MODELING AND SIMULATION IN 2004: AN INDUSTRIAL PERSPECTIVE

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Abstract

The use of advanced modeling and simulation tools for both design and operations has long since become routine in industry, and their development has been well documented at previous FOCAPD meetings. Nevertheless many long-existent needs and new requirements are not met, and both the enabling technologies and application of these tools continues to evolve. This paper provides an industrial perspective on the current state of modeling and simulation technology, with an emphasis on recent developments, emerging technologies, and new industrial applications that promise to have a significant impact on industrial practice and economic effectiveness, as well as gaps requiring further research. Three main subject areas are covered. The first is physical property modeling, the technology for representing the properties and phase behavior of material. The second is systems and architectures for modeling and simulation. The third is design environments that enable effective use of models.

Keywords

Modeling, Simulation, Optimization, Physical Properties, Process Design, Real-Time Optimization.

Introduction

The topics in this paper have been the focal point of FOCAPD meetings since their inception. Many of the technologies discussed here were presented at FOCAPD meetings in the 1980s, with an expectation of rapid adoption. In fact, with the exception of steady-state simulation, adoption has been relatively slow and limited, and only recently has progress been made on unified environments for the development and application of consistent models throughout the plant lifecycle.

In this paper, we present our perspective on the current state of modeling and simulation technology and related applications. We discuss recent developments, industrial applications that can now be successfully addressed, areas where more work is needed, and our thoughts on future directions.

Physical Property Modeling

From pharmaceuticals and polymers to extraction and refining, industrial processes hinge upon the physical and chemical properties of materials. Without accurate, consistent thermophysical properties, engineers cannot reliably simulate, compare, design, optimize, and estimate the cost of industrial processes and new products.

Most industrial processes involve complex mixtures of chemicals, i.e., products, byproducts, isomers, solvents, catalysts, entrainers, and more. Compositions never remain constant. They change with variations in feedstocks, operating conditions, and product specifications. Even small changes in product properties can have critical processing and product quality consequences. Without access to reliable physical property models and data, companies cannot take full advantage of their process and economic models to reduce capital and operating costs, meet regulatory requirements, and achieve product quality goals.

Although large physical and chemical property databases exist, they cannot supply all the data industrial enterprises require. The best approach is to leverage databases with powerful, consistent, first principles

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modeling tools that interpolate, extrapolate, and predict properties from laboratory data or validated parameters.

The ability to generate consistent property data with first principles models delivers many benefits. Companies that start with accurate, consistent data develop better products, processes and designs and reduce time to market. They can rapidly assess the performance and manufacturability of new products. They can run virtual tests for dangerous chemical reactions, design new product grades, and optimize processes and equipment during design and operation. Equally important, companies that standardize on property models and data ensure consistency throughout the process asset lifecycle.

Traditional methods for physical property modeling are well understood (Chen and Mathias, 2002) and will not be considered in this paper. Instead, we will briefly consider recent and current developments in six areas that we believe will have a significant impact on the practice of physical property modeling over the next several years. Collectively, these developments extend the range of systems and properties that can be effectively modeled in industrial practice, given the data available.

Achievements in Modeling Electrolyte Systems

The presence of ionic species and the related solution chemistry make modeling the properties and phase behavior of electrolyte systems unique. However, progress over the past two decades enables rigorous modeling of chemical processes with electrolytes. Of particular significance is the continuing development of the electrolyte NRTL (eNRTL) model, a semi-empirical Gibbs energy expression that has been developed and proven for aqueous strong and weak electrolytes (Chen et al., 1982) and ionic liquids (Belveze et al., 2004). Recently the model has been extended for aqueous organic electrolytes (Chen et al., 2001) and generalized for mixed-solvent electrolytes (Chen and Song, 2004), including electrolytes in non-aqueous solvents. The eNRTL model has evolved into a comprehensive thermodynamically consistent framework for modeling virtually all types of electrolyte systems encountered in industry today.

The eNRTL model contains two contributions: one from local interactions that exist in the immediate neighborhood of any species, and the other from the long-range ion-ion interactions that exist beyond the immediate neighborhood of an ionic species. The model uses the segment-based NRTL expression (Chen, 1993) to account for the local interactions and the unsymmetric Pitzer-Debye-Hückel (PDH) formula (Pitzer, 1980) to account for the long-range interactions

Similar to the NRTL model for chemical systems, the eNRTL model is a correlative model, not predictive. While there are no adjustable parameters in the PDH term, the local composition term requires binary parameters that must be determined from experimental data before the model can be reliably used to interpolate and extrapolate phase behavior of multi-component systems. Another consideration is that the solution chemistry must be accurately represented in terms of ionic species and association / dissociation reactions.

