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Research article

Sensitivity of NO_x formation to nitrogen release and char surface area: An estimation approach for CFD modelling of pulverized coal combustionAndreas Johansson^{a,*}, Alexey Sepman^a, Johannes Fernberg^a, Fredrik Normann^b, Henrik Wiinikka^{a,c}^a RISE AB, 94128 Piteå, Sweden^b Division of Energy Technology, Chalmers University of Technology, Göteborg, Sweden^c Division of Energy Engineering, Luleå University of Technology, 97187 Luleå, Sweden

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ABSTRACT

To effectively mitigate NO_x emissions in pulverized coal combustion, Computational Fluid Dynamics (CFD) is frequently employed as a predictive tool. Because fuel-bound nitrogen is the primary source of NO_x in these applications, modelling largely relies on coal characterization—data that are often uncertain even with costly experimental measurements.

This study introduces a systematic framework for estimating missing fuel-nitrogen characteristics from standard proximate and ultimate analyses based on correlations from rapid coal devolatilization experiments. Utilizing a conventional CFD approach, we simulated coal combustion in a 150-kW facility, which mimics rotary kiln conditions. A sensitivity analysis evaluates the impact of uncertainties in volatile nitrogen yields, precursor compositions (HCN/NH₃), and char surface reactivity on NO_x predictions. Results indicate that input uncertainties may account for up to 25% of the total predicted NO_x. The ratio of nitrogen released as volatiles versus char-bound nitrogen and the initial char surface area of the coal particles are both critical parameters, while variations in volatile precursor ratios had a negligible effect (<1%). The model was validated against measured NO_x emissions from the 150-kW facility, demonstrating that while the framework provides a robust estimation tool, high-fidelity characterization of char properties remains vital for precise emission modelling.

1. Introduction

Combustion of nitrogen containing fuels, such as pulverized coal and biomass, generates nitrogen oxides (NO_x) emissions [1]. In the atmosphere, NO_x is an environmental hazard, as it has been shown to deplete ozone layers, generate smog and cause acidic rainfall [2]. Computational Fluid Dynamics (CFD) as a tool has been successfully deployed to evaluate NO_x emissions in combustion processes utilizing pulverized coal and biomass for decades [3]. In coal combustion, NO and NO₂ are mainly produced through conversion of fuel bond nitrogen released during devolatilization and char oxidation [4,5]. The amount of nitrogen released in the volatile matter or bound in the char is specific for each coal [5,6]. The type of nitrogen containing molecules released depends not only on the coal, but also on the conditions in the flame [5,7]. Generally, fuel bound nitrogen from a coal particle releases either as intermittent species in the form of HCN and NH_x compounds (mainly NH₃), or directly as NO and N₂ [8]. The intermittent species HCN and

NH₃ either oxidize further into NO or reduce NO back to N₂ depending on the temperatures and availability of NO/O₂ inside the flame.

The remaining nitrogen in the coal particle after devolatilization is bound in the char. The primary fate of char-bound nitrogen is conversion to NO through oxidation [5]. However, the char also reduces NO_x through char reduction [8,9]. Char reduction is the process where carbon in the char particle reacts with NO to form N₂. In addition to fuel bound nitrogen conversion, so called “thermal NO_x” may form in pulverized coal flames [11,12]. Thermal NO_x involves the splitting of N₂ in the air and the following oxidation to NO in the flame described by the Zeldovich mechanism [13]. The thermal NO_x production is heavily dependent on the flame temperature [14].

Since the composition of nitrogen species released from the coal particle affects the NO produced in a coal flame, NO_x modelling requires prediction of the fuel nitrogen compounds released. X-ray Photoelectron Spectroscopy (XPS) have been used to study the release of nitrogen species during devolatilization and char oxidation [6,15–17]. While XPS

* Corresponding author.

E-mail address: andreas.h.johansson@ri.se (A. Johansson).<https://doi.org/10.1016/j.fuproc.2026.108594>

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provides detailed information on nitrogen functionalities in coal, it does not directly predict the yields of volatile nitrogen species such as NH_3 , HCN , and N_2 . These yields depend on pyrolysis conditions and coal-specific behavior [11,18]. Kambara et al. studied coal nitrogen chemistry and the formation of NO_x precursors during rapid pyrolysis at high heating rates ($\sim 10^4$ K/s) and inert atmospheres for 20 coals [15]. The volatile nitrogen composition is generally composed of approximately 80% HCN , 15% NH_3 and 5% N_2 . The experiments showed that the yield of NH_3 and HCN correlate with quaternary, pyridine and pyrrole type nitrogen species in coal. However, experimental yields also depend on pyrolysis temperature, heating rate, the coal-specific reactivity and secondary reactions [15,18]. The composition of nitrogen released during char oxidation, on the other hand, is more difficult study. Molina et al. reviewed the mechanisms which account for the formation of NO_x from the char-bound nitrogen [11]. They found that during char oxidation, the nitrogen functionalities in chars have a weak correlation with the formation of NO and N_2O from the char-N [11]. This means that even when complicated and costly coal characterization is available, the analysis can often only provide rough estimation of nitrogen yields from the char.

The reducing interactions of NO with char have been extensively studied [8–10,19–21]. According to Jones et al. there are two experimental studies of char NO reduction at coal combustion temperatures [20]. In the first study, Levy et al. described the reaction rate as an Arrhenius rate expression proportional to the partial pressure of NO and to the external area of the char particle with an activation energy determined as 147 kJ/mol [9]. The expression is presented in the NO_x modelling section of this study. In the second study, Song et al. proposed a similar expression with slightly lower activation energy [8]. Aarna and Suuberg also reviewed the available kinetics of the NO/Char reaction [21]. The authors agree that the reaction is generally of the first order in respect to NO but with some catalytic effects of minerals and further complexities when oxidizing gases (CO , H_2O and O_2) are present.

While modelling techniques vary, a consolidated set of numerical frameworks has become standard for simulating contemporary pulverized coal combustion. Most models of larger scale industrial applications involve solving the RANS equations with a lagrangian-euler approach for tracking the reactive coal particles, see examples [22,23]. Volatile and char combustion is treated as a one or two step reaction and the NO formation calculations are also often detached from the combustion calculations, as the N-species reactions have only minor impact on the coal flame. The standard approach in research and development is to split NO formation into fuel NO_x , thermal NO_x and sometimes also prompt NO_x [24]. A few examples of coal combustion studies from this year that utilized these techniques for NO_x analysis include: a cement rotary kiln, 125 MW and 660 MW coal-fired boilers, and a lab-scale study on the effects of particle size [25–28]. In addition to applying the general modelling framework described above, all these examples utilize the same NO pathways discussed previously which also chose to split the volatile N into $\text{N}_2/\text{HCN}/\text{NH}_3$ while assuming all char N oxidize into NO .

Coal combustion is typically used to heat induration grate kilns (GK) in the iron and steel industry for iron ore pelletizing [28]. The kilns in the GK induration machine operate at much higher stoichiometric ratios than typical boilers and other combustion applications. To oxidize iron ore from magnetite to hematite, the kiln operates at an air-to-fuel equivalence ratio (ϕ) of 4–6 with highly preheated air (>1073 K). Due to the high combustion temperature caused by the preheated air and the high air-to-fuel ratio NO_x reduction is challenging. Edland et al. [29] investigated the contribution of volatile- and char bound nitrogen in this process. A 1D model for NO_x formation was developed and used to perform a sensitivity study on the modelling parameters and some other conditions in the kiln. They found that early ignition is important to minimize NO_x formation.

To model NO_x formation in pulverized coal combustion, existing literature generally follows two distinct research lines. The first line

focuses on detailed coal-nitrogen chemical mechanisms, where high-fidelity network models (e.g., CPD, FG-DVC) and spectroscopic techniques (e.g., XPS, NMR) provide deep insights into coal-structure evolution and nitrogen functional groups [30]. However, these approaches require structural parameters rarely available in industrial contexts, forcing users to estimate inputs from literature correlations and thereby shifting rather than eliminating input uncertainty. The second line relies on simplified industrial CFD frameworks, using RANS-based turbulence, global reaction schemes, and decoupled NO_x post-processing to keep computational costs manageable for large-scale systems. Meanwhile, practitioners are forced to supply coal-nitrogen inputs based on arbitrary or unverified assumptions.

