components; and (iv) the process of combustion and evaporation of droplet arrays, groups, and sprays. He also examines these occurrences for their various interconnections. The text briefly mentions several more problematic areas. Future direction recommendations are proposed. The researcher examined multiple NO_x configurations and demonstrated that only the turbulence-chemistry interaction model based on mixture fraction could produce satisfactory results. All other models significantly underestimated the maximum levels of nitric oxide. Using the mixture fraction-based turbulence chemistry interaction, the combustion model accurately predicted the amount of nitric oxide in the combustor. Both O modelling with omission and OH modelling demonstrated a strong correlation with the data. Prior studies investigated how burner arrangement and oxidizer temperature affect NO_x release from a liquid kerosene-powered small-scale furnace operating under high-temperature air combustion conditions. At temperatures equal to or greater than 823 K, the emission of NO_x decreased as the distance between the spray and oxidizer nozzles increased. At oxidizer temperatures below or equal to 623 K, the emission of NO_x initially rose and then declined as the inter-nozzle separation increased. Gradually increasing the inter-nozzle distance led to flame extinction and a subsequent reduction in NO_x output. Kaneko, et al. [14] conducted a diverse range of experiments and numerical simulations. The results showed that the low intensity of mixing in the spray tip area, where the flow and turbulence structure significantly differ from those of continuous jet flames, is responsible for the significant production of NO_x in diesel engines. It is possible to reduce NO_x emissions from diesel engines by increasing the mixing intensity at the spray tip area to match that of a continuous jet flame. Additionally, the study indicated that the flame's luminosity appeared to decrease as a result of the nitrogen pre-injection, and the NO_x emission index was two-thirds of that observed in the non-injection scenario. Numerical simulation also demonstrated the impact of pre-injection on NO_x reduction. The research shows the experimental and numerical simulation results, together with photographic analysis, of the improved mixing of the spray tip region when water was injected as a pre-injection to boost mixing. Many prior studies investigated centers on comparing the NO_x properties of methane/air and heptane/air PPFs. The authors use a detailed study of the main routes and patterns of distribution of important radical species to explain the differences in the quality and amount of NO_x emitted by the two flames at different levels of partial premixing. Furthermore, the authors investigated the impact of fuel blends on NO_x emissions using methane/hydrogen and heptane/hydrogen

blends. In n-heptane flames, the amounts of C_2H_2 and CH radicals produced are significantly higher than in methane flames. These higher quantities are the primary cause of the observed differences in NO_x properties between the two fuels. Scholars investigated the impact of the NCN radical pathway on the generation of NO in flames, focusing on thermochemistry and reaction kinetics. The sensitivity analysis revealed that the specific value of the NCN formation heat heavily influences the contributions of individual steps to the creation of NO and NCN. The NCN thermochemistry applied in all studied flames have a significant impact on the simulated mole fractions of NO and NCN. The results of this study show that thermochemistry has limits on NCN chemistry that need to be taken into account in order to make model predictions for NO levels in fires more accurate. Hampartsoumian, et al. [12] Understanding the design factors that result in reduced NO_x emissions from combustion systems are essential, as is the examination of chemical reactions that occur within flames and include nitrogenous species. This study incorporates data from both experimental and modeling research on the nitrogenous emissions produced by an oil-fueled furnace. The furnace uses staged combustion to control the release of NO_x emissions. The NO concentration profiles within the flame are measured and compared for the same burner operating in both the unstaged and staged modes. When the effects of super equilibrium radical production and turbulence/chemistry interaction are considered, the predictions show that the emission of NO is in satisfactory qualitative accordance with the values reported in experiments. Prior literature presents an analysis of the emissions and combustion properties of a lean-lean two-stage combustor model. The authors tested the combustor in both single-stage and two-stage modes, utilizing the typical input conditions of a stationary gas turbine in a simple cycle. They demonstrated that using appropriate air splits, we could achieve a high level of combustion efficiency and maintain low NO_x emissions, even when the overall equivalency ratios varied widely. When the primary mixture was sufficiently lean, we observed that combustion oscillation was rare in lean-lean two-stage combustion. However, significant combustion oscillation occurred at higher overall equivalence ratios (usually above 0.8) in single-stage combustion. Li, et al. [18] The study investigates how starting conditions affect premixed moderate or intensive low-oxygen dilution (MILD) combustion from a single jet burner in a small-scale furnace. To achieve this, the study uses Reynolds-averaged Navier-Stokes (RANS) modeling and experiments. The numerical results indicate that premixed MILD combustion is only possible in the current furnace and burner setup when the Reynolds number (Re) surpasses a critical threshold (Rec). When the Reynolds number (Re) is more than or equal to the critical Reynolds number (Rec), it is possible to generate stable MILD combustion, regardless of the variations in A , Φ , or f . W The authors also include a diagram that illustrates the stability boundaries for premixed MILD combustion, highlighting the relationship between boiler temperature and recirculation rate. Doppalapudi and Azad [9] studied utilized computational fluid dynamics (CFD) to examine the combustion patterns and their impact on nitrogen oxide (NO_x) emissions. This study created a diesel engine model with a flat combustion chamber (FCC) for simulation purposes. This study suggests that implementing lean fuel mixture combustion, adjusting the chamber, and optimizing fuel spray can improve complete combustion. Altering the fuel injection profile, spray angle, and injection timing can achieve this. The current study used large-eddy simulations (LES) to look at how an n-dodecane spray, which is a diesel substitute, can self-ignite in a mixture of methane and air that is not very rich. The primary objective is to examine the generation of NO_x , CO, and the precursor C_2H_2 for soot formation in dual-fuel (DF) spray combustion. The experiment investigates the impact of different ambient

oxygen concentrations (13%, 15%, and 21%). The extensive chemical kinetic analysis reveals that the process of thermal NO creation primarily generates NO_x. Furthermore, the first reactions that result in the production of both CO and C₂H₂ have demonstrated the pivotal role of C₂H₃. Sahu and Srivastava [28] studied a numerical investigation of the combustion and emission properties of n-heptane, dimethyl ether, and their blends (with 10%, 25%, and 50% dimethyl ether mixed with n-heptane) in a constant volume chamber. The results indicate that n-heptane spray combustion has the highest rate of heat release, characterized by a highly intense premix combustion phase. On the other hand, dimethyl ether spray combustion has the lowest rate of heat release and the shortest premix combustion phase. The premixed phase and heat release rate diminish as the dimethyl ether mass percentage in the blends increases. The emissions of soot, carbon monoxide (CO), unburned hydrocarbon (UHC), and nitric oxide (NO) decreased as the mass fraction of dimethyl ether in the blends increased, reaching their lowest levels. Yang, et al. [34] Ammonia is a potential zero-carbon fuel that can reduce carbon emissions from IC engines. Ammonia compounds contain nitrogen, which increases NO_x output in internal combustion engines. In addition to thermal NO_x generation in petrol and diesel, ammonia combustion synthesizes NO_x fuel. This complicates ammonia engine NO_x emissions. Separating fuel and heat NO_x emissions helps understand how nitrogen oxides develop and evolve in ammonia engines. The researchers want to explain that. The simulations show that ammonia oxidation produces the fuel NO_x as an intermediate species. The nitrogen temperature and residence time significantly influence the concentration of Thermal NO_x in the burned zone. As expected, these results show fuel and atmospheric nitrogen separation. Nitrous oxide (N₂O) from the fuel's NO_x process diffuses mostly throughout the liner walls. Later in the oxidation process, fissures release ammonia for partial oxidation. Researchers also conducted a three-dimensional direct numerical simulation (DNS) to investigate the production of nitric oxide (NO) and nitrous oxide (N₂O) in turbulent NH₃/H₂/N₂-air premixed flames. Using comprehensive chemical kinetics, the study seeks to understand the influence of equivalency ratio and pressure on these reactions. This study found that the specific shape of the flame often greatly influences the generation of NO, while curvature, particularly under high pressure conditions, does not significantly affect the creation of N₂O. The researchers look at these numbers while considering changes in thermo-diffusive effects and the rise in certain important radicals, like atomic hydrogen, during the N₂O consumption. Beige and Mardani [3] conducted large eddy simulations (LES) of a Gas Turbine Model Combustor (GTMC) using a five-step global mechanism that incorporates distinct thermal and non-thermal NO_x generation components. The LES results indicate a strong correlation between the vertical structures within the chamber, the temperature field, and chemical reactions. These structures play a significant role in facilitating rapid premixing and the subsequent reduction of NO_x emissions. However, they also contribute to the generation of NO_x by creating localized high-temperature areas that contain chemical radicals. Moreover, careful analysis of specific data reveals that the majority of heat release occurs in samples with mixture fractions close to the overall value, while the powerful vortices and the stoichiometric mixture fraction predominantly influence the production of NO. Luo, et al. [20] conducted an analysis on the combustion parameters and NO_x emission of a turbocharged hydrogen engine using the available test data. The findings indicated that the combustion duration, namely the crank angle at which 10% to 90% of the fuel is consumed, was identical at both 1500 rpm and 2000 rpm. Furthermore, when the brake mean effective pressure (BMEP) reached 0.27 MPa, the combustion duration was much greater compared to other

loads. The NO_x emission exhibits varying trends under different operating circumstances. These findings are used to develop effective control strategies for turbocharged hydrogen internal combustion engines that balance power, brake thermal efficiency, and NO_x emissions. Ilbas, et al. [13] studied a low-eddy and premix burner to investigate the characteristics of unstable combustion in mixed fuels containing methane and ammonia. This study aims to investigate the effects of adding ammonia at various sound frequencies, dynamic pressure amplitudes, and light emission intensities on combustion instability. Additionally, the authors examined the effects of adding ammonia to methane fuel gas on temperature and emissions. The authors conducted an analysis using pure methane and three methane-ammonia mixes as fuel, all at a ratio of 0.7 equivalents. The analysis also considered three different acoustics. The addition of ammonia to methane fuel did not result in any noticeable changes in combustion performance. The presence of nitrogen bonded to ammonia significantly increased the anticipated levels of NO_x emissions. Khazraii, et al. [16] focus on the numerical simulation of NO_x emissions in turbulent liquid fuel spray flames using thermal and fuel models. An investigation is conducted to examine the impact of fuel spray angle and inlet air temperature on the emission of nitric oxide. The results show that as the spray angle increases, combustion becomes more efficient, and the maximum flame temperature rises. Furthermore, the highest temperature influenced an increase in the concentration of NO_x. The findings indicate that the use of fine droplet sprays resulted in increased NO_x emissions. Through a review of the literature, researchers have demonstrated that an ideal temperature range can enhance the rate of NO_x generation. Table 1 provides a concise overview of the relevant publications this study analyzed. All of the prior studies described in this research used thermal and/or prompt NO_x production. In this study examines NO_x emissions under equilibrium oxygen conditions, specifically focusing on the comparison between thermal and prompt NO_x generation. It also investigates the situations that occur prior to NO_x prediction. A numerical calculation demonstrates that thermal NO_x will generate less NO_x than prompt NO_x creation. Elevated temperatures, typically over 1500 °C, strongly influence thermal NO_x emissions. It mostly happens after the flame, where temperatures peak. The process is based on the extended Zeldovich mechanism, which entails the conversion of nitrogen in the air (N₂) into NO through oxidation. Thermal NO_x generation occurs at a relatively slow pace, requiring more time than prompt NO_x generation. Thermal NO_x is the primary source of NO_x emissions in combustion processes characterized by high flame temperatures. At lower temperatures compared to thermal NO_x, prompt NO_x generation occurs. It happens in the first stage of the flame front, when the temperature is relatively lower. Hydrocarbon radicals (like CH) and nitrogen molecules (N₂) interact in the process, creating HCN. This is then changed to NO. Although prompt NO_x does contribute to total NO_x emissions, its impact is often minor in comparison to thermal NO_x, particularly in combustion processes with high temperatures. Ultimately Within high-temperature combustion settings, those seen in C₅H₁₂, the principal mechanism for the formation of NO_x is through thermal processes. Nitrogen oxides (NO_x) have a greater impact at lower temperatures or when there is an excess of fuel. To control thermal NO_x emissions, it is necessary to implement techniques that reduce the highest temperatures reached during combustion, such as flue gas recirculation or staged combustion. Modifying the fuel composition or improving fuel/air mixing can result in a rapid reduction of NO_x. Understanding these differences is important for coming up with effective NO_x control strategies in combustion systems that use pentane or similar hydrocarbons.

