ON THE SIMPLIFICATION OF KINETIC REACTION MECHANISMS OF AIR–ETHANOL UNDER HIGH PRESSURE CONDITIONS

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ABSTRACT

In the last decade, the interest towards non-petroleum based fuels is strongly increased due to the current concerns about the impact of the transport system on atmospheric pollutions, mainly due to CO2 emissions. Ethanol, either blended with conventional fuels or in its pure form, is one of such fuels already in use in the automotive industries. As an example, the flex-fuel engines are designed to employ gasoline from 10% up to 85% of ethanol (E10, E85). In this work, the oxidation kinetics of ethanol with air has been considered and analyzed in an ambient at high pressure, ranging from 4 to 6 MPa, by means of a Computational Singular Perturbation methodology. This study starts from a detailed kinetic reaction mechanism, which is extensively used in the literature and is made up by 235 reversible reactions among 46 chemical species. This mechanism has been used to get several families of simplified (skeletal) mechanisms by considering equivalence ratios in the range 0.2–2.0 and two sets of initial temperatures (900–1200 K and 1200–1700 K). The skeletal mechanisms have been validated by comparing the temperature and major chemical species profiles and the ignition delay time with those obtained by employing the detailed mechanism. Advantages and limitations of these mechanisms are highlighted. The accuracy of the skeletal mechanisms is very good in the range of equivalence ratio and temperature considered in the simplification procedure. Moreover, it is shown that a further simplification of the reaction mechanism is obtained by narrowing the range of equivalence ratio instead of the range of temperature. The most simplified skeletal mechanisms show an error in the prediction of temperature and fuel profiles lower than 3%, except for the case of low temperature and lean mixtures, where the maximum error increases up to 14%. Finally, the main reaction pathways are analyzed to show how the most important intermediate chemical species and products characterize the skeletal mechanisms for different values of equivalence ratio and temperature. The skeletal mechanisms are given as Supplementary data. The reader can refer to such data for the entire set of the retained reactions and species for each skeletal mechanism.

REFERENCES