Sandia National Laboratories
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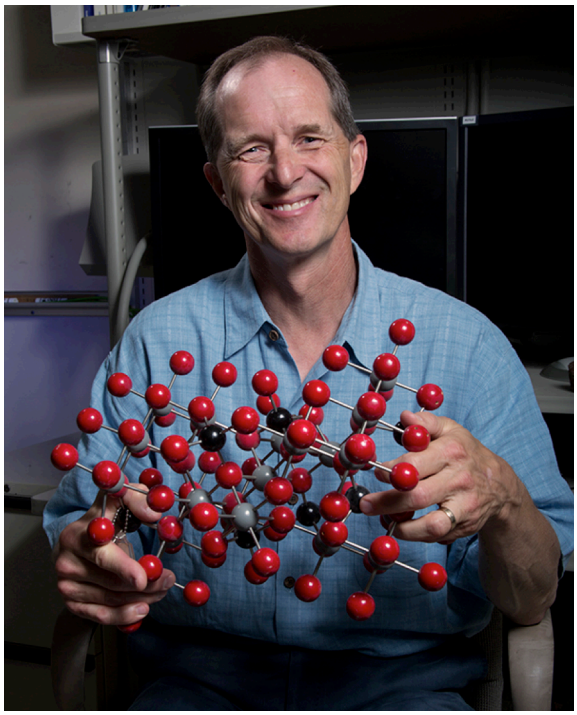
Computer Power Clicks with Geochemistry

Sandia is developing computer models that show how radioactive waste interacts with soil and sediments, shedding light on waste disposal and how to keep contamination away from drinking water. "Very little is known about the fundamental chemistry and whether contaminants will stay in soil or rock or be pulled off those materials and get into groundwater," said Sandia geoscientist Randall Cygan (Geoscience Research and Applications Dept.).

Clay minerals are made up of aluminosilicate layers held together by electrostatic forces. Water and ions can seep between the layers, causing them to swell, pull apart, and adsorb contaminants. "It's very difficult to analyze what's going on in the interlayers at the molecular level through traditional experimental methods," Cygan said.

Cygan and his colleagues turned to computers. "On a computer we can build conceptual models," he said. "Such molecular models provide a valuable way of testing viable mechanisms for how contaminants interact with the mineral surface."

Molecular modeling describes the characteristics and interaction of the contaminants in and on the clay minerals. "We've developed a foundational understanding of how the clay minerals interact with contaminants and their atomic components," Cygan said. "That allows us to predict how much of a contaminant can be incorporated into the interlayer and onto external surfaces, and how strongly it binds to the clay."



Sandia geoscientist Randall Cygan uses computers to build models showing how contaminants interact with clay minerals. (Photo by Lloyd Wilson)

The computer models quantify how well a waste repository might perform. "It allows us to develop performance assessment tools the Environmental Protection Agency and Nuclear Regulatory Commission need to technically and officially say, 'Yes, let's go ahead and put nuclear waste in these repositories,'" Cygan said.

Molecular modeling methods also are used by industry and government to determine the best types of waste treatment and mitigation. "We're providing the fundamental science to improve performance assessment models to be as accurate as possible in understanding the surface chemistry of natural materials," Cygan said.

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