Table 1: Overview of the Chosen Studies that Were Surveyed.

Types of NOx	Source of study	Research methodology	Temp range	enhancement
Thermal	Ilbas, et al. [13]	Numerical	400 -600 K	–
		Numerical and experimental	423 – 1023 K	–
		Experimental	–	Reduce NOx by 30%
	Tajik, et al. [31]	Numerical	1200 – 1770 K	Reduce NOx by 15%
Thermal and prompt	Cerinski, et al. [7]	Numerical	650 -2200 K	Reduce NOx up to 60%
	Hampartsoumian, et al. [12]	Numerical and experimental	22 – 2008 K	–
			300 – 2100 K	–
	Khazraii, et al. [16]	Numerical	300 – 1500 K	–

Mathematical Models

The numerical model is based on a classical description of the Lagrangian liquid phase and the Eulerian gas phase. The Lagrangian technique uses data from the liquid phase as a source for the interaction terms that connect the two phases.

Liquid Phase

Liquid-phase droplets establish the beginning of solutions using a combination of the Lagrangian approach and force balance. This method focuses primarily on the mostly spherical, appropriately diluted, and smaller liquid droplets present in the region of interest. This text elucidates a collection of ordinary differential equations pertaining to mass, momentum, and heat transfer. The determination of the equilibrium force of the droplet particles is established [6].

$$\frac{du_p}{dt} = f_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + \frac{\rho}{\rho_p} u_p \frac{\partial u}{\partial x_i} \quad (1)$$

$$f_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D Re}{24} \quad (2)$$

$$Re = \frac{d_p \rho |u_p - u|}{\mu} \quad (3)$$

The gravitational force acting on the droplets is given by the equation $g_x (\rho_p - \rho) / \rho_p$, where g_x is the acceleration due to gravity, $\rho_p - \rho$ is the density of the droplets, and (ρ_p) is the density of the medium. The velocity of the droplets is represented by u in m/s^2 . The drag force per unit mass of the particle is represented by (f_D) and is given by the equation $(u - u_p)$ in m/s^2 . The fluid's pressure differential generates the third term, an extra force on the opposite side. The derivative of the function p with respect to t is denoted as (du_p/dt) . The term refers to the pace at which a particle evaporates. The acceleration due to gravity is denoted as g_x and is measured in metres per second squared (m/s^2). The diameter of a droplet is represented as d_p . The drag coefficient is shown as CD . The heat equilibrium is used to quantify the quantity of heat transferred from the liquid to the gaseous phase. An important factor to consider is the impact of the drag force exerted by the particles. In order to ascertain the characteristics of the drag force coefficient, the drag correlation is used.

$$CD = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} \quad (4)$$

(a_1), (a_2), (a_3) When vapour concentrations change from the gas phase to the surface of a droplet, the vaporization rate changes as well. One way to determine the volumetric source's term is by using the formula:

$$s_h = \left[\frac{\bar{m}_p}{m_{p.o}} cp \Delta T_p + \frac{\Delta m_p}{m_{p.o}} (-h_{fg} + \int_{T_{ref}}^{T_p} C_{p,i} dt) \right] \dot{m}_{p.o} \quad (5)$$

Gas Phase

The Eulerian multiphase is characterized by the preservation equations of momentum, continuity, and energy. Each phase is handled independently. Furthermore, a persistent model is used to represent the gaseous state. The mass conservation equation is valid at any point in the system's function. Initially, the model just considers the gas phase of a process and does not analyses the interaction between several phases [24]. The source term is determined by the particle's trajectories. Ansys Fluent is capable of resolving the gas phase by including the source term in the equation.

$$\frac{\partial}{\partial x_i} (\rho u_i) = S_m \quad (6)$$

Momentum

$$\rho u_i \frac{\partial u_i}{\partial x_i} = \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \left(\frac{\partial u_j}{\partial x_j} \right) \delta_{ij} \right] + \rho g_i - \frac{\partial p}{\partial x_i} + F_i \quad (7)$$

Energy

$$\rho u_i \frac{\partial e}{\partial x_i} = -p \frac{\partial u_i}{\partial x_i} + \Phi v + \frac{\partial}{\partial x_i} \left(k \frac{\partial T}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \quad (8)$$

$$\rho u_i \frac{\partial m_i}{\partial x_i} = -p \frac{\partial J_i}{\partial x_i} + S_m \quad (9)$$

$$J_i = -\rho D_{i,m} \frac{\partial m_i}{\partial x_i} \quad (10)$$

Standard k- ε Model

Practical and industrial contexts use turbulence flow, a computational model that represents turbulence. By using the turbulence model, we successfully calculated the anticipated fluctuations in turbulence with considerable simplicity. The flow field of the combustor was solved using the k-ε model. This model can effectively forecast complicated swirls of low to medium intensity, including shear flow, divided flow, and whirling flow. It is also suitable for calculating swirl and segregated flow wells in the combustion chamber. The Boussinesq assumption serves as the primary premise in this model's computation, initially establishing a correlation between the Reynolds stress and the average velocity gradient. The calculation of the eddy viscosity coefficient may be achieved by including a formula and a new transport equation into the dissipation rate. The following are the equations that describe the transport of turbulent substances, The model's

dissipation rate and kinetic energy [6].

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \epsilon - Y_m + sk \quad (11)$$

$$\frac{\partial}{\partial t} \rho \epsilon + \frac{\partial}{\partial x_i}(\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k} + S_\epsilon \quad (12)$$

$$\mu_t = \rho C_m \frac{k^2}{\epsilon}, G_k = -\rho u'_i u'_j \frac{\partial u_j}{\partial x_i}, G_b = \beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i} \quad (13)$$

The constants model is:

$$C_{1\epsilon} = 1.44, C_{2\epsilon} = 1.92, C_m = 0.09, \sigma_k = 1, \sigma_\epsilon = 1.3, \sigma_{3\epsilon} = -0.33$$

Combustion Model

The current study used the probability density function (pdf) to examine different combustion characteristics. The mixture fraction can yield two probability density functions: a truncated Gaussian function and a beta function [23]. These may be used to demonstrate how turbulence affects the values of the conservation scalar. The present investigation often employs a beta function owing to its cost-effectiveness and adaptability. Computing the beta function via mathematical methods:

$$p(f) = \frac{f^{\Psi-1} (1-f)^{B-1}}{\int_0^1 f^{\Psi-1} (1-f)^{B-1} df} \quad (14)$$

$$f = \frac{z_i - z_{i,ox}}{z_{i,fuel} - z_{i,ox}} \quad (15)$$

The coefficients Ψ and B are functions that explicitly depend on the average mass mixture fraction (f) and the concentration variation (g)

$$\Psi = f \sim [(f \sim (1-f \sim)) / g - 1] \quad (16)$$

$$B = (1-f \sim) \Psi \quad (17)$$

Rescaling these numbers based on a specific probability Once we determine the finite difference solutions for each grid point, we can use the values of f and g to compute the average values of species concentration, as well as the resulting temperature, density, and enthalpy. the ratio of the combination the $p(f)$ functions may have suitable parameters. The variables $y_i(f)$, $H_i(f)$, $T(f)$, and (f) represent the instantaneous mixture fraction (f). The amount Q , which represents the average of the Favre values, may be computed using these given values. The user's text remains unchanged.

$$Q = \int_0^1 \check{p}(f) Q(f) df \quad (18)$$

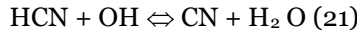
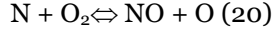
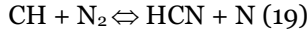
Equations (16) and (17) were used to calculate Ψ and p based on the given values of f and g . The beta PDF is dependent solely on the mixture fraction. Various quantities of $Y_i(f)$, $T(f)$, and others were tabulated and estimated for $N = 100$ using state equations for the mixture fraction ranging from 0 to 1.

Nox Model

Prompt Nox Formation

Nitric oxide (NO), nitrogen dioxide (NO₂), and nitrous oxide (N₂O) are the three

primary constituents of nitrogen oxide (NO_x) emissions. Fenimore [10] first discovered the occurrence of "prompt NO_x," which refers to a secondary process that results in NO_x production. The burning of hydrocarbon fuels quickly generates a tiny quantity of NO_x in the laminar premixed flame region before thermal NO_x forms. We refer to this phenomenon as prompt NO_x [17]. Strong evidence suggests that low temperatures, fuel-rich conditions, and short residence time during combustion can produce significant amounts of fast NO_x. Rich flames are the most common locations for quick NO_x to occur. The actual production involves a complex series of actions and numerous potential intermediary species. Nitrogen molecules and hydrocarbon radicals often combine to produce amines or cyano compounds under conditions of low temperature (below 750 °C) and sufficient fuel supply. Subsequently, these nitrogen-containing particles react with the nitrogen present in the atmosphere, resulting in the formation of nitric oxide (NO). The following reactions frequently lead to the creation of immediate Nox [16].



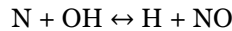
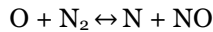
Equations (22) and (23) demonstrate that CH and CH₂ are the primary constituents that actively contribute to the generation of immediate NO_x. Prompt NO_x is more susceptible to fuel chemistry than thermal NO_x. The concentration of hydrocarbon radicals increases with higher equivalent ratios, resulting in an increase in hydrogen cyanide (HCN). As the equivalent ratio increases, the prompt creation rate of NO_x increases, reaches a maximum point, and then decreases when there is a scarcity of oxygen. Thermal NO_x production has a greater impact on the total combustion system than prompt NO_x. Studies, including combustion modelling, tend to underestimate the overall amount of nitrogen oxide (NO_x) emissions because they fail to consider the rapid NO_x mechanism [2]. If we make the assumption that the rate at which prompt-NO is formed, denoted as [NO]_p, may be described by the following equation:

$$\frac{d[\text{NO}]}{dt} = k_{pr} [\text{O}_2]^a [\text{N}_2] [\text{FUEL}] e^{-E_a/RT} \quad (24)$$

$$k_{pr} = 1.2 * 10^7 (RT/p)^{a+1}; E_a = 251151 \text{ J/gmol}$$

Thermal NO_x Formation

Thermal NO_x, which results from the dissociation of nitrogen and oxygen molecules at very high temperatures, is one of the primary reasons for NO_x generation. The Zeldovich mechanism is a collection of extremely temperature-dependent chemical processes that control the generation of thermal Nox [16, 36].



