Kinetic Modeling of Hydrogen-Light Hydrocarbon-Air Mixtures Combustion

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Abstract

In 2000, fossil energies represented 80 % of the primary energy offer and might reach 87 % in 2030. However, their reserves are quite limited in time and their conversion into secondary energy induces the release of various pollutants. One solution to reduce the impact of human activities on earth climate might be the utilization of hydrogen as an energy vector. However, the shift from a fossil energy to a hydrogen based economy faces several major issues including production, storage, transportation, distribution and utilization. The use of hydrogen-natural gas-air mixtures would constitute an intermediate step toward a hydrogen based economy. A good knowledge of the combustion properties of these mixtures is thus required. A first step toward this, is to possess a robust detailed kinetic scheme. The purpose of the present study is to compare 3 detailed kinetic schemes, that of Konnov, that of Dagaut and the GRI-mech 3, with existing experimental data.

The validation data set includes shock-tube, flame speed, jet-stirred reactor and detonation cell size data. For shock-tube, the experimental data of Chaumeix, Petersen, Lifshitz and Cheng are considered. The dilution varies between 75 and 99 %. The equivalence ratio is between 0.75 and 1.5 for different hydrogen to methane ratios. The pressure and temperature behind the shock waves are between 168 and 2000 kPa and between 1100 and 2300 K, respectively. For flame speed, the experimental data of Milton, Yu, Law, Halter, Huang and Ilbas are used. The equivalence ratio varies between 0.5 and 3.2 for hydrogen content in the fuel from 0 to 100 %. The initial temperature is between 300 and 500 K and the initial pressure is around atmospheric pressure. Air is used as the oxidant. The jet-stirred reactor data come from Dagaut. The hydrogen content in the mixture is between 0 and 1.75 %. The equivalence ratio varies between 0.3 and 2. The temperature and the pressure are between 900 and 1400 K and between 100 and 1000 kPa, respectively. The nitrogen dilution is from 78.4 and 98.2 % and the residence is either 120 or 250 ms. For detonation cell size prediction, the experimental data of Matignon and Chaumeix have been taken into account. The equivalence ratio is either 0.75 or 1. The hydrogen content varies from 0 to 100 % of the fuel. The initial pressure and temperature are respectively between 10 and 200 kPa and between 293 and 473 K. The nitrogen dilution is from 0 to 71 %. The evaluation is achieved by using the correlation of Ng.

For shock-tube data, each model present some advantages according to the composition and the temperature ranges considered. The mean relative error on delay times is whithin 60%. The model of Konnov predicts the shortest delay times. For flame speed data modeling, the three models are as reliable and allow prediction of the flame speed within 14 %. The maximum of deviation is for stoichiometric mixtures with a mean value around 23 %. This discrepancy comes from the inability of all the models to predict the experimental data of Milton which have been obtained on a wide range of initial temperature and pressure. For jet-stirred reactor data, the model of Dagaut furnish significantly better results. The three models predict in general quite well the reactant mole fractions, H_2, CH_4, C_2H_6, C_3H_8 and O_2. The stable intermediate mole fraction, CO, CH_2O, C_2H_4 and C_2H_2, are very well reproduced by the model of Dagaut whereas the two other models can involve large error on the predictions. The CO_2 and H_2O, the products, mole fractions are satisfactory predicted by the model of Dagaut whereas the two other schemes give usually poor results. For detonation cell size, the model of Konnov is the best with predicted cell size within 50 % of the experimental data.

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