Despite extensive work in both domains, an informational gap remains: the extent to which uncertainties in input parameters propagate into final 3D NO_x predictions remains largely unquantified. To bridge this gap within the standard modelling framework used in industrial practice, this work develops a transparent estimation workflow requiring only routinely available proximate and ultimate analyses. Specifically, this study delivers four key contributions:

1. **Framework Development:** Synthesizes empirical correlations into a simple, cohesive CFD input workflow to derive fuel-nitrogen release and char reactivity parameters alongside their uncertainty bounds solely from routine laboratory analyses.
2. **Uncertainty Propagation:** Maps estimated fuel-N input uncertainties into the 3D combustion model to determine overall impact on predicted NO_x emissions.
3. **Experimental Validation:** Benchmarks the predicted emissions against measurements from a 150-kW test facility operating under industrial rotary kiln conditions.
4. **Sensitivity & Hierarchy:** Conducts a systematic sensitivity analysis to establish the relative hierarchy of fuel-N input parameters, identifying which coal-nitrogen properties govern emission predictions within the chosen conditions and CFD framework, and which can be safely simplified.

2. Mathematical modelling

Simulations of the turbulent coal combustion were made with the commercial CFD software ANSYS Fluent. A Reynolds Average Navier-Stokes approach was selected, using the realizable $k-\epsilon$ model [30] to model turbulence. The coal particles were modelled using an Euler-Lagrangian approach with the Discrete Phase Model (DPM) [25, p. 451]. Devolatilization of coal was modelled according to the two-competing-rate model [25, pp. 480]. Volatile gas combustion is modelled with a two-reaction mechanism using the Eddy Dissipation Concept (EDC). The char combustion was both kinetically and diffusion-controlled, where the slowest rate of the two was chosen. Turbulent combustion was modelled with the Eddy Dissipation Concept. An uncoupled version of the Discrete Ordinances Model was used to model the radiation heat transfer [32]. In addition to the modelling procedures described in this section, the default water drying model in Fluent was used for evaporation and boiling of water in the coal particle. Since the pulverized coal has a low water content (0.5%), the drying model was not considered important and hence not further discussed. The NO_x modelling is described in detail below while the detailed description of the rest of the modelling is available in the supplementary material. The supplementary material also includes the relevant modelling constants and the rate constants are presented in Table S1.

Reaction and devolatilization constants are generally set as default coal combustion values in fluent.

The NO_x formation was computed based on the temperature and species concentrations provided by the reactive CFD flow modelling of gaseous and solid phases. This conventional approach does not directly account for N-radical species in the gas phase kinetics, thus reducing the computational cost of the simulation significantly. This is beneficial for

the simulation of real-world systems and engineering applications. The schematical overview of the NO formation pathways in the model is presented in Fig. 1.

This simplification is only valid when NO and intermittent-N concentrations are sufficiently low inside the flame, and their effect on the flame temperature and the gas composition is negligible. Since the expected concentrations of NO and N-radicals was significantly lower than 1% in all areas of the domain, we consider this assumption as valid.

The Zeldovich mechanism (see reactions of the extended mechanism R1-R3) predict the thermal NO_x production.



The nitrogen release in the coal is modelled such that a fraction of the nitrogen is released with volatiles and the remaining nitrogen is released proportionally to the oxidation of char. Volatile nitrogen can be released as NO, or as one of the intermittent species HCN and NH₃. The rate of nitrogen devolatilization is assumed to be proportional to the total volatile mass loss ($dm_N/dt \propto dm_{vol}/dt$) and with a constant partitioning of HCN and NH₃. While it is well-established that nitrogen release can lag general particle mass loss during early devolatilization before accelerating in later stages [32], this simplification introduces minimal error in the present application. Because the grate kiln operates under a highly oxidative environment (~15% O₂ at the outlet) with high-quality coal, devolatilization occurs extremely rapidly within a very compact near-burner zone, minimizing the impact of temporal release delays on downstream NO_x predictions. HCN and NH₃ may then either react with O₂ to form NO or with NO to form N₂, see Fig. 1. The temperature and availability of O₂ and NO in the zone of devolatilization determines if the oxidation of HCN/NH₃ forms NO or N₂. R4-R7 below shows the volatile intermittent species reactions.



The model assume that all char bound nitrogen N_{Char} is converted into NO during the char oxidation reaction (R8).



The model assumes that no nitrogen remains in the ashes and that the nitrogen is uniformly distributed within the char matrix. Then the rate of char nitrogen oxidation becomes proportional to the char burnout times the mass fraction of nitrogen in the char [31]. The char particles may also reduce NO according to the reaction (R9).



Using the expression of char NO reduction for R9 developed by Levy et al. [8] and the burnout rate, then the total contribution of the from coal particle (R8-R9) to the local NO_x formation can be described as (1)

$$R_{NO,particle} = m_{N,char} \cdot R_{burnout} - c \cdot A_{N_2-BET,char} \cdot P_{NO} \cdot \exp\left(-\frac{E}{RT_p} R\right) \quad (1)$$

Where $m_{N,char}$ is the mass fraction of nitrogen in the char, $R_{burnout}$ is the burnout rate in kg/s, c is the particle concentration kg/m³, A_{N_2} is the N₂ surface area of the char particles after devolatilization, P_{NO} is the partial pressure of NO in atm, E is the activation energy, R the gas constant and T_p is the particle temperature.

The net NO formation of gas and particle reactions is determined by reactions R1-R9 according to the relation:

$$\begin{aligned} \frac{d[NO]}{dt} = & k_{f,1}[O][N_2] - k_{r,1}[NO][N] + k_{f,2}[N][O_2] - k_{r,2}[O][NO] + k_{f,3}[N][OH] \\ & - k_{r,3}[NO][H] + k_4[HCN][O_2] - k_5[NO][HCN] + k_6[O_2][NH_3] \\ & - k_7[NO][NH_3] + \frac{R_{NO,particle}}{M_{w,NO}} \end{aligned} \quad (2)$$

where k_f and k_r is the forward reaction rates found in Table 1. and $M_{w,NO}$ is the molecular weight of NO. $R_{NO,particle}$ corresponds to the

Table 1

Reaction rate constants in NO chemistry.

Reaction constant	Forward rate	Backward rate
k_1	$1.8 \cdot 10^8 \cdot e^{-\frac{38379}{T}}$	$3.8 \cdot 10^7 \cdot e^{-\frac{425}{T}}$
k_2	$1.8 \cdot 10^4 \cdot e^{-\frac{4680}{T}}$	$3.81 \cdot 10^3 \cdot e^{-\frac{20820}{T}}$
k_3	$7.1 \cdot 10^7 \cdot e^{-\frac{450}{T}}$	$1.7 \cdot 10^8 \cdot e^{-\frac{24560}{T}}$
k_4	$1.0 \cdot 10^{10} \cdot e^{-\frac{280451}{RT}}$	—
k_5	$3.0 \cdot 10^{12} \cdot e^{-\frac{251151}{RT}}$	—
k_6	$4.0 \cdot 10^6 \cdot e^{-\frac{133800}{RT}}$	—
k_7	$1.8 \cdot 10^8 \cdot e^{-\frac{113000}{RT}}$	—

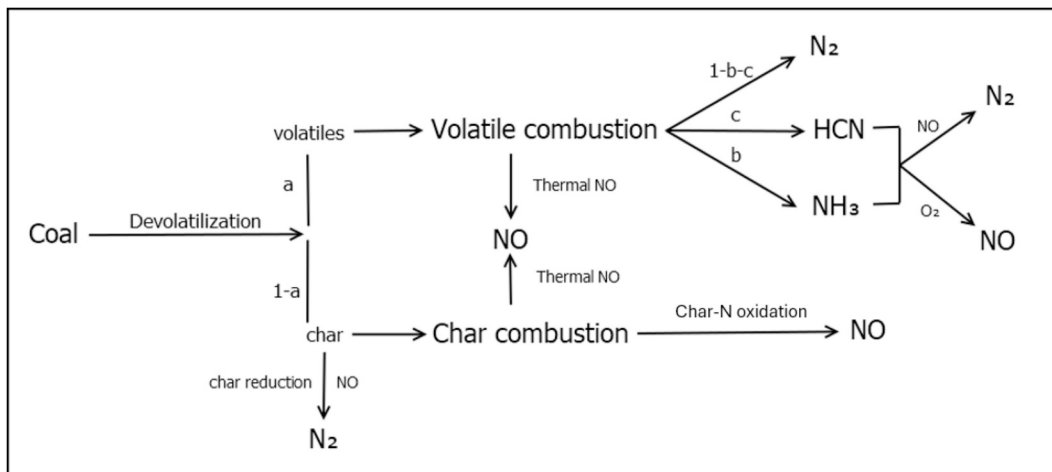


Fig. 1. Schematics of the NO formation modelling of coal combustion.