The following formula is used to determine the thermal-NO creation rate:

$$\left(\frac{d[NO]}{dt}\right) = 2k_{f,R14}[O][N_2] \frac{\left(1 - \frac{k_{r,R14}k_{r,R15}[NO]^2}{k_{f,R14}[N_2]k_{f,R15}[O_2]}\right)}{\left(1 + \frac{k_{r,R14}[NO]}{k_{f,R15}[O_2]k_{f,R16}[OH]}\right)} \quad (25)$$

Experimental investigations have determined the rate coefficients for the chemical equations included in the NOx model, as well as the rate constants for chemical reactions as follows:

$$\begin{aligned} k_{f,i} &= 1.8 \cdot 10^8 e^{-38370/T} \quad k_{r,i} = 3.8 \cdot 10^7 e^{-425/T} \\ k_{f,2} &= 1.8 \cdot 10^4 T e^{-4680/T} \quad k_{r,2} = 3.81 \cdot 10^3 T e^{-20820/T} \\ k_{f,3} &= 7.1 \cdot 10^7 e^{-450/T} \quad k_{r,3} = 1.7 \cdot 10^8 e^{-24560/T} \end{aligned}$$

(k_f) and (k_r) represent forward reactions rate constants and their units ($m^3/gmol \cdot s$), so the NOx formation rate must be calculated using the concentrations of (O), (OH), and (H). The mass transport equations of the nitrogen-containing species have source terms that return the total rates to the fluent solver via the Pollute structure [2, 33].

$$\frac{\partial}{\partial t}(\rho\gamma_{HCN}) + \nabla \cdot (\rho\vec{v}\gamma_{HCN}) = \nabla \cdot (\rho D \nabla \gamma_{HCN}) + S_{HCN} \quad (26)$$

$$\frac{\partial}{\partial t}(\rho\gamma_{NO}) + \nabla \cdot (\rho\vec{v}\gamma_{NO}) = \nabla \cdot (\rho D \nabla \gamma_{NO}) + S_{NO} \quad (27)$$

$$\frac{\partial}{\partial t}(\rho\gamma_{NH3}) + \nabla \cdot (\rho\vec{v}\gamma_{NH3}) = \nabla \cdot (\rho D \nabla \gamma_{NH3}) \quad (28)$$

$$[O] = 3 \cdot 97 \cdot 10^5 T^{-1/2} [O_2]^{1/2} e^{-31090/T} \quad (29)$$

$$[OH] = 2 \cdot 129 \cdot 10^2 T^{-0.57} e^{-4595/T} [O_2]^{1/2} [H_2O]^{1/2} \quad (30)$$

Numerical Method

Ansys Fluent 15.0 is capable of solving the governing equations. Within the Cartesian coordinate system, the pressure-based stable solver has successfully resolved two-dimensional geometry [2]. Figure 1 illustrates the flowchart outlining the processes of the numerical simulation. The primary focus of the present investigation was on stream lines' operating conditions. The SIMPLE method has shown a correlation between pressure and velocity. Equations involving momentum and mixing fractions use the power law to separate the variables. This approach discretizes the energy equation, resulting in second order accuracy of the outcomes. Following the solution's conclusive grid independence test, conducting separate simulations for the discrete-phase and continuous-gas phases. conducting 350 consecutive-phase iterations for each discrete-phase iteration. Additionally, we carried out 200 iterations in accordance with the NOx prediction. This study focuses on investigating spray combustion inside a turbulent combustion process that does not include premixing. To verify our results, we performed a comparison between the test cases and the experimental data obtained by Mao, et al. [21]. The n-pentane-air spray (Figure 2) generates a flame consisting of two distinct regions. The lowermost part is identified as the flame cone, and the larger region above it is the development zone. This is similar to the discoveries documented by Mao, et al. [21]. The combustion chamber has a cylindrical shape with dimensions of 10 metres in length and 1 meter in diameter. A 0.2-metre-diameter injector is used to bring n-

pentane fuel into the system, while a 0.49-micron-diameter injector is used to introduce air. Figure 2 illustrates the geometric characteristics, while Table 2 presents the boundary conditions. The boundary conditions used in the measurements done by Mao, et al. [21] are the basis for a thorough simulation of a 2-D test scenario. One way to verify the results obtained from the computational fluid dynamics (CFD) simulation is to compare them with the measurements and experimental data. The validation computation takes into account the spray droplet's input parameters. The parameters and gas phase readings are similar in magnitude. Table 3 presents the pertinent boundary and operating conditions for the liquid and gas properties. In accordance with the Cartesian coordinate system, the arrangement displays symmetry. The "GAMBIT" program is utilized to establish the geometry and create the 2D grid. The study was mostly about finding the best ways to observe and study different things that might happen in the areas around the burner output, specifically the changes in features shown in Figure 3 (a). The study does calculations on multiple grids. We evaluate the grid's convergence, consider its impact on the results, and select the most suitable grid for this investigation. We conduct numerous experiments by altering the grid's dimensions, amount, and arrangement within the computational domain. For each research instance, we performed a series of calculations using three modified structured grids that covered the full domain. Instance C has a total of 83,200 cells, 167,304 nodes, and 84,105 faces. Table 4 displays the grid's parameters. Figure (3b) displays a comparative examination of the experimental results derived from several grid adjustments. The diagram depicts the temperature curve of a gas flame under different conditions. The density of the grid has a substantial influence. Therefore, we can deduce that the solution depends on the grid.

Table 2: Experimental Condition.

Fuel	n -Pentane	
Injection pressure	2.67	<i>MPa</i>
Injection duration	steady	<i>ms</i>
Injection quantity	4	<i>ml</i>
Sauter mean diameter	28	μm
Maximum-drop diameter	79	μm
Injector diameter	0.2	μm
Spray injection velocity	69	<i>m/s</i>
Ambient pressure	3.2, 6.3, 9.4	<i>MPa</i>

Table 3: Operating Condition.

parameters	value	units
Injector inlet	296	<i>K</i>
Ambient temp.	296	<i>K</i>
Injector diameter	1.194	<i>mm</i>
Initial velocity of air	11.6	<i>m/s</i>
Initial velocity of fuel	69	<i>m/s</i>
Reynolds number	3600	—
Air temp.	1255	<i>K</i>
Air mass flow rate	0.08-0.225	<i>Kg/s</i>

Table 4: The Grid Details.

Details	Coarse mesh	Medium mesh	Refine mesh
CELL	5200	20800	83200
Faces	10626	42052	167304
Nodes	5427	21253	84105

Results and Discussions

This study investigated the production of nitrogen oxides (NO_x) from C₅H₁₂ fuel using two methods: thermal and prompt NO_x formation. The results were compared to the case prior to NO_x formation, which were obtained from Mao, et al. [21]. experimental investigation.

Temperature

The Figure 4 illustrates the relationship between temperature (T) in Kelvin (K) and location (y) in meters (m) at a constant x-positions. The data is displayed for three distinct scenarios: "Prompt NO_x" and "thermal NO_x" are both types of NO_x that are present when there is no absence of NO_x. for (x = 0.0 m) Devoid of nitrogen oxides (NO_x) The temperature remains consistent at around 295 K over the y-axis range of 0 to 0.1 m. Nitrogen oxides (NO_x) This line is not discernible on the graph, indicating that it aligns with the temperature profile of "Without NO_x." As a result, it remains constant at a temperature of 295 K over the y-axis range. High temperatures form nitrogen oxides (NO_x), known as thermal NO_x. The "prompt NO_x case" mirrors the situation where no NO_x data is available, yet the temperature remains constant at Steady temperature: The temperature remains consistent at 295 K for all three circumstances throughout the y-axis range. This indicates that the presence or absence of NO_x (either prompt or thermal) does not influence the temperature at this particular x-position. Under the specified circumstances, the intersecting lines suggest that NO_x (both prompt and thermal) does not have a noticeable effect on the temperature distribution. The consistent temperature may suggest a certain state in the system, such as thermal equilibrium, where the introduction of NO_x does not affect the thermal dynamics at x = 0.0 mm. the graph indicates that in this specific case, the presence or absence of NO_x has no effect on the temperature at the given point. At 295 K, the temperature remains constant. When x is equal to 0.1 meters, the lack of NO_x leads to a rise in temperatures from 1800 K to 1850 K, whereas the immediate presence of NO_x causes an increase in maximum temperatures and an early reduction in temperature. The temperature profile begins at 1800 K and exhibits a slower rate of increase compared to the scenario without NO_x. The diagram also demonstrates that both prompt and thermal NO_x emissions have a significant impact on temperature distribution. Prompt NO_x exacerbates peak temperatures and accelerates their decline more rapidly than both thermal NO_x and the scenario without NO_x emissions. At a distance of 0.05 m, the temperature reaches its maximum value of 1850 K. It then falls, but remains above the temperature profile of the "without NO_x" condition until it reaches a distance of 0.08 m. When the distance y is equal to 0.1 m, the temperature decreases to 1350 K from 0.08 m at the beginning. The temperature profile increases gradually until reaching y = 0.06 m, and then decreases fast. The maximum temperature recorded here is around 1850 K. Temperature elevation produces thermal NO_x, which are nitrogen oxides. In comparison to the situation where NO_x is absent, the temperature rise is more slow, reaching its highest point at a comparable temperature but at a later time (about y = 0.05 m). The early reduction is not as apparent, but it aligns with the "Without NO_x" profile at y = 0.08 m before experiencing a sudden decrease. At x = 0.2m, we observe that all cases progress at a rate equal to their differences.

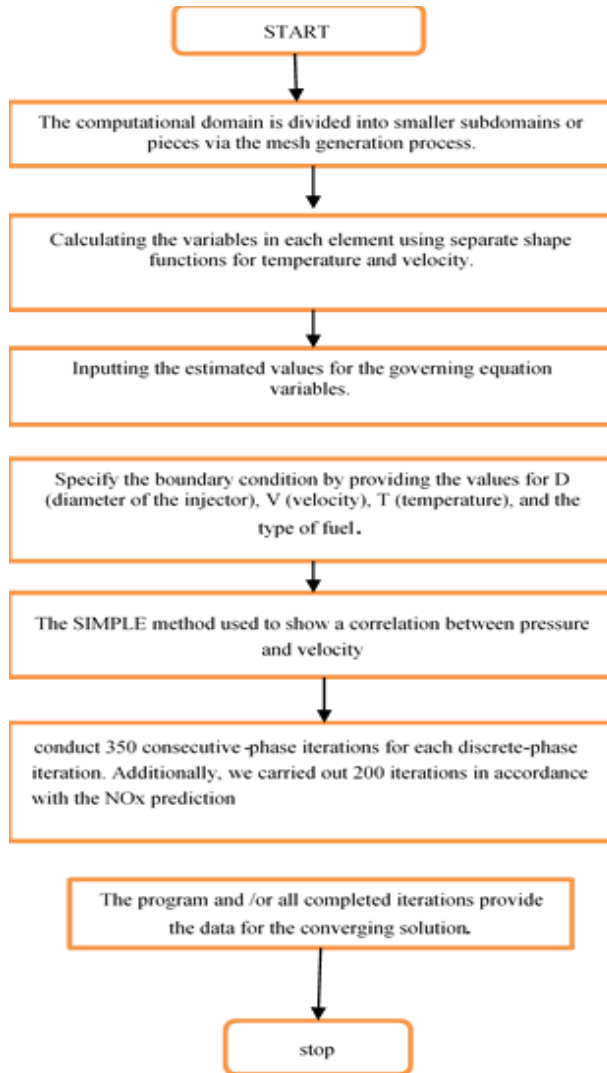


Figure 1: Flow Chart for the Numerical Solution.

