Numerical and experimental engine study of HCCI combustion. Validation of a reduced n-heptane/iso-octane chemical kinetic mechanism.

A skeletal (27 species, 29 reactions) chemical reaction mechanism for iso-octane and a skeletal (27 species, 21 reactions) chemical reaction mechanism for n-heptane are constructed respectively from a semi-detailed iso-octane mechanism (84 species, 412 reactions) and a semi-detailed n-heptane mechanism (57 species, 290 reactions) of the Chalmers University of Technology in Sweden. The construction of the reduced mechanisms is performed by using reduction methods such as the quasi-steady-state assumption and the partial equilibrium assumption. Subsequently these reduced mechanisms are forged into one chemical reaction mixture mechanism for mixtures of iso-octane and n-heptane (39 species, 48 reactions). The obtained mixture mechanism is numerically compared to the Chalmers mechanisms and to other more detailed mechanisms provided by ENSIC-CNRS (Nancy) and LLNL (Curran et al.). The compression ratio, inlet temperature and equivalence ratio are varied and ignition delays are calculated from pressure curves and heat release curves, obtained by modelling calculations. The comparison of the ignition delays, pressure curves and heat release curves, calculated using the mixture mechanism show, at the mentioned conditions, good coherence with the other mechanisms (Chalmers, Nancy and Curran). For this comparison detailed mechanisms of Nancy (473 species, 2411 reactions for iso-octane and 559 species, 2593 reactions for n-heptane) and Curran (857 species, 3606 reactions for iso-octane and 561 species, 2539 reactions for n-heptane) are used in addition to the ones Chalmers provided. A numerical and experimental parametric study of this mechanism with regard to the ignition delays, pressure curves and heat release curves are determined for several engine parameters adhering to HCCI conditions : inlet temperature (290-350 K), equivalence ratio (0.2-0.6) and compression ratio (8-14).

Furthermore the results obtained from the reduced mixture mechanism are compared to the experimental results obtained from experiments performed on a CFR engine, using the same parameters.