Figures 1 and 2 show the ability of the eNRTL model to represent aqueous organic electrolytes and mixed-solvent electrolytes, respectively.

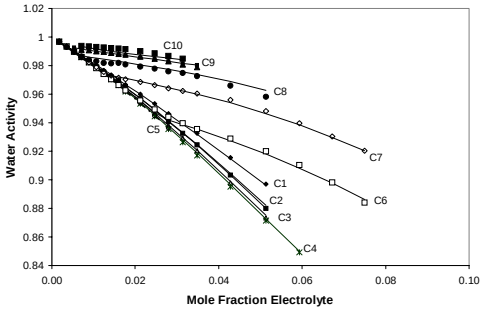

Figure 1. Water activity vs. electrolyte concentration for various aqueous sodium carboxylates and model representation (from Chen et al., 2001).

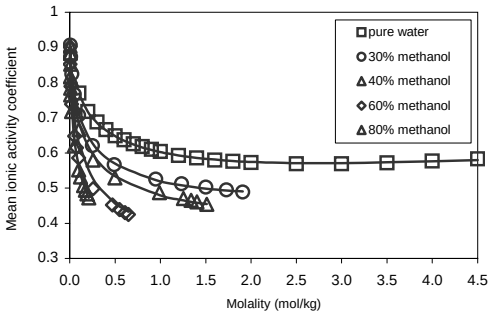

Figure 2. The best fit with the eNRTL model and the experimental data for potassium chloride in methanol-water mixtures (from Chen & Song, 2004).

In spite of the success in modeling electrolyte thermodynamics, there are a number of important areas that require new developments and innovations. For example, more high quality experimental data are needed to identify binary interaction parameters. A critical related issue is the proper identification and scientific validation of the actual chemical species that exist as a result of the electrolyte solution chemistry. The arbitrary introduction of nonexistent chemical species that are sometimes created to fit and reconcile experimental data (called the "speciation approach") puts into question the validity of the entire compilation of interaction parameters.

A strong need remains unfilled for a predictive model for electrolyte thermodynamics. Recent attempts to extend UNIQUAC and UNIFAC to model electrolyte solutions

are less than satisfactory (Iliuta et al., 2002). Proper molecular insights and theoretical rigor are yet to be structured into the UNIQUAC/UNIFAC equations to account for the presence of ions. Other un-met needs include engineering models for viscosity and densities of electrolyte solutions (Gorensek et al., 2003).

Perhaps the biggest opportunity lies in the development and compilation of public databanks for electrolyte solution chemistries and model interaction parameters. This effort would require skilled thermodynamicists to take measurements, compile, review, and selectively include experimental data for use in the determination of interaction parameters. Such a public, validated databank would be of tremendous, lasting value.

Advances in Polymer Process Modeling

Polymer process modeling is another area in which there have been tremendous accomplishments. Merely ten years ago, few engineers would have foreseen the possibility of rigorously modeling polymer processes with conventional process simulators. When heat and mass balance calculations were needed, polymers were often approximated as heavy hydrocarbons. When engineers attempted to model polymerization chemistries, they either had to limit their efforts to modeling only single-phase reactions or use polymer thermodynamic models with composition-dependent interaction parameters that offered little extrapolation capability. Lack of experimental data and engineering models for polymer thermodynamics gravely limited the value of early polymer modeling efforts. Consequently, these models offered only limited value in describing the behavior of industrial polymers, especially for multiple phase reaction systems. Typically, even these simple reactor models could not be integrated into process simulators for process studies.

Today, proven polymer thermodynamic models, such as the polymer NRTL activity coefficient model of Chen (1993) and the PC-SAFT EOS of Gross and Sadowski (2002), with composition-independent model parameters, have become available for use in process simulators to allow for interpolation and extrapolation of phase behavior. Rigorous mathematical equations that describe the development of polymer molecular structure are an integral part of unit operation models (reactors, mixers, flashes, etc.) to allow for computation and tracking of polymer molecular structure and the corresponding product quality. Numerous polymerization kinetic models have been integrated into commercial simulators. Multi-phase equilibrium calculations are an integral part of unit operation models including reactor models.

