

Modeling MgO Particle Passivation during Carbonization

VITALII STARCHENKO, KE YUAN, ANDREW G. STACK
AND JULIANE WEBER

Oak Ridge National Laboratory

Presenting Author: starchenkov@ornl.gov

In recent studies on mineral reactivity for the application of CO₂ capture from the atmosphere (for instance in mineral looping process) one of the open questions is a possible passivation of reactive surface area during the carbonation process. Passivation can dramatically reduce the CO₂ uptake by the reactive mineral and prevents the application of mineral looping.

In this study we present numerical analysis of the transport properties of the inert solid layer which grows on the reactive mineral in combination with microscopic analysis of samples from long-term (decades) carbonation experiments. In ex-situ characterization studies using transmission electron microscopy and time-of-flight ion mass spectrometry of reacted MgO minerals we measured the thickness of the carbonated layer, which, assuming dominantly diffusive nature of reactive species transport, can be converted into the effective diffusion rate. We demonstrate that the diffusivity of the passivation layer is in the range of 10^{-8} - 10^{-9} cm²s⁻¹ which is much higher than the diffusivity of solid material. This indicates that the transport is potentially enhanced by porosity generation during the carbonation process or via the grain boundaries in a polycrystalline solid. Furthermore, we will discuss the use of pore scale modeling for multiple solid phase dissolution-precipitation problem.