

Time-dependent 3-D modelling of contact-regional metamorphism suggests reactions occur in < 1 Ma

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Metamorphic rocks develop through a complex series of thermal, chemical and mechanical processes that contain feedback effects. The integrated outcome of these processes is an assemblage of minerals with a specific texture that forms a spatial distribution pattern consistent with the heat source. The rates, magnitudes and duration of the various controlling processes are difficult to extract from the natural rock system in part because of the feedback effects. However, recent advances in high-resolution 4-D computational modeling provide a powerful tool for investigating complex systems and constraining the rates of governing processes, their durations, and their relative importance during a thermal event.

A series of time-dependent 3-D computational experiments of heat and mass transport for contact-regional metamorphic systems with variable host-rock and intrusion properties allows rates and duration of processes to be examined in the context of a controlled environment throughout the entire system's history. For example, for a system with a 3-km thick pluton intruded at 12 km depth into metapelitic host rocks that vary along a geothermal gradient of 36°C/km and with anisotropic permeability (K) of $K_{x,y} = 10^{-15} \text{ m}^2$, $K_z = 10^{-16} \text{ m}^2$, fluid flow is the dominant heat-transport mechanism. Within 1 km of the contact, convective flow maintains temperatures above 560°C (staurolite in) for about 0.6 Ma above 525°C (garnet in) for ~0.75 Ma and above 500°C for ~1.2 Ma. For isotropic K (10^{-16} m^2), the duration of time the rocks remain at high temperature is about 30% longer for $T > 525^\circ\text{C}$ and nearly double for 500°C. Consequently, these thermal data constrain the time available for garnet and staurolite nucleation and growth and set boundaries for duration of metamorphic reactions.

When extracting parameters from real rocks for use in kinetic models, the rates and their duration should also be consistent with values derived from high-resolution simulations of metamorphic events.

Metal speciation dynamics in dispersions of soft colloidal ligand particles under steady-state laminar flow condition

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In this presentation, a theory is reported for metal speciation dynamics in a swarm of soft, spherical core-shell colloidal ligand particles (like biocolloids, microgel particles) under steady-state laminar flow condition. Mass transfer and subsequent complexation of metal species within the reactive, permeable particle shell are governed by the interplay between (i) convective-diffusion of free metal ions M within and around the shell where ligands L are distributed, and (ii) kinetics of ML complex formation/dissociation in the shell. The local concentrations of metal M and complex ML are determined by the convective-diffusion equations with appropriate chemical source term and full account of radial and angular concentration polarization contributions. The steady-state flow field is determined from the solution of Navier-Stokes equation including convective acceleration term for the fluid external to the particle, and from Brinkman equation for the internal fluid flow. The confined location of ligands within the particle shell leads to ML formation/dissociation rate constants (denoted as k_a^* and k_d^* respectively) that differ significantly from their counterparts (k_a and k_d) defined for homogeneous ligand distribution throughout the solution. The relationship between k_{ad}^* and k_{ad} is derived from the numerical evaluation of the spatial, time-dependent distributions of free and bound metal within and/or outside the particle. The dramatic dependence of k_{ad}^* on hydrodynamic particle softness, Péclet number, soft surface layer thickness and particle radius are analyzed in the steady-state non-equilibrium chemical regime within the context of dynamic features for colloidal complexes. The analysis covers the limiting cases of hydrodynamically impermeable, hard particles where binding sites are located at the very surface of the particle core (e.g. functionalized latex colloids) and free draining, polymeric ligand particles devoid of a hard core (e.g. porous gel particles). The formalism further applies to any values of the Péclet number, i.e. for speciation dynamics determined by kinetic processes coupled to diffusion and/or convection metal mass transfer(s). A discussion is provided for the comparison between the exact numerical results and the analytical formulation based on the approximate Levich expression for convective-diffusion metal flux at the surface of hard ligand particles.