Central to the task of polymer modeling is the ability to compute and track the development of molecular structure such as polymer chain length, polymer molecular weight distribution (MWD), copolymer composition, polymer particle size distribution, etc. Fig. 3 shows the representation of MWD using a four-site Ziegler-Natta polymerization model that computes the MWD from the reaction mechanism, reaction rate constants, and reactor conditions.

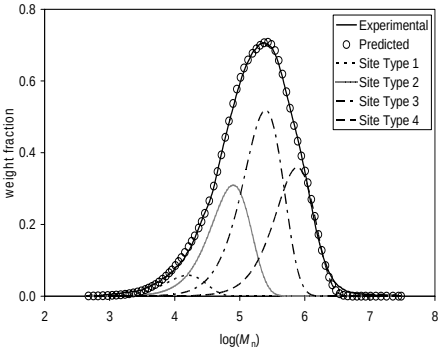

Figure 3. Representative MWD and deconvolution results indicating that a four-site kinetic model is sufficient (from Khare et al., 2004).

Today's process simulators provide innovative modeling capabilities to address additional polymer modeling issues, i.e., mass transfer and structure-property relationship. Mass transfer plays a more important role in polymer systems than in conventional chemical systems. For example, the addition polymer propagation reaction rate is controlled by the mass transfer rate of monomers through the viscous polymer melt. Polymer producers define product quality in terms of specific end-use properties rather than polymer molecular structure. For example, polyolefin producers are concerned about Melt Index (MI) or Melt Flow Ratio (MFR). Therefore, it is essential that polymer modelers find ways to relate end-use properties to polymer molecular structure.

Process simulators are now routinely used to model practically all major polymer production processes. Engineers and chemists use process models to help them develop new catalysts, design new processes, monitor and control polymer production and grade transitions, and design new product grades. Numerous publications have appeared recently that describe achievements in polymer process modeling. Examples include modeling of low-density polyethylene tubular reactor process (Bokis et al., 2002), modeling of gas-phase polypropylene processes with stirred-bed reactors (Khare et al., 2004), modeling of nylon-6 polymerization processes (Seavey et al., 2003), modeling of slurry high-density polyethylene processes (Khare et al., 2002), etc. Chen (2002) lists some additional success stories reported by industry.

Polymer process models are increasingly used online to serve as monitoring systems and to improve existing control systems (Froisy et al., 1999; Schmidt and Mähling, 2001). This is due to advancements in integrated process modeling systems and on-line state estimation technology for large-scale first principle models (Papastratos et al., 1999). It is now straight forward to build and validate a steady state polymer process model, to convert the steady

state model to a dynamic one that incorporates controllers, to bring the steady state model online as online calculators for process monitoring purposes, to bring the dynamic model online and have the model state variables validated with real time data, to apply the dynamic model on line as look-ahead predictors, to apply the dynamic model as operator training simulators, etc. The online validated dynamic model can then be used to generate linear state-space models to be used with model predictive controllers.

While polymer process modeling is becoming widely used, innovations in polymer process modeling technology are needed to address unsolved challenges and new opportunities resulting from the inherently complex polymer chemistry and physics.

One problem that has drawn attention recently is the computation of phase equilibrium for polymer systems while taking into account the distribution of polymer molecular weight distribution in various phases (See Fig. 4). Industrial polymers are polydisperse. After the feed polymer phase separates, the molecular weight distribution of polymer in the light phase will be different from that in the heavy phase. Recently, Behme (2003) introduced an efficient algorithm for solving two-phase (VL and LL) phase equilibrium calculations for polymer systems with molecular weight distribution. Research is on-going to enhance robustness of the algorithm.

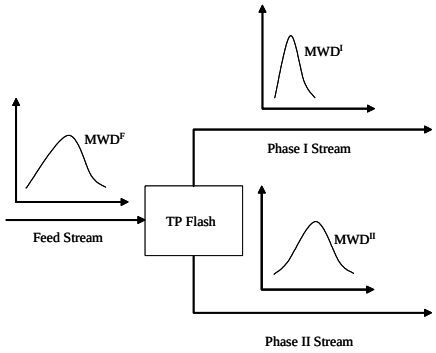

Figure 4. A two-phase TP flash for a mixture containing a polydisperse polymer (from Behme et al., 2003).

Another important area is the modeling of polymer solution viscosity. Recent works of Song et al. (2003) and Novak (2003) have provided useful models that accurately correlate available viscosity data for polymer systems. However, it is not known whether such models provide the predictive power to extrapolate beyond available data ranges or simple polymer-solvent systems. Fig. 5 shows the correlation of viscosity data for a polystyrene-styrene solution.

