Documenting the physical changes and thermodynamic effects of geochemical reactions: a metasomatic example in Gale vector space

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Metasomatic reactions associated with many geological processes (e.g., hydrothermal alteration, diagenesis, weathering, etc.) are typically difficult to specifically define because some reactants and products (soluble species) may be added or removed by the fluid, and evidence for their involvement in a reaction may thus be absent from a suite of rocks. As a result, given a known (observed) reactant and product mineral assemblage, one is commonly able to identify a myriad of possible geochemical reactions. Determining which reaction actually operated to produce the observed change in mineral assemblage may thus be intractable without other mineralogical, geochemical, or physical constraints.

Matrices of row and column vectors may be used to describe both the compositions of minerals and aqueous species, and the coefficients of these minerals and species in geochemical reactions. As a result, a number of matrix operations can be undertaken to provide insight into the nature of geochemical reactions involving minerals and species. One important result is a geometric representation of the geochemical reactions in a multi-dimensional Gale vector space. This space hosts points defining all possible reactions among the minerals and species under consideration, and thus can be used to systematically describe the feasible geochemical reactions. Because changes to physical characteristics (mass, volume, and density), and thermodynamic properties (ΔG_r, ΔH_r, ΔS_r) can be determined for each possible reaction, Gale vector space can be used to conclusively identify all possible reactions consistent with constant volume, density, mass, adiabatic, or isothermal constraints. As a result, investigation of geochemical reactions in a Gale vector space provides a comprehensive and systematic way to identify all feasible chemical reactions using such constraints. An example involving the serpentinization of olivine is used to illustrate the features and power of using a Gale vector space in this application.