

Abstract Submitted
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A Gibbs Formulation for Reactive Materials with Phase Change¹

D. SCOTT STEWART, Mechanical Science and Engineering, University of Illinois, Urbana, IL — A large class of applications have pure, condensed phase constituents that come into contact, chemically react and simultaneously undergo phase change. Phase change in a given molecular material has often been considered to be separate from chemical reaction. Continuum modelers of phase change often use a phase field model whereby an indicator function is allowed to change from one value to another in regions of phase change, governed by evolutionary (Ginzburg-Landau) equations, whereas classic chemical kinetics literally count species concentrations and derive kinetics evolution equations based on species mass transport. We argue the latter is fundamental and is the same as the former, if all species, phase or chemical are treated as distinct chemical species. We pose a self-consistent continuum, thermo-mechanical model to account for significant energetic quantities with correct molecular and continuum limits in the mixture. A single stress tensor, and a single temperature is assumed for the mixture with specified Gibbs potentials for all relevant species, and interaction energies. We discuss recent examples of complex reactive material modeling, drawn from thermitic and propellant combustion that use this new model.

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