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A Gibbs Formulation for Reactive Condensed Phase Materials with Phase Change[1] D. SCOTT STEWART, University of Illinois, Urbana-Champaign — 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 evolution equations based on species mass transport. We argue that the latter is fundamental and is the same as the former, if all species, phase or chemical are treated as distinct chemical species. A self consistent continuum-thermomechanical model, must account for all significant energetic quantities and have correct molecular and continuum limits in the mixture. The use of Gibbs potentials for all relevant species, chemical and phase does this neatly and allows the use of classical potentials, while allowing for modeling of phase interaction terms and reaction rate and phase change kinetics. The phase field quantities are the mass fractions. One has a single stress tensor, and a single temperature.

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