Metadynamics technique offers insight into mineral growth and dissolution

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By using a novel technique to better understand mineral growth and dissolution, researchers at the Department of Energy's Oak Ridge National Laboratory are improving predictions of mineral reactions and laying the groundwork for applications ranging from keeping oil pipes clear to sequestering radium.

The mineral barite was examined to understand mineral growth and dissolution generally, but also because it is the dominant scale-forming mineral that precipitates in oil pipelines and reservoirs in the North Sea. Oil companies use a variety of compounds to inhibit scale formation, but a better understanding of how barite grows could enable them to be designed more efficiently.

Additionally, barium can trap radium in its crystal structure, so it has the potential to contain the radioactive material.

In a paper featured on this month's cover of the Journal of the American Chemical Society, the ORNL-led team studied barite growth and dissolution using metadynamics, a critical technique that allows researchers to study much slower reactions than what is normally possible.

"When a mineral is growing or dissolving, you have a hard time sorting out which are the important reactions and how they occur because there are many things that could be happening on the surface," said Andrew Stack, ORNL geochemist and lead author on the paper. "We can't

determine which of many possible reactions are controlling the rate of growth."

To overcome this hurdle, ORNL Chemical Sciences Division's Stack started with molecular dynamics, which can simulate energies and structures at the atomic level. To model a mineral surface accurately, the researchers need to simulate thousands of atoms. To directly measure a slow reaction with this many atoms during mineral growth or dissolution might take years of supercomputer time. Metadynamics, which builds on molecular dynamics, is a technique to "push" reactions forward so researchers can observe them and measure how fast they are proceeding in a relatively short amount of computer time.

With the help of metadynamics, the team determined that there are multiple intermediate reactions that take place when a barium ion attaches or detaches at the mineral surface, which contradicts the previous assumption that attachment and detachment occurred all in a single reaction.

"Without metadynamics, we would never have been able to see these intermediates nor determine which ones are limiting the overall reaction rate," Stack said.

To run computer simulations of mineral growth, researchers used the Large-scale Atomic/Molecular Massively Parallel Simulator, a molecular dynamics code developed by Sandia National Laboratories. Co-authors on the paper are the Curtin University (Australia) Nanochemistry Research Institute's Paolo Raiteri and Julian Gale.

Provided by Oak Ridge National Laboratory