

Abstract

Moderate or intense low oxygen dilution (MILD) combustion is an advanced technology aimed at increasing the thermal efficiency of the combustor and reducing major pollutant emissions such as NO_x , CO, and soot. MILD combustion is achieved by the exhaust gas recirculation technique, in which the reactants undergo high preheating and extreme dilution by the combustion products. The gas turbine combustors are operated at elevated pressure to increase their thermodynamic efficiency and decrease their size. However, they emit major pollutant emissions like NO_x , CO, and soot. These emissions pollute the atmosphere and are hazardous to health. Also, soot tends to increase with pressure. The MILD combustion technology can suppress these emissions and is preliminarily implemented with all modes of fuels operating at atmospheric pressure. However, its implementation at high pressure is complicated and needs a detailed investigation. In the present dissertation, numerical investigations are conducted to study the effect of pressure on the MILD combustion of gaseous fuels.

The complexity of achieving MILD combustion at elevated pressure for premixed methane-air mixtures in a cylindrical combustor is computationally studied under highly preheated and diluted conditions. The simulations are conducted considering various ranges of operating conditions, including reactant preheat temperature of 1100-1500 K, combustor pressures of 1-10 atm, and mixture dilution of 21% O_2 to 3% O_2 (volume basis) in air. Also, ignition delay times are calculated as a function of pressure, temperature, and mixture dilution level. Ignition delay times increase with the decrease in O_2 content; however, they substantially decrease with increasing combustor pressure and reactant temperature. A regime diagram is prepared to show the three different modes of combustion: HiTAC (High-temperature air combustion), MILD, and no ignition. An increase in pressure requires a very high level of N_2 dilution or low oxygen content to achieve MILD combustion. However, MILD combustion at elevated pressure can be achieved under a low preheat reactant temperature compared to the atmospheric pressure.

In the subsequent study, numerical simulations are conducted to study the effect of pressure on the soot formation of methane fuel under MILD combustion environment up to 20 atm. The investigation is conducted using a one-dimensional counterflow diffusion flame-type burner under a strain rate of 200 1/s. Soot volume fraction and

particle number density increase with pressure, and their peak values are positioned near the stagnation plane. A rise in pressure increases the major precursors for soot formation, such as benzene (A1), naphthalene (A2), pyrene (A4), and coronene (A7). At the same time, it also enhances the nucleation rate, HACA rate, condensation rate, and oxidation rate for soot. The soot nucleation rate has a larger value than both the HACA rate and condensation rate towards their contribution to the overall soot mass growth rate.

The numerical study is carried out further to evaluate the effect of pressure and gravity on soot formation and flame structure for turbulent methane-air diffusion flame. The CFD study is conducted under a traditional combustion environment so that the result obtained for soot chemistry can be compared with that of the MILD combustion environment. The soot volume fraction, surface growth rate, mass nucleation rate, and oxidation rate increase with increased operating pressure, regardless of gravity. The soot mass addition is observed more by surface growth rate than nucleation rate. Zero-gravity flames have a higher soot volume fraction, a wider soot-containing zone, and a lower flame temperature than normal-gravity flames while maintaining constant pressure.

The investigation is further extended to explore the chemical kinetics of CO and CO₂ formations for higher hydrocarbon alkanes (C₁-C₄) under a MILD combustion environment. The fuel jet comprises three cases of fuel mixture (Case 1: CH₄ + H₂, Case 2: C₃H₈ + H₂, and Case 3: C₄H₁₀ + H₂) having constant mixture density and operating under a fixed jet Reynolds number. The formation of CO is reported as maximum for Case 3 (C₄H₁₀ + H₂) and minimum for Case 1 (CH₄ + H₂). However, the reverse trend is observed in the case of CO₂ formation. The reacting flow analysis from the CFD work suggests that the reaction $C_2H_2 + O = CH_2 + CO$ strongly influences CO formation in all three fuel mixture cases. Likewise, the formation of CO₂ is majorly influenced by the reaction $CO + OH = CO_2 + H$. The ethylene route in the reaction pathway substantially plays a vital role in the CO formation in all three fuel mixtures.

Keywords: *MILD combustion, gaseous fuel, pressure, soot, CO, CO₂, CFD, chemical kinetics*