NHR4CES NHR for Computational Engineering Science

CLAIX / Lichtenberg2 Projects

High Performance Computing at NHR4CES

October 15, 2023 - February 01, 2025

1 Project title

Numerical Study of Biomass Ignition, Combustion, and Pollutant Formation in Laminar Jet Flows

2 Project ID

p0021020

3 DFG classification

404, Heat Energy Technology, Thermal Machines, Fluid Mechanics

4 (List of) Involved people

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5 Project report

5.1 Introduction

Replacing coal with biomass holds great potential to reduce global CO_2 emissions due to its closed carbon cycle. However, controlling harmful NO_x emissions from solid biomass combustion is one of the major challenges, which necessitates complex and costly exhaust gas after-treatment systems. To analyze NO_x formation pathways, it is crucial to accurately model the complex sub-processes and interactions of the solid particles and the gas phase. High-fidelity simulations can generate datasets that are fundamental for analyzing these formation pathways, providing insights that are beyond the reach of experimental techniques.
This project investigated the formation pathways of NO_x from solid pulverized biomass flames. We conducted several direct numerical simulations (DNS) of pulverized solid biomass combustion under different atmospheric conditions to compare the flame behavior and examine the effect on NO_x formation pathways. As atmospheric conditions directly impact the combustion process, an optimized combustion strategy can be developed to minimize NO_x formation from solid pulverized biomass flames.
To address the high computational cost associated with modeling solid biomass flames, we employed an existing simplified modeling approach to study the influence of the released volatile composition on NO_x formation. The predictions of this simplified modeling approach were evaluated against the predictions of detailed DNS. Based on these comparisons, we proposed a modified formulation of the existing model that offers improved accuracy in predicting NO_x formation. This enhanced method can be effectively integrated into reduced-order flamelet modeling frameworks for solid fuel combustion.

5.2 Methods

The thermochemical conversion of solid fuels involves mass, momentum, and energy transfer between the particles and the gas phase. To model these interactions, the Euler-Lagrangian approach is employed, where the solid particles are described in the Lagrangian framework using a point-particle assumption and the gas phase is modeled in the Eulerian framework. The governing equations in the Euler-Lagrangian framework are solved using the in-house semi-implicit finite element solver CIAO.
Second order accuracy in space and time is used to solve the Eulerian equations. The scalar transport is solved using the WENO5 scheme for the convective and a second order central difference scheme for the diffusive terms. Species mass fractions and temperature are solved using Strang splitting for scalar equations. A backward differential formula from the CVODE solver is used to integrate the chemical subsystem. To advance the particles in time, a two stage Runge-Kutta solver with second order accuracy is used to update the dispersed phase state, position, and source terms for the Eulerian equations.

5.3 Results

This section presents the results of the parameter study to analyze the NO_x formation pathways using DNS. Note that additional simulations with different biomass types have also been performed to validate the particle and gas phase model and to analyze the NO_x formation pathways within this project, but are not shown here for brevity. The analysis presented focuses on flames of pulverized Miscanthus biomass under a variety of atmospheric conditions, in order to evaluate the influence of these conditions on NO_x production.

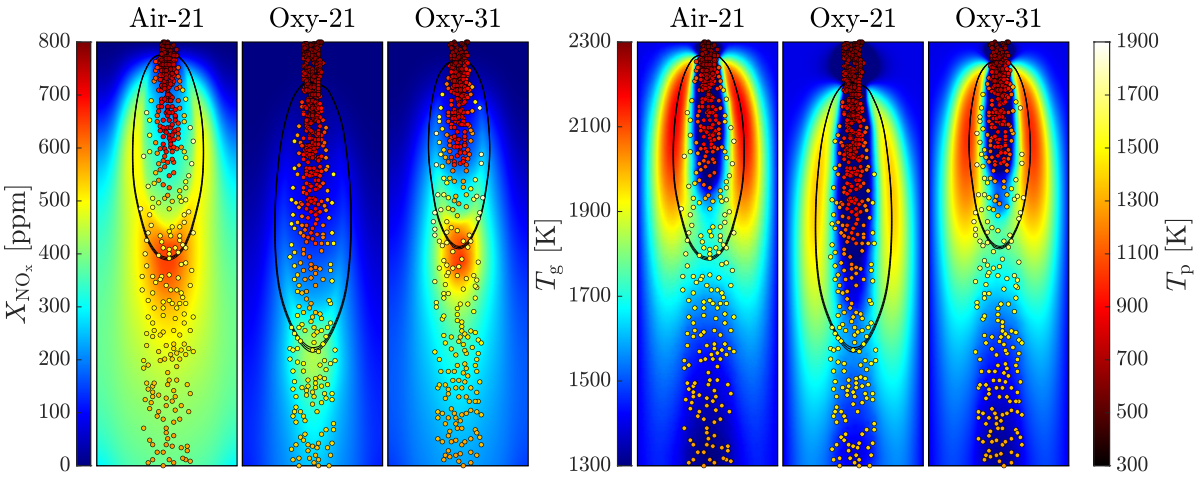

Figure 1: Comparison between NO_x mole fractions (left) and gas temperature (right) in different atmospheres around the statistically steady-state. Particles are colored by the particle temperature. Stoichiometric mixture fractions for each flame are visualized by black isolines.

