

Modeling at Sasol - An Interview with Dr Petrie Steynberg, Chief Scientist, Research and Development, Sasol Technology (Pty) Ltd.

The website of Sasol Technology (Pty) Ltd. (www.sasol.com) states: "The Sasol Group of companies comprises diversified fuel, chemical and related manufacturing and marketing operations, complemented by interests in technology development and oil and gas exploration and production."

Its principal feedstocks are obtained from coal, which the company converts into value-added hydrocarbons through Fischer-Tropsch process technologies. Sasol also uses various petrochemical feedstocks in its chemical plants outside of South Africa. It also has interests in crude oil refining and chemical production and marketing through a number of global strategic partners or joint ventures. More recently, Sasol has embarked on developing international gas-to-liquids ventures, based on its unique slurry phase distillate process."

The Interview

What follows is the transcript of an interview conducted by Accelrys with Dr Petrie Steynberg (or Petrus J. Steynberg), Chief Scientist, Research and Development, Sasol.

1. *What computational modeling, simulation, and/or informatics tools does your company use?*

In our R&D environment we have a stern focus on homogeneous and heterogeneous catalysis research. Quantum calculation tools applicable to single site and surface catalysis are used.

2. *What do you use them for? How does this work fit in with your company's long-term goals?*

From a catalysis perspective, we use computer simulation to predict chemical structures, thermochemistry, and reaction barriers. In the quest to stay abreast in international fast tracked technological areas, molecular modeling is of strategic importance to speed up product/process development and to guide experiment.

Industry Sectors

Petrochemicals
Chemicals

Organization

Sasol Technology (Pty) Ltd



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

Intellectual property permitting, we do publish in open scientific literature, either as part of experimental work or pure theoretical publications. For example, see:

Dalton Transactions, 2003, 10, 2036-2042

Dalton Transactions, 2003, 4669-4677

Organometallics, 2004, 23, 1207-1222

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

Modern R&D efforts don't have the same time luxuries like perhaps a few years back. Implementation and correct application of molecular modeling software saves time. In certain instances where experimental data is lacking, theoretical alternatives is the only cost effective alternative.

5. What would you say are the main scientific advantages of using computation to drive, refine and/or even replace experimentation? Likewise any financial advantages? Did its use save resources - i.e. time, money...?

We believe that computation will not replace experimentation in the foreseeable future. It has however, found commonplace in our R&D projects. Unless a unique modeling based discovery/suggestion translates into commercial operation, financial advantages are difficult to realise. However, the use of molecular modeling has saved time and thus money for Sasol.

6. Did the use of the computational chemistry/biology techniques result directly in refinements to existing processes? And, if so, how much has it saved your company? And in the future?

Unravelling the fundamentals of industrial important existing technologies, has resulted in unique IP positions for Sasol and is thus a key component in establishing Sasol's position for selected technological areas. To translate e.g bargaining value into monetary terms can be done; however, we haven't gone that far. We wish to continue with the current value adding to applicable projects in the medium and long term horizon.

7. How long would you say that it took for your company/organization to recoup the initial investment in the software (including initial, installation and running costs) with any cost savings mentioned in the previous question?

With the success rate of R&D efforts in the international arena at best 10-15%, it is not straight forward to calculate a return on investment for any R&D expense, let alone for one of the essential enabling tools. From an international survey published in 2002, sustainable investment for the commodity/petrochemical industries should be 1 modeling specialist per \$1-4 B/yr revenue. From the outset, our investment was very conservative in human capital as well as hard- and software and we will continue along this road.

8. What do you and your organization plan to use the software for in the future?

We wish to maintain our current Status Quo where the mainstay of our activities will be in the catalysis area.

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

Yes.