Chemicals case study

Modeling at Corning - An Interview with Jim Dickinson, Glass Research Department, Corning Science and Technology Division

The website (www.corning.com) of Corning Incorporated states: "Corning is a global, high-technology company that has been changing the world through research and technological innovation for more than 150 years. By integrating scientific discovery with market need, the company has developed leading positions in the telecommunications, information display, and advanced materials industries.

The company is an industry leading manufacturer and supplier of optical fiber, cable systems, photonic components and networking devices for the telecommunications industry; and high-performance flat glass for television, information display and other communications industries. The company also develops advanced materials for the scientific, semiconductor, environmental and ophthalmic markets.

With research centers around the world and more than 90 manufacturing locations, Corning employs more than 32,000 employees in 34 countries. Its diverse portfolio of businesses are aligned under two major business sectors: Corning Optical Communications and Corning Technologies. The company's revenues for 2001 were \$6.3 billion."

The interview

What follows is the transcript of an interview conducted by Accelrys with Jim Dickinson, Glass Research Department, Corning Science and Technology Division.

1. Which modeling, simulation and/or informatics product(s) does your company use and what role do they play in your research process?

We have Cerius² materials science modules and Materials Studio. We have no formal molecular modeling group here at Corning so the use of computational products is up to the individual scientist. We use them for anything from basic visualization of crystalline materials to high-level ab initio based molecular dynamics calculations using DMol³ and CASTEP. In most cases the role the software plays is in testing a new idea or reaction for its probability of occurrence or confirming an assignment of a vibrational band to a particular species in the material.

2. What do you use these applications for? How does this work contribute to your company's long-term goals?

In general we use computational techniques for studying the dynamic and electronic properties of materials — in particular glassy materials. We are a glass company, so understanding at a fundamental level the origin of defects, for example, and how they effect the optical properties of glass, will lead us to better design processes to eliminate their effects.

3. Have you published work in the scientific literature and/or general press that uses computational software? If so, when and where?

Yes. In 2001 at the Internatinal Congress on Glass in Scotland

4. What did the software enable you to do that experimentation didn't?

The research reported involved looking at the dynamics of the interaction of different gas species with amorphous silica. We were able to show that these interactions can result in non-intuitive structural changes that were previously unrecognized.

5. What would you say are the main scientific advantages of using computation over experimentation?

You can obviously carry out computational experiments at conditions that are unavailable in the laboratory. The main advantage I feel, though, is the ability to pick apart the data and understand the exact origin of the what you have calculated.

6. Did the use of computational techniques save resources in terms of time or money as compared to experimentation?

Yes, in several cases the use of computational methods led us to experiments that would either not have been done or would have been done at a later stage in the project.

7. How quickly did your company/organization re-coup the initial investment in the software (including initial, installation and running costs) in terms of cost savings mentioned in the previous question?

I don't have an answer to this in concrete numbers. I would say within 6 months.



8. Did the use of the computational chemistry techniques result directly in refinements to existing processes? And, if so, how much has it saved your company? If yes, how much do you predict the techniques will save your company in the future?

Yes, computational methods have resulted in refinements to processes. I don't know how much money has been saved exactly, but I would say in the 5-10 million dollar range if all costs were considered. Of course this can vary from company to company depending on the particular application.

9. Would you recommend the use of modeling/simulation to your peers?

Yes.

