Internal combustion engines presently power the majority of applications because of their dependability, power production, and fuel efficiency. With the ability to blaze cleaner gaseous fuel at a thermal efficiency exceeding that of a diesel-only engine but with significantly lower emissions, alternative, zero-carbon fuels (such as hydrogen) are currently attracting attention. Tragically, IC engines cause economic and ecological harm by emitting high levels of pollutants and greenhouse gases. Using numerical modeling and simulation, this thesis aims to improve the fundamental knowledge of the best way to use hydrogen in internal combustion engines that use diesel-hydrogen dual-fuel and premixed fuel combustion (PFC) technologies, in which a specific percentage of the original diesel fuel is replaced with hydrogen. In order to simulate hydrogen-enhanced n-heptane combustion, this thesis designs, executes, and evaluates the computational tools required for premixed fuel, dual fuel direct injection in the cylinder, and hydrogen swallowed into the engine's intake air. A three-dimensional cylinder sector was used for the combustion modeling using ANSYS FLUENT, and the engine speed was varied between 1500 and 2000 revolutions per minute (rpm). The simulation duration ranged from 570° to 833° crank angles. The n-heptane and H2 interaction stages and the CO and NOx generation processes were incorporated into a reaction mechanism. It comprises 165 reactions and 40 species. According to the simulation results it is found that boosting the hydrogen mixing significantly improves the heat release rate, brake thermal efficiency, and peak cylinder pressure, all contributing to improved performance. In the case of premixed fuel combustion at 1500 rpm, cylinder pressure rises by 8.2% to 24%, thermal efficiency improves by 7.1% to 21.3%, CO emissions decrease by 16.2% to 38.7%, and CO2 emissions are reduced by 32.3% to 45.1% when 10% to 20% VI of H2 is premixed with the fuel, respectively. Similarly, at 2000 rpm, the cylinder pressure increased by 3.9% to 14.5%, thermal efficiency improved by 10.4% to 27.6%, CO emissions decreased by 31.8% to 45%, and CO2 emissions were lowered by 17.6% to 22.3% when 10% to 20% of H2 was premixed with fuel, respectively. Regarding to the case of diesel-hydrogen dual-fuel combustion. At 1500 rpm, mixing 10% to 20% of H2 with the fuel results in an 14.8% to 29.3% increase in cylinder pressure, a 12.4% to 23.2% improvement in thermal efficiency, a 28.9% to 59.2% decrease in CO emissions, and a 6.3% to 18.3% reduction in CO2 emissions. Comparably, at 2000 rpm, when 10% to 20% of H2 was mixed with fuel, the cylinder pressure rose by 4.1% to 15.9%, thermal efficiency climbed by 23.7% to 37%, CO emissions dropped by 57.1% to 64.2%, and CO2 emissions came down by 25.1% to 39.1%. Finally, hydrogen injection via the air intake manifold (AIM) to the engine will be discussed. At 1500 rpm, adding 10% to 20% of H2 through the air intake manifold increases cylinder pressure by 23.3% to 36.9%, improves thermal efficiency by 13.3% to 23.2%, reduces CO emissions by 19.6% to 49.1%, and reduces CO2 emissions by 42.8% to 57.1%. At 2000 rpm, the introduction of 10% to 20% H2 through the air intake manifold resulted in a cylinder pressure increase of 3.5% to 15.4%, a thermal efficiency enhancement of 32.2% to 56.3%, a reduction in CO emissions by 45.3% to 61.8%, and a decrease in CO2 emissions by 35.5% to 66.3%. Furthermore, due to enhanced combustion, there has been a slight increase in NOx emissions.