An *a priori* thermodynamic data analysis based chemical lumping method for the reduction of large and multi-component chemical kinetic mechanisms

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A chemical species lumping approach for reduction of large hydrocarbons and oxygenated fuels is presented. The methodology is based on an *a priori* analysis of the Gibbs free energy of the isomer species which is then used as main criteria for the evaluation of lumped group. Isomers with similar Gibbs free energy are lumped assuming they present equal concentrations when applied to standard reactor conditions. Unlike several lumping approaches found in literature, no calculation results from the primary mechanism have been employed prior to the application of our chemical lumping strategy. An 807 species and 7807 individual reactions detailed mechanism comprising *n*-decane, α-methylnaphthalene and methyl-decanoate has been used. The thermodynamic data have been analysed and 74 isomer groups have been identified within the oxidation of *n*-decane and methyl-decanoate. The mechanism reduction has led to a mechanism size of 463 species and 7600 reactions. Thereafter the lumped mechanism has been checked under several reactor conditions and over a broad range of temperature, pressure and equivalence ratio in order to quantify the accuracy of the proposed approach. In all cases, very good agreement between the predictions obtained using the lumped and the detailed mechanism has been observed with an overall absolute error below 12%. Effects of the lumping procedure on sensitivities and on isomer concentrations were taken into account to further demonstrate the validity of the proposed approach.