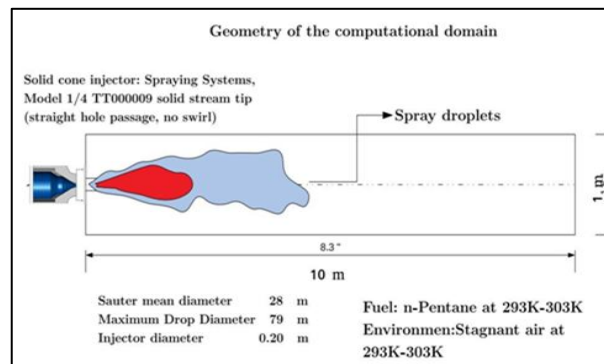


Figure 2: The Case's Schematic for the Spray Combustor.

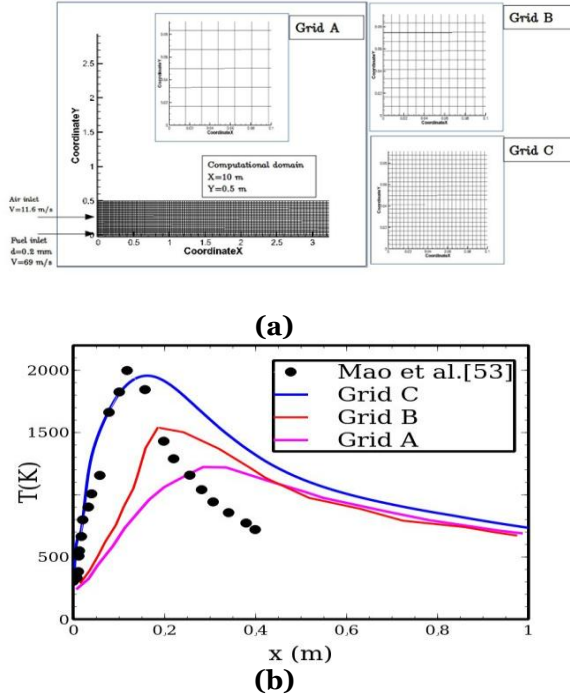


Figure 3: (A) Grid Independence and (B) Comparison Between the Gas Temperature With Experimental Data of Mao, et al. [21] At Different Grid Resolutions.

At $y = 0$, the values for temperature are around 1650 K for without NOx and 1750 K for thermal, while the value for prompt is around 1900 K. All instances progress uniformly at a rate equal to the difference between them at $x = 0.3\text{ m}$. At $y = 0$, the values are around 1400 for without NOx, 1495 for thermal, and 1600 K for prompt. In the case of NOx findings, the temperature discrepancy between the numerical simulation for prompt NOx and Mao, et al. [21] is 0.076%. The Figure 5 displays temperature contour plots along the symmetry axis for three distinct scenarios: absence of NOx, presence of thermal NOx, and presence of prompt NOx. In the absence of NOx, the graphic illustrates the spatial variation in temperature within the combustion system, excluding the generation of nitrogen oxides (NOx). The zone with the highest temperature is located near the flame front and gradually decreases as the distance increases along the axis. The maximum temperature seen is approximately 1600 K, and it decreases progressively as we move towards the downstream area. Figure (b) shows the temperature's spatial arrangement in the presence of thermal NOx. The temperature profile closely resembles that of the case without NOx; however, the region of highest temperature extends further downstream. Thermal NOx seems to affect temperature distribution, possibly leading to higher temperatures persisting over a longer distance. Plot (c) This graphic displays the spatial variation of temperature in relation to the generation of nitrogen oxides (NOx). The temperature distribution exhibits a more prominent and wider high-temperature area in the vicinity of the combustion zone, in contrast to the scenario without NOx. The maximum temperature remains elevated, but its influence does not extend as far downstream compared to the thermal NOx scenario. Thermal NOx and prompt NOx have differing effects on high-temperature

areas. Thermal NOx leads to a broader area of high temperature, while prompt NOx creates a more focused zone of high temperature close to the flame front. The presence of NOx influences the temperature gradients. Thermal NOx has a tendency to sustain higher temperatures over a greater distance, whereas quick NOx has a more significant impact on the immediate combustion zone. These temperature profiles aid in comprehending the combustion dynamics and the influence of various NOx types on the temperature distribution within the combustion system. This knowledge is essential for the development of combustion systems that aim to reduce NOx emissions and maximize efficiency.

CO Mass Fraction

CO generation during the spray combustion of pentane (C_5H_{12}) is a major problem due to its toxicity and role as a precursor to other dangerous chemicals. Understanding the mechanics of carbon monoxide (CO) production and the various factors that affect it is essential for improving combustion processes and reducing emissions. Pentane Combustion Chemistry (C_5H_{12}) Pentane combustion is the process by which fuel droplets vaporize, blend with air, and oxidize. Due to the heterogeneous fuel-air mixture, spray combustion may not achieve full oxidation, resulting in CO-producing incomplete combustion. Hydrocarbon content and complexity may increase the number of intermediate molecules, such as carbon monoxide. Increasing volatility not only increases vaporization, but also concentrates CO creation. Incomplete combustion increases carbon monoxide production under ideal combustion circumstances. Lower combustion temperatures may hinder the conversion of CO to CO_2 . By improving vaporization and mixing, smaller droplets may reduce carbon monoxide production by permitting more complete burning.

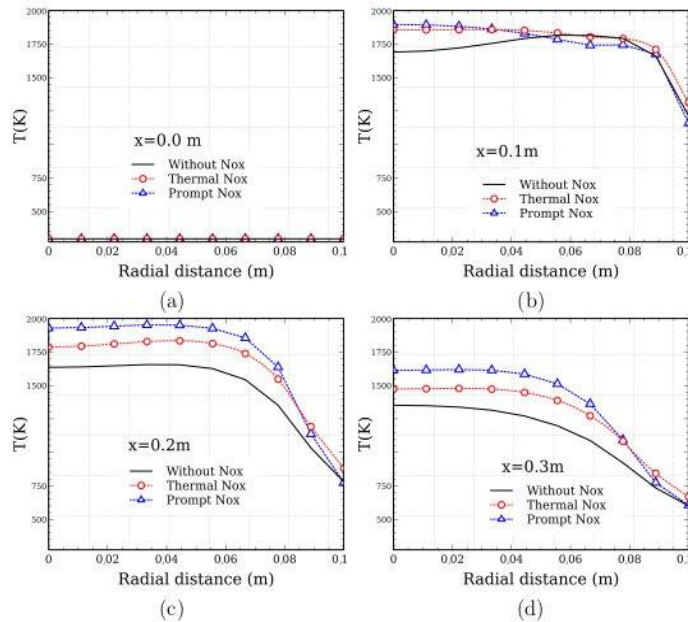


Figure 4: Radial Profiles of Flame Temperature Without NOx, Thermal NOx and Prompt NOx at (a) $x = 0.0$ m, (b) $x = 0.1$ m, (c) $x = 0.2$ m and (d) $x = 0.3$ m.

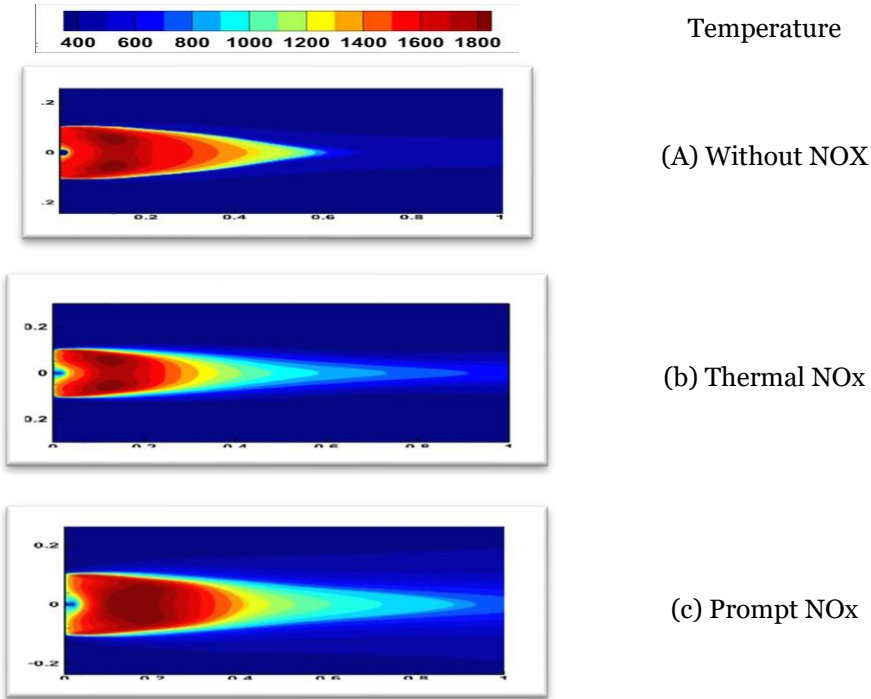


Figure 5: Temperature Contour Plots for Thermal(A) Prompt(B) and Before(C) Along the Axis of Symmetry.

Figure 6 displays contour plots of the CO mass fraction for three different scenarios: absence of NO_x, thermal NO_x, and prompt NO_x. In Figure a, the plot represents the CO mass fraction when NO_x formation is absent. Near the flame front, observing the highest concentration of CO, which decreases as we move away from it, indicating very low CO levels. Figure b plots the CO mass fraction during the formation of thermal NO_x. Thermal NO_x formation occurs at temperatures above 1800 K as nitrogen and oxygen react in the air. The distribution of CO is slightly different compared to the first plot, with more pronounced high concentration regions that extend further downstream along the axis, indicating the influence of thermal NO_x on CO distribution. In Figure c, the presence of hydrocarbons in the combustion process influences the occurrence of prompt NO_x at lower temperatures. Similar to the thermal NO_x case, high concentrations of CO are observed. Figure 7 shows the mass fraction along the axis of symmetry, revealing NO_x production differences between the thermal and fast models before and after. For $x = 0.0$ m, the carbon monoxide (CO) mass fraction increases rapidly to 0.1 at $y = 0.014$. After that, all three models grow slightly until they reach their maximum CO mass fraction of 0.124 at $y = 0.09$ m. On the x axis, the radial lines are at $x = 0.0, 0.1, 0.2$, and 0.3 m. These placements connect research variables to flame locations. The highest difference occurs at $y = 0.07$ m and $x = 0.1$ m, when prompt, thermal, and NO_x conditions produce mass fractions of 0.122, 0.08, and 0.065, respectively. At $x = 0.2$ and 0.3 m, the carbon mass percentage drops until it hits zero at $x = 0.3$ and $y = 0.1$. In the case of NO_x findings, the CO mass fraction discrepancy between the numerical simulation for prompt NO_x and thermal NO_x is 0.04%.

