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Optimizing Simplified One-Step Chemical Models for High Speed Reacting Flows ALP OZGEN, RYAN W. HOUIM, ELAINE S. ORAN, University of Maryland College Park — One of the most important and difficult parts of constructing a multidimensional numerical simulation of a hydrocarbon reacting flow is finding a reliable and affordable model of the chemical and diffusive properties. Full detailed chemical models of these systems contain too many reactions and chemical species to be practical for realistic scenarios. The objective of our work is to create the simplest model possible that can reproduce the time-dependence of the energy input and the conversion from fuel to products. To that end, we are developing a procedure optimizing parameters in the most simplified "one-step" model. An important requirement of this model is that it reproduces known flame and detonation properties. Multidimensional numerical simulations using the new model are compared to deflagration-to-detonation experiments in channels containing ethylene and oxygen.

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