# Geochemical modeling of lung fluid-mineral interactions: Highlighting fundamental knowledge gaps

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Minerals respired into lungs are known, from a number of epidemiological studies and historical accounts, to have significant human health effects when the dose is high. These health effects often have latency periods of tens of years before symptoms manifest. Geochemists and mineralogists can contribute towards an understanding of how these diseases work in considering mineral interactions in the lung as a fluid-mineral interaction problem. We have performed a series of fluid-mineral interaction models utilizing the Geochemist's Workbench modeling platform, considering thermodynamic, kinetic, and fluid flow parameters towards the dissolution of a set of commonly encountered minerals. Employing rate laws from the literature, we calculated possible residence times of minerals in the lung and found that those times and possible mineral reactions products were sensitive to dose, particle size, lung fluid composiiton, and the flushing rates of fluid across particles in the lung [1].

These calculations bring into light some fundamental parameters that are poorly defined but are important in our ability to define how minerals behave in human lungs over decadal scales. While some reaction rates for minerals are defined in fluids of similar composition to lung fluids [2], many mineral rate laws are not well defined for these conditions. The composition of lung fluid itself is also not well defined with respect to some fundamental chemical speciation, noteably the speciation of phosphorus, and the organic speciation of many key cations for whose activity these calculations of mineral reactivity need to be defined. Additionally the physiological role of fluids flushing past minerals is largely undefinined in the human lung, and may have a significant role in the biodurability of minerals.

Within this context as well we can consider how mineral reactivity may be linked to cellular damage and the initiation of fibrotic diseases and cancers. Mineral reactivity can affect cells directly or can affect the biochemical environment cells function in through possible surface reactions that generate reactive molecules (often readicals), sorption of key biomolecules, or changes in the surrounding pysicochemical environment these cells reside in. Some of these reactions may be quite different if we consider the immediate reactivity of a mineral when it enters the lung and becomes whetted by lung fluid v. the reactivity of a mineral and potential secondary minerals forming on dissolution of that mineral over decades. We will discuss the results of our modeling study and what they have brought us to consider about the future state of mineral reactivity and lung fluid interactions.

[1] Taunton et al. (2010) American Mineralogist 95, 1624-1635. [2] Jurinski and Rimstidt (2001) American Mineralogist 86, 392-399.

# Effect of fertilizing soil with Selenium on trace element uptake by kenaf (*Hibiscus cannabinus*)

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Fertilizing food and feed crops with Selenium (Se) fertilizers can result in an increased uptake of Se by the crops, which may be beneficial for humans and animals consuming these crops. However, assessing nutritional quality of Se-enriched crops includes not only studying uptake of Se by the crops, but also how the uptake of other trace elements is affected by fertilizing the soil with Se fertilizer. Therefore, we fertilized three types of soils with two types of Se (Selenate and Selenite, 1 mg Se $kg^{-1}$ added to the soil) and studied the uptake of Se, Cd, Cu, Mn, Ni, Pb, Al, Fe, and Zn by kenaf (*Hibiscus cannabinus*), an indicator plant species for Se, grown on these soils. The three soils were clayey, loamy and sandy, and originally contained 0.50, 0.28 and 0.29 mg Se $kg^{-1}$ dry mass, respectively. Afterwards, we conducted this experiment again on loamy soil using different application doses (0.5, 1, 2 and 4 mg Se $kg^{-1}$ added to the soil).

Applying Selenate resulted in the highest increase of Se concentrations in the crop, with the highest accumulation being obtained on sandy (477 ± 77 mg $kg^{-1}$) and loamy (518 ± 97 mg $kg^{-1}$) soil, whereas Selenite performed best on a sandy (107 ± 17 mg $kg^{-1}$) and a clayey (122 ± 23 mg $kg^{-1}$) soil. Applying Selenate affects also significantly the concentrations of the other metals in crops grown on the loamy soil, but not in crops grown on the clayey and the sandy soil. When the Se application dose is varied on the loamy soil, Zn is already affected from an application dose of 0.5 mg Se $kg^{-1}$. The concentration of Al starts to be also affected from 1 mg Se $kg^{-1}$, and the concentrations of Fe, Mn and Pb also from 2 mg Se $kg^{-1}$. The Cu concentration is affected from a dose of 4 mg Se $kg^{-1}$ onwards. The Al concentration clearly decreases with increasing application dose of selenite, whereas changes are less clear upon application of selenate. Zn, Pb and Fe concentrations are always reduced when applying selenite. Upon application of selenate, they are also lower than the control concentrations at the lower application doses (until 2 mg Se $kg^{-1}$), but they are elevated at the highest application dose (from 4 mg Se $kg^{-1}$). This may be related to reduced plant growth observed when selenate is used at its highest application dose. Mn concentrations are not affected when applying selenite, but they are reduced when applying selenate. Our findings illustrate that different metals respond to Se application in a different way.

Experiments with other crops and other Se fertilizers, including Se nanoparticles, that also focus on effects on Se mobility in the soil and the effects of ageing, are still ongoing. Results of these experiments will also be presented.