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

PI, Prof. Dr.-Ing. Heinz Pitsch (Institute Director), Institute for Combustion Technology (ITV), RWTH Aachen University, Germany
PI, Dr.-Ing. Michael Gauding, Institute for Combustion Technology (ITV), RWTH Aachen University, Germany
PM, Dr.-Ing. Pooria Farmand, Institute for Combustion Technology (ITV), RWTH Aachen University, Germany
R, Christian Boehme, Institute for Combustion Technology (ITV), RWTH Aachen University, Germany

# 5 Project report

## 5.1 Introduction

Replacing coal with biomass offers significant potential for reducing global $CO_2$ emissions due to biomass's closed carbon cycle. However, controlling harmful $NO_x$ emissions in solid biomass combustion remains a major challenge, often requiring costly exhaust gas after-treatment systems. Accurate modeling of particle–gas interactions is crucial for understanding $NO_x$ formation pathways, and high-fidelity simulations provide insights beyond the reach of experimental techniques.
This project investigates $NO_x$ formation in pulverized biomass flames using direct numerical simulations (DNS) under varying operating conditions to analyze flame behavior and its influence on $NO_x$ emissions. As combustion is highly sensitive to operating conditions, the findings support the development of optimized strategies for emission reduction.
Given the importance of fuel-$NO_x$ pathways, the effect of volatile composition on $NO_x$ formation was also examined. To this end, a fixed volatile composition, which is typically assumed in reduced-order models, was employed and compared with reference DNS results that included dynamically released volatiles. Based on these comparisons, a refined reduced-order model with improved $NO_x$ prediction accuracy was proposed, which is suitable for integration into flamelet modeling frameworks for solid fuel combustion.

## 5.2 Methods

The thermochemical conversion of solid fuels involves complex mass, momentum, and energy exchange between solid particles and the gas phase. This is captured using an Eulerian–Lagrangian approach: the gas phase is treated in an Eulerian framework, while solid particles are modeled as point particles in a Lagrangian formulation.
The governing equations are solved with CIAO, an in-house semi-implicit finite element solver. The Eulerian equations use second-order discretization in space and time, with scalar transport handled via a fifth-order WENO scheme for convection and second-order central differences for diffusion.
Species mass fractions and temperature are integrated using Strang splitting to separate transport and chemistry. Chemical source terms are computed via finite-rate chemistry using the CVODE solver. Solid particles are advanced with a two-stage, second-order Runge–Kutta scheme that updates their state, position, and source terms.

## 5.3 Results

This section presents the results of the parametric 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 presented analysis focuses specifically on solid pulverized Miscanthus biomass flames

under varying atmospheric conditions, aiming to assess the impact of these conditions on $NO_x$ production in a drop tube furnace (DTF) configuration.
Figure 1 illustrates the correlation between $NO_x$, mixture fraction, and gas-phase temperature in air atmosphere. Distinct high- and low-temperature zones can be identified around the stoichiometric mixture fraction. The peak $NO_x$ production rate aligns with the maximum consumption rate of nitrogen-containing volatiles (NFuel), which are released from the solid particles. This occurs in the high-temperature, fuel-rich regions near the particles, emphasizing the critical role of fuel-bound nitrogen in $NO_x$ formation during biomass combustion.

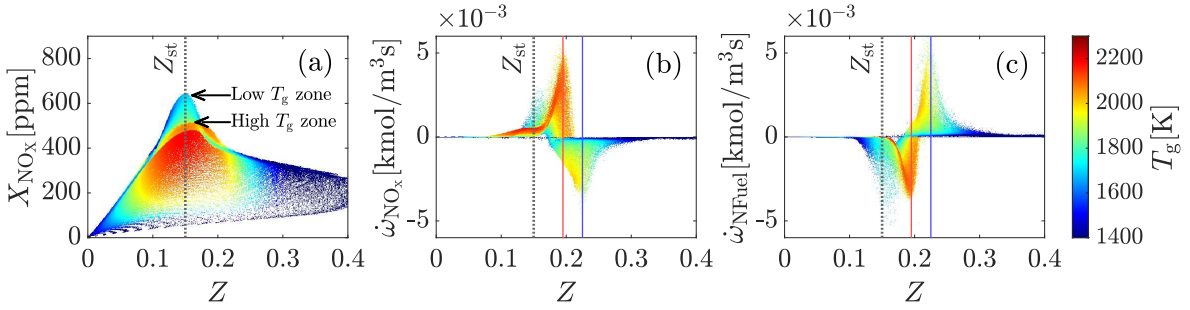


Figure 1: (a) $X_{NO_x}$, (b) $\dot{\omega}_{NO_x}$, and (c) $\dot{\omega}_{NFuel}$ of the Miscanthus flame in air atmosphere in mixture fraction space, colored by gas phase temperature. The peak production and consumption rates for $NO_x$ and NFuel are marked with solid red and blue lines, respectively.

