# HIGH-FIDELITY MODELING OF AMMONIA DROPLET BURNING IN MICROGRAVITY

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## Abstract

This work presents a comprehensive numerical investigation of the evaporation and combustion of isolated ammonia droplets in microgravity, using a one-dimensional spherically symmetric model. The simulation framework includes detailed multicomponent transport in the gas phase, detailed chemical kinetics, radiative heat transfer via the P1 model, and adaptive mesh refinement. In the liquid phase, Maxwell–Stefan theory is used to model species diffusion, including the absorption of water vapor from the surroundings. Thermodynamic equilibrium at the gas–liquid interface is computed using the Peng–Robinson equation of state. Model validation was carried out using the microgravity experimental data of Matsuura et al. (Proc. Comb. Inst. 40, 2024), demonstrating excellent agreement in droplet regression rates and flame standoff distances.

Once validated, the model was used to analyze the flame structure and the impact of ambient pressure and $O_2$ concentration. Emphasis was placed on droplet burning rates, flame diameter evolution, and formation of nitrogen oxides (NOx). The analysis quantified the relative importance of $N_2$, $N_2O$, HNO, $NO_2$, and thermal pathways under different conditions. It was found that higher ambient $O_2$ concentrations significantly enhance NOx formation via the thermal pathway, especially at elevated pressures, whereas the $N_2O$ and $N_2$ pathways play a key role in NO consumption, acting as DeNOx pathways.

## Introduction

Ammonia ($NH_3$) is emerging as a promising carbon-free fuel for energy and propulsion applications, particularly where storage, transport, and decarbonization are critical, such as maritime transport, power generation, and aerospace. Its high hydrogen content, established infrastructure, and potential for carbon-free combustion make it an attractive alternative to hydrocarbons. However, ammonia combustion presents challenges, including low flame speeds, high ignition temperatures, and complex nitrogen chemistry leading to NOx formation.

Among various configurations, droplet combustion provides fundamental insight into spray combustion relevant to practical devices. More specifically, microgravity droplet combustion offers an idealized setting to isolate the key physical and chemical phenomena. Recent experiments by Matsuura et al. [1] provided valuable data on ammonia droplet burning under microgravity and high-pressure conditions, but detailed numerical studies resolving both gas and liquid phases remain scarce.

In this work, we present an advanced numerical investigation of isolated ammonia droplet combustion under microgravity using a one-dimensional, spherically symmetric model. The model includes detailed multicomponent gas-phase diffusion, detailed kinetics [2], adaptive mesh refinement, and radiative heat transfer (P1 model). The radiating species included in the model are $H_2O$, along with $NH_3$, NO, and $N_2O$ [3]. A key novelty in the droplet model is the liquid-phase treatment, accounting for water absorption, Maxwell–Stefan diffusion, and non-ideal thermodynamic equilibrium via the Peng–Robinson equation of state.

Simulations were carried out using the OpenSMOKE++ Suite framework [4] across pressures from 10 to 30 bar and $O_2$ molar fractions from 0.21 to 0.60, capturing flame structure evolution and the influence of ambient conditions on burning rates, flame diameter, and NOx formation. The model was first validated against the experimental data of Matsuura et al. [1], then employed to explore key features of $NH_3$ droplet combustion and NOx chemistry under extreme conditions.

## Results and discussion

The numerical model was first validated against the experimental data of Matsuura et al. [1] under microgravity conditions at 15 bar and 21% $O_2$. Excellent agreement was achieved in terms of droplet diameter evolution and flame standoff ratio (Fig. 1). The model also correctly predicted water absorption from the flame into the droplet, which eventually leads to surface overheating and puffing observed in the experiments. Importantly, the inclusion of liquid-phase transport and non-ideal thermodynamics proved essential to capture this behavior.

After validation, systematic parametric studies were conducted by varying ambient pressure from 10 to 30 bar and $O_2$ molar fraction from 0.21 to 0.60. Higher pressure led to more compact and intense flames, with increased peak temperatures and shortened droplet lifetimes. Similarly, increasing the $O_2$ concentration enhanced flame reactivity, leading to faster evaporation and burning rates. The flame diameter initially increased, then decreased as the droplet approached the end of its life.

The model revealed the presence of an endothermic region preceding the flame front,

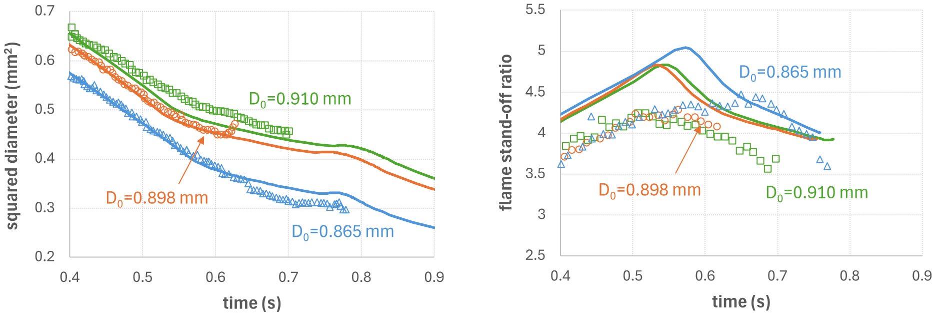

**Figure 1.** Temporal evolution of squared droplet diameter (left panel) and flame standoff ratio (right panel).

especially at elevated pressures and $O_2$ levels. As $O_2$ increased, this region became more intense, shifting the flame inward and altering the flame structure.

A detailed chemical analysis of NOx formation was also performed, identifying and quantifying the contributions from $N_2$, $N_2O$-intermediate, HNO, $NO_2$, and thermal pathways. The thermal mechanism played a minor role at low $O_2$ levels but became increasingly important at high $O_2$ and pressure. The $N_2$ and $N_2O$ pathways consistently acted as NO-consuming (DeNOx) mechanisms, while HNO contributed to NO formation. Under high-pressure, oxygen-rich conditions, the thermal pathway significantly contributes to total NOx emissions.

## Conclusions and future works

This work presented a comprehensive numerical study of ammonia droplet evaporation and combustion in microgravity, using a detailed one-dimensional model incorporating advanced gas-phase transport, detailed chemical kinetics, radiative heat transfer, adaptive meshing, and a rigorous description of liquid-phase thermodynamics and mass transport. Validation against recent experimental data demonstrated the model's ability to accurately reproduce droplet regression rates, flame structure evolution, and NOx formation trends across a wide range of pressures and oxygen concentrations.

The results provide a valuable framework for interpreting and predicting ammonia combustion behavior under microgravity and high-pressure conditions. The modeling approach can support the design of advanced ammonia-fueled propulsion systems, guide future experiments by highlighting key phenomena such as water absorption and endothermic zones, and contribute to the development of low-emission technologies for space and terrestrial applications. Further extensions to multi-droplet systems and transient instabilities will broaden its applicability to realistic spray combustion environments.

## References

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