A critically evaluated database of kinetic parameters for polymerization would have tremendous value. The industry needs the rate constants as a basis for development of high quality polymer process models, but individually they lack the resources to measure, regress, evaluate and compile the kinetic parameters. The IUPAC's continuing efforts in developing such a database for free-radical polymerization (Buback et al., 1995 and 2002) are an excellent contribution.

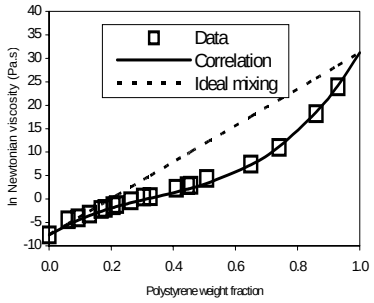

Figure 5. Newtonian viscosity of polystyrene-styrene solutions at T = 333.15 (K) and M_w = 366000 (g/mol) (from Song et al., 2003).

Modeling in the Pharmaceutical Industries

Process modeling is not practiced extensively in the pharmaceutical industry except for solvent recovery and emission reduction studies. Recently we identified a new application area where physical property modeling can bring much benefit to the pharmaceutical industry. The industry deals with hundreds of new drug candidates each year. Chemists and engineers need to develop process recipes for these new molecules and the recipes often involve multiple reaction steps and separation steps such as crystallization or extraction.

A critical consideration in the pharmaceutical process design is the choice of solvents and solvent mixtures, from among hundreds of typical candidates, for reaction, separation, and purification (Frank et al., 1999; Kolar et al., 2002). Phase behaviors, such as solubility, of the new molecules in solvents or solvent mixtures weigh heavily in the choice of solvents in the recipe development. Little if any experimental data are available for the new molecules. Although limited solubility experiments may be taken as part of the trial and error process, solvent selection is largely dictated by researchers' preferences or prior experiences. Predictive models that allow for computation of phase behavior are desperately needed. Existing solubility parameter models such as that of Hansen (Hansen, 1999) offer little predictive power. Group contribution models such as UNIFAC (Fredenslund et al., 1975) are also inadequate due to missing functional groups and the collapse of functional group additivity rule with large, complex molecules.

We have developed a NRTL-based segment contribution activity coefficient (NRTL-SAC) model for fast, qualitative estimation of solubility of organic nonelectrolytes in common solvents and solvent mixtures. Conceptually, the approach suggests that one account for the liquid nonideality of mixtures of small solvent molecules and complex pharmaceutical molecules in terms of a few pre-defined conceptual segments with pre-

determined binary interaction characteristics. Examples of the conceptual segments are hydrophobic segment, polar segment, and hydrophilic segment. The number of conceptual segments for each molecule, solvent or solute, is not determined from molecular structure, but rather from regression of available experimental phase equilibrium data for systems that contain the molecule. The molecular make-up in terms of these conceptual segments becomes molecular descriptors for the solvent and solute molecules: hydrophobicity X, polarity Y- and Y+, and hydrophilicity Z. In practice, we first develop a molecular descriptor databank for common solvents. Then we determine molecular descriptors for new drug molecules from the limited experimental data that may become available.

Once the molecular descriptors are identified for solvent and solute molecules, the model offers a practical tool for chemists and engineers to qualitatively estimate activity coefficients and compute solubilities in pharmaceutical process design (Bakken et al., 2003). The model is:

$$\ln \gamma_I = \ln \gamma_I^C + \ln \gamma_I^R \qquad (1)$$

where the combinatorial term, γ_I^C is computed from the Flory-Huggins term for the entropy of mixing and the residual term, γ_I^R, is set equal to the local composition (lc) contribution of the polymer NRTL model (Chen, 1993).

As an example, Fig. 6 shows the calculated solubilities vs. the experimental solubilities for hydrocortisone in 11 different solvents at 298.15 K. The chemical structure of hydrocortisone is represented by the molecular descriptors, (X, Y-, Y+, Z), of (0.401, 0.970, 1.248, 0.611).

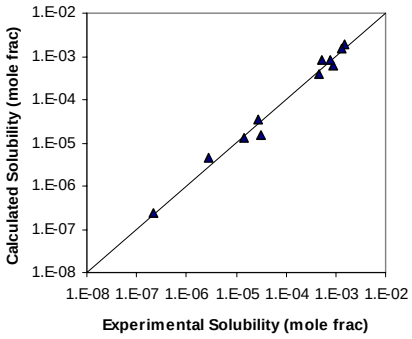

Figure 6. Hydrocortisone Solubility in 11 Different Solvents at 298.15 K (from Chen and Song, 2004).

