

## BP, Modeling, Data, Catalysis, and Me - an Interview with Dr Joseph T. Golab, BP Chemicals

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BP Chemicals ([www.bp.com](http://www.bp.com)) activities include the exploration, production, transportation, and refining of crude oil and natural gas, and the manufacture and marketing of petrochemicals. Products and services cover three main areas - on the road (e.g. fuels and stations), for the home (e.g. gas (LPG)), and for business (e.g. fuels and lubricants).

This multi-national company operates in four business segments: exploration and production; petrochemicals; refining and marketing; and gas, power, and renewables. It comes as no surprise that applying, maintaining, and developing a computational chemistry research program across such a large, diverse organization not only presents many challenges, but also plenty of opportunities.

Michael Francis, Accelrys, caught up with the scientist tasked with this challenge, Dr Joseph T. Golab, Technology Manager for Chemistry Modeling, Global Technology & Engineering Department, BP Chemicals, at AccelrysWorld 2004 to find out more.

BP Chemicals uses molecular modeling for a number of purposes. Perhaps most obviously, BP scientists use modeling to understand chemistry on a molecular level. But they go beyond this, aiming to enhance research by creating new work processes at the molecular scale, transferring science from the model to the lab to the plant. Modeling must generate chemical and engineering data that is useful in making technical business decisions. An interesting trend is the need to link chemistry modeling results to engineering simulation tools. The data generated from all of these efforts requires effective informatics systems.

"The overall goal of BP's modeling and simulation efforts is to ensure that valuable, valid, and relevant information is provided to the scientist and engineer in a timely manner," explained Dr Golab. "To effectively achieve this goal my role is split into three areas - introducing and maintaining chemistry modeling tools across the company, introducing a 'network program' to share information, and designing and introducing effective informatics systems to

store data and information generated by modeling so that it can be mined and used beyond the immediate future."

The introduction of modeling programs involves far more than simply telling people what tools to use, explained Dr Golab. "We want to ensure that we continue to keep up with the best tools available, so we do a lot of evaluations and alignment of new tools that are similar to what we already use." Dr Golab discussed the resource aspect, "Other sectors in BP have greater computer resources than we do. We try to tell them our needs and advise on what tools to buy."

BP is structured in 'vertical' units by business and along product lines. So it is vital that communication flows across the organization between chemists and engineers with connected interests. Dr Golab explained how this has been tackled. "We introduced a network programme that slices across these different silos, to share the information."

"Twice a year the five networks meet - a modeling and simulation network, a high throughput experimentation network, a catalysis network, a process technology engineering network, and a materials science network - to ensure the sharing of information."

"In the molecular modeling network, for example, discussions often include specification and competencies requirements, and the training and equipment people need."

"We work as a team to review every single business unit in a 2-3 year cycle, looking at what kind of modeling and simulation they're using, and advising on and demonstrating new tools that have been released since previous meetings."

The third aspect of Dr Golab's role involves the effective company-wide storage of data and information in a way that can be used in both the short and long-term future. "We strive to bring about a standard common paradigm for a scientist to capture and share the context around the data that they've collected, be it from models or from experimentation."

"It's not just so that the data can be shared with people down the hall, but with the person two years or three years from now. How is that person going to understand why and where this data originated? The problem we want to avoid is someone knowing that the experiment was done because they have the data, but not knowing why the experiment was done. The original data-collector may no longer be around to be quizzed."

Directed by Dr Golab, it is clear that computational chemistry plays an important role in BP. One major application is in the understanding and design of more efficient industrial catalysts. "Catalysts underpin almost all the processes that we do today. With a few exceptions, for example, explosions, every process requires a catalyst to do it more efficiently or more selectively."

"Many of our products are small gas phase molecules, produced via catalytic mechanisms, which makes them extremely amenable to calculation." Catalysts investigated using modeling include those involved in methane to methanol conversion and a catalyst used to control polymer properties by modifying stereoblock microstructure. "We are now using computation to investigate a wide range of chemicals and processes - studying mechanisms and reaction schemes, kinetic effects, what happens if metals are interchanged, inhibitor effects, chemical neighborhood, active sites, the effect of time, and whether or not modeling efforts can be linked with high-throughput experimentation."

And the practical applications of these end products? The majority of BP's products are raw materials that are sold on and refined by third parties.

Dr Golab gave some examples. "Purified terephthalic acids are used in wide-ranging everyday applications. For example, fibers in clothes and in plastic drinks bottles. Acrylamides, after further processing, are made into fertilizers. Gas phase products, for example ethylene and propylene, are used in energy production. Polypropylene, after cracking, gives polyethylene that can be made into car bumpers for example."

But what about the advantages of the use of modeling and simulation tools? "The tools have enabled a better understanding of reaction mechanisms so that we have more efficient processes which lead to less waste," said Dr Golab. "Computation enables the prioritization of experiments, in some cases eliminating non-starters, resulting in substantial resource savings."

"It is easier to delete a file than clean tar out of a pilot plant," concluded Dr Golab.