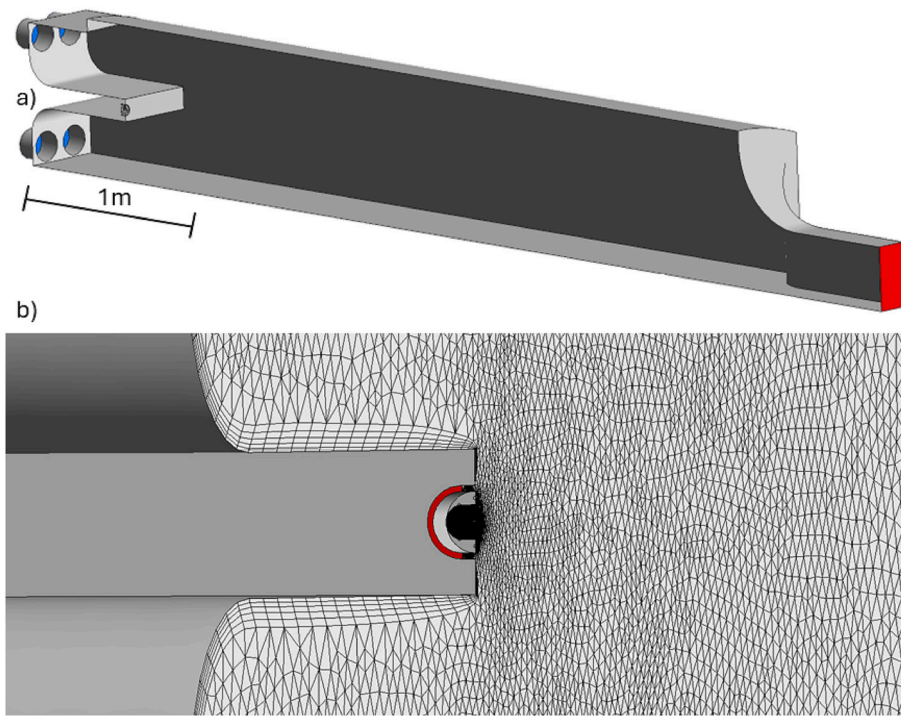


Fig. 2. a) symmetrical plane view of the computational domain. The blue surfaces to the left in the image are the secondary air inlets. The red surface to the right is the outlet of the combustion chamber. b) view of the burner and mesh from the upstream direction. The red circular inlet is the primary air inlet and the black surface in the middle is the coal + transport air inlet.

contribution from the solid-gas reactions R8 and R9. Breaking the strong N_2 requires much larger activation energies than the oxidation reactions of atomic N [31]. In most combustion conditions except extremely fuel rich conditions, there is sufficient oxygen available to react with the available atomic N. The concentration of [N] can be considered quasi-steady state ($\frac{dN}{dt} = 0$). With this assumption, eq. (2) can be rewritten as an expression which is independent of the atomic nitrogen concentration [31]:

$$\frac{\partial[NO]}{\partial t} = 2k_{f,1}[O][N_2] \frac{\left(1 - \frac{k_{r,1}k_{r,2}[NO]^2}{k_{f,1}[N_2]k_{f,2}[O_2]}\right)}{\left(1 + \frac{k_{r,1}[NO]}{k_{f,1}[O_2] + k_{f,3}[OH]}\right)} + k_4[HCN][O_2] - k_5[NO][HCN] + k_6[O_2][NH_3] - k_7[NO][NH_3] + \frac{R_{NO,particle}}{M_{w,NO}} \quad (3)$$

The first term of eq. (3) represents the thermal NO_x formation. The kinetic parameters k_1 - k_6 ($m^3/mol \cdot s$) are presented in Table 1. The O and OH concentrations are estimated using a partial equilibrium assumption, which is an extension of the equilibrium assumption [33]. The underlying assumption is that NO kinetics are much slower than the main combustion reactions and chemical equilibrium concentrations can be used for the O and OH concentrations in the flame. The remaining terms in eq. (3) represents the fuel induced NO_x formation.

The NO species transport equation is given by eq. (4) below:

$$\frac{\partial}{\partial t}(\rho Y_{NO}) + \nabla \cdot (\rho \vec{v} Y_{NO}) = \nabla \cdot (\rho D \nabla Y_{NO}) + S_{NO} \quad (4)$$

where Y_{NO} is the species concentration of NO, ρ is the gas density, D is the effective diffusion coefficient and S_{NO} is the NO source term. Since the intermediate species NH_3 and HCN are solved, transport equations for the intermediates are included as presented in eqs. (5) and (6) respectively

$$\frac{\partial}{\partial t}(\rho Y_{NH_3}) + \nabla \cdot (\rho \vec{v} Y_{NH_3}) = \nabla \cdot (\rho D \nabla Y_{NH_3}) + S_{NH_3} \quad (5)$$

$$\frac{\partial}{\partial t}(\rho Y_{HCN}) + \nabla \cdot (\rho \vec{v} Y_{HCN}) = \nabla \cdot (\rho D \nabla Y_{HCN}) + S_{HCN} \quad (6)$$

Fluent does not natively store or report the NO production rate for individual reactions (R1-R9). Therefore, a custom python code was made to calculate NO production from R1-R9 based on results from the fluent combustion simulation.

3. Kiln conditions

The simulated kiln is a 150-kW facility designed to mimic the combustion conditions inside rotary kilns. Further description of the kiln and experimental work is available in [34].

To limit the computational effort, we take advantage of the symmetry in the domain. The kiln is symmetrical in a vertical, centered plane which allows us to only include one half of the geometry. The kiln is approximately 4.3 m long and is presented in Fig. 2a. The secondary air is injected by 8 fan driven preheaters located behind the burner. The burner is centrally located in the beginning of the kiln which and thereby cut in half by symmetry plane applied in the CFD simulation.

In the experimental setup, the exhaust gases travel through the kiln outlet into a boiler where the gases are cooled before released through the flue gas system. The computational mesh constructed in the domain consists of 1.3 million cells of varying size. A finer mesh is constructed at the burner inlet and in the near burner region where gradients are sharper, and the flow is more complex. A schematic closer look of the nozzle design of the burner is found in Fig. 3. A refined mesh consisting of 5.0 million cells was evaluated to ensure grid independence. The resulting solution was qualitatively identical to the original, with predicted NO_x emissions at the outlet differing by less than 4%. The temperature and major combustion species (O_2 , H_2O and CO_2) differ by less than 1%. The meshes, temperature field and NO field using both the mesh in this study and the refined version can be found in Figs. S1-S6 in the supplementary material. These show insignificant spatial differences in the temperature and NO concentration field between the meshes despite a considerable increase in grid resolution. To reduce the

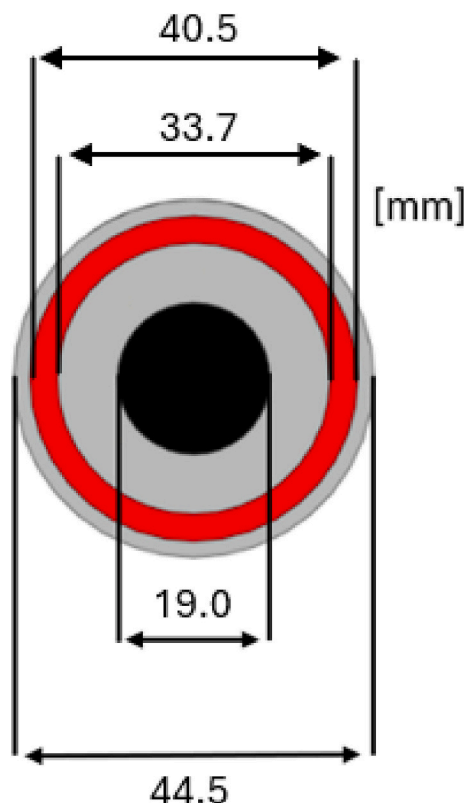


Fig. 3. Illustration of the burner, viewed from inside the kiln. Red areas represent primary air slit and black areas represent the coal injection. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

computational effort, the 1.3 million cell mesh were chosen. The burner consists of a coal injection register and a primary air injection. Coal is transported through a pipe with transport air at an average flow velocity of 16 m/s. A more detailed description of the experimental system modelled is available in the experimental study [34].

The proximate and ultimate analysis as well as the particle size distribution of the coal powder used is presented in Table 2. The table also includes the relative uncertainties and references to the methods involved to acquire the results. Uncertainties in the fuel analysis are not investigated.

