A NOVEL MACHINE LEARNING BASED LUMPING APPROACH FOR THE REDUCTION OF LARGE KINETIC MECHANISMS FOR PLASMA-ASSISTED COMBUSTION APPLICATIONS

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Abstract
This work focuses on the reduction of a detailed isooctane plasma-assisted combustion (PAC) mechanism, consisting of 2805 species and 18457 reactions, by combining two techniques. Using the well-established plasma-specific direct relation graph with error propagation (P-DRGEP) method, a reduced mechanism of 415 species and 4716 reactions is produced. The mechanism has excellent predictive capabilities over a wide range of initial conditions for: initial pressure equal to 10 atm, temperatures from 750 K to 1200 K and equivalence ratios from 0.75 to 1.50. In addition, a plasma-specific isomer lumping approach is proposed and its viability and accuracy demonstrated. With the gradient boosting machine learning method and data from 0D reactor simulations that employ the reduced mechanism, predictive regression models are trained, which are found to describe accurately the lumped reaction rate coefficients. A lumped mechanism is developed, which contains 300 species and 3827 reactions. Two variations of this method are presented: one with models that use just gas temperature as input feature and another with two-input models, which apart from gas temperature also employ one of the radicals O, H or OH as a second input feature. In the former approach and over the broad range of initial conditions used to test the reduced mechanism, absolute errors fall within 6% on time to ignition, when compared to simulations with the detailed mechanism. The latter approach produces even lower errors, which do not exceed 3%.