



e-Science Points to Pollution Solutions (A Press Release from NERC)

Results from a UK e-Science project are helping to solve two pressing environmental problems. One finding could help to avoid arsenic contamination of drinking water extracted from man-made wells. Another could lead to improved methods of removing the now-banned industrial chemical, dioxin, from soil. The results were obtained using e-Science techniques and grid computing to simulate all the possible interactions between these contaminants and rock or soil.

Arsenic often appears in minerals rich in iron and sulphur, such as pyrite (fools' gold). Scientists working as part of eMinerals, a major project funded under the Natural Environment Research Council's (NERC) e-Science programme, have found out precisely how arsenic is taken up and held in the pyrite structure and the factors likely to lead to its release. "We now know that arsenic replaces the sulphur in pyrite rather than the iron, and that pyrite is likely to dissolve more easily when arsenic is present," says Dr Kate Wright, who worked on the project. Further work could identify ways of stabilising arsenic-containing iron sulphide rock by introducing additives that slow the rate at which it dissolves.

The eMinerals project found that a dioxin molecule will bind more strongly to clay surfaces the more chlorine atoms it contains, irrespective of the position of the chlorine atoms in the dioxin molecule. It also found that binding is

stronger the greater the electrical charge on the surface. However, water competes with dioxin to bind to surfaces and, in practice, a dioxin molecule's ability to bind to a surface is a balance between the binding strength of the dioxin to the surface, the water to the surface, and the dioxin to the water.

Both examples involved performing numerous simulations of the interactions between the different minerals in soil and rock with all the known variants of the contaminants. For example, there are 76 different variants of the dioxin molecule and numerous mineral surfaces in the environment to which they can attach, so hundreds of serious calculations are necessary.

The project has developed a grid infrastructure consisting of clusters and condor pools (including campus grids) at the collaborating institutions and resources held on the National Grid Service and the North West Grid. High performance computing resources can also be accessed for particularly large simulations if necessary.

Without access to such grid resources, researchers would have to perform all of the simulations sequentially, taking too much time to be practicable. Using the eMinerals infrastructure, they can submit all these jobs at once and see the results within a few hours. Results are automatically returned to a distributed data store with an interface that shows the files as if they are part of a single system. The data can be

accessed remotely by collaborating scientists, as well as by those who originally submitted the job.

“We’re doing grid properly. We can submit hundreds of jobs from the user’s desktop to a number of different compute grids, and get the data back with metadata attached and with the analysis done - and in a state that enables collaborators to understand what the simulations are saying. We’re giving control back to the user,” says Professor Martin Dove, eMinerals principal investigator.

Further information

See Web site at

<http://www.eMinerals.org> .

Martin Dove and other members of the eMinerals team will be talking about results from the project and demonstrating the eMinerals technology at the 7th UK e-Science All Hands Meeting in Nottingham on 10-13th September 2007

<http://www.allhands.org.uk>

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