Figure 1 shows the NO_x mole fractions and gas temperature for three different atmospheres for Miscanthus. It can be seen that the global maximum of NO_x mole fractions occurs at the flame tip in all investigated atmospheres in weaker temperature regions due to a longer residence time, while the local maximum of NO_x occurs around the stoichiometric conditions in high temperature regions. Comparing the flames to each other, it can be seen that the oxidizer conditions have a significant effect on the flame topology and the overall NO_x formation, which is highest in air due to the presence of thermal-NO_x.

Figure 2 presents the correlation between the NO_x mole fraction and the gas phase temperature. As discussed previously, distinct high- and low-temperature zones are visible around the stoichiometric mixture fraction in Fig. 2a. Moreover, the peak NO_x production rate coincides with the maximum consumption rate of NFuel - the total nitrogen-containing volatiles released from the particles - in the high-temperature, fuel-rich region near the particles themselves. This highlights the critical role of fuel-bound nitrogen in the overall formation of NO_x during biomass combustion.

Figure 3 presents an analysis of NO_x formation pathways through a rate of production

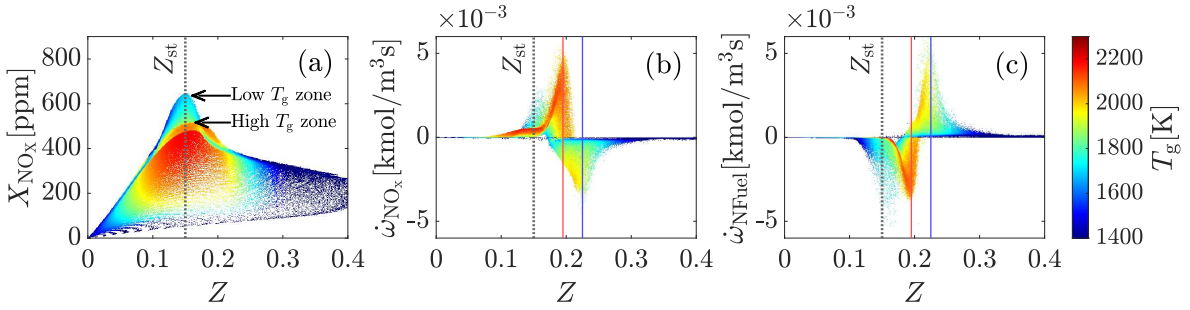

Figure 2: (a) X_{NO_x}, (b) $\dot{\omega}_{NO_x}$, and (c) $\dot{\omega}_{NFuel}$ of the Miscanthus flame in air atmosphere in mixture fraction space, coloured by gas phase temperature. The peak production and consumption rates for NO_x and NFuel are marked with solid red and blue lines, respectively.

analysis (ROPA) of all nitrogen element fluxes, integrated across both the entire numerical domain and simulation time to provide a comprehensive overview. The influence of atmospheric conditions on NO_x formation is evident in the role of N and HNO in NO production. Under oxy-fuel conditions, the contribution of the N radical to NO formation decreases, while the influence of HNO becomes more significant, causing a shift in the dominant formation pathways. Additionally, an increase in oxygen content in the oxidizer composition results in an overall higher production OH radicals, which in turn enhances NO production.

An existing modeling approach assumes a fixed volatile composition (FVC) release with reduced computational cost compared to the detailed dynamic volatile composition (DVC) release model. Figure 4 shows a good agreement for gas-phase temperature prediction, while the NO_x mole fraction field cannot be captured by the FVC model.

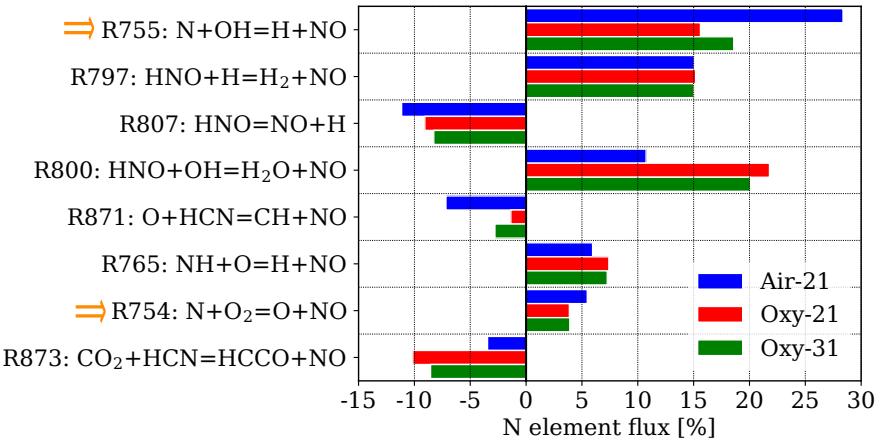

Figure 3: Effect of different atmospheres on the ROPA of NO integrated over the entire computational domain and simulation time. The extended Zeldovich reactions are marked with (⇒).

