Kinetic Monte Carlo models: A powerful tool to predict mineral reaction kinetics

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In many branches of Earth sciences we are currently observing a major change, as researchers quantifying the chemical behavior of complex systems must now supply predictions of the future state of these systems. Specifically, the prediction of coupled mineral dissolution and precipitation processes are critical for a large number of applications.

In our view, this challenging task requires a comprehensive re-evaluation of our current way of doing business, as it will become increasingly expensive and time-consuming to study the systems of interest only in an inductive way, i.e., by taking measurements and conducting simplified experiments. These results may be extrapolated at best.

At the same time, increasing and cheap computer power in combination with more sophisticated software provides a complementary tool [1]. We have started to employ kinetic Monte Carlo (KMC) simulations to model and predict mineral dissolution behaviour, 3-D grain systems and pore-system evolution even in multi-grain systems. We will provide some examples of current results. Of particular interest is the combination of KMC results with the new rate spectra concept [2]. Having said this, we are convinced that the value of experiments will further increase because the predicted results must be tested independently. KMC results will thus determine which experiments are critically important to conduct.

[1] Luttge et al (2014), *Elements* **43**, 132-157 [2] Fischer et al. (2012), *GCA*, **98**, 177-185