The boundary conditions replicate the experimental conditions from coal combustion experiments performed in [34]. These experimental conditions in turn mimic the conditions found inside an industrial GK induration machine for manufacturing iron ore pellets. The kiln is operated at fuel lean conditions ($\lambda \sim 3.5$) as oxygen is required in the process of oxidizing magnetite (Fe_3O_4) to hematite (Fe_2O_3) in the grate. The main operating parameters are listed in Table 3. Note that the mass flows are divided by two compared to the experimental conditions due to symmetry boundary condition in the middle of the furnace.

The inner walls of the furnace are modelled with a mixed thermal boundary condition. This is a shell heat transfer modelling assumption. The wall thickness was 0.275 m with conductivity within the material of 0.047 W/mk. The external heat transfer coefficient on the outer wall due to natural convection was 10 W/m²K, the emissivity constant was assumed to be 0.9 while the room temperature outside the kiln was 20 °C.

4. Sensitivity study

A sensitivity study is made to investigate the impact of uncertainties of Fuel-N properties on the predicted NO_x by the CFD model. The

relevant coal properties required by the NO_x model are summarized below:

- The amount of volatile nitrogen.
- The amount of char bound nitrogen.
- The composition of volatile nitrogen. The amount of HCN, NH₃ and N₂.
- The composition of char bound nitrogen (assumed NO).
- The reactive surface area of the char particles.

Since the proximate and ultimate analysis (Table 2) are known, and all fuel nitrogen is assumed to reside in the volatiles/char (i.e. no nitrogen remaining in the ash), the required coal properties can be rewritten as:

1. $Y_{N,VM} = \frac{\text{Vol-N}_{\text{combustion}} [\%]}{\text{VolProximate} [\%]} = \text{Fraction of N in volatiles at combustion conditions} / \text{VM in proximate analysis.}$

$$R_{HCN/NH_3} = \text{Volatile} \frac{HCN}{NH_3} \text{ Ratio.}$$

2. $X_{N_2} = \text{Volatile N}_2 \text{ molar fraction (\% of } N_{\text{vol}}\text{).}$
3. $A_{\text{Char}} = \text{Char BET surface area [m}^2\text{/g].}$

$Y_{N,VM}$ is introduced as the ratio between the volatile nitrogen yield and the volatile matter in the proximate analysis. By estimating $Y_{N,VM}$ instead of the volatile and char bound nitrogen in coals directly, we remove variations in volatile nitrogen yields due to volatile proximate matter content and total nitrogen content in the coal. High-temperature, fast pyrolysis studies show that volatile yields and by association volatile nitrogen often exceed proximate VM because of rapid devolatilization

Table 2
Coal fuel analysis.

	Unit	Measure	Analysis method
Particle size distribution			
<1 μm	%	2.1	Sieve
<5 μm	%	15.6	Sieve
<10 μm	%	29.2	Sieve
<15 μm	%	39.5	Sieve
<20 μm	%	47.6	Sieve
<45 μm	%	71.7	Sieve
<63 μm	%	81.3	Sieve
<90 μm	%	89.8	Sieve
<125 μm	%	95.2	Sieve
<180 μm	%	98.5	Sieve
<250 μm	%	99.6	Sieve
Proximate analysis (as received)			
Moisture	%	0.5 ± 0.05	ISO 589:2018 mod
Volatile matter	%	19.2 ± 1	ISO 562:2010 mod
Fixed carbon*	%	68.2 ± 5	ISO 562:2010 mod*
Ash	%	12.1 ± 0.6	ISO 1171:2018
Ultimate analysis (as received)			
Cl	%	< 0.01	ASTM D4208–2019 mod
S	%	0.3	ASTM D4239–2018
C	%	77.0	ASTM-D5373:2016
H	%	3.9	ASTM-D5373:2016
N	%	1.33	ASTM-D5373:2016
O*	%	5.3	ASTM D3176–2015*
Calometric analysis (as received)			
LHV	MJ/kg	30.473	ISO 1928:2020

* calculated values, by difference.

Table 3
Operating flows used in the study.

Boundary condition	Unit	Measure
Coal feeding rate	kg/h	7.7
Coal injection velocity	m/s	16.0
Transport air	kg/h	7.2
Primary air	kg/h	14.4
Secondary air	kg/h	236.3
Transport air temperature	°C	100
Primary air temperature	°C	230
Secondary air temperature	°C	850

[35]. This can be demonstrated using experimental data by Kambara et al. [15]. Using data from the coal samples, a linear regression was constructed between the volatile nitrogen yield and the proximate volatile matter. The relationship is presented in Fig. 4.

Calculations for the average, maximum and minimum values are repeated for parameters R_{HCN/NH_3} and X_{N_2} . On average $Y_{N,VM}$ was 1.40, meaning that volatile nitrogen release is approximately 40% higher than predicted by proximate analysis. The average R_{HCN/NH_3} was 6.06 and X_{N_2} was 7.5% on average. Using parameters 1–3 together with the fuel analysis of the present coal, a baseline representation of average nitrogen release behavior in coal combustion was constructed, referred to as Case 0. The underlying experimental data covers a wide range of coal covering from semianthracite to blown coal with a carbon content span from 65 to 88% on a dry, ash free basis.

Determination of the char surface (A_{Char}) after devolatilization also requires advanced in-flame measurements. The estimation of the char surface area (A_{Char}) in this work was based on the model proposed by Williams et al. [5]

$$A_{Char} = 1546.3C^2 + 2834.9C + 1301.7 \quad (7)$$

where A_{Char} is the initial char N_2 BET surface area in m^2/kg and C is the

fixed carbon content of the parent coal. Based on the ultimate analysis for the coal in this study (see Table 2) the surface area was estimated to be $33.8 \text{ m}^2/\text{g}$. In experiments used to develop the relation (7), the deviation between measured surface area and the relation is large for some coals [27]. Out of 19 coals tested, the largest measured deviation from the correlation was found to be in the order of $100 \text{ m}^2/\text{g}$. For all coals, the remaining char particles had a surface area greater than $10 \text{ m}^2/\text{g}$. Without further coal characterization or in-flame measurements, the reasonable range of uncertainty of $10\text{--}100 \text{ m}^2/\text{g}$ was selected.

The parameter sensitivity study is presented in Table 4. The Cases $1 \pm$ investigate the estimated upper and lower limit of $Y_{N,VM}$. In cases $2 \pm$ isolate variation in R_{HCN/NH_3} . Cases $3 \pm$ alters X_{N_2} and Cases $4 \pm$ investigates the effect of A_{Char} on the NO_x emissions. The Min case is constructed by the combination of parameters which individually result in the lowest NO_x emissions. The Max is constructed by the parameter values which individually results in the highest emissions.

Based on Table 4, the workflow to estimate of the inputs required to model NO_x is described as three steps: first, partitioning nitrogen based on a volatile-yield multiplier; second, assigning species based on the Kambara database [15]; and finally, initializing char reactivity via fixed-carbon correlations.

1. Calculate the volatile and char nitrogen yields for the coal,

$$N_{vol,total} = N_{fuel} * VM_{proximate} * Y_{N,VM}$$

$$N_{char,total} = N_{fuel} - N_{vol,total}$$

where N_{fuel} is the total coal nitrogen from the ultimate analysis, $VM_{proximate}$ is the volatile matter from the proximate analysis and the average, $Y_{N,VM} = 1.4$. This assumes there is no nitrogen in the ash.