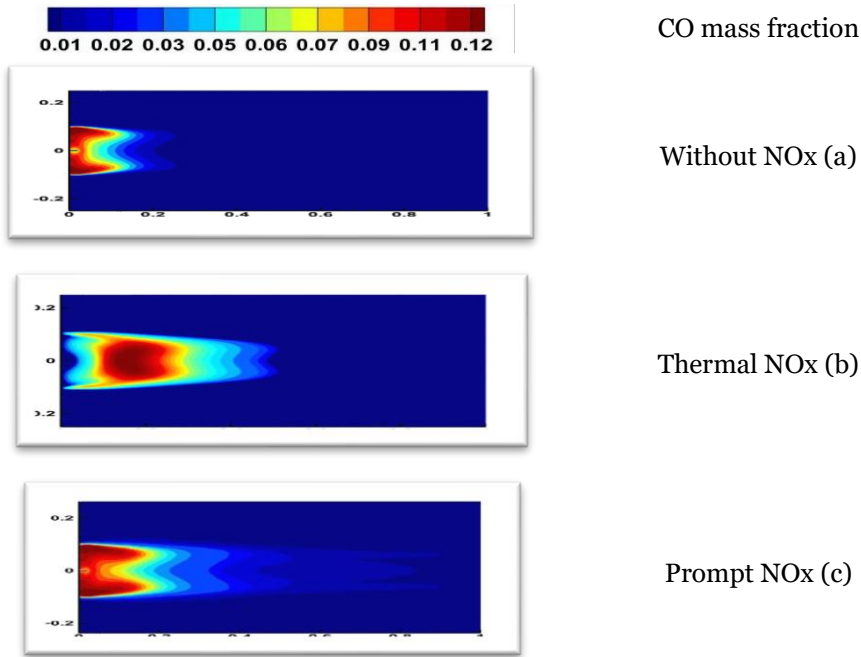


Figure 6: Shows CO Mass Fraction Contour Plots for Thermal(A) Prompt(B) and Before(C) Along the Axis of Symmetry.

OH Mass Fraction

hydrocarbons like pentane requires the hydroxyl (OH). It is an important intermediate species in the oxidation process, affecting fuel breakdown as well as the production of CO and NOx. To improve efficiency and reduce emissions, it is critical to understand the production and behaviour of OH in spray combustion. Pentane Combustion Chemistry (C₅H₁₂) Pentane combustion produces OH radicals via high-temperature reactions involving fuel molecules and intermediates. Several conditions, including high temperatures, accelerate fuel breakdown and chain branching reactions, producing OH. Equivalence ratio is the stoichiometric condition that maximizes OH production by balancing fuel and oxygen. Fuel-rich conditions may lower OH concentrations due to oxygen shortages. Spray characteristics Measure the droplet size Reduced droplet size promotes vaporization and mixing, raising temperatures and distributing OH molecules more evenly. Spray angle and velocity alter fuel and air distribution, which impacts local combustion conditions and OH production. Finally, increasing turbulence and mixing improves fuel-air mixing, thereby facilitating the production and dispersion of OH. Figure 8 contour plots show the mass fraction of OH. These graphs align along the axis of symmetry. (Platform A): This graph displays the percentage of OH molecules in the absence of NOx compound formation. The flame front exhibits the highest concentration of OH. Moving away from the flame front results in lower OH concentrations. This is seen in Figure b: Figure b illustrates how the mass proportion of OH varies during the formation of thermal NOx. There are minor changes to the OH distribution compared to the first plot. The thermal NOx affects the OH distribution, indicating that the high-concentration spots move further downstream along the axis. Lower temperatures

influence the production of nitrogen oxides (NOx) from hydrocarbon combustion (Figure c). The NOx-free case, like the thermal NOx case, shows that regions with high OH concentrations are more widely elongated along the axis. In the vicinity of the flame front, rapid NOx creation influences the dispersion. The flame front consistently exhibits the highest OH mass percentages. When heat and rapid NOx generation are present, OH disperses more widely downstream from the flame front, in contrast to situations where NOx is absent. The colour bar at the top of the graph represents the scale for OH mass fraction, ranging from a very low value of 7.54038×10^{-5} to a high value of 0.0005. There are four subplots in the Figure 9 that show the radial profiles of the OH mass fraction in three different situations: NOx is not present, thermal NOx is present, and prompt NOx is present. Four different axial points ($x = 0.0$ m, 0.1 m, 0.2 m, and 0.3 m) display these profiles. Subplot (a) is located at $x = 0.0$ meters. The OH mass fraction is initially negligible under all conditions. At this juncture, the production of OH radicals is minimal, irrespective of the presence of NOx. At $x = 0.1$ m, the value of (b) remains unchanged. The mass fraction of OH exhibits a modest rise in comparison to its initial value. It's easy to see the differences between the conditions because thermal NOx has a higher percentage of OH mass than environments without NOx and prompt NOx. At this distance from the origin, the generation of thermal NOx appears to increase the presence of OH radicals more than quick NOx. At position x, the value of (c) is equal to 0.2 meters. When $x = 0.1$ m, the mass percentage of OH is higher. The largest OH mass fraction occurs in thermal NOx, followed by quick NOx and no NOx. The influence of NOx on OH radical generation becomes more noticeable at this distance, particularly when considering the contribution of thermal NOx. The value of (d) is 0.3 metres at $x = 0.3$ m. The mass fraction of OH remains substantial. Thermal NOx consistently exhibits elevated OH levels in comparison to prompt nitrogen oxides and in the absence of NOx. The observed trend at $x = 0.2$ m remains unchanged, indicating that heat NOx consistently amplifies the presence of OH radicals at longer distances. Overall Patterns at all radial distances, thermal NOx consistently produces the largest OH mass fraction. Nitrogen oxides (NOx) exhibit a greater proportion of OH mass compared to a scenario without NOx, but a lower proportion than in the presence of thermal NOx. The absence of NOx results in the lowest OH mass fraction in all places. The changes in the OH mass fraction suggest that NOx, specifically thermal NOx, has a big effect on how the OH radicals spread out and how strong they are during combustion. The presence of OH radicals can significantly impact combustion efficiency and emissions, as they play a crucial role as intermediates in numerous combustion reactions. In the case of NOx findings, the OH mass fraction discrepancy between the numerical simulation for prompt NOx and thermal NOx is 0.5 %.

Nox Mass Fraction

Figure 10 shows how the prompt and thermal NOx mass fraction changes as the distance between the two points ($x = 0.0$ m and $x = 0.1$ m) increases during the combustion of C_5H_{12} . The x-axis represents the horizontal distance from the center, measured in meters. At $x = 0.0$ m, the mass fraction of NOx remains at zero and then rapidly climbs to 0.1. Subsequently, all three models see a gradual increase in size until they reach their peak mass fraction of 1.5×10^{-5} . Radial lines mark the x-axis at $x = 0.0$, 0.1 , 0.2 , and 0.3 meters. These placements provide a connection between research variables and flame positions. When considering prompt and thermal factors, the maximum discrepancy arises at the coordinates ($x = 0.1$ m, $y = 0.07$ m) when considering the factors of prompt and thermal. As the radial distance increases,

the NOx mass fraction diminishes. The center section contains a substantial amount of NO, indicating that hydrocarbons and radicals produce a significant quantity of NOx. As you move away from the center in a radial direction, you observe a decrease in concentration and a decrease in the speed of reflexes. In the case of NOx findings, the NOx mass fraction discrepancy between the numerical simulation for prompt NOx and thermal NOx is 1 %. Figure 11 contour plot displays the NOx mass fraction, which represents the concentration of NOx at different locations inside the combustion chamber. The combustion chamber's most thermally intense regions often exhibit elevated NOx levels due to the strong correlation between NOx generation and temperature.

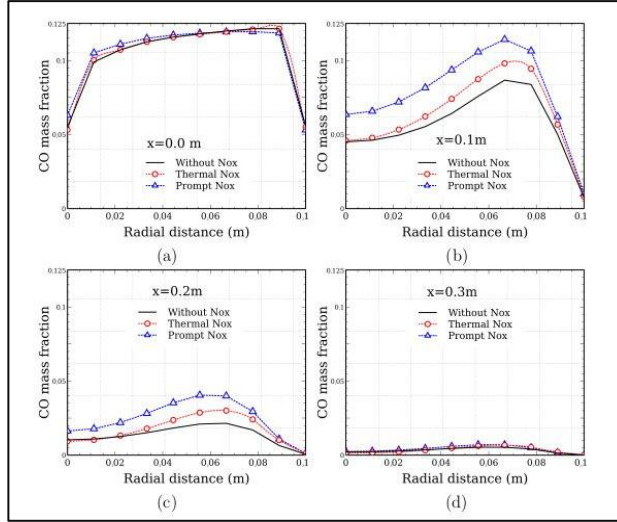


Figure 7: Radial Profiles of CO Mass Fraction Without NOx, Thermal NOx and Prompt NOx at (a) $x = 0.0$ m, (b) $x = 0.1$ m, (c) $x = 0.2$ m and $x = 0.3$ m.

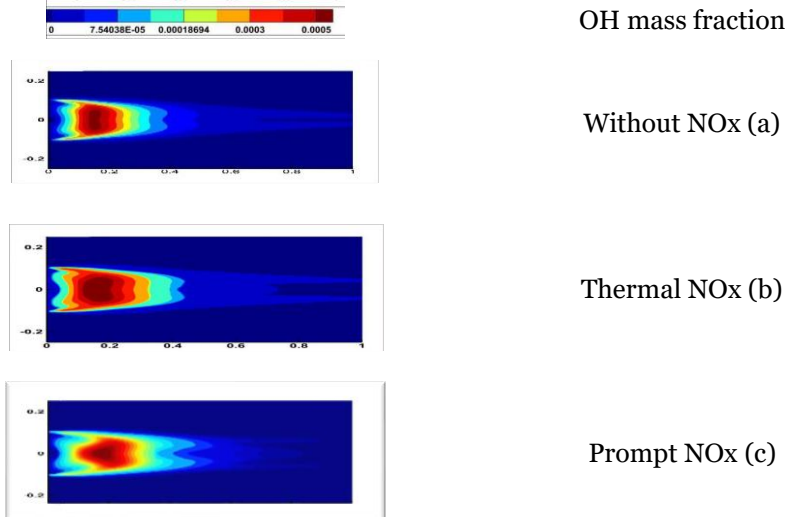


Figure 8: OH, Mass Fraction Contour Plots for Thermal(a) Prompt(b) and Before(c) Along the Axis of Symmetry.

The largest concentrations of NOx occur in regions with the highest temperatures. This is because the reaction rates of the Zeldovich mechanism exhibit exponential growth as the temperature increases. Engineers use mass fraction contours to design combustion systems that aim to minimize NOx emissions. By comprehending the locations where large concentrations of NOx are generated, they may include modifications in the design to reduce these areas of intense pollution. Possible adjustments might include altering burner layouts, optimizing fuel-air ratios, or using new materials that have enhanced resistance to high temperatures while minimizing the production of excessive NOx. Minimizing NOx emissions is crucial for complying with environmental requirements. Nitrogen oxides (NOx) play a role in the creation of smog and acid rain, resulting in notable health and environmental consequences. Enhancing combustion processes is critical for enterprises to meet strict emission limits and effectively manage NOx emissions. Enhancements in Efficiency: Enhancing the combustion process to reduce NOx emissions may also improve combustion efficiency overall. Reducing peak temperatures may decrease the likelihood of generating additional emissions and enhance the longevity of combustion equipment. The contour graph is a useful tool for analyzing the geographic pattern of NOx emissions within a combustion chamber. It identifies areas where NOx accumulates significantly and links these areas to regions with elevated temperatures. By comprehending these distributions.