Figure 2 compares $NO_x$ mole fraction and gas-phase temperature across three atmospheric conditions. In all cases, the global $NO_x$ maximum occurs near the flame tip, where lower temperatures and longer residence times promote accumulation. Local maxima also appear near stoichiometric, high-temperature regions. Oxidizer composition strongly affects flame structure and $NO_x$ formation, with air yielding the highest $NO_x$ due to enhanced thermal $NO_x$ production.
To analyze the $NO_x$ formation mechanisms in detail, Figure 3 presents a rate of production analysis (ROPA) of nitrogen-containing species. The analysis integrates nitrogen element fluxes across the entire computational domain and simulation duration to offer a comprehensive overview. The results reveal that atmospheric conditions significantly alter $NO_x$ formation pathways. Under oxy-fuel conditions, the contribution of atomic nitrogen (N) to NO formation decreases, while the role of HNO increases, indicating a shift in dominant reaction pathways. Additionally, a higher oxygen content in the oxidizer leads to increased production of hydroxyl (OH) radicals, which further enhances NO formation.
As Fuel-$NO_x$ pathways dominate $NO_x$ formation, the impact of volatile composition on prediction accuracy is evaluated. The fixed volatile composition (FVC), required in reduced-order models, is compared with the detailed dynamic volatile composition (DVC) model. While FVC accurately predicts gas-phase temperatures, it fails to capture $NO_x$ distribution (Figure 4). To address this, a modified FVC model (FVC-N)

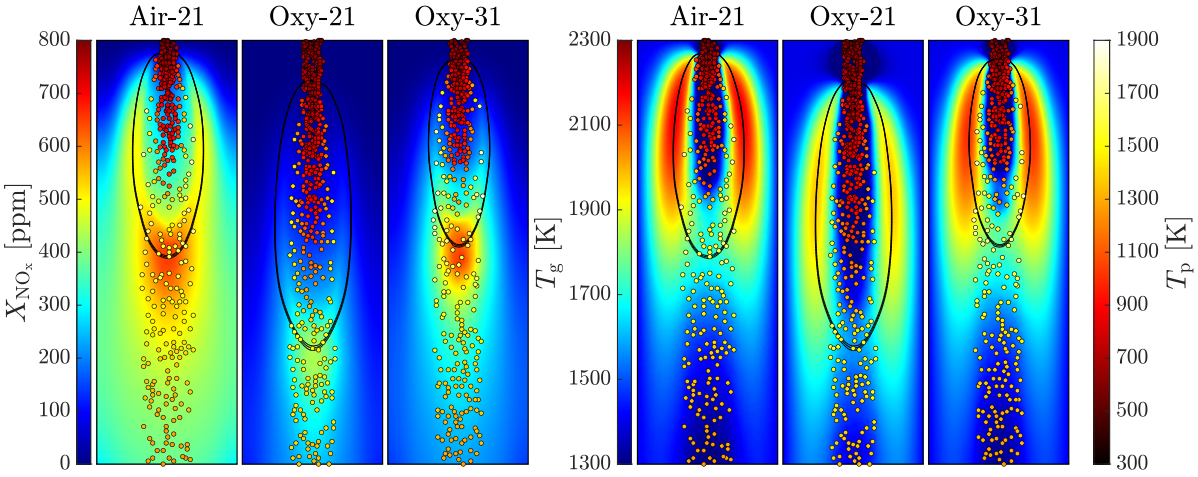


Figure 2: Comparison between $NO_x$ mole fractions (left) and gas temperature (right) in different atmospheres around the statistically steady-state. Particles are colored by the particle temperature. Stoichiometric mixture fractions for each flame are visualized by black isolines.

is proposed, which separates nitrogen-containing volatiles due to their distinct release timescales. This improves $NO_x$ prediction, as confirmed by closer agreement with DVC results in Figure 4.