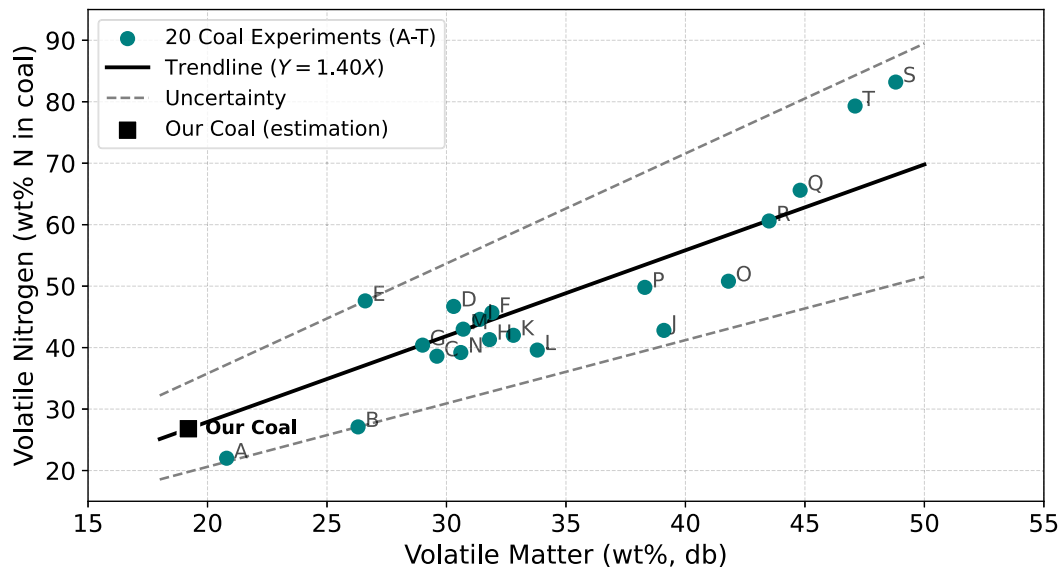


Fig. 4. Volatile yields of nitrogen fraction compared to volatile matter fraction from the proximate analysis. Circles represent data from 20 coal samples (A-T) studied by Kambara et al. The trendline represents a linear regression between volatile nitrogen yield and VM in the proximate analysis. The uncertainty is calculated from samples E and B. The black square is the estimation for our coal with 19.2% VM.

Table 4

Summary of the parameters investigated in the sensitivity analysis within appropriate uncertainty ranges.

Case	0	1+	1-	2+	2-	3+	3-	4+	4-	Min	Max
$Y_{N,VM}$ [–] (1)	1.40	1.79	1.03	1.40	1.40	1.40	1.40	1.40	1.40	1.79	1.03
R_{HCN/NH_3} [–] (2)	6.06	6.06	6.06	8.45	3.60	6.06	6.06	6.06	6.06	3.60	8.45
X_{N_2} [%] (3)	7.5	7.5	7.5	7.5	7.5	10	5	7.5	7.5	5	10
A_{Char} [m ² /g] (4)	33.8	33.8	33.8	33.8	33.8	33.8	33.8	10	100	100	10

Table 5

The parameters varied with their respective baseline values and uncertainty ranges used to predict nitrogen partitioning and char surface area for pulverized coals in combustion conditions.

Parameter	Symbol	Baseline	Uncertainty Range	Source
Volatile-N multiplier	$Y_{N,VM}$	1.4	1.03–1.79	Kambara et al. [15]
HCN/NH ₃ ratio	R_{HCN/NH_3}	6.06	3.60–8.45	Kambara et al. [15]
Volatile N ₂ fraction	X_{N_2}	7.5%	5–10%	Kambara et al. [15]
Char Surface Area	A_{Char}	Eq. (7)	10–100 m ² /g	Williams et al. [24]

- Split the volatile nitrogen into the released species. Char nitrogen was assumed to be released as NO.

$$N_{N_2} = N_{vol,total} * X_{N_2}$$

$$N_{HCN} = N_{vol,total} * (1 - X_{N_2}) * \frac{R_{HCN/NH_3}}{(R_{HCN/NH_3} + 1)}$$

$$N_{NH_3} = N_{vol,total} * (1 - X_{N_2}) - N_{HCN}$$

Where on average, $X_{N_2} = 7.5\%$ and $R_{HCN/NH_3} = 6.06$.

- The initial char surface area for the coal can be found with relation (7) which gives 33.8 m²/g using the fixed carbon content for the coal in this study.

The same approach is repeated using the upper and lower uncertainty estimates of $Y_{N,VM}$, X_{N_2} and A_{Char} . Table 5 summarizes the baseline values and the physical basis for the uncertainty ranges used in this framework. This systematic structure allows the methodology to be applied to other coal types.

5. Results

The temperature field of a vertical, central plane from the CFD combustion simulations of the kiln is presented in Fig. 5. The flame is detached from the burner with ignition at approximately 0.7 m from the burner tip. In the experiments performed, the ignition point of the flame location was slightly fluctuating back and forward in axial direction [37]; however, the time-average observed flame location is found approximated at the location predicted by the CFD simulation. The near burner region is defined by a black line in Fig. 5.

Fig. 6 includes scalar fields of temperature, velocity, major gas species and NO precursors for the near burner region. The concentrations of

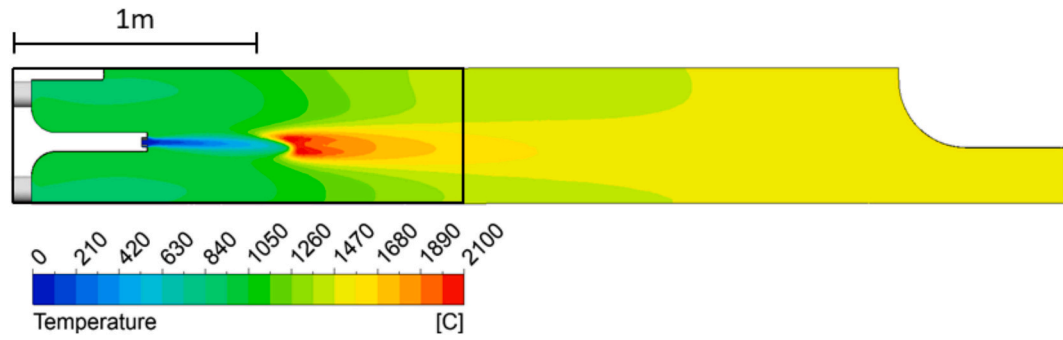


Fig. 5. Contour views of simulated temperatures in a vertical central plane of the kiln. The black line indicates the area defined as near burner presented in Fig. 6.

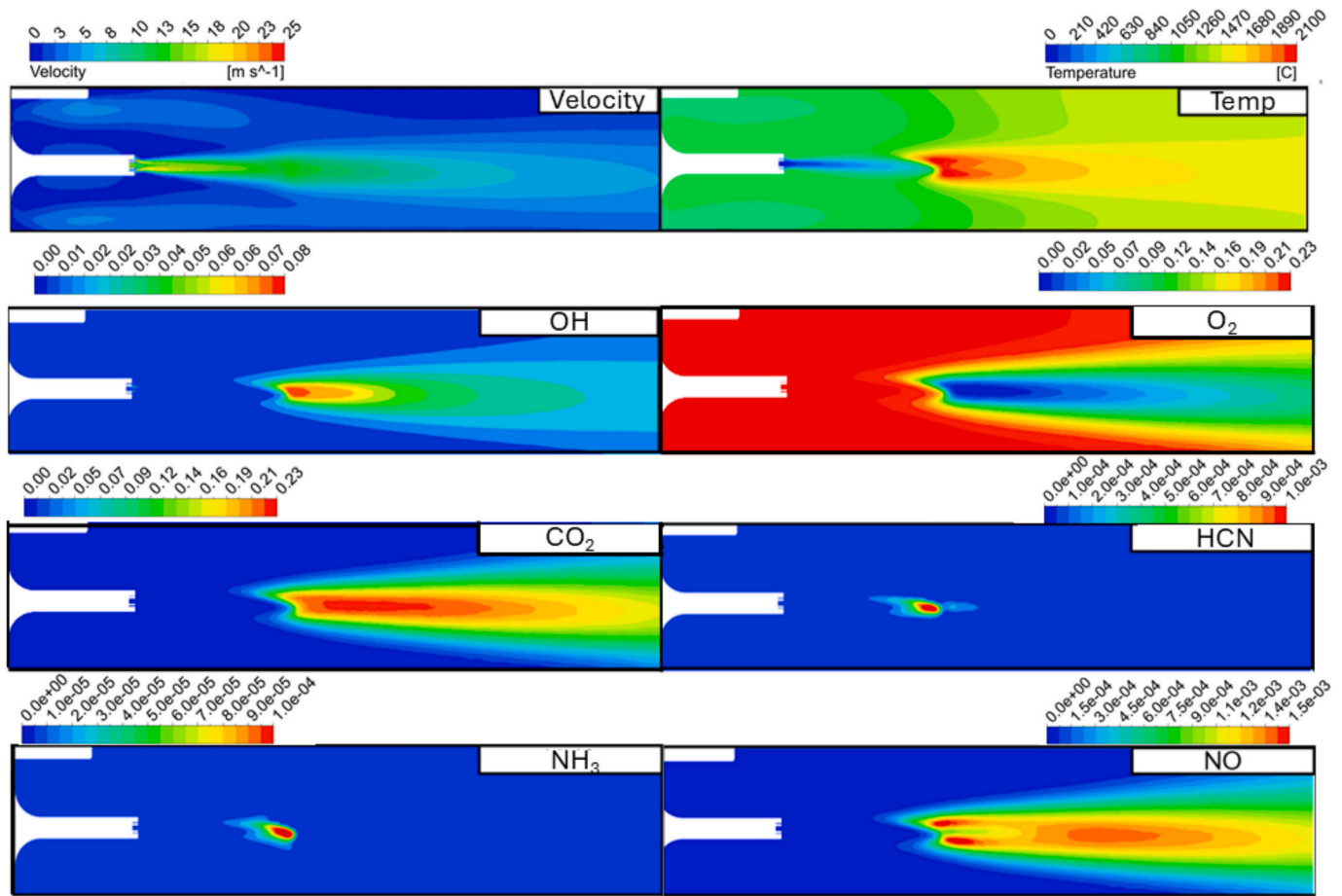


Fig. 6. Scalar fields from the center of the kiln in the near burner region (see caption in Fig. 5). Scalar fields from left to right: Velocity [m/s], Temperature [°C], OH mass fraction [–], NO mass fraction [–], NH₃ mole fraction [–], HCN mass fraction [–], O₂ mass fraction [–] and CO₂ mass fraction [–].

