Abstract

The decarbonization of aviation requires a fundamental shift in propulsion technologies, with hydrogen emerging as a promising zero-carbon fuel for gas turbine engines. Although hydrogen possesses unique combustion characteristics, such as high flame speeds and wide flammability limits, it also presents susceptibility to flashback and the potential for NO_x production due to high combustion temperatures, posing significant design challenges that demand efficient computational tools for practical engineering applications. This thesis develops and validates computational methodologies that enable accurate and efficient analysis of hydrogen combustion in jet engines, addressing the critical challenges of flashback prevention and nitrogen oxide emission control.

Research progresses along three complementary fronts. First, system-level thermodynamic analysis using the Numerical Propulsion System Simulation (NPSS) software demonstrates the feasibility and performance benefits of hydrogen-fuelled turbofan cycles. By modelling the complete cryogenic fuel system from tank to combustor, this work evaluates alternative thermodynamic configurations exploiting hydrogen's heat sink capacity, revealing potential improvements in cycle efficiency.

Second, Reynolds-Averaged Navier-Stokes (RANS) simulations are employed to characterize hydrogen flame behaviour in two configurations: a micromix combustor with converging nozzle geometries and the AHEAD lean premixed swirl-stabilized burner featuring radial swirl generation and axial air injection for flashback mitigation, investigated with both two-dimensional axisymmetric and three-dimensional RANS. A multi-fidelity modelling framework is used to integrate computationally inexpensive two-dimensional axisymmetric RANS simulations with limited experimental data for flame position prediction. This approach achieves accurate flame position assessment with a number of calibration points comparable to the size of the

input parameter space, outperforming more complex surrogate modelling techniques at small training set sizes.

Third, representing the core contribution of this work, a Chemical Reactor Network (CRN) methodology is developed for rapid prediction of NO_x emissions without requiring the full resolution of the combustor flow field. The methodology employs an optimization algorithm for network calibration against high-fidelity data and incorporates physically motivated reactor topologies derived from fundamental swirl combustion structures. Validation on a non-premixed hydrogen combustor with water injection demonstrates the model's capability to capture the exponential NO_x reduction achieved through steam dilution. Application to the AHEAD premixed combustor shows that the calibrated network successfully predicts emission trends across wide operating ranges. A comparison against two-dimensional and three-dimensional RANS demonstrates that the CRN achieves accuracy competitive with or superior to RANS simulations, with a cost separation exceeding five orders of magnitude against 3D RANS. The robustness of these predictions is further assessed through a Polynomial Chaos Expansion (PCE) uncertainty analysis, which identifies inlet flow-rate measurement accuracy as the dominant contributor to NO_x prediction variance, rather than the calibrated model parameters. In both test cases, the CRN exhibits the ability to generalize results far from the conditions used for its calibration, enabling design space exploration that would otherwise be computationally prohibitive.

The computational tools and methodologies developed in this thesis provide a foundation for emissions-conscious preliminary design of hydrogen aviation propulsion systems, balancing accuracy, physical insight, and computational tractability, essential for industrial design processes.