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Toward a New Paradigm for Reactive Flow Modeling BOB SCHMITT, Sandia National Laboratories — Traditional reactive flow modeling provides a computational representation of shock initiation of energetic materials. Most reactive flow models require ad hoc assumptions to obtain robust simulations. These assumptions result from partitioning energy and volume change between constituents in a reactive mixture. These models assume pressure and/or temperature equilibrium for the mixture. Many mechanical insults to energetic materials violate these assumptions. Careful analysis is required to ensure that the model assumptions and limitations are not exceeded. One limitation is that SDT is replicated only for strong planar shocks. These models may require different parameters to match data from thin pulse, ramp wave, or multidimensional loading. This approach fails for complex loading. To accurately simulate reaction under non-planar shock impact scenarios a new formalism is required. The continuum mixture theory developed by Baer and Nunziato is used to eliminate ad hoc assumptions and limitations of current reactive flow models. This modeling paradigm represents the multiphase nature of reacting condensed/gas mixtures. Comparisons between simulations and data are presented.

Dave Crawford
Sandia National Laboratories

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