THE ENGINEERS TOOLBOX

A review of modelling and analysis tools

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Technical Summary

A range of software tools for process modelling are available at modest cost to operate on desktop PCs. The different types of modelling activity and their relationship are outlined, and the question of the availability of resources and knowledge raised. The different tools are discussed and their application illustrated with practical examples from the sugar industry.

MODELLING ACTIVITIES

The diagram below shows the information flows between various types of modelling activity.
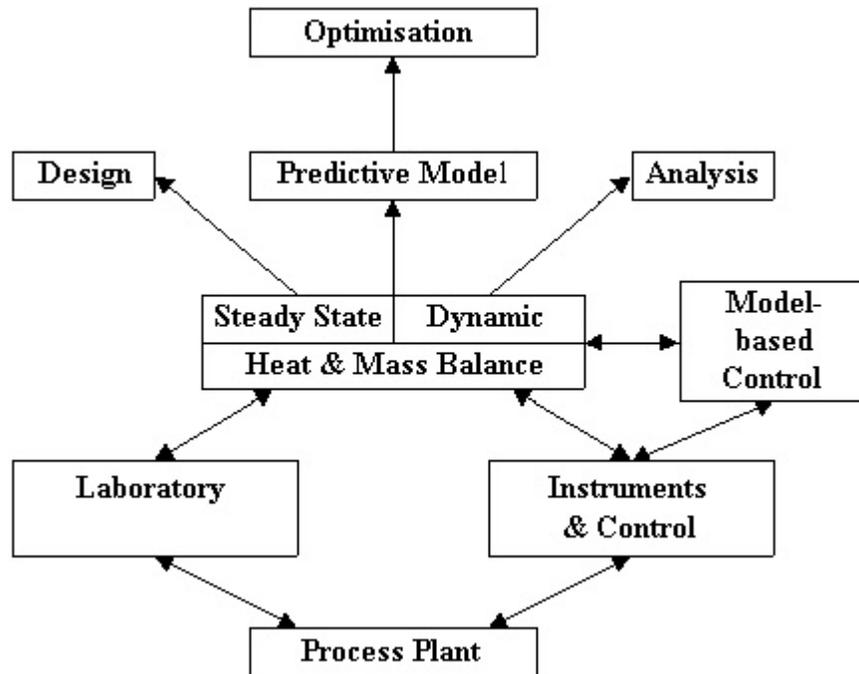

Figure 1. Information flow diagram

Heat and mass balances: This forms the foundation for further work and provides a comprehensive basis for process design. A model is built up from knowledge of the process and uses existing plant or laboratory data to calculate mass and energy flows.

Predictive model. A development of the heat and mass balance that models each unit operation based on physical plant dimensions or known performance. This allows the effect of changing feed materials or operating parameters to be predicted.

Optimisation: A mathematical technique to find the combination of parameters that gives the most favourable outcome from a model. The parameters are usually constrained to an acceptable range and the outcome is defined as an objective function such as "minimise annualised cost" or "maximise throughput".

Design: using the heat and mass balance data to design plant items or processes. Examples include pipe sizing, pump selection, heat exchange design.

Analysis: Using the heat & mass balance data to analyse some particular aspect of process performance. A good example of this is "Pinch Technology" analysis of energy requirements.

Dynamic modelling: An extension of the steady state heat and mass balance to include rate of change equations and introduce dynamic factors such as dead time and plant characteristics like vessel volumes. A dynamic model can predict the behaviour of plant in real time, to allow the investigation of plant stability or reaction to changes. Dynamic simulation concerns itself with second by second data, rather than perhaps hourly or daily averages.

Model based control: This is a slightly different activity to the others in that the "model" need not be a rigorous mathematical description of the process but can be an empirical equation or approximation, for example $y = mx + c$. Model based control software monitors a process to determine its behaviour and fit an empirical model to that behaviour, ideally this process should be continuous or repeated often to ensure the model remains valid as throughputs change and equipment wear takes place.

Skills and knowledge
Developments in software packages mean that it is no longer necessary to be a computer scientist to perform modelling work. This has created both problems and opportunities.

