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Chemical Kinetics and Computational Fluid-Dynamics Analysis of H2/CO/CO2/CH4 Syngas Combustion and NOx Formation in a Micro-Pilot-Ignited Supercharged Dual Fuel Engine

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Abstract : A chemical kinetics and computational fluid-dynamics (CFD) analysis was performed to evaluate the combustion of syngas derived from biomass and coke-oven solid feedstock in a micro-pilot ignited supercharged dual-fuel engine under lean conditions. For this analysis, a new reduced syngas chemical kinetics mechanism was constructed and validated by comparing the ignition delay and laminar flame speed data with those obtained from experiments and other detail chemical kinetics mechanisms available in the literature. The reaction sensitivity analysis was conducted for ignition delay at elevated pressures in order to identify important chemical reactions that govern the combustion process. The chemical kinetics of NOx formation was analyzed for H2/CO/CO2/CH4 syngas mixtures by using counter flow burner and premixed laminar flame speed reactor models. The new mechanism showed a very good agreement with experimental measurements and accurately reproduced the effect of pressure, temperature and equivalence ratio on NOx formation. In order to identify the species important for NOx formation, a sensitivity analysis was conducted for pressures 4 bar, 10 bar and 16 bar and preheat temperature 300 K. The results show that the NOx formation is driven mostly by hydrogen based species while other species, such as N2, CO2 and CH4, have also important effects on combustion. Finally, the new mechanism was used in a multidimensional CFD simulation to predict the combustion of syngas in a micro-pilot-ignited supercharged dual-fuel engine and results were compared with experiments. The mechanism showed the closest prediction of the in-cylinder pressure and the rate of heat release (ROHR).

Keywords : syngas, chemical kinetics mechanism, internal combustion engine, NOx formation
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