

gPROMS: a model system?

Vicky Ashley, Richard Jarvis and Scott Owens give their verdict on this process modelling package



(Left to right):
Richard Jarvis,
Vicky Ashley
and Scott Owens
at Nexia
Solutions, Risley
Background:
The Nexia
Solutions
Technology Centre
flagship building

gPROMS is an advanced process modelling (APM) environment from Process Systems Enterprise (PSE). It looks similar to the traditional steady-state flowsheeting packages, but uses an equation-oriented architecture to represent equipment, chemistry, physics, operating procedures and other relationships as mathematical equations, to whatever degree of accuracy is required (or possible!).

The main advantage of this architecture is that once the model is created, any solution technique can be applied. It can be used for steady-state or dynamic simulation, optimisation (including dynamic optimisation), parameter estimation and experiment design. gPROMS provides facilities for managing all of these activities.

At Nexia we adopted the package in 2005 as a replacement for our existing APM and flowsheeting software, which we felt was not developing in the way that we wanted, and had some modelling and

robustness limitations.

Our year-long evaluation involved testing various modelling tools on the market against a rigorous list of "ideal software" criteria. We also investigated the working relationship with the suppliers, as this is important to us. gPROMS and PSE came out highly in all areas; there were some limitations, but – crucially – no "show stoppers".

how and why do we use it?

We use gPROMS as a modelling and solution framework. The software is used primarily by process modellers and chemical modellers; each has different requirements, but both need powerful modelling and solution tools that are easy to understand and work with.

Process modellers typically work with a process flowsheet representation that sees the process in chemical engineering "unit-and-stream" terms. Chemical modellers use gPROMS as a dynamic solver, developing detailed chemistry models that are delivered back into the chemical engineering environment to provide increasingly-accurate predictive models.

In the past we tried mathematical solver software for the chemistry side, but this led to complex and uncheckable models for large sets of dependent reactions. It was much more difficult to access information and maintain models than it is in gPROMS. Another big advantage of our current setup is that both the process and chemical modelling groups can work with a common tool.

A typical "project lifecycle" involves developing and conducting quality assurance (QA) tests on them, performing sensitivity analyses, performing parameter estimations to adjust model parameters to laboratory or pilot data, and analysing model results. Only when this has been done do we deploy models and scale up results. An essential requirement is that the environment can cope with all these activities.

Because of the type of applications we have, most of our models need to be custom built. PSE does provide a library of standard models, but we tend to use these just as a starting point for our own.

Another key aspect is the linking of modelling with experimental work and pilot plant trial data. Because of the costs and safety implications of running

radioactive experiments and pilot plant trials, we build existing knowledge into models that are then used to reduce the number of experiments required to a safe minimum. We also use models to interpret experimental data to provide accurate parameter values and confidence information, which is important in risk management. Once we have sufficiently accurate parameters, we can use this information to reliably scale-up the process.

In the future we will apply gPROMS' formal model-based experiment design techniques to design optimal subsequent experiments, minimising the number of factors to be considered and thus the experiment time, costs and materials requirements.

example

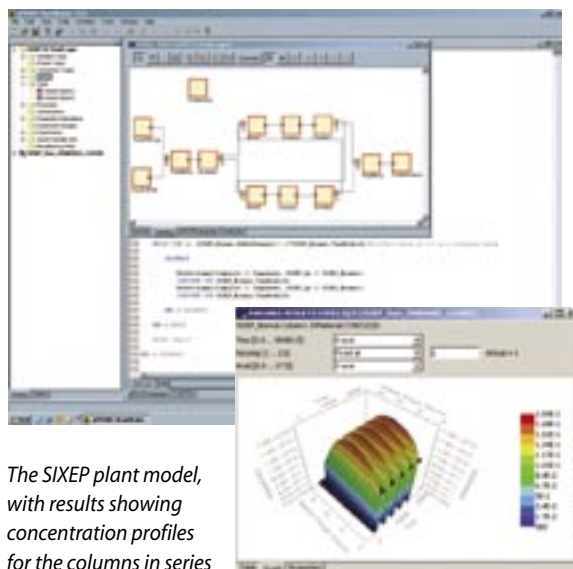
A typical application is the Sellafield ion exchange effluent treatment (SIXEP) plant, an ion exchange process designed and commissioned in the 1970s to remove radioactivity from a particular effluent stream.

In recent years, the decommissioning of plants means that there is a strong commercial motivation to use SIXEP to treat additional effluents. However, before our customer does this, they need to prove to themselves and the Environmental Agency that the process will still perform effectively and reliably.

Though the original engineering was very sound, there is no obvious way to extrapolate the original data to validate performance for new feed compositions and process conditions. This is where predictive modelling can help.

Over the years we have built a high-level chemical engineering description coupled with increasingly accurate chemistry models. The current gPROMS model now embodies the SIXEP engineering, physics and chemistry (down to ion exchange levels) in a mixture of first-principles and empirical models backed up with experimental data.

Before any recommended changes to the plant, we go through a rigorous modelling procedure, which includes a whole raft of experiments and QA to test model validity. The customer now considers this model as an essential requirement for their plant operations. The components of the model have since been applied to new ways of deploying



The SIXEP plant model, with results showing concentration profiles for the columns in series

ion exchange technology and in the evaluation of new materials.

impressions

Our major impression is that gPROMS is numerically very powerful, and provides all the process modelling capability that we need. This is the number one requirement.

