Abstract

The characteristics of C_0-C_4 series hydrocarbon oxidation is of great interest in the field of combustion in practical applications. The combustion of gaseous fuels like liquefied petroleum gas (LPG) involves oxidation of hydrocarbon-based fuels. LPG as a transition fuel, an abundant and relatively cheap energy source, encourages the search for the optimal burner configuration to provide stable, efficient, and clean combustion for the gas turbine applications. Motivated with an idea of simulating a complex combustion problem with a limited computational resource, the present dissertation is focused on the development of a reduced skeletal model for studying the high-temperature ignition and combustion characteristics of H_2/CO/ C_1-C_4 hydrocarbons and its blend compositions. The reduced skeletal model is then further utilized to elucidate the physicochemical aspects of flames stabilized inside the newly proposed design methodologies of high intensity burner configurations for the industrial applications.

In order to investigate the combustion and ignition characteristics, a reduced 50 species 373 elementary chemical mechanism is being developed for the high-temperature combustion of H_2/CO/C_1-C_4 compounds. It is found that the reduced skeletal mechanism can reproduce the results from the detailed USC 2.0 mechanism with maximum error of less than 12% in the ignition delay times under a wide ranges of operating conditions. The applicability of the reduced skeletal mechanism is then demonstrated numerically through computational fluid dynamics (CFD) simulation in an industrial gas swirl burner for a non-premixed swirl-stabilized propane/air flame. The central processing unit (CPU) time cost of the skeletal mechanism is about one-third of the detailed USC Mech 2.0 mechanism for the ignition delay, laminar flame speed simulations, and is about half of the detailed USC Mech 2.0 for non-premixed CFD simulations.

The chemical kinetics of conventional single fuel and binary fuel, relevant to gas-turbine engines, are extended to explore in the tri-fuel (TF) context, with the help of TF blends of LPG+CH_4+H_2 at the pressure and temperature range of 1-20 atm and 900-2000 K, respectively. The blending of hydrogen with hydrocarbon fuels improves flame propagation, reduces emissions, and increases the combustion performance of the engine. The numerical investigation is conducted to explore the characteristics of TF mixture over a wide range of operating conditions by considering eight different test mixtures (M1-M8). The test mixtures (M2 to M4) contain higher hydrogen content and thus hydrogen kinetics will tend to dominate,

while test mixtures (M6 to M8) contain a higher concentration of hydrocarbons, thus the methyl radical chemistry plays a prominent role in the oxidation process. Such contrasting trends were further explored by extensive chemical kinetic modeling with the help of the reduced USC Mech_50 species model to analyze the ignition delay time, laminar flame speed, flame temperature, and heat release rate characteristics.

In the subsequent study, an experimental and numerical model to determine the exergy balance based on flow availability and availability transfer in the process of LPG/ air combustion in meso-scale gas turbine combustor is developed to elucidate the second law efficiency and total thermodynamic irreversibility. In terms of developing an energy and exergy efficient combustor design, this work highlights the influence of vortex shedding and recirculation in the volumetric entropy production and the exergy efficiency. It is performed in a heat recuperative high-intensity LPG-fuelled mesoscale combustor for mini-gas turbine applications. The design methodology, total volumetric entropy generation, exergy efficiency, flow recirculation and mixing characteristics are reported. The entropy generation rate due to thermal conduction is approximately more than 50% of the total entropy generation, while its contribution percentage due to chemical reaction is the smallest. Exergy efficiency reaches its peak under fuel-rich condition at higher thermal input, while its minimum value is obtained at lower thermal input under fuel-lean condition.

The experimental and numerical investigations are further extended to study the flame stabilization of premixed LPG/air mixtures in a zirconia-based stack porous media (PM) burner with 10 PPI foams at higher thermal inputs of 16.63, 19.95 and 23.28 kW under fuel-rich conditions. A detailed chemical model with 67 species and 475 elementary reactions is developed and implemented to elucidate the chemical aspect in the work. Flame morphology, effects of PM on flame temperature and its reaction zone, and major emissions like NOx and CO are analysed to design an ultra-high intensity burner for mini-gas turbine applications. Chain branching reaction ($H + O_2 \leftrightarrow O + OH$) accounts for consuming 5-10% of the combustion heat, and its contribution percentage slightly predominant towards stoichiometry due to more O_2 availability that accelerates the chain branching reaction. Flame temperature and the residence time are the dominant factors affecting CO and NOx formations.

Keywords: *Reduced Mechanism, LPG, Ignition delay time, Laminar flame speed, Heat release rate, Mesoscale, Porous burner*