nitrogen compounds in Fig. 6 represent concentrations of case 0. The peak NO concentration is in the outer boundary of the flame. The coal and corresponding transport air generates a jet in the center of the kiln with an inlet velocity of approximately 25 m/s. The HCN and NH₃ released during devolatilization are quickly consumed. The peak HCN concentration is an order of magnitude larger than NH₃ because the volatile HCN/NH₃ ratio (parameter 2) is 6.06. The contours show that all HCN and NH₃ are depleted in the hot flame region.

The particle tracks from the coal burner are presented in Fig. 7a and b. The mass fraction of char in the coal is initially 68% and the mass fraction of volatile matter is 19%. Some small particles in the outer part of the coal jet are devolatilized early (see Fig. 7a), and some larger ones are devolatilized closer to the middle of the kiln.

Fig. 7b shows that most of the char has burned out at the outlet. The remaining unburned char content corresponds to, on average 2% of the weight total remaining in the particles leaving the chamber. The high burnout is at least consistent with indirect experimental observations of low CO concentrations (<200 ppm) and lack of visible char in the downstream boiler indicating near complete char burnout.

The predicted NO_x at the furnace outlet is presented in Fig. 8. As seen from the parameter sensitivity study, increasing $Y_{N,VM}$ (cases 1±) reduces total NO_x produced by 7.9% whilst decreasing the ratio to the lower limit increases the total NO_x by 8.2%. Changing the ratio of HCN/NH₃/N₂ in the volatiles (cases 2± and 3±) within ranges of the sensitivity study has no significant effect <1% on the overall NO_x production in the kiln. The Char N₂ BET surface area (cases 4±) affects the predicted

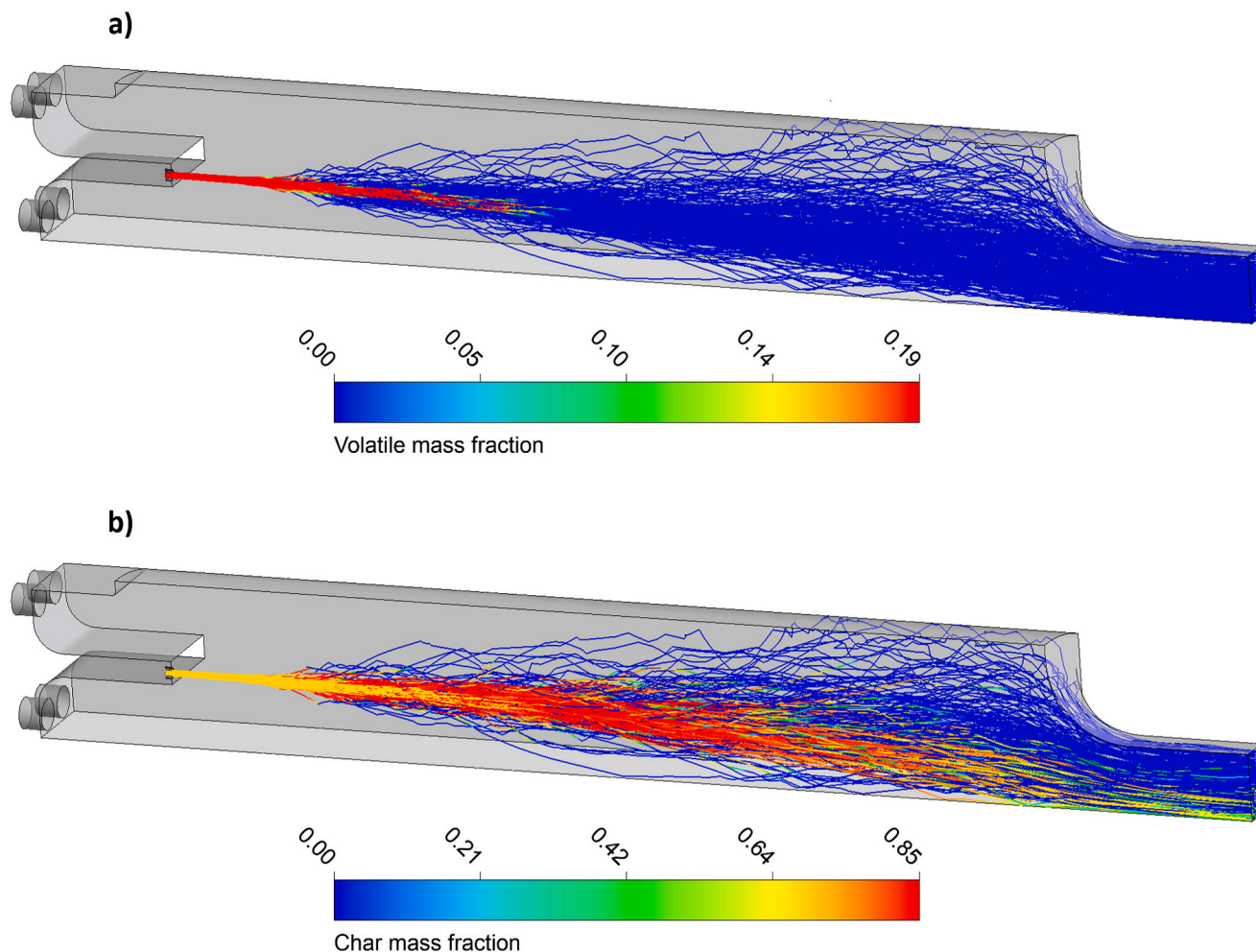


Fig. 7. The path of 300 out of 8000 particles simulated. In a), particles are colored by the volatile mass fraction and in b), particles are colored by the char mass fraction of each particle.

outlet NO_x the most. Decreasing the surface area increases NO_x at the outlet by 10.1% compared to the reference surface area, while the largest area decreases NO_x by 19.7%.

The minimum predicted emissions are attained with the largest $Y_{N,VM}$ in combination with the largest char surface area. The maximum emissions are instead found using the smallest $Y_{N,VM}$ and the smallest char particle surface area. These cases are presented as the Min and Max lines in Fig. 8. In total, an uncertainty of +20% and – 26% of predicted NO_x can be attributed to uncertainties in the input parameters alone. Simultaneously changing several parameters for the min and max lines produces NO emissions changes nearly identical to additively stacking the individual contributions as purely uncorrelated parameters. It can be visually seen in Fig. 8 that the changes from the parameters 1+, 2-, 3- and 4- stacked together roughly produce the min line NO_x value. Similarly, the combined increases from cases 1-, 2+, 3+, 4+ would roughly equal max line NO_x levels. This suggests that there is low correlation between the parameters. The measured values are presented as the green bar in Fig. 8. The average experimental NO_x measurement is within the uncertainty range. Case 4- is closest to the measured emissions while baseline model (Case 0) overpredicts NO_x compared to experimental data by 15%, placing the base case just outside of the standard deviation of the NO_x measurements. It is important to emphasize that we do not necessarily expect case 0 to give the best prediction. In addition, there are also structural model limitations to consider when assessing the deviation to measurements. For example, the use of a simple two-reaction gas phase model in this work lacks endothermic dissociation,

which leads to elevated peak temperatures that inflate the thermal NO_x component of the model [36].

The contribution to the overall NO_x formation from each reaction in the NO_x modelling framework is presented in Fig. 9.