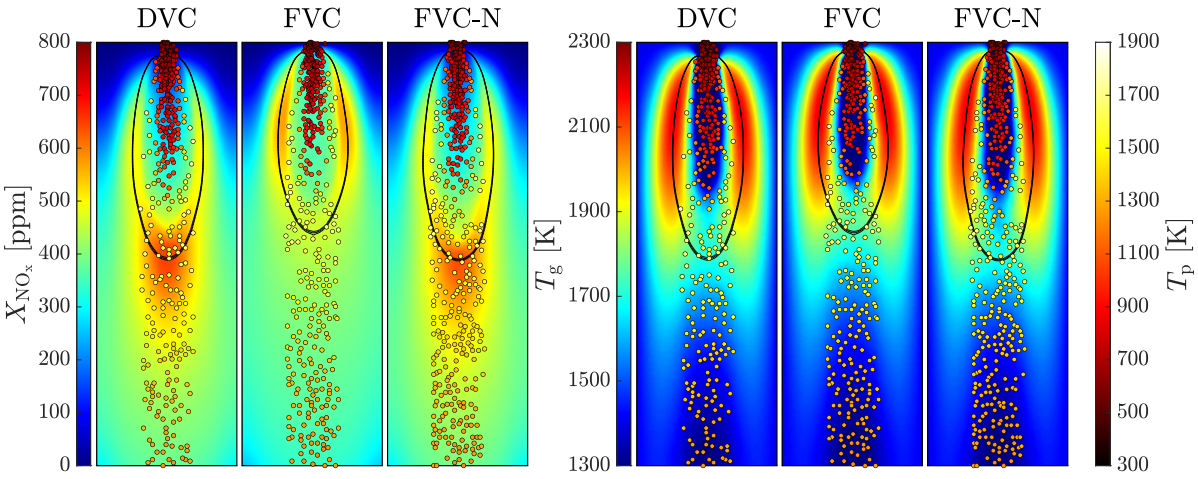

Figure 4: Comparison between the DVC, FVC, and FVC-N modeling assumptions for the NO_x mole fractions (left) and the gas temperature (right) in air. Particles are colored by the particle temperature and stoichiometric mixture fractions are visualized by black isolines.

Assuming a separate release of the N-containing volatiles from the other volatiles (FVC-N), due to the different release time scales of the N-containing volatiles, leads to a significant improvement in NO_x formation predictions as shown in Fig. 4.

5.4 Discussion

A parameter study was performed to analyze the NO_x formation pathways under different atmospheric conditions in biomass jet flames. Overall, lower NO_x emissions were observed under oxy-fuel conditions, where HNO is the major direct precursor of NO, while the N-radical is the most dominant direct precursor of NO in air.
Finally, a modification of the FVC model using a separate release of N-containing volatiles is able to capture the NO_x formation of the DVC model. These model assumptions lead to a significant improvement in the reduced-order modeling of NO_x formation in solid pulverized biomass flames.

5.5 Keywords

Biomass Combustion, NO_x Formation Modeling, Reaction Pathway Analysis, Direct Numerical Simulation

5.6 Software

The simulations have been performed using the in-house flow solver CIAO. All codes are parallelized using MPI.

6 Pictures

See Section 5.3

7 Awards, cooperations, publications

7.1 Selected honors, prizes, awards (up to ten) related to your project.

None.

7.2 Selected conference participations (e.g. invited keynote lectures or online conferences) during 2021 related to your project.

P. Farmand, C. Boehme, H. Nicolai, F. Loffredo, P. Debiagi, M. Gauding, C. Hasse and H. Pitsch. Modeling of NOx emissions in laminar solid pulverized biomass fuels flames. In 19th International Conference on Numerical Combustion, Kyoto (Japan), 2024.
P. Farmand, C. Boehme, A. Niazmehr, M. Gauding, H. Pitsch. Numerical Study of Ignition, Combustion, and Pollutant Formation of Biomass Compared to Coal. 5th International Workshop on Oxy-Fuel Combustion, Aachen (Germany), 2025.

7.3 Selected national and international cooperations (up to five) related to your project

None.

7.4 Publications related to your project

P. Farmand, C. Boehme, P. Steffens, H. Nicolai, F. Loffredo, P. Debiagi, S. Girhe, H. Chu, M. Gauding, C. Hasse, H. Pitsch. Numerical investigation and modeling of NOx formation in pulverized biomass flames under air and oxyfuel conditions. Combustion and Flame (under review).

7.5 Thesis (bachelor, master, PhD) related to your project

Christian Boehme, Numerical investigation and model assessment of NOx-formation pathways during coal and biomass combustion, Master Thesis, Aachen (Germany), 2024.
Pooria Farmand, Numerical Study on Ignition, Combustion, and Pollutant Formation Processes Using Solid Pulverized Fuels, PhD Thesis, Aachen (Germany), 2025.

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8 Support by NHR4CES

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