It is also well-structured to the way that an organisation such as ours works, with a lot of interaction between different technology groups and rigorous QA procedures. Important features here are the model management capabilities, the "openness" of the gPROMS models, and the powerful audit facilities.

We also like the gO:Run facility, which allows gPROMS models to run in "execution mode" behind an Excel interface. This means that we can deliver packaged models (encrypted for confidentiality) for end users to

carry out their own investigations. We are prototyping this capability at the moment, and expect it to increase in importance as we deal with a wider range of clients.

A seemingly minor but important aspect for us is that we can run the software on our own server, which means that gPROMS can be used on any PC. Updates are downloaded from the web straight onto the server, where they are immediately available to all users. We can also execute applications in batch mode if necessary.

Naturally we have a few grumbles. For a start, parameter estimation facilities in gPROMS are too strongly geared towards expert users. Quite often, all chemists want to do is a quick least-squares fit to data; there needs to be more default options for the infrequent user. To some extent this could be addressed by better and more accessible documentation.

Nexia Solutions

NEXIA Solutions, the research and technology (R&T) subsidiary within the British Nuclear Fuels (BNFL) group of companies, uses Process Systems Enterprise's gPROMS advanced modelling package for modelling of complex nuclear and chemical systems.

The company specialises in nuclear chemistry and chemical engineering processes, in areas such as waste management, fuel reprocessing, asset maintenance and treatment of radioactive effluent. Its main function is to provide R&T support to nuclear sites to ensure their continued safe operation. Nexia Solutions is also currently gearing up to become a national nuclear laboratory. The role of the process and chemical modelling team is to underpin these services by providing model-generated data for decision support, using a variety of software tools.

As a supplier to the nuclear industry, it faces particular challenges. Nexia has to deal with complex chemistry that can involve two-thirds of the periodic table. Its customers' plants cannot be accessed or modified easily, and it is virtually impossible to add instrumentation. In addition to this, safety is critical.

the role of modelling

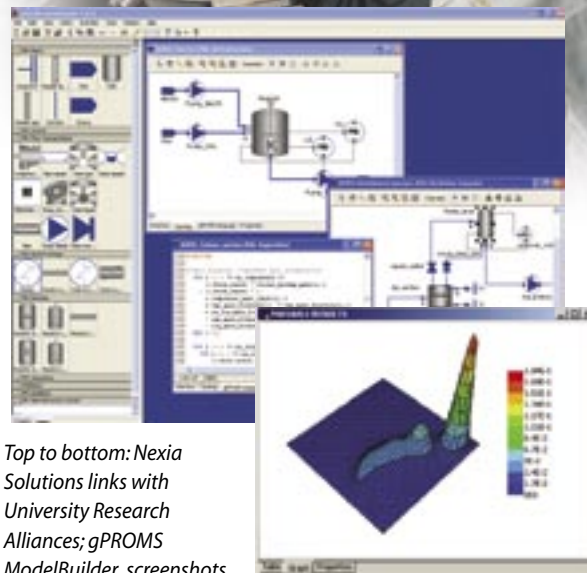
As a provider of services in this complex technology area it is essential that Nexia can justify decisions quantitatively to its clients. Modelling enables the company to do this, in a reproducible way. Equally important, it allows it to capture and build on that knowledge to make increasingly accurate predictions.

To model effectively, Nexia first needs to understand the science which underpins its customers' plants and processes and capture this knowledge in model form. Once this is done, the models support front-end and detailed design to improve design, safety, operations and economics by investigation and resolution of plant problems, as well as to develop and scale-up new processes.

In particular, modelling is used to minimise risk by removing uncertainties. It also provides a quality assurance (QA) audit trail, to demonstrate that Nexia has done the analysis, and to show how it came to its conclusions. This is essential in the nuclear industry.

Nexia uses a wide range of modelling software, including tools for process modelling, chemistry modelling, computational fluid dynamics (CFD), structural and impact analysis, operational research, environmental and seismic modelling. Increasingly modelling is becoming a differentiator in the service the company offers, for applications both inside and outside the nuclear industry.

gPROMS, a modelling and solution environment originally developed within Imperial College London in the 1990s and developed and marketed since 1997 by Process Systems Enterprise of London, is Nexia's key tool for process modelling.



Top to bottom: Nexia Solutions links with University Research Alliances; gPROMS ModelBuilder screenshots

Another current limitation is the fact that we cannot use named chemical species in model arrays (for example, the ability to refer to Mass ("U") rather than Mass (1)), which is a problem, as we sometimes deal with hundreds of species. At our request, PSE is introducing this in the next version.

Also, we'd like to be able to perform runs interactively from within the gPROMS ModelBuilder environment; currently this can only be done via the Excel interface. Similarly, sensitivity analyses require working from Excel or programming a task using the task language. We have discussed this with PSE.

One of the things we are very happy with is the relationship with PSE, which provides us with excellent support and regular modelling assistance. Also important to us is the fact that, as a key user in a key sector, we are members of the PSE Strategic Advisory Council. This gives us a strong say in development priorities, and confidence that our requirements will be taken into account.

the future

The potential impact of modelling on research and technology is something that we will exploit much more in the future, using the full power of gPROMS for model-based data analysis and experiment design. PSE is working with us to introduce these capabilities. **tce**

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