In Fig. 9, reactions R1-R3 represent the NO_x produced through the thermal mechanism. Reactions R4 and R5 are the net contribution of HCN while reactions R6 and R7 are the contribution of NH_3 . For volatile HCN release, the reduction with NO through R5 is greater than the oxidation to NO , resulting in a net reduction in the system. For volatile NH_3 , the oxidation R6 is greater than the reduction through R7. Oxidation of nitrogen in the char in reaction R8 is the largest contribution of NO produced. Since the coal in the study has 68% char, this is unsurprising. For case 0 ($Y_{N,VM} = 1.4$), 73% of the fuel N is released with the char. Fig. 4 shows that on average this value is around 50%, hence for most other coals the contribution of R8 would be smaller. The difference in net contribution from the intermittent volatile species explains the slightly larger NO_x emissions in Case 2+ with elevated NH_3 and slightly lower emissions in case 2- with elevated volatile HCN. The oxidation of nitrogen residing in the char is the dominant source of NO formation (R8). Viewed in combination with the effects of volatile fuel nitrogen, the total Fuel-N contribution to NO formation surpasses the thermal NO formation in the flame. The total amount of N in coal is hence important in coal combustion modelling. Fortunately, the total nitrogen in the coal is easily obtained with relatively good accuracy through traditional fuel analysis. That said, the thermal NO_x still produces a significant share of the NO_x generated by the coal flame and

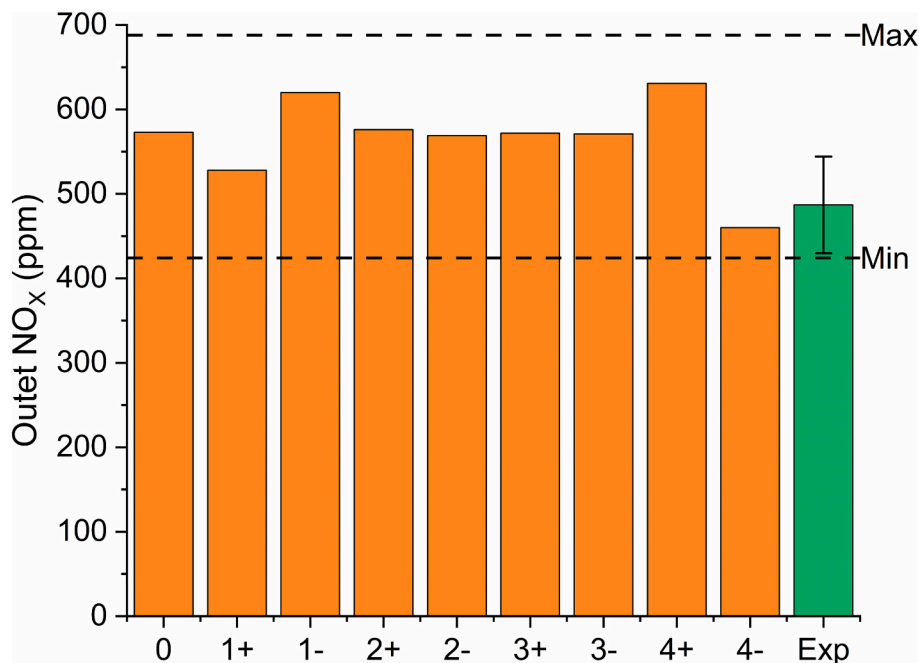


Fig. 8. Predicted outlet NO_x concentration by the simulations for each case of the sensitivity analysis. Min/Max lines indicate NO_x concentrations from the combination of parameters that yields the minimum/maximum predicted NO_x emissions. The Max line is found using parameters 1-, 2+, 3+ and 4+. The Min line is found using parameters 1+, 2-, 3- and 4-. Measured outlet NO_x concentration is given as the green bar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

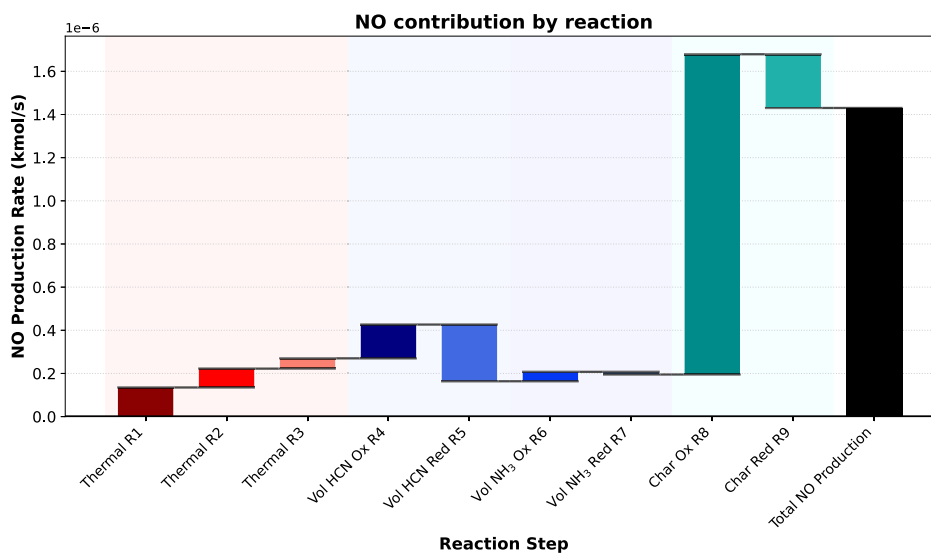


Fig. 9. NO_x production rate of reactions R1-R9 for the base case (case 0). The red colored bars represent thermal NO_x reactions, The purple/blue bars represent production of NO_x due to volatile HCN/NH₃ reactions, while the teal bars are NO_x production associated with coal char. The black bar is the total NO_x produced by case 0. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

should not be neglected. The char NO reduction, reaction R9, is the largest (net) NO reducing reaction. The importance of char reduction is comparable to the thermal NO_x produced by the flame. The direct proportionality of char surface area to NO char reduction reaction rate in combination with a large uncertainty of the char surface area makes the quality of the estimation crucial in NO_x modelling. The rate of production for the other cases in the sensitivity study is provided with the Figs. S7-S14 in the supplementary material.

In Figs. 10 and 11, the mass flow weighed average concentration of NO_x and the intermittent nitrogen in the kiln is presented. The mass flow average over a surface (in this case the combustion chamber cross

section) is the averaged scalar field over a surface normalized by mass flow rate. The concentrations in the base case (case 0) and the upper and lower range of char surface area (cases 4±) are compared in Fig. 10. Since the fuel nitrogen release during devolatilization is the same in the three cases, virtually no differences are found for HCN/NH₃ content. Devolatilization starts around 0.3 m from the burner inlet, where the concentration of HCN, NH₃ and NO_x rapidly increases. Already at 0.5 m from the burner inlet, the devolatilization slows down and the temperature of the flame increases, and the concentration of HCN and NH₃ declines rapidly. The rapid oxidation of HCN and NH₃ into N₂ and NO is exponentially related to the temperature. At this location, NO formation

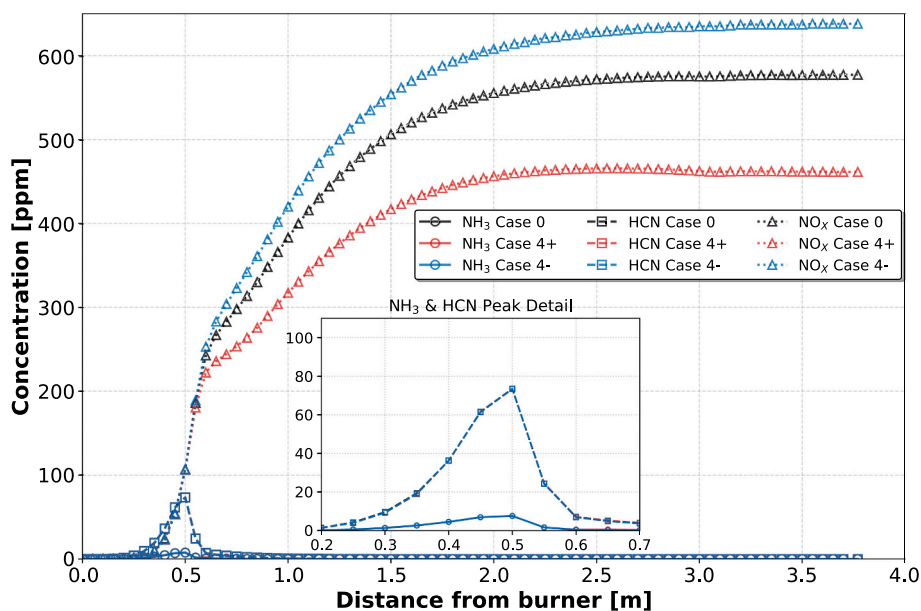


Fig. 10. Mass flow weighted average concentrations of HCN, NH_3 and NO_x in the kiln. Comparison of cases 0, 4+ and 4-. The concentrations are mass flow normalized averages reported at cross-sectional planes at presented locations in the kiln.

