



Modeling at Halliburton - An Interview with Jim Weaver, Ph.D., Senior Scientific Advisor, Duncan Technology Center, Halliburton

Introduction

The website of Halliburton reads, "Halliburton, founded in 1919, is one of the world's largest providers of products and services to the petroleum and energy industries. The company serves its customers with a broad range of products and services through its Energy Services Group and Engineering and Construction Group business segments. In 2001 the company had revenues of \$13 billion and employed approximately 85,000 people at year-end. Halliburton conducts business operations in over 100 countries throughout the world and in 2001 revenues from locations outside the United States represented 62 percent of the company's revenues."

The interview

What follows is the transcript of an interview conducted by Accelrys with Jim Weaver, Ph.D., Senior Scientific Advisor.

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

The principle softwares used in our Duncan Technology Center are Cerius 2 , Gaussian, and Chemoffice.

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

We are committed to being the leaders in our industry. This requires both the ability to efficiently study molecular systems and to be able to communicate our findings.

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

We have a number of publications that presents data generated using molecular simulations. Most of this has been in the Society of Petroleum Engineers publications.

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

Visualization of molecular simulations significantly impacts our ability to communicate and demonstrate molecular concepts at a level that is more easily understood by non-chemists. It allows us to 'fill-in' data to supplement experimental data.

5. *What would you say are the main scientific advantages of using computation over experimentation? Likewise financial advantages? Did its use save resources - i.e. time, money...?*

I do not support the concept of computational over experimental. I do find that there is a significant synergy gained by using both together and appropriately. The synergy results in better understanding, which provides shorter product development times and superior products. Time to market and products with fewer problems is real money.

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

Probably five years or more, but recall that when we started, high speed computing was very expensive and unstable, software was difficult to use and not very flexible as to the problems that could be addressed. Now computing power is cheap and software is tolerant and easy to use.

7. 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? And in the future?

Computational chemistry has contributed significantly. Several products have been developed where molecular simulation played a principle part. Many others where the contribution was smaller, but still important.

8. Did the use of the computational chemistry techniques allow you to gain a competitive advantage?

It improves our time to market in product development, and it often provides support to product marketing efforts.

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

We plan to increase our effort and are expanding number of users and providing appropriate training.

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