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CHEMICAL KINETIC MODELING OF COMBUSTION IN INTERNAL COMBUSTION ENGINES USING REDUCED CHEMISTRY

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A general method for automatically reducing detailed kinetic mechanisms for complex fuels is applied. The method is based on the simultaneous use of sensitivity, reaction-flow, and extended lifetime analyses. The sensitivity analysis detects species to which the overall combustion process is sensitive. Small inaccuracies in calculating these species result in large errors in the characteristic behavior of the chemical scheme. Redundant species are detected by applying a simultaneous reaction-flow and sensitivity analyses. The sensitivities are transported through the reacting flow and each species is assigned an importance according to the importance of the species itself and the flow of atoms to and from the important species. The redundant species are removed from the detailed mechanism (74 species and 510 reactions) resulting in a skeleton mechanism (63 species and 386 reactions). The skeleton mechanism is in turn the object for a further reduction by applying extended species sensitivity and lifetime analyses. These analyses are the basis for a reduction by means of a quasi–steady-state assumption. By introducing the quasi–steady-state assumption, the skeleton mechanism is reduced further to 19 species and 16 global reactions. The skeleton and reduced mechanisms generated using different cutoff levels of ''relative species importance'' and ''lifetime,'' respectively, are validated against the detailed mechanism to find

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