## 5.4 Discussion

With the computing time on CLAIX, we conducted a parametric study to investigate $NO_x$ formation pathways under different operating conditions in pulverized solid

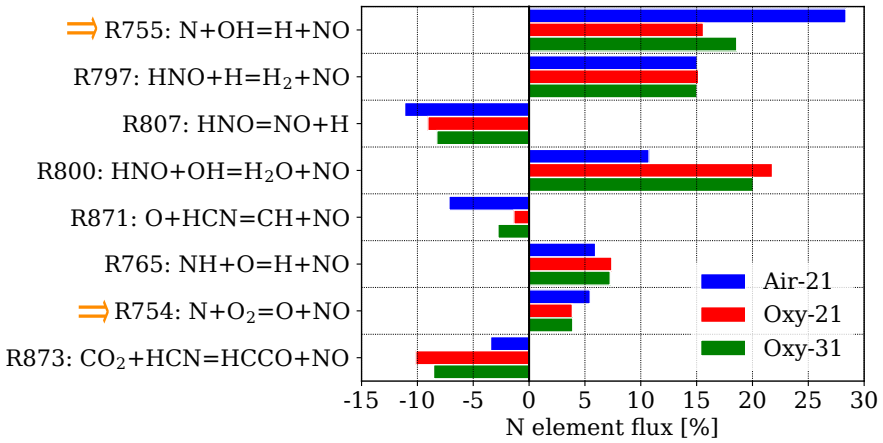


Figure 3: Effect of different atmospheres on the ROPA of NO integrated over the entire computational domain and simulation time. The extended Zeldovich reactions are marked with (⇒).

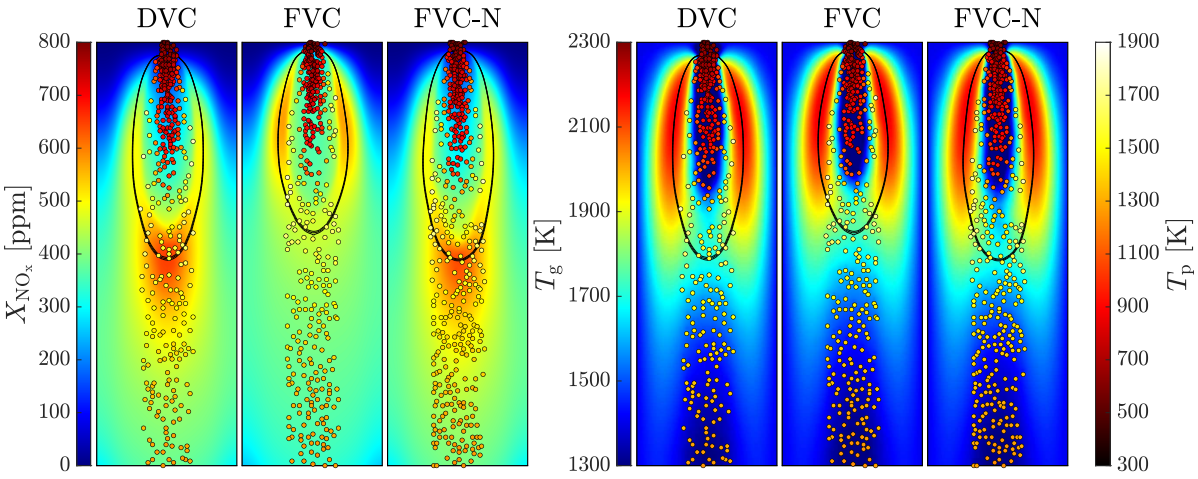


Figure 4: Comparison between the DVC, FVC, and FVC-N modeling assumptions for the $NO_x$ mole fractions (left) and the gas temperature (right) in air. Particles are colored by their temperature, and black isolines visualize stoichiometric mixture fractions.

biomass laminar jet flames. The analysis revealed that the surrounding atmosphere plays a significant role in $NO_x$ production. Specifically, lower $NO_x$ levels were observed under oxy-fuel conditions, where HNO serves as the primary direct precursor to NO. In contrast, in air, the N-radical is the dominant direct precursor for NO formation.
Finally, a modification of the fixed volatile composition (FVC) model, which separately accounts for the release of nitrogen-containing volatiles, successfully captures $NO_x$ formation predictions similar to those of the dynamic volatile composition (DVC) model. This modification significantly improves 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 $NO_x$ 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 $NO_x$ formation in pulverized biomass flames under air and oxyfuel conditions. Combustion and Flame (accepted).

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

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

# 8 Support by NHR4CES

Funded member of NHR4CES.

NHR4CES NHR for Computational Engineering Science

**By sending this information, I agree to its publication by NHR4CES (including RWTH Aachen and TU Darmstadt) and the NHR Verein for the purpose to report on the scientific use of NHR4CES infrastructure, in print and online.**