NO Density

Figure 12 displays NO density contour plots for two distinct scenarios: thermal NOx and prompt NOx. (Figure a): This graphic illustrates the spatial distribution of NO density during thermal NOx formation. As the distance from the flame front increases, the concentration of NO falls, resulting in a change that ultimately indicates extremely low NO levels. The flame's high-temperature areas concentrate the distribution pattern. (Figure b): This graphic illustrates the spatial distribution of NO density in the presence of quick NOx. Similar to thermal NOx, the flame's front displays the highest concentration of NO. Nevertheless, the dispersion is more extensive in comparison to thermal NOx, as the zones with higher density reach further downstream along the axis. Thermal NOx leads to a more focused and confined distribution of NO density around areas with high temperatures. On the contrary, prompt NOx has a broader distribution of NO density, extending to a greater distance downstream from the flame front. The display's top colour bar illustrates the NO density scale, which ranges from very low ($5E-07$) to higher (1). The generation of NOx, whether through thermal or rapid mechanisms, has a substantial impact on the distribution of NO density during the combustion process. Elevated temperatures produce thermal NOx, which forms a concentrated zone with high NO density towards the front of the flame. Hydrocarbon radicals affect the formation of NOx at lower temperatures, which leads to a wider spread of NO density further downstream. The disparities in NOx generation and subsequent distribution mechanics highlight the importance of regulating combustion conditions to efficiently control NOx emissions. thermal NOx indicate Low density when a substance's bulk or concentration is low compared to its volume or area. Throughout The density of NO from thermal NOx is consistently lower than that from prompt NOx, staying close to 10^{-5} across the radial range. NO density decreases steadily with radial distance. We evaluate the nitrogen oxide (NO) concentration quantitatively at a distance of 0.1 meters from the reference point. For Figure 13. There are two clear axial points on the graphs ($x = 0.0$ m and $x = 0.1$

m) that show the density profiles of NO for quick NOx and thermal NOx as a function of radial distance. The vertical axis depicts the density of nitrogen oxide (NO). The x-axis displays the radial distance from the central axis in metres, with $x = 0.0$ m representing prompt NOx. At the center axis (where the radial distance is equal to zero), the density of NO is relatively high, around 4.5×10^{-4} . As the distance from the center increases, it decreases. The concentration of NO declines gradually with increasing radial distance, reaching a stable level of around 4×10^{-4} up to a distance of about 0.07 m. Beyond this point, there is a significant decrease in NO concentration towards the edge at 0.1 m. The elevated NO density in close proximity to the center signifies substantial immediate NOx production as a result of heightened local levels of hydrocarbons and radicals. The drop indicates a dilution and decreasing rate of reaction as one moves towards the outside edges. The density of NO resulting from thermal NOx is constantly lower than that of quick NOx, maintaining a value close to 10^{-5} throughout the whole radial range. Minor reduction: NO density exhibits a gradual and consistent decline with increasing radial distance. Thermal NOx formation is less significant at this location, possibly because the total temperatures are lower near the injection point, where rapid NOx formation is more common. The density at $x = 0.1$ m exhibits a modest decrease relative to $x = 0.0$ m, commencing at around 4×10^{-4} . The density of NO falls gradually as the distance from the center increases, in a more consistent manner compared to the previous figure. Beyond 0.07 m, there is a significant decline in density. The level of NOx emissions remains substantial, but there is a more consistent decrease, indicating a more uniformly distributed combustion process as the fuel spray spreads out and combines with air.

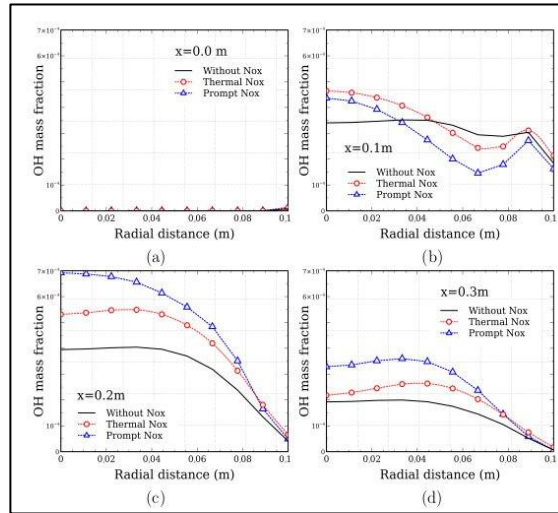


Figure 9: Radial profiles of OH mass fraction without NOx, Thermal NOx and prompt NOx at (a) $x = 0.0$ m, (b) $x = 0.1$ m, (c) $x = 0.2$ m and (d) $x = 0.3$ m.

The density of NO generated by thermal NOx remains extremely low, approximately 10^{-5} , which is comparable to the profile at $x = 0.0$ m. Marginally more reliable, at this axial distance, there is a negligible decrease, suggesting that thermal NOx generation remains minimal and consistent. The low concentration of thermal NOx indicates that temperatures have not reached the necessary levels for substantial thermal NOx generation, even at a distance of 0.1 m from the injection point. In

both graphs, the density of prompt NOx is significantly higher than that of thermal NOx. This implies that prompt NOx primarily contributes to NOx production during the initial stages of spray combustion. The distribution of NOx shows a strong correlation with radial distance, with a larger concentration observed near the center that gradually decreases towards the outside regions. In the case of NOx findings, the NO density discrepancy between the numerical simulation for prompt NOx and thermal NOx is 1 %. The term thermal NOx refers to thermal processes' consistent production of nitrogen oxides (NOx). At low densities, thermal NOx stays in both axial directions. This implies that the early stages of combustion fail to meet the necessary conditions for thermal NOx production, such as high temperatures. Consequences Understanding the primary role of rapid NOx generation might inform optimization techniques for fuel injection and combustion chamber design, aiming to minimize NOx emissions. Implementing precise temperature control measures to minimize the development of thermal NOx, particularly in areas where temperatures may increase, is a crucial technique for reducing emissions. In conclusion The NO density profiles provide valuable insights into the spatial dynamics of NOx production during C₅H₁₂ spray combustion.

Rate of NOx

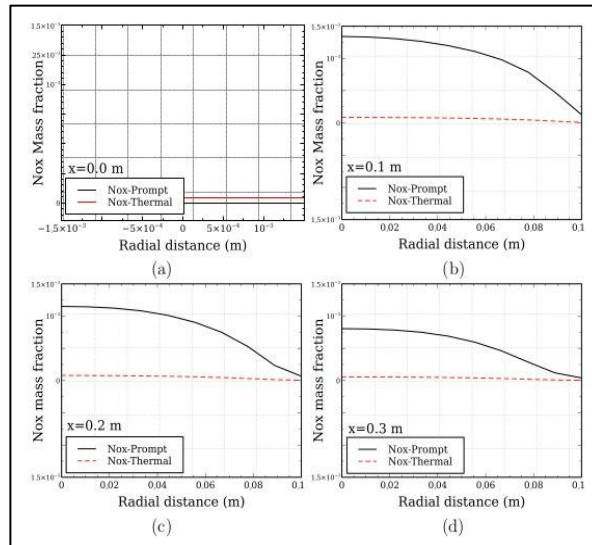
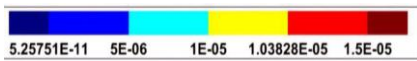


Figure 10: Radial Profiles of NOx Mass Fraction for Thermal NOx and Prompt NOx at (a) $x = 0.0$ m, (b) $x = 0.1$ m, (c) $x = 0.2$ m and $x = 0.3$ m.

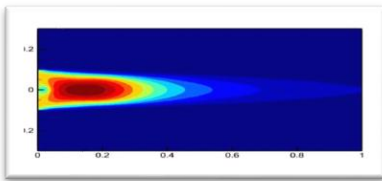
The chemical interactions between nitrogen (N₂) and oxygen (O₂) in the combustion air at elevated temperatures generate thermal NOx. Formations of great importance occur at temperatures over 1800 K. The production rate shows exponential growth. As the temperature rises, the production rate increases exponentially. It usually happens in the area of the flame front and the regions behind the flame when temperatures are at their maximum. There are various methods available to control or manage a situation. For example, exhaust gas recirculation or lean combustion can lower the flame's temperature. Alternatively, staged combustion can be used to create areas with elevated fuel concentrations and

areas with reduced fuel concentrations. The prompt formation of NO_x occurs at the flame front as a result of the interaction between hydrocarbon radicals and nitrogen. Unlike thermal NO_x, it manifests at lower temperatures. Situations with a high fuel concentration frequently observe this phenomenon. This phenomenon is prevalent in the initial stages of combustion, especially when hydrocarbons are present.

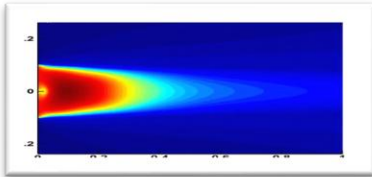
To prevent excessive fuel concentration, the process entails adjusting the air-fuel combination, employing alternative fuels that have a lower tendency to produce NO_x right away. Figure 15 depicts the rates of nitrogen oxide (NO) production, both through prompt and thermal-induced mechanisms, during the combustion of a C₅H₁₂ fuel spray. The production of quick NO_x is significantly higher than that of thermal NO_x over the measured distances, suggesting considerably faster rates of NO creation. About 0.2 metres away, the rate of immediate nitrogen oxide (NO_x) production is at its highest point, with a magnitude of about 1.6 times ten to the power of negative four (1.6×10^{-4}). This suggests that the critical regions for controlling the levels of NO_x are the initial stages of combustion, characterized by a significant presence of hydrocarbon radicals. The rates of thermal NO_x are rather low, with the highest value occurring at approximately 0.1 metres and remaining close to zero for all radial points. In the case of NO_x findings, the NO_x rate discrepancy between the numerical simulation for prompt NO_x and thermal NO_x is 1 %.



NO_x mass fraction



Thermal NO_x mass fraction(a)



Prompt NO_x mass fraction (b)

Figure 11: NO_x Mass Fraction Contour Plots for Thermal(a) and Prompt(b) Along the Axis of Symmetry.

Thermal and prompt rate of NO_x formation

Figure 16 demonstrates the contrasting rates of prompt and thermal NO creation. It reveals that prompt NO_x formation is considerably greater than thermal NO_x formation at the measured distances, which suggests significantly elevated levels of NO production. The maximum rate of immediate NO_x production occurs at a distance of around 0.2 metres, with a value of approximately 1.8×10^{-4} . This implies that the early phases of combustion, characterized by a high concentration of hydrocarbon radicals, are crucial areas for managing NO_x emissions. The formation of localized thermal NO_x is rather low, reaching its maximum at approximately 0.1 meters. This suggests that the early stages of the combustion process do not generally have the widespread presence of high-temperature conditions that are required for large-scale NO_x generation. In this combustion

scenario, the formation of thermal NOx is more concentrated and less severe, indicating its subordinate significance in comparison to prompt NOx. Distance The generation of NOx increases as the distance increases, up to 0.2 metres, and then progressively decreases. This suggests that reactive hydrocarbon radicals are most active around this specific area. The limited and early peak of thermal NOx creation indicates that the spray combustion process does not reach the appropriate temperature parameters for its early production. The implications for combustion strategies should focus on reducing the amount of quick NOx produced by achieving the best air-fuel mixture and controlling combustion so that areas with too much fuel don't form. By manipulating the timing and blending of fuel and air, it is possible to decrease the presence of hydrocarbon radicals, which are responsible for the formation of prompt NOx. While not as crucial in the initial phases, it is beneficial to keep combustion temperatures low in the entire chamber to reduce the generation of thermal NOx. Methods such as exhaust gas recirculation (EGR) and staged combustion are efficient in controlling temperatures and minimizing overall NOx emissions. The plot shows the significant influence of quick NOx generation in the burning of C₅H₁₂ spray and emphasizes the necessity for specific techniques to reduce NOx emissions.

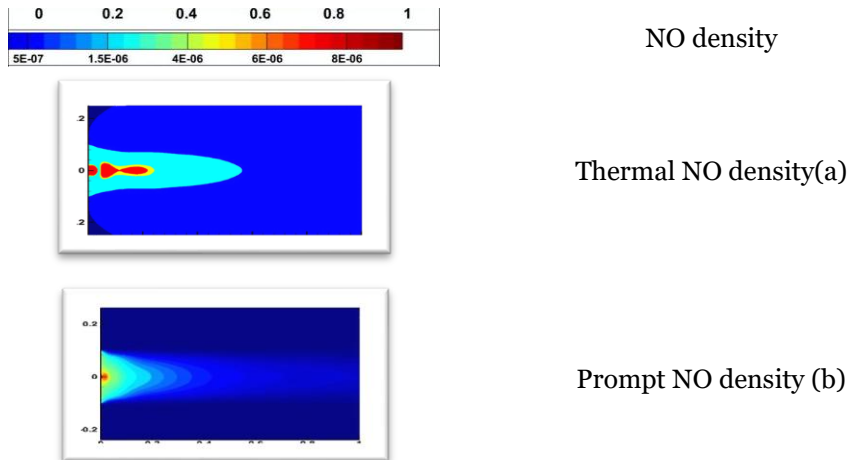


Figure 12: NO Density Contour Plots for Thermal(a) and Prompt NOx (b) Along the Axis of Symmetry.

Prioritizing the initial reactions and effectively controlling temperature can lead to substantial decreases in total NOx emissions, enhancing environmental results and ensuring adherence to emission laws. Figure 17 show contour plots representing NOx generation rates. Figure (a) displays the thermal NOx rate, while Figure (b) displays the prompt NOx. This suggests that the early phases of the combustion process do not have widespread high-temperature conditions that are required for large thermal NOx generation. In this combustion scenario, the formation of thermal NOx is more concentrated and less severe, indicating its subordinate significance in comparison to prompt NOx. The generation of NOx rises as the distance increases, up to 0.2 metres, and then progressively decreases. This suggests that reactive hydrocarbon radicals are most active around this specific area. The early and low peak of thermal NOx creation indicates that lowest rate. The spray combustion process does not reach the appropriate temperature parameters for its

production at an early stage. The storyline emphasizes the significant influence of prompt NOx generation in the combustion of C₅H₁₂ sprays, as well as the need for specific efforts to reduce NOx emissions. By prioritizing the first reactions and effectively controlling temperature, it is possible to obtain substantial decreases in total NOx emissions, leading to better environmental results and adherence to emission laws. Prompt NOx rate a color scale visualizes the thermal NOx rate with red representing the highest rate and blue representing the lowest rate. The graph's lower part concentrates the highest levels of thermal NOx generation, which expand horizontally and gradually diminish as they ascend. This location is most likely to have the greatest temperature since the creation of thermal NOx is highly dependent on temperature. The distribution exhibits a degree of symmetry along the vertical axis, suggesting a consistent state in the combustion process. Figure (b) represents the rate of nitrogen oxide (NOx) emissions. The graph's lower part contains the regions with the highest rates of immediate NOx generation, which are more densely clustered than the rate of NOx formation due to thermal processes. The middle red zone is where the most intense immediate NOx production occurs. Hydrocarbon radicals and nitrogen, commonly present in combustion areas with high fuel-to-air ratios, influence NOx generation. The distribution has a denser and tapered structure, suggesting certain areas where the rapid synthesis of NOx is very active, possibly correlating to places with an excess of fuel. The rates of both thermal and prompt NOx reach their highest levels towards the lower section of the plots, indicating that the formation processes are most active in this area, maybe when the flame is at its highest temperature and/or the fuel concentration is high the distribution of NOx is highly localized, indicating specific locations where the required conditions for its generation exist. High temperatures produce the nitrogen oxides (NOx. known as thermal NOx.

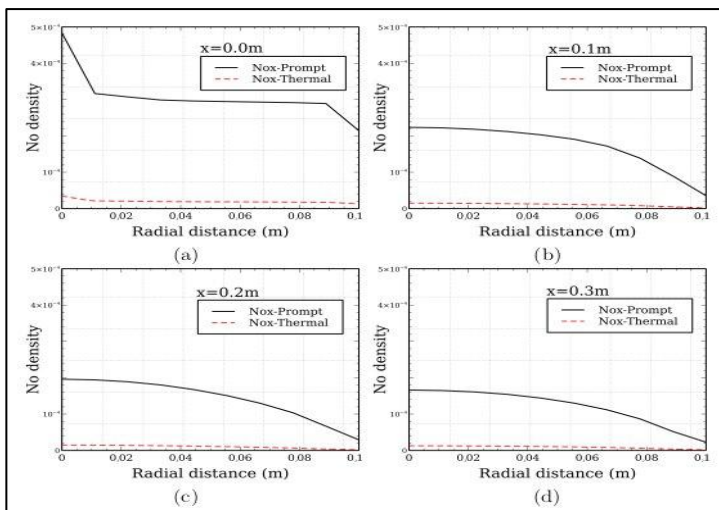


Figure 13: Radial Profiles of NO Density for Thermal NOx and Prompt NOx at (a) $x = 0.0$ m, (b) $x = 0.1$ m, (c) $x = 0.2$ m and (d) $x = 0.3$ m.

This substance's formation is highly temperature-dependent, occurring at a much greater rate in hot places. Nitrogen oxides (NOx) form in fuel-rich zones even at lower temperatures compared to thermal NOx; the formation of hydrocarbon radicals and nitrogen is a key factor. Overall, the thermal NOx rate has a greater

distribution, indicating its reliance on elevated temperatures across a larger area. The prompt NOx rate exhibits a higher concentration, indicating its formation in specific areas with a high fuel-to-air ratio. Both figures provide valuable information on NOx generation's geographical attributes throughout the combustion process

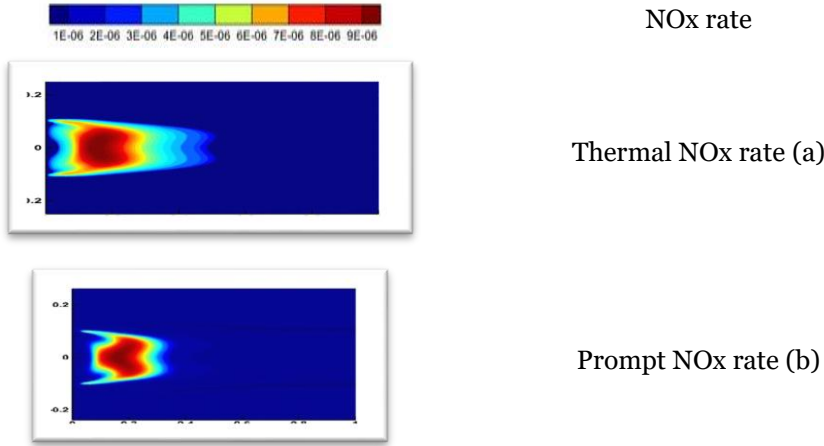


Figure 14: Contour Plots of NOx Rate in ((a)Thermal and (b) Prompt Model).

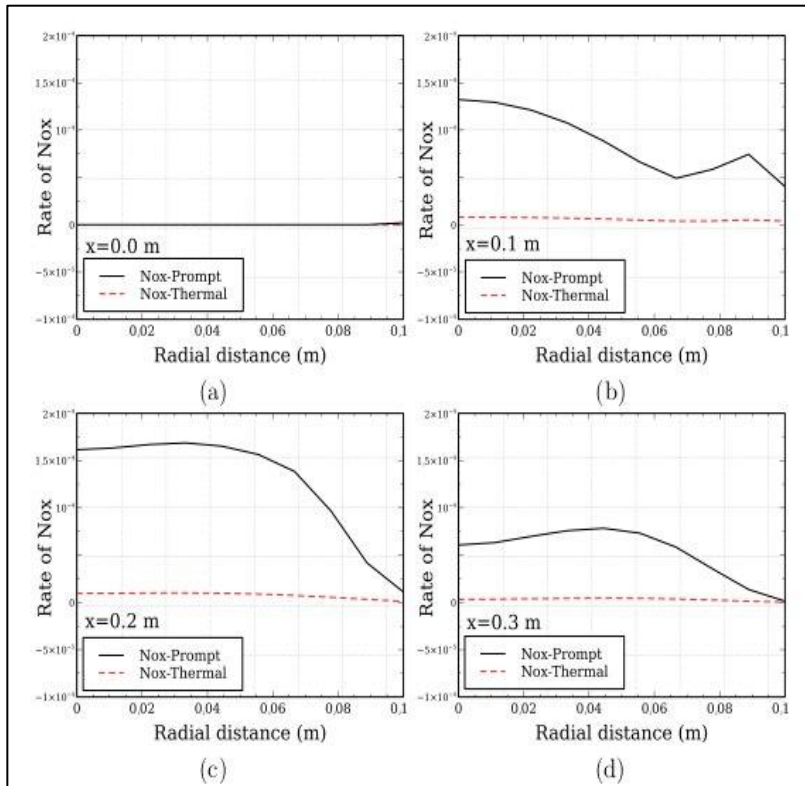


Figure 15: Radial Profiles of NOx Rate for Thermal NOx and Prompt NOx at (a) $x = 0.0$ m, (b) $x = 0.1$ m, (c) $x = 0.2$ m and $x = 0.3$ m.

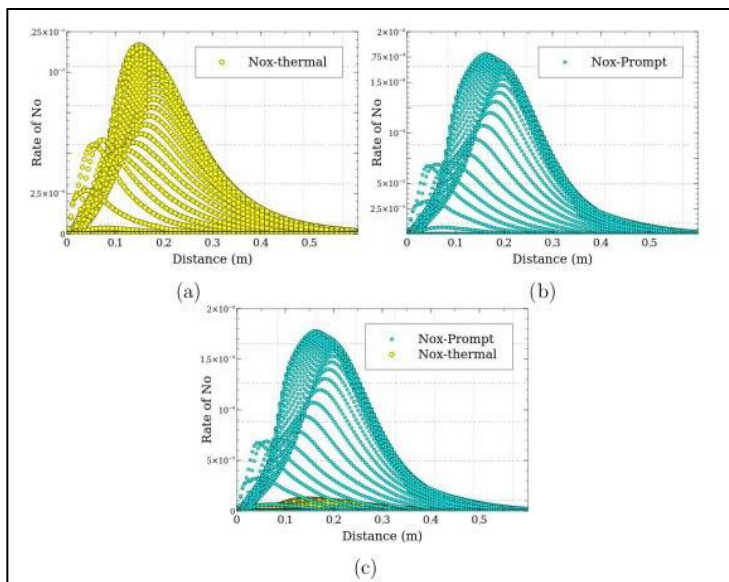


Figure 16: the NOx Rate for ((a) Thermal, (b) Prompt and (c) Thermal-Prompt)) NOx Formation Along the Axis of Symmetry.

