ABSTRACT

As the global energy sector moves toward low-carbon fuels, most energy still relies on fossil combustion, driving CO2 emissions that account for nearly 30% of global warming. Hydrogen has grown rapidly as a clean-energy option, but its high burning velocity (3 m/s) and very low ignition energy (0.02 mJ) pose storage and safety challenges. Ammonia (NH3) has therefore emerged as a carbon-free alternative due to its ease of storage, higher volumetric energy density (11.5 MJ/L), and convenient boiling point (-33.4 °C). However, its slow kinetics and fuel-bound nitrogen led to low flame speeds, long ignition delays, high autoignition temperatures, narrow flammability limits, low thermal intensity, and significant NOx/NH3 emissions.

This dissertation develops optimized combustion strategies for hydrocarbon-assisted ammonia flames to achieve clean, stable, ultra-low-NO_x operation. Machine-learning models were first developed to predict combustion characteristics of hydrocarbons and their blends with NH_3 and H_2, enabling the selection of appropriate mathematical and kinetic frameworks for ultra-low-NO_x modelling. A detailed parametric study then examined flame stabilization, NO_x pathways, and fuel-cracking behaviour in pure and assisted NH_3 flames. Insights from CRN analysis, numerical simulations, and literature led to the design of a novel two-stage burner combining fuel-staging and porous-media-assisted combustion. The fabricated burner was experimentally evaluated for temperature fields, flame structure, and NO/NH_3 emissions over a wide operating range, while validated numerical models quantified flame sensitivity to staging configurations and clarified the key kinetic routes controlling NO formation and reduction.

Initially, several ML models were developed to predict fundamental combustion characteristics of hydrocarbon fuels, using large datasets of experimental and simulation-based laminar burning velocity (LBV) measurements for isooctane and a wide range of alternative and green-fuel blends (NH_3, H_2, alcohols, DMF, syngas, etc.). A hybrid GA-ANN framework achieved the highest accuracy ($R^2 \approx 0.991$- 0.997), outperforming GLR, SVM, RF, and XGBoost models, and enabling a generalized LBV correlation valid across diverse operating conditions.

Building on these insights, the study extended the ML framework toward predicting exhaust emissions of staged NH_3 - LPG combustion systems. Multiple models RF, XGBoost, Decision Tree, Voting, Stacking, and ANN were benchmarked, with the ANN achieving the best performance ($R^2 = 0.998$, RMSE = 4.46), while ensemble models exhibited comparable accuracy. These models demonstrated strong capability in capturing nonlinear emission

behaviour and identifying optimal operating conditions for reduced NO_x, CO, and NH_3 slip, providing a rapid diagnostic tool for evaluating staging strategies.

Guided by ML-based insights into staging effectiveness, experiments were conducted on a novel two-stage radial injection burner over equivalence ratios of 0.7–1.4 at 20 kW. Multiple staging strategies were assessed to control flame stability, heat release, and emissions in hydrocarbon-assisted ammonia flames. Fuel staging and sequential premixing achieved the lowest NO_x by shifting heat release downstream, reducing peak temperatures, and enhancing $DeNO_x$ chemistry, with kinetic analysis identifying HNO and NH_i species as key NO pathways.

To further improve lean-flame stability and reduce emissions, zirconia-based porous-media combustion was investigated in a two-stage burner, demonstrating extended stability limits, enhanced heat recirculation, and significant reductions in NO, CO, and unburned NH_3 across LPG-NH_3 conditions. Reaction-zone migration into the porous matrix enabled high thermal intensities with minimal pollutants, while flame color transitions and kinetic analysis clarified underlying reaction mechanisms.

Overall, the work validates an integrated ML-staging-porous-media framework for low-NO_x, stable, and efficient ammonia–hydrocarbon combustion, providing a robust basis for next-generation clean combustor design and real-time emission optimization.