Kinetic Monte Carlo models: How can sensitivity analysis improve our understanding of pyroxen dissolution anisotropy ?

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For decades, the development of mineral dissolution rate laws has been based on an important diversity of laboratory experiments, analytical characterizations and numerical studies. Even if new analytical advances, such as the use of Vertical Scanning Interferometry to study mineral dissolution rates, have allowed for a better understanding of the dissolution processes, they still fail to precisely explain the atomic scale mechanisms occurring at the mineral-solution interface. Complementary numerical approaches such as molecular dynamics or kinetic Monte Carlo (kMC) simulations are therefore required to gain knowledge on the elementary steps controlling mineral reactivity. In particular, kMC simulations are valuable method to gain insights into the dissolution process without dealing with complex modeling. Many studies have demonstrated their interest on simple Kossel crystals and some real minerals such as calcite and muscovite or silicate glasses. In our study, we applied kinetic Monte Carlo simulations to enstatite dissolution. The main objective is to understand the extent to which these models can reproduce the dissolution anisotropy measured in laboratory for four different faces: (100), (010), (001) and (210). We show that sensitivity analysis (SA) on these models can provide many different information on dissolution and that, without using any scaling parameters, they can reproduce laboratory results, within errors. Furthermore, we will show that the SA makes it possible to propose a general analytical expression for the dissolution of each studied face, which depends on the probability of detachment of the various atoms from the crystal surface.