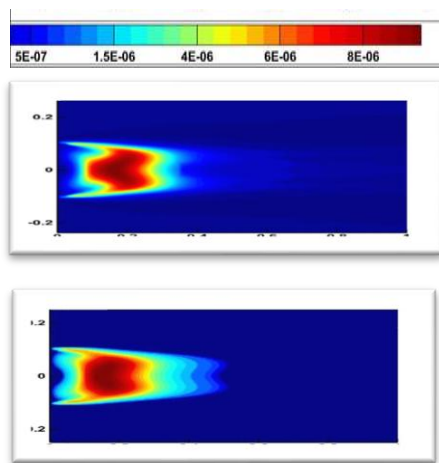


Figure 17. Contour Plots of ((a)Thermal NOx Rate and (b) prompt NOx Rate).

CONCLUSION

This study provides a comprehensive numerical analysis of the steps leading to the release of nitrogen oxides (NOx) during the spray combustion of C_5H_{12} . It specifically emphasizes the different effects of thermal and prompt NOx processes. The results underscore that:

- High temperatures, through the Zeldovich mechanism, primarily cause thermal NOx, which is significantly lower than prompt NOx under all investigated circumstances. This decrease is crucial for formulating strategies to comply with rigorous emission standards.

- The research also clarifies the crucial function of OH mass fraction in both the creation and reduction of NOx species. OH, have a dual function in the combustion process, as they impact the decomposition of intermediate hydrocarbons and influence temperature distributions. Understanding the behavior of OH is essential for optimizing combustion conditions in order to minimize NOx emissions.
- There is a 1% difference in NOx mass fractions and rates between the thermal and prompt models, highlighting the thermal model's advantage in terms of emission reduction.

Finally, this study demonstrates the need for accurate temperature regulation and proactive control of chemical processes in the early stages to effectively decrease NOx emissions. These findings improve the overall understanding of NOx production in spray combustion and provide a foundation for future research focused on creating combustion technologies that are both cleaner and more efficient. Further investigation into the dynamics of OH and the implementation of temperature management measures will play a crucial role in developing the field of combustion research and promoting environmental protection.

References

- [1] W. Amjad, M. Imtiaz, I.-G. Lim, *Computational Study of Different Factors in Nox Formation*, Kosco Symposium Journal (2008), 110-114.
- [2] Ansys Fluent, *Ansys Fluent Theory Guide*, Ansys Inc., USA, 2011.
- [3] A. A. Beige, A. Mardani, *An investigation on flame structure and NOx formation in a gas turbine model combustor using large eddy simulation*, Phys. Fluids **35** (2023), 075133.
- [4] L. Bo, W. Yuanhua, X. Hong, *Numerical Study of Air Nozzles on Mild Combustion for Application to Forward Flow Furnace*, China Refining and Petrochemical Industry (English Edition) (2016), 108-122.
- [5] M. D. Bohon, W. L. Roberts, *NOx emissions from high swirl turbulent spray flames with highly oxygenated fuels*, Proceedings of the Combustion Institute **34** (2013), 1705-1712.
- [6] B. T. Bojko, P. E. DesJardin, *On the development and application of a droplet flamelet-generated manifold for use in two-phase turbulent combustion simulations*, Combustion and Flame **183** (2017), 50-65.
- [7] D. Cerinski, M. Vujanović, Z. Petranović, J. Baleta, N. Samec, M. Hriberšek, *Numerical analysis of fuel injection configuration on nitrogen oxides formation in a jet engine combustion chamber*, Energy Conversion and Management **220** (2020), 112862.
- [8] S. P. Cooper, C. R. Mulvihill, O. Mathieu, E. L. Petersen, M. W. Crofton, K. Y. Lam, *CH Kinetics Measurements and Their Importance for Modeling Prompt NOx Formation in Gas Turbines*, Journal of Engineering for Gas Turbines and Power **142** (2020), 041007.
- [9] A. T. Doppalapudi, A. K. Azad, *Advanced Numerical Analysis of In-Cylinder Combustion and NOx Formation Using Different Chamber Geometries*, Fire **7** (2024), 35.
- [10] C. P. Fenimore, *Formation of nitric oxide in premixed hydrocarbon flames*, Symposium (International) on Combustion **13** (1971), 373-380.
- [11] B. Golchert, P. Ridenour, W. Walker, N. K. Selvarasu, M. Gu, C. Q. Zhou, *Effect of Nitrogen and Oxygen Concentration on NOx Emissions in an Aluminum*

- Furnace, in: ASME 2006 International Mechanical Engineering Congress and Exposition, Energy Conversion and Resources, 2006, 323-333.
- [12] E. Hampartsoumian, W. Nimmo, M. M. Pourkashanian, A. Williams, M. Missaghi, *The Prediction of NO_x Emissions from Spray Combustion*, in: Combustion Technologies for a Clean Environment, CRC Press, 2022, 237-256.
 - [13] M. Ilbas, O. Kumuk, B. Alabas, *Experimental investigation of the combustion instability behaviors and NO_x emissions in an ammonia/methane fueled low eddy premixed burner*, Journal of the Energy Institute **108** (2023), 101241.
 - [14] T. Kaneko, T. Fujii, Y. Matsuda, T. Chikahisa, *NO_x Reduction in Diesel Combustion by Enhanced Mixing of Spray Tip Region*, JSME International Journal Series B Fluids and Thermal Engineering **48** (2005), 665-670.
 - [15] R. A. Keller, *Studies of parametric emissions monitoring and DLN combustion NO_x formation*, Doctoral dissertation, Kansas State University, 2011.
 - [16] Y. Khazraii, K. Daneshvar, H. PoorkhademNamin, *Numerical Simulation on NO_x Emission in Liquid Fuel Spray Flames*, International Journal of Modeling and Optimization **1** (2011), 334-339.
 - [17] L. Lazić, A. Varga, J. Kizek, *An experimental and numerical study of the influence of FGR on NO_x formation*, Materials and Technologies **38** (2004), 269-274.
 - [18] P. Li, J. Mi, B. B. Dally, R. A. Craig, F. Wang, *Premixed Moderate or Intense Low-Oxygen Dilution (MILD) Combustion from a Single Jet Burner in a Laboratory-Scale Furnace*, Energy & Fuels **25** (2011), 2782-2793.
 - [19] G. Löffler, R. Sieber, M. Harasek, H. Hofbauer, R. Hauss, J. Landauf, *NO_x formation in natural gas combustion—a new simplified reaction scheme for CFD calculations*, Fuel **85** (2006), 513-523.
 - [20] Q.-h. Luo, J.-B. Hu, B.-g. Sun, F.-s. Liu, X. Wang, C. Li, L.-z. Bao, *Experimental investigation of combustion characteristics and NO_x emission of a turbocharged hydrogen internal combustion engine*, International Journal of Hydrogen Energy **44** (2019), 5573-5584.
 - [21] C.-P. Mao, G. Szekely Jr, G. Faeth, *Evaluation of a locally homogeneous flow model of spray combustion*, Journal of Energy **4** (1980), 78-87.
 - [22] B. M. Masum, H. H. Masjuki, M. A. Kalam, I. M. Rizwanul Fattah, S. M. Palash, M. J. Abedin, *Effect of ethanol–gasoline blend on NO_x emission in SI engine*, Renewable and Sustainable Energy Reviews **24** (2013), 209-222.
 - [23] M. J. Mohsen, M. F. Al-Dawody, *The combustion characteristics of compression ignition engine fuelled partially by LPG-Diesel blends (Simulation study)*, Al-Qadisiyah Journal for Engineering Sciences **15** (2022), 157-164.
 - [24] S. A. Morsi, A. J. Alexander, *An investigation of particle trajectories in two-phase flow systems*, J. Fluid Mech. **55** (1972), 193-208.
 - [25] S. Nehr, B. Bohn, A. Wahner, *Prompt HO₂ Formation Following the Reaction of OH with Aromatic Compounds under Atmospheric Conditions*, The Journal of Physical Chemistry A **116** (2012), 6015-6026.
 - [26] S. Park, *Pressure effect on NO emission in methane/air lean-premixed flames*, Journal of Mechanical Science and Technology **33** (2019), 3031-3038.
 - [27] D. Perrone, T. Castiglione, P. Morrone, S. Barbarelli, M. Amelio, *NO_x emissions for oxy-mild combustion of pulverized coal in high temperature pre-heated oxygen*, Energy Procedia **148** (2018), 567-574.
 - [28] B. Sahu, D. K. Srivastava, *A Numerical Study on Spray Combustion and Emissions Characteristics of n-Heptane, Dimethyl Ether, and Their Blends in a Constant Volume Combustion Chamber*, Journal of Energy Resources Technology **145** (2023), 062301.

- [29] W. A. Sirignano, *Fuel droplet vaporization and spray combustion theory*, Progress in Energy and Combustion Science **9** (1983), 291-322.
- [30] A. Stagni, A. Frassoldati, M. Pelucchi, T. Faravelli, *Chapter 13 - Chemistry of nitrogen oxides (NOx) formation in flameless combustion*, in: S.E. Hosseini (Ed.) Fundamentals of Low Emission Flameless Combustion and Its Applications, Academic Press, 2022, 421-451.
- [31] A. R. Tajik, T. Shamim, A. F. Ghoniem, R. K. Abu Al-Rub, *CFD Modelling of NOx and Soot Formation in Aluminum Anode Baking Furnace*, in: ASME 2018 International Mechanical Engineering Congress and Exposition, Volume 8A: Heat Transfer and Thermal Engineering, 2018.
- [32] J. Warnatz, U. Maas, R. W. Dibble, *Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation*, Springer Berlin, Heidelberg, 2006.
- [33] M. Xu, Y. Tu, G. Zeng, Q. Wang, A. Zhou, W. Yang, *Numerical study of further NOx emission reduction for coal MILD combustion by combining fuel-rich/lean technology*, International Journal of Energy Research **43** (2019), 8492-8508.
- [34] R. Yang, Y. Yan, Z. Liu, J. Liu, *Formation and evolution of thermal and fuel nitrogen oxides in the turbulent combustion field of ammonia internal combustion engines*, No. 2023-01-0192, SAE Technical Paper, 2023.
- [35] Y. B. Zeldovich, P. Y. Sadvnikov, D. Frank-Kamenetskii, *Oxidation of Nitrogen in Combustion*, Academy of Sciences of the USSR, Institute for Chemical Physics, Moscow-Leningrad (translated by M. Shelef), 1947.
- [36] Y. B. Zeldovich, *The Oxidation of Nitrogen in Combustion and Explosions*, Eur. Phys. J. A, Hadrons Nuclei **21** (1946), 577-628.
- [37] S. Zhong, S. Xu, X.-S. Bai, Z. Peng, F. Zhang, *Large eddy simulation of n-heptane/syngas pilot ignition spray combustion: Ignition process, liftoff evolution and pollutant emissions*, Energy **233** (2021), 121080.