# Dynamic response of microbial activity to intermittent stress: Effects of dormancy in biogeochemical simulations

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## Motivation

Microorganisms are known to be able to switch between active and dormant states, thereby allowing them to endure periods of unfavorable environmental conditions. To our knowledge, the effects of dormancy and reactivation on microbial transformation processes have not been addressed in biogeochemical simulations of environmental systems.

## Approach

Microbial respiration and population dynamics are modeled using the numerical simulation software BRNS (Biogeochemical Reaction Network Simulator). Active and dormant biomasses are included as state variables, and kinetic expressions are derived to account for the deactivation and reactivation of the microorganisms. The kinetic expressions are functionally linked to the energy yields of the corresponding respiration pathways, as well as to the maintenance requirements of the organisms. The model further allows for variations in the yield factor, depending on the energy budget, and considers loss of biomass during reactivation.

## Results

The model is used to simulate the concentrations of key redox species, rates of respiration and changes in biomasses, for a number of time-dependent scenarios. In particular, the response of the geomicrobial reaction system to intermittent stress conditions due to the periodic lack of energy substrates or electron acceptors is compared for simulations including dormancy or not. The results indicate that the ability to switch to and from the dormant state increases the overall resilience of the microbial system, and leads to enhanced, long-term levels of substrate utilization.

# Oxidation of biofluid constituents by higher valent (hydr)oxide nanoparticles

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Biological mechanisms that have evolved for inactivating reactive oxygen species may provide protection against nano-sized oxidant particles. To explore this further, molecular-level mechanisms must be compared. As far as reactive oxygen species are concerned, the identities and concentrations of antioxidants vary substantially from organism to organism. Glutathione is common to all organisms, while the ovothiol family of antioxidants is only employed by invertebrates. Primates, which lack the ability to biosynthesize ascorbic acid, must also rely upon the antioxidant properties of uric acid. Concerted action can be important. The amphiphilic antioxidant α-tocopherol, for example, requires regeneration by the hydrophilic antioxidant ascorbic acid.

Adsorption/desorption reactions are key features of nanoparticle/water interfaces. We have established that ascorbic acid, uric acid, and glutathione readily reduce and dissolve nano-sized hydrous manganese(III,IV) oxide (HMO), $MnO_2$(pyrolusite), and $PbO_2$(plattnerite). Prior studies of carboxylic acid and substituted phenol adsorption provide analogies to the adsorption of ascorbate ($pK_a$ = 4.17) and its oxidation product dehydroascorbate ($pK_a$ ~ 8). Purine adsorption has not been extensively investigated. As a consequence, extents of adsorption for uric acid ($pK_a$ = 5.61) and its oxidation product allantoin are difficult to estimate.

Blood, sweat, tears, and mucus are complex assemblages of biochemical constituents. Mucins and other macromolecules may adsorb yet be relatively resistant towards oxidation. Resistant macromolecules may block access by hydrophilic antioxidants and at the same time facilitate access and reaction by amphiphilic biochemicals. Major cations ($Ca^{2+}$, $Mg^{2+}$) and anions ($HCO_3^-$) may alter the aggregation state of mucins and other macromolecules.

The re-oxygenation of $Mn^{2+}$(aq), $Fe^{2+}$(aq), and other dissolution products under biofluid conditions is poorly understood. If re-oxygenation rates are significant, catalytic redox cycling can occur, with adverse toxicological consequences.