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# Modeling Autoignition and Combustion Characteristics of Monodisperse Ammonia Droplet Clouds

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As a promising carbon-neutral fuel, ammonia ($NH_3$) is often combusted in spray form, where droplet interactions critically influence combustion performance and emissions. To elucidate these interactions, this study conducts detailed numerical simulations of evaporation, autoignition, and combustion in monodisperse ammonia droplet clouds. A unit cell approach is adopted, simulating a representative droplet and its surrounding gas phase under transient boundary conditions that mimic the broader cloud environment, providing computational tractability while capturing local physics. Interfacial dynamics are resolved using the Volume-of-Fluid (VOF) method, with evaporation rates derived directly from species concentration gradients at the interface, thus avoiding empirical correlations. The simulations incorporate detailed ammonia–air chemistry and solve the full set of conservation equations. We systematically investigate the effects of inter-droplet spacing, ambient pressure, temperature, and oxygen levels on transient evaporation, autoignition delay, critical ignition conditions, and subsequent flame dynamics. Particular emphasis is placed on quantifying NOx emissions and performing detailed pathway analyses to identify the key NO formation and destruction mechanisms within the cloud configuration. The findings provide fundamental insights into ammonia cloud combustion and offer essential data for refining sub-models used in larger-scale ammonia spray combustion simulations.