# Comprehensive kinetic modeling and experimental study of a fuel-rich, premixed *n*-heptane flame

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An existing comprehensive kinetic hydrocarbon oxidation model has been augmented and revised for a detailed analysis of *n*-heptane flame chemistry. The analysis was enabled by experiments in which the detailed species composition in a fuel-rich flat premixed ($\Phi$=1.69) *n*-heptane flame at 40 mbar has been studied by flame-sampling molecular-beam mass spectrometry using electron impact ionization. Mole fraction profiles of more than 80 different species have been measured and compared against the new detailed kinetic model consisting of 349 species and 3686 elementary reactions. For all major products and most of the minor intermediates, a good agreement of the modeling results with the experimentally-observed mole fraction profiles has been found. The presence of low- and intermediate-temperature chemistry close to the burner surface was consistently observed in the experiment and the simulation. With the same kinetic model, *n*-heptane auto-ignition timing [1,2], flame speeds [3,4] and species composition in a jet-stirred reactor [5] have been successfully simulated for a broad range of temperatures (500-2000 K) and pressures (1-40 bar). The comprehensive nature and wide applicability of the new model were further demonstrated by the examination of various target experiments for other $C_1$ to $C_7$ fuels.

The reaction scheme is based on previous works for butane and butene isomers [6-7] as well as for *n*-heptane [8]. During the development of the new *n*-heptane reaction scheme the prediction for $C_1$-$C_7$ fuels was systematically compared against experimental data. To achieve this a minimal data format for various reactors (shock tube, jet-stirred reactor, laminar flames and burner stabilized flames) was developed. This format serves as input for automatic validation of the reaction scheme and is still human readable. This minimal format can support the discussion of the WG4 (Standard definition) in the SMARTCATS action.

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