In silico, physiological, and proteomic cost-benefit analysis of resource-limited microbial growth

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Evolutionary selection has produced fit microbes with robust and often redundant metabolic network functionality. Maintaining and regulating network redundancy represents a substantial resource burden especially in nutrient limited environments and therefore needs to be off set by fitness advantages. A genome enabled *in silico* methodology was developed and experimentally tested which quantifies molecular-level, resource allocation tradeoff strategies that permit competitive cellular functioning under a continuum of nutrient availabilities. The approach decomposed a metabolic network into a complete listing of non-divisible, mathematically-defined biochemical pathways which were then used to identify all potential strategies for investing limiting resources like iron and nitrogen into the genome encoded metabolic machinery. The tabulated enzymatic resource investment requirements for each distinct biochemical pathway were examined in concert with the pathway's efficiency at converting substrate into biomass. The analysis identified the most competitive molecular-level tradeoffs between pathway resource requirements and metabolic efficiency; allocating limiting resources to perform one function well came at the cost of performing another metabolic function well. *In silico* predictions were evaluated experimentally using physiological and proteomic data collected from iron- or nitrogen-limited *Escherichia coli* chemostat cultures. Experimental chemostat data was consistent with *in silico* theory and illustrated that under iron- and nitrogen-limited conditions *E. coli* regulates its metabolism to invest the limiting resource competitively at the cost of optimal biomass yields on electron donor. The study highlights a fundamental evolutionary and metabolic design paradigm for competitive network structure and control.

Solubility as a determinant of rates of intergranular diffusion in metamorphic rocks

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Rates of intergranular diffusion in metamorphic rocks are principally determined not by temperature, but instead by the properties of the intergranular medium, particularly those properties that govern the solubility of the diffusing species.

Quantitative comparison of length scales and time scales for metamorphic reaction in natural examples reveals extremely large variations in rates of intergranular diffusion for Al among systems with different H_2O activities. For instance, at 600 °C the effective diffusion coefficient for Al ($m^2{\cdot}sec^{-1}$) is $10^{-18.8}$ in fluid-saturated systems, $10^{-22.5}$ in hydrous-but-fluid-undersaturated systems, and $10^{-25.4}$ in anhydrous systems. Thus even at constant temperature, Al diffusivities can range across 6 to 7 orders of magnitude depending on the character of the intergranular medium.

In fluid-saturated systems, garnet zoning—which monitors the length scale of chemical equilibration during growth—shows that intergranular solubilities controlled by characteristics of the fluid itself (H_2O/CO_2 ratios, availability of ligands for complexation, pH) can exert greater influence on diffusivities than temperature. As a case in point, the nature of compositional zoning in garnet from Harpswell Neck, Maine, varies markedly from cores to rims. For Mn, Fe, and Mg, many crystals have irregular, patchy distributions in their cores that give way to smooth, concentric zoning in their outer rims. In contrast, zoning of Ca and Y is comparatively smooth and concentric throughout these crystals. Rims of all crystals share equivalent concentrations of all elements. Raman spectrometry of fluid inclusions demonstrates that growth of garnet cores took place in the presence of a CO_2-rich fluid, whereas growth of garnet rims took place in the presence of an H_2O-rich fluid. Thus the patterns of garnet zoning imply that low solubility for Mn, Fe, and Mg and high solubility for Ca and Y in a CO_2-rich fluid restricted the length-scales of equilibration for the former and expanded them for the latter during the growth of garnet cores; transition to an aqueous fluid with relatively high solubility for all elements then led to rock-wide equilibration for all during growth of garnet rims. Differential solubility of cations in fluids of variable composition is therefore a fundamental control on rates and scales of intergranular diffusion.