Knowledge
The capabilities of modern software may result in the user being exposed to a stage where he usually meets a problem – often lack of knowledge. If the chosen package can model a rotary vacuum filter the user may want to try a model of the filters in a sugar factory but find he is bombarded with input screens requiring particle size distribution, physical properties etc.
The level of fundamental knowledge in the sugar industry may not be sufficient to fulfil the potential that modelling has to offer. If one were to start a modelling project on the issue of colour formation in the sugar end or non-sugars extraction in diffusion it would soon become apparent that the knowledge required is not readily available, if at all.

Sugar industry R&D has tended in the past to be more concerned with process chemistry than with process engineering aspects. In recent years there has also been both an apparent decline in the volume of research done by the sugar industry and a shift in its focus towards diversification and customer-related product application work. It now seems likely that the sugar industry's knowledge has reached or will soon reach something of a plateau and that this will ultimately constrain the application of modern modelling techniques.

As examples of this shift are the research laboratories of British Sugar and of American Crystal Sugar, both of who have shifted a significant proportion of their efforts away from the sugar production process. The contribution of the Braunschweig Institute to the public knowledge base also seems set to decline as their funding is reduced, potentially a significant loss of engineering research and mathematical understanding of the sugar process.

The pressures of environmental legislation are also "tying down" research, engineering and capital resources for little tangible benefit to the environment.

Skills
In the past a modelling task may have been too difficult because either the computer power or specialist programming skills were not available. The increase in computing power and storage capacity, which has been accompanied by falling hardware costs, has eliminated computer power as constraint. Similarly the growth in software tools means that one doesn't have to code FORTRAN to solve a mass balance, although it can be an advantage to do so and may be necessary to use some of the advanced functionality on offer.

Packages currently on the market require 1-5 days formal training and perhaps a further 5 days of exploration and self-teaching to give the user the necessary skills to start to use the package in earnest. This assumes an engineer with an aptitude for computers and for mathematics is the user and that support from colleagues or software vendors is available. Regular use of a package for a few hours each month is probably the minimum required to keep the skills fresh and ready to use.

Large-scale users of modelling, for example petrochemical companies, often have teams of modelling specialists working on a range of projects. The have made the commitment to this level of resource on the basis of the benefits to efficiency or plant productivity that are to be expected from in-depth analysis and optimisation of process plant.

The sugar industry has a potential level of saving that is sufficient to fund modelling activities but in general has not taken up the challenge fully. In some cases this may be due to the unavailability of skilled engineers, or the inability to recruit and retain them.

Resources
A feature of the EU sugar regime is that it endows companies with sufficient profitability to fund capital investments, research and engineering activities, yet the quota system denies companies the ability to increase their output and hence their profits. This can result in a prevailing climate

of cost reductions in order to sustain profit growth-not necessarily a climate conducive to recruitment or to investing in modelling skills and systems.

Companies tend to spend too much time agonizing over software purchasing decisions and too little time considering the human resources required. Most of the bigger packages operate on the basis of an annual fee, combining license payments with upgrades and support.

The ongoing cost of owning two or three high-powered tools is unlikely to exceed the cost of a single engineer and may be as little as half that cost. To make use of the tools requires at least one and probably two engineers dedicated to the task, it therefore makes little sense to invest in software and not support that investment with the necessary manpower.

It may be appropriate to "buy in" the process modelling skills from the software vendor or from an independent consultant/contractor. This is done in the sugar industry to good effect and is one way of securing the necessary resource commitment. The investment decision must include costs of both software and personnel; one without the other is unlikely to be viable.

Using an external resource inevitably raises the issues of continuing support and maintenance of the models. External consultants/contractors can be paid to produce a level of documentation that an internal modeller may not have the time to produce, this can actually improve the long term support of a model. On the other hand, the lack of "in house" expertise can reduce the benefits and ease of application of modelling as part of the day to day business.

To be successful in the longer term a sugar company needs to be able to depend on an external resource continuing to be available, this will certainly be the case if sufficient work is placed externally but may not be if the quality of work is variable and unpredictable.

A survey showed that with most packages at least 5-10 days are required for a new user to be able to use the package. To this time one may need to add time to build in physical properties or to code models for specific unit operations, before any practical benefits ensues. The survey also showed that many of the respondents have been using a particular package for at least a year and many spend more that 50 days per year using it. This is further evidence of the need to dedicate resource to modelling if it is to be effective.

SOFTWARE TOOLS

 Spreadsheets: It is relatively easy to build a steady state mass and heat balance using a spreadsheet package available on most corporate desktops. Incorporating the physical properties data will take some time and it may be necessary to code some mathematical methods in a macro language to ensure convergence. A useful model can be produced although in many cases the documentation and testing will be less than perfect and the user friendliness verging on the hostile to anyone other than the author.

It is possible to produce a useful dynamic model in a spreadsheet too, although in reality the macro language/programming functions are paramount and the spreadsheet is primarily acting as a familiar user interface and data integration tool.

Add-in modules for spreadsheets are not commercially available to provide physical properties data for water and steam, and templates for boiler and turbine calculations can also be purchased. Mathematical routines and statistical analysis add-ins are available and growth of the Internet will only help the development of this source of tools and productivity aids.

Process simulators: A wide range of process simulation software is on the market, most of which specializes in hydrocarbon processing or petrochemical applications. This can make the packages poor value for the sugar industry customer as much of the cost has been invested in rigorous distillation and reaction models or comprehensive physical property databases. Many of the packages have difficulty handling the concepts of solids or aqueous solutions. In some cases requiring optional extensions to the package. Similar limitations apply to the unit operations models-one may have the choice of several distillation or reactor models but the chances of finding a sugar beet diffuser or a centrifugal model are limited. In these cases a model of a unit operation can be constructed from several building blocks (such as component splitters) or there may be a facility to code a model in a high level language.

In general it is the more sophisticated and costly packages, such as AspenPlus™ , that provide sufficient flexibility and functionality to allow sugar processes to be modeled effectively. One exception to this is Sugars™**,** which is a specialist PC simulation package specifically developed for the sugar industry. While Sugars™ provides sugar-specific unit operation models and physical properties it would be of little vale to an oil refinery or chemical plant.

Equation based simulators such as Speedup™ provide a high level language environment where processes and unit operations are defined by sets of equations which are then solved by a powerful mathematical engine. This is the ultimate in flexibility but brings with it a degree of complexity and a significant initial effort requirement, which may not be to everyone's taste. Potential purchasers of simulation software should concentrate on the issues of industry specific unit operations, physical properties, aqueous solutions and solids processing. Only the more powerful or the more specialist packages are likely to be adequate in these areas.

Prediction
The process simulators all possess some degree of predictive ability, particularly in the well-researched areas such as heat transfer. Most allow the user to input existing plant data to determine heat transfer coefficients and then goon to use the coefficients in predictive mode. Some contain rigorous models such as shell and tube heat exchangers where the effect of flow rate and process conditions on a given heat exchanger are calculated from first principles. Most spreadsheet tools developed by engineers are retrospective heat and mass balances rather than predictive. Using skill and judgement together with the back-solving/goal-seeking abilities of the spreadsheet they can be used for prediction to a limited extent.

Where predictive methods use empirical or plant measured parameters it is useful to have a software package that can calculate these parameters using techniques such as data reconciliation or parameter estimation. The routines are available in Speedup™, and Sugars™ uses

characterisation routines for centrifugals and solubility/saturation data for vacuum pans and crystallisers.

Optimisation

Prediction is a pre-requisite for optimisation. Once a robust predictive model is developed an optimisation routine can be applied to it with constraints to keep the search area in a practical zone. Optimisation is standard in a number of packages, including Speedup™ and AspenPlus™; some can do "what-if" table generation without locating the optimum.

A real time optimiser is a combination of an optimising model with a scheduler and plant interfaces. These allow periodic optimisation using plant data and a model, with the ability to feedback new optimum settings into the plant control system or offer them as advice.

Design

A number of tools are available that start from the foundation of a heat and mass balance. Netmate™ can calculate pipeline sizes and friction losses in a network of piping including control valves and pumps. Alfa Laval's CAS program will size plate heat exchangers and a range of packages is available to size shell and tube heat exchangers. Pump selection can be done with Netmate™ or with proprietary selection tools from the pump manufactures.

All of these packages have a common feature – they rely on a valid heat and mass balance to provide the process parameters that allow them to work. Ideally the mass balance should be determined for a range of conditions and the skilled engineer should test the flexibility of the systems designed to cope with process variations.

Analysis

Again using the foundation of heat and mass balance data, these packages look at a particular aspect of process performance and offer guidance on improving or optimising the design or operation of the plant.

The most developed field of application is that of Pinch Technology, analyzing the flows and temperatures to determine targets for minimum energy consumption or total annualized cost. Two packages in this market Supertarget™ and Advent™, include tools to directly extract process data from a number of simulation packages. Lower cost pinch packages such as Hero™ published by the IChemE in the UK are available for as little as $400, obviously with restricted functionality but perhaps providing a useful first step at a few percent of the cost of the heavyweight applications.

Dynamic modelling

Many sugar companies have yet to develop steady state heat and mass balances for their processes, so dynamic modelling may not be of immediate interest. Of the commercial packages, Speedup™ offers a real time simulation engine that is fully integrated with steady state modelling and optimisation tools. This allows a model to be developed and validated in steady state and then enhanced into a dynamic model by addition of rate of change equations, controller models and additional parameters such as tank volumes and time delay in pipelines.

Specific areas of the process have been dynamically modelled to solve problems or improve process control. Often this is done with specialist applications software (e.g. for dryers) or with a programming language such as FORTRAN.

Model based control
This is an area where both freestanding tools and add-ons to commercial control systems are available. The real time and multitasking nature of the application favours use of mini computers rather than PCs, although the growth in processor power and emergence of operating systems like Windows NT may accelerate the move to PCs.

Model based control does not require a rigorous mathematical model as the "model" used can consist of a set of gain and dead-time relationships between process inputs and outputs. It is quite possible to use a dynamic model.

A model based control system, such as Predictive Control's Connoisseur package, is equipped with interfaces for a range of control systems and the software tools required to input small disturbances into the process and monitor the results. In this way the package "learns" from the process response, reducing the need for detailed knowledge of the process dynamics.

As the complexity of the tools and mathematics employed increases the level of training and education necessary to use the techniques successfully also rises. Skilled practitioners in dynamic modelling or model based control are likely to have some form of postgraduate qualification have build up considerable experience of a range of processes. Increasingly this type of activity is become the preserve of the "expert" and many process operating companies buy in the services of consultants or the software companies to carry out studies for them.

Practical applications
This section describes successful applications along with some ideas for using models to simulate the reader into considering how modelling might be applied.

Updated heat and mass balance
One application of steady state modeling is to act as a reference data source. Some sugar companies do this by maintaining an updated process model of each factory, which reflects the current state of the plant and its recent investments.

This model then acts as a reference library to provide flow, temperature, physical property and composition data for any stream in the factory. When an engineer needs to specify a pump, heat exchanger, control valve etc. the basic data is readily available and he does not need to build a spreadsheet to determine the operating conditions.

These models are also used to determine the cost benefits of capital investment projects and to provide a common data interface to engineering companies who use the models at the basis of their design work for the sugar company.

Sugar house/refinery monitoring

The energy and extraction performance of a sugarhouse or refinery is largely determined the unit efficiency of vacuum pans, crystallisers and centrifugals. If solubility data is updated regularly the performance of each of these operations can be determined from the process laboratory data and mass balance model. By comparing these parameters with good practice or with previous results at the same factory it is possible to see where performance is deteriorating and take corrective action.

Similarly a regular colour balance calculation would aid diagnosis of sugar colour increases. Example parameters for regular monitoring would include massecuite saturation levels, centrifugal wash water % massecuite, and centrifugal crystal yield.
In addition to identifying performance issues the model could illustrate the benefit of correction by calculating the effect of changing any given parameter.

Pulp press optimisation

Where a number of presses of different size, design or characteristic are used there is a need to determine the optimum combination of operating speeds. This is a classic optimisation problem with constraints of meeting total throughput and speed/power limits on individual presses. This has been done with Speedup™ and with spreadsheet models.

As well as finding a steady state optimum the model can be used to assess the impact of slice rate or marc variations, or the effect of taking one press off line. This helps determine the number of variable speed drives that should be provided and the required speed turndown.

The outcome of these studies can be contrary to conventional wisdom, for example if a single layer press is added to a battery of small ones it should probably be run at its maximum speed.

Pulp Dryer Control

An alternative approach to dynamically modelling a drier is to use a model based control system where the model is an empirical one derived from plant responses. This has been done to good effect, using inputs such as drum inlet and outlet temperature, fan damper position, feed screw speed etc. By adding additional measurements such as pressed pulp moisture and dried pulp moisture the derived model can achieve a closer tolerance to the required set point.

A controller for dried pulp moisture evolves whish is predictive rather than simply feedback, overcoming the problems of the dead time in the drier drum. As pressed pulp feed moisture changes the model makes adjustments to prevent a deviation in product moisture occurring. The advantage of this approach over feedback control is clear – problems can be avoided or minimised rather than acted upon after they have happened. The same technology has also been applied to control of thick juice pH and to diffuser acidification, significantly reducing the process variability and hence saving money on chemicals and improving extraction.

Heat recovery optimisation

A real time optimiser system has been used to distribute process condensate between a number of heat recovery exchangers. The system modelled the heat exchangers by predicting

temperatures from known heat transfer coefficients and used this information to allocate the available condensate to achieve the best economic return. In building the model and determining the economics it became apparent that the value of the recovered heat was different for each type of heat recovery situation. This was due to the use of a number of fuels and to interaction with the steam turbine and the evaporators.

For example, if steam cost £5/tonne to generate in the boilers and passed through a backpressure turbine requiring 8kg/kWh, there would be 125kWh generated per tonne. This electricity generated would displace imported power costing £5 during the daytime or £2.50, making the "net cost" of the steam zero during the day or £2.50/t at night. If the optimiser increased the heat recovery and reduced the exhaust steam demand during the day it would not improve the operating costs, but it would during the night.

Alternatively an equivalent amount of heat could be added to the boiler combustion air, reducing the fuel burn but not affecting power generation. The optimiser effectively had a choice between routing condensate to an exchanger where heat was worth £5, or to one where it was worth zero in the day and £2.50 at night. As a result the algorithm always pushed the maximum quantity of condensate towards the boiler air preheater, the constraint being the pipeline hydraulics (control valve was driven fully open).

Having learned from the optimiser a pipe work change was made to send the condensate from the preheater to the cooling tower, giving a lower back pressure and hence more flow.

With hindsight the above will not be surprising, but it was only discovered during the process of building the model and optimising it in steady state. People often say of modelling or of pinch technology that "it does noting we couldn't do conventionally", although this may be true in theory the reality is that people do make advances and do save money by applying the available tools to their process.

In this application the change of electricity tariff with the time of day does create an "event" which could change the optimum way to run the plant. In this situation a real time optimiser is the ideal tool to take in the tariff data and act accordingly on a continuous basis; it is unlikely that an engineer is going to do this manually perhaps 6 times per day.

It is a common view that a significant, occasionally all, proportion of the benefits of any modelling activity are realised during the focused study of the process system and development of the model.

CONCLUSIONS

A wide range of modelling tools are available, some of which meet the needs of the sugar industry with its solids phases, aqueous solutions and specialist unit operations.

In general the cost of skilled human resources t use the tools is higher than the cost of the tools themselves, this should be fully considered before seeking to purchase software. Modeling is nevertheless a profitable activity if properly resourced. Part of the sugar industry does make effective use of some of the available tools, and the operating costs of the industry are sufficiently high to justify this type of effort.

P D Thompson, Ceng MIChemE May 1997.
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