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Coupled thermo-chemo-mechanical modelling of reactive solids for thermochemical energy storage materials

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Extended Abstract

Abstract

A continuum-scale thermo-chemo-mechanical modeling framework is developed to investigate the coupled multiphysics behavior of thermochemical energy storage (TES) materials undergoing reversible hydration and dehydration reactions during thermal cycling. This framework integrates species diffusion, reaction kinetics, heat generation and transport, and mechanical deformation to capture the spatial and temporal evolution of temperature, stress, species concentration, and reaction progress across TES domains. Constitutive models are proposed to replicate experimentally observed material responses under cyclic storage conditions. To isolate the chemo-thermal contributions, pellet-scale case studies are conducted without mechanical coupling. Non-dimensional parametric studies are performed to assess the sensitivity of key material properties, such as thermal conductivity, diffusivity, and kinetic rate constants, on energy storage efficiency and transformation dynamics. A representative simulation, calibrated against thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) data, demonstrates the model's ability to capture transient behaviour of TES materials. Additionally, a fully coupled simulation is presented to illustrate how mechanical stresses influence reaction evolution. Mechanical stresses generated by differential expansion/contraction, or constrained boundary conditions, modify local reaction equilibria. This work offers a mechanistic understanding of TES behavior under realistic operating conditions and lays the groundwork for designing more efficient and mechanically robust energy storage systems.

Keywords:

Thermochemical energy storage Continuum thermo-chemo-mechanics Chemical reactions