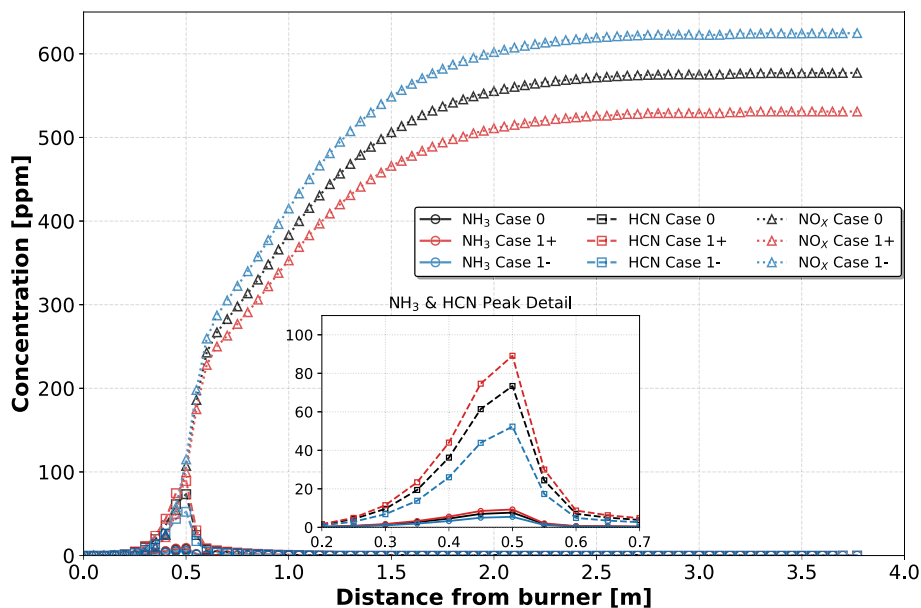


Fig. 11. Mass flow averaged HCN, NH_3 and NO_x concentration in the kiln as a function of the distance from the burner. Comparison of Cases 0, 1+ and 1-. The concentrations are mass flow normalized averages reported at cross-sectional planes at presented locations in the kiln.

increases more than the destruction of HCN and NH_3 . This is likely due to the formation of additional thermal NO_x in the hot flame. Since only a small portion of char leaves the kiln unburned, we expect declining generation of NO_x due to char oxidation.

If we compare cases 0, 4+ and 4- in Fig. 10, the effect of char initial surface on the NO_x concentration starts when char is formed after the devolatilization. Since the volatile nitrogen release is the same for all cases, the HCN/ NH_3 / NO concentrations are essentially the same before devolatilization is complete. The difference in NO_x emissions between 10, 34 and $100 \text{ km}^2/\text{kg}$ is initially small, but cumulatively amount to a large difference at the end of the kiln. For the case 4+ ($100 \text{ m}^2/\text{kg}$), the conditions at around 3 m into the kiln allows char reduction to slightly outpace char-N oxidation and thermal NO_x formation, decreasing the total NO_x concentration at this segment.

The cases with different amounts of volatile and char nitrogen (cases

0, 1+ and 1-) are presented in Fig. 11. Interestingly, the simulation predicts that less nitrogen released as volatiles favors NO_x concentration in the entire length of the kiln, even region of rapid devolatilization. At approximately 0.6 m from the burner, where char combustion starts, the case with the least volatile nitrogen (case 1-) results in the largest NO_x emissions. The net effect of additional NH_3 /HCN/ N_2 released during devolatilization can suppress thermally induced NO_x production in the flame through reduction. The reaction analysis in Fig. 9 additionally suggests this, with a net destruction of NO through reactions with the intermittent species. As expected, this difference is exacerbated during char combustion as more nitrogen is released during char burnout for the low volatile case.

6. Conclusions

The study provides a systematic framework for estimating fuel-nitrogen release and char reactivity from standard coal analyses for CFD modelling of pulverized coal flames. Using a CFD model with the proposed framework, the NO_x emissions of a 150 kW kiln are predicted and compared to measurements. Additionally, the uncertainty of the emissions is examined through a sensitivity analysis, which also investigates the impact of various NO_x formation pathways in coal combustion. The key findings of this study are summarized as follows:

- 1. Framework Usability:** A systematic methodology to estimate fuel-nitrogen yields and initial char physical surface area during pulverized coal combustion was established using standard laboratory analyses. This framework offers a reliable alternative for CFD practitioners when high-fidelity coal characterization is unavailable.
- 2. Uncertainty Propagation:** Propagating realistic fuel-N input uncertainties through the CFD model revealed that volatile-N yield and char surface area variations combine to produce an overall emission prediction band of approximately $\pm 25\%$.
- 3. Experimental Validation:** Baseline CFD predictions overestimated flue gas emissions by approximately 15% compared to pilot-scale measurements. Crucially, this places the experimental data safely within the calculated input uncertainty bounds of the model.
- 4. Sensitivity & Parameter Hierarchy:** Systematic parameter sweeps established a clear hierarchy of fuel-N inputs, confirming that thermal NO_x and fuel-bound nitrogen both contribute significantly under high-temperature kiln conditions, while parameter sensitivity varies widely:
 - Char surface area (A_{char}) dominates: Accounting for heterogeneous char-NO reduction is essential, with char surface area identified as the single largest source of uncertainty in predicted NO_x concentrations.
 - Volatile-N yield ($Y_{\text{N,VM}}$) is secondary: The fraction of nitrogen released with volatiles has a secondary, yet noticeable, impact on total predicted NO_x.
 - Precursor split ($\text{HCN}/\text{NH}_3/\text{N}_2$) is negligible: The ratio of volatile nitrogen precursor species has a negligible effect on final burner NO_x concentrations.

The results indicate that the case with the lowest char surface area within the uncertainty range provides the closest agreement with experimental data. To achieve high-fidelity NO_x predictions in these applications, an accurate description of volatile nitrogen yields, and in-flame char surface area is necessary. Furthermore, the significant impact of char-NO reduction suggests that adopting a more detailed modelling of the intrinsic surface area than the approach by fluent—which does not assume a linear relationship between char surface area and burnout—could improve CFD modelling accuracy for these systems. Studies of coal refired several times have shown that the intrinsic char surface area can stay similar or even increase until substantial char mass has burned out [37]. The simple approach used by Fluent likely underestimates the impact of NO reduction by char. For future work we acknowledge that complementing this study with not only more experimental kiln measurements, but also include the state of the art coal analyses and drop tube experiments necessary to accurately describe the coal for combustion modelling. With all those relevant parameters experimentally obtained for our coal (such as volatile matter composition, volatile nitrogen composition, char reactivity etc.), the estimation framework used in this study can be tested. This would also allow the NO_x emission predictions from the high-fidelity industry approach adopted in this study to be compared with state of the art mechanisms and coal combustion models. Ultimately, this study could

serve as a “Modeler's Roadmap” for predicting emissions in industrial systems with this popular modelling approach where fuel sources are diverse and data is sparse.

Beyond the modelling implications, these findings have significant practical relevance for the operation of industrial kilns. Given that fuel-nitrogen uncertainty can lead to a 25% variance in predicted emissions, relying solely on baseline CFD results for environmental compliance or burner optimization may be misleading. This study demonstrates that for industries using diverse coal sources, a robust sensitivity analysis is essential for interpreting CFD data and ensuring that NO_x reduction strategies are based on realistic emission ranges rather than single-point estimates.

AI tool use

During the documentation of this work into this article, the internet chatbots Gemini and ChatGPT have been used to review the document and suggest changes to language of the article. The authors take full responsibility for the content of the published article.

CRediT authorship contribution statement

Andreas Johansson: Writing – original draft, Methodology. **Alexey Sepman:** Writing – review & editing. **Johannes Fernberg:** Writing – review & editing. **Fredrik Normann:** Writing – review & editing, Funding acquisition. **Henrik Wiinikka:** Writing – review & editing, Supervision, Funding acquisition.

Declaration of competing interest

All the authors declare that no known competing financial interests or personal relationships have influenced the work published in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fuproc.2026.108594>.

Data availability

Data will be made available on request.

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