NRTL-SAC works well not only for small molecules, but also for oligomers and polymers. We are extending the NRTL-SAC model to cover organic salts so that the model can be applied to all pharmaceutical molecules.

Impact of Molecular Simulation

With the ever-increasing computing speed, molecular simulation has evolved dramatically over the past twenty years. It has impacted process modeling in a number of ways: 1) help elucidate fundamental physical and chemical interactions and support development of new theories and models, 2) complement experiments for data generation especially for systems that are not readily amenable to existing experimental procedures, and 3) provide an alternative approach to extend and improve on existing applied thermodynamic models (Chen and Mathias, 2002).

While we do not foresee use of rigorous *ab initio* calculations any time soon for process modeling and simulation, we see other benefits from molecular simulation. One example is the recent use of the COSMO-SAC quantum mechanical model (Lin and Sandler, 2002) for the prediction of activity coefficients of highly non-ideal chemical systems. The model computes thermodynamic properties in three steps:

1. The screening charges originating from the solvation of the solute molecule are determined from quantum mechanical calculations with the "Conductor-like Screening MOdel" (COSMO).
2. The screening charge density is discretized into finite surface elements to produce the σ-profile, which represents the number of surface elements with a given charge density.
3. The σ-profile enables prediction of the excess Gibbs energy of any mixture and the activity coefficients of various components through exact statistical thermodynamics.

The activity coefficient of a molecule *i* in solution *S* is determined solely from the σ-profiles of the component molecules and the surface segment interactions

$$\ln \gamma_{i/S} = \frac{A_i}{a_{\text{eff}}} \sum_{\sigma_m} p_i(\sigma_m)\left[\ln \Gamma_S(\sigma_m) - \ln \Gamma_i(\sigma_m)\right] + \ln \gamma_{i/S}^{SG} \qquad (2)$$

where $\gamma_{i/S}^{SG}$ is the Staverman-Guggenheim combinatorial activity coefficient of component *i* in solution *S*, and $\Gamma_j(\sigma_m)$ is the activity coefficient a surface segment with charge density σ_m in a solution *j*.

While COSMO-SAC is generally less accurate than the UNIFAC group contribution method, COSMO-SAC has proven to be a viable predictive model that is complementary to UNIFAC, especially for systems where UNIFAC methodology fails either due to missing UNIFAC groups or inadequacy with the functional group additivity rule. The application of COSMO-SAC requires a library of σ-profiles for each molecule of interest. Such a library could be as valuable to industry as the DIPPR or UNIFAC databanks. We strongly encourage its development.

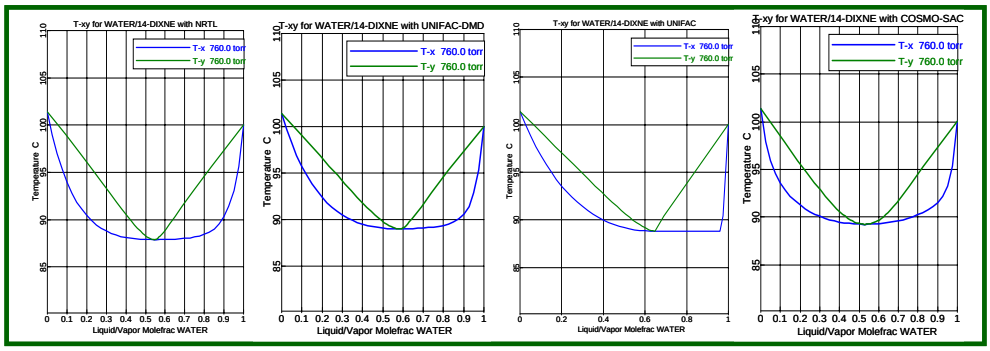

Figure 7. Comparison of TXY phase diagram prediction results for water - 1,4-dioxane at 760 mmHg with NRTL (left), UNIFAC-Dortmund (mid-left), UNIFAC (mid-right) and COSMO-SAC (right). NRTL practically duplicates the experimental data. All four models correctly represent the minimum azeotrope, but UNIFAC incorrectly predicts a liquid phase split (from Oba et al., 2003).

Opportunities with Cellular Process Modeling

The emergence of bioinformatics promises an unprecedented volume and complexity of data. Such biological data reflect highly complex relationships in multiple scales, from gene sequence, to proteomics, to protein-protein interaction, to sