

The World's First Virtual Centre for Simulation



Sim-Serv Survey

**Current Trends in Computer Aided Process
Engineering**

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Sim-Serv

1.0 Introduction

Process simulators are clearly an essential part of process engineering. They are used in variety of ways; from the modelling of single unit to modelling of the whole plant in different phases of plant life cycle; process development, design, process integration and training of personnel.

The study on current trends in process engineering was done by looking the trends in process simulation congresses and by studying the recruiting advertisements in web.

2.0 Current trends

The current trend analysis was done by studying the articles in process simulation congresses and in international discussion forums. The information from the recruiting advertisements in web supported the findings.

Background

Process simulation has been used over 30 years in oil, chemical and petrochemical industry. Most of the time computing power and simulation methods allowed only steady-state simulation; flowsheeting and simulation of single equipment such as distillation columns. Dynamic simulation was used only for modeling of single units mostly by in-house programs. Especially in the beginning, many simplifications had to be made, such as ideal models, mean physical property values and bulk concentrations. Improvement to all this has already occurred and further changes are coming as discussed in the following sections.

More rigorous models

More rigorous modeling is obviously a clear trend. This applies to the simplifications required in unit operation modeling itself but also calculation of physical properties and non-ideal flow conditions. This is discussed in more detail in the following.

Molecular modeling

Computational chemistry and molecular modeling are developing quite rapidly; even their status now is still in quite impractical level from process engineering point of view. The first semi-practical applications have already been shown. The benefit is that they allow in future a mechanistic modeling approach to physical properties instead of the current empirical or semi-empirical modeling. This is relating to physical properties such

as viscosity, vapor liquid equilibrium (VLE) and maybe also reaction kinetic data. The time scale for practical developments is possibly 10 years.

Physical property models

In simulation there is a constant need for physical property models. They also take most of the simulation time (maybe 80% in chemical applications). The need is to calculate them over wide range of temperature and pressure, also near the critical point. Even though the methods are semiempirical and mostly nonpredictive they have still been improving all the time. Traditionally predictive VLE calculations have been possible to the quite ideal compounds and mixtures such as hydrocarbons, light bimolecular gases and some organic compounds, but not for polar molecules or electrolyte solutions. This is basically still true. New methods can predict some special situations such as VLE in presence of hydrogen and compounds near supercritical point. Still all non-ideal VLE methods are based on measurements directly or indirectly, even both models have improved. New groups have all the time been added to group contribution methods such as UNIFAC, which predict VLE or LLE (liquid-liquid equilibrium) values based on functional chemical groups. This development will continue, but it doesn't change the fact that real predictive methods probably require a different approach i.e. molecular modeling even the practical results are still waiting.

Rate based mass transfer models

Rate-based models are an important trend in unit operation modeling. Traditionally most mass-transfer equipment models (such as distillation, absorption, extraction etc.) have been based on ideal stage concept because computational simplicity. The more advanced approach is to use real mass transfer calculation to predict the mass transfer rates. This however requires the knowledge of diffusion coefficients for prediction of mass transfer coefficients. Also specific mass transfer areas need to be calculated. The improvement is that there is no longer need for arbitrary and fully experimental stage efficiency estimates. On the other hand the experimental diffusion coefficients are needed.

Models for combined phenomena

Traditional thinking was that one phenomenon is done in one operation. For example this means that the reaction is done in a reactor and separation a separation operation, which

are different equipment and not combined. Nowadays the requirements for more intensified operation often demands different phenomena to take place simultaneously. For example reaction and separation are combined into one operation where both phenomena take place simultaneously; for example in reactive distillation. Some examples are; combined reaction / separation, mass transfer / heat transfer, reaction / phase change etc. These operations have been difficult to design and implement earlier, since suitable software has not been available commercially. Now more and more models and software for these operations is coming available.

Computational fluid dynamics

Computational fluid dynamics (CFD) allows calculating real flow patterns and concentration values in vessels etc. This is required e.g. for more exact prediction of reaction yields in reactors, since the real driving force behind chemical reactions can be used instead of average concentrations. In separation equipment, real concentrations and back flow effects affecting on separation results can be predicted. The benefit is that the product yields & qualities can be improved and the overall efficiency of process improved by more realistic design. Therefore the application of CFD is a very important trend.

There are still problems in multi phase systems and in incorporation of reactions in CFD calculations. The making and calculation of a CFD simulation is still time consuming and it requires specialized staff. Future will probably see CFD becoming more of an every engineer's tool in about 5 to 10 years such as flowsheeting is now.

Optimization methods

Process design has always been considered more as an art than science. Since design is in fact multicriteria optimization, it is clear that advancing optimization methods have also touched this domain. In an ideal case a process design can be done fully in a computer, if the process can be modeled and there is an optimization program that allows both real and uncontinuous values to be used. The latter is for making selections on equipment types and connectivity. This problem is being tackled with mathematical algorithms such as mixed integer nonlinear programming (MINLP) and genetic algorithms (GA). The design is still not fully automatic since both methods require a superstructure of alternatives to be made by hand. Also it is very difficult to take into account all soft criteria needed in design (such as safety, operability etc.). Also the current algorithms

don't manage the combinatorial explosion of real problems. Therefore the methods are now used for limited scale problems (planning of paper roll cutting etc.). Future will probably widen the application area, but this is not solely an optimization algorithm problem but also question of how to measure the many criteria required in engineering.

Dynamic

Simple dynamic simulation has been used for tens of years for simple batch processes in chemical industry. The real problem has been, how to make tools for dynamic process simulation, which look like flowsheeting programs and would include easy made dynamic models and a physical property package. The problem has been both the robustness of algorithms and the computation time improved. Not until in recent years dynamic flowsheeting simulators have become available for chemical processes. Still the problem is that the dynamics is more of simple residence time dynamics and not very rigorous. The future will see dynamic simulation to become a standard tool for every process engineer resembling existing flowsheeting. The user can choose the level of rigorousness from simple residence time dynamics to rigorous equipment dimension based dynamics with all control loops. Implementation of dynamic simulation in the design of chemical processes is an important development taking place in about five years.

Simulation in some special process industry areas

Simulation in process industry has to date been limited mostly to chemical and power processes. Advancements of simulation in these areas have lead to higher interest also in other areas such as food, biotech, mineral processing, inorganic chemistry, pulp and paper industry, where solids and difficult chemical properties have prevented or made modeling more difficult. The key question in these areas is often, how to deal with physical properties, since the compounds are difficult to model. The equipment models and phenomena in them are mostly the same as elsewhere. The use of simulation in these areas will certainly increase as more dedicated models become available.

Micro-scale phenomena

Simulation for micro-scale phenomena is becoming more important when micro equipment (micro reactors etc.) is used more commonly in future. In this equipment there

are other dominant phenomena than in the large-scale equipment, since the ratio of surface area to volume is very different.

Batch process scheduling

Since batch industry will probably increase, because more dedicated small-scale products are being used, also need for batch process scheduling and optimization is increasing. At the moment such programs exist, but they are often not much related to process phenomena i.e. the equipment performance may vary with time, which should be considered.

Sources of information

ESCAPE 1-12; European symposium on computer aided process engineering series

ECCE European congress of chemical engineering

<http://capenet.chemeng.ucl.ac.uk/>

<http://cape-alliance.ucl.org.uk/>

3.0 Study on simulation job advertisements in web

A study on simulation job advertisements was done by searching with 'simulation' key word in the web and in specific company web pages (the list of companies is included). Altogether 19 process simulation related recruiting advertisements were found all over the world. Most of the advertisements were related to recruiting process design engineers with simulation knowledge (11 cases). Three advertisements for simulation program / model developers, two for offshore oil production design / simulation engineers and three for control engineers developing model based control systems for process industry were also found.

Summary of the recruiting advertisements

1. Process design engineers with simulation knowledge (11 cases)
 - using commercial (mostly) steady-state process flowsheeting software as a tool for process design, operation or troubleshooting
 - programs mentioned Hysys / Hysim, Pro/2, Aspen
 - mostly steady state simulation, even some programs include nowadays dynamic features
 - dynamic simulation mentioned specifically only once
 - two advertisements mention distillation column design
 - industry areas mostly oil refining but also petrochemicals and chemicals

2. Simulation program or model developers (3 cases)
 - development of either commercial or in-house simulation models, user interfaces subroutines for commercial simulators
 - program types dynamic, batch and steady state
 - programs mentioned Prosim, Aspen, gProms and in-house programs

3. Offshore oil production design / simulation engineers (2 cases)
 - simulation of offshore pipe hydrodynamics (two-phase flow) and heat transfer

4. Control engineers making model based control systems for process industry (3 cases)
 - models for model based or neural control in process industry

Analysis of recruiting advertisements

In process industry the market of simulation program users is large. Most process design engineers are required to be able to use commercial simulation programs. These programs are mostly steady state but many contain also dynamic and batch process features. Because dynamics was mentioned only once, it is obvious, that the main use is steady-state flowsheeting (+ distillation column design). The main industry areas are mostly oil refining but also chemical and petrochemicals industry.

In program and model developers the dynamics and batch process orientation is high. It is obvious that the program and model development is directed more to these areas, when the practical program usage is more in steady-state flowsheeting.

In offshore area the process simulation is directed to simulation of pipe hydrodynamics. These models are partly available in commercial chemical engineering simulators (such as Pro/2) but specific petroleum industry tools are also used.

Control engineers are making model-based control systems for process industry. The tools used are specific control programs and Matlab. No conventional process simulation programs were mentioned

The search was done by simulation-oriented keywords, obviously therefore no CFD etc. recruiting was found.

List of the company web pages studied

Novartis
ICI
Aventis (Hoechst)
Borealis
Dow
BASF
ExxonMobil
Abb
Atofina
Basel
Bosch
Algol
Kemira
Henkel

Unilever
Nestle
Rocher
Sulzer
BP
Huber
Chemopetrol
Aga
Linde
Huntsman
MW Kellogg Ltd
Uponor
UPM Kymmene
PKN Orlen SA
Teknos
Slovnaft
Myllykoski
Stora Enso
Forchem
Raisio
Shawgroup Inc
Outokumpu
Omya
Orion
OMG
Finnish Chemicals
Fortum
Technip-Coflexip
CTS Engineering
Arizona Chemical
Associated Octel
Crombton