Synergies and Uncertainties in the Combustion Chemistry of Fuel Blends

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Recent efforts for a clean and efficient combustion translate into the development and interaction of novel technologies operated on novel fuels. Novel technologies often involve either the combustion of fuel mixtures consisting of components with significantly differing properties (e.g. RCCI) or the combustion of highly diluted mixtures (e.g. EGR, MILD combustion). Moreover, most of these technologies operate at conditions (low temperatures, lean stoichiometries, high pressures) that may lie outside the working range of several detailed kinetic mechanisms.

Combustion of mixtures exhibits complex synergistic effects, with respect to both heat release and molecular growth processes, which cannot be predicted solely from the behaviour of the constituent components. In practice this implies that kinetic models developed for single fuel components may be inadequate in resolving all the necessary chemical timescales and, also, that accurate predictions will require more accurate determinations of rate parameters.

The first part of the present work aims to quantify synergies in the combustion chemistry of small hydrocarbons. A comprehensive detailed kinetic mechanism [1, 2] is used to numerically reproduce the structure of laminar premixed flames of C1-C6 hydrocarbon mixtures and quantify synergistic effects. The second part deals with uncertainties related to mechanism development with reference to neat and blended flames of C_3H_4 isomers. Through specific examples, the study tries to quantify the level of mechanism complexity that is appropriate/necessary for accurate predictions also taking into account practical requirements.

[1] G. Vourliotakis, G. Skevis, M.A. Founti, Proc. Combust. Inst. (2014) doi: 10.1016/j.proci.2014.06.060.
[2] A. Gazi, G. Vourliotakis, G. Skevis, M.A. Founti, Combust. Sci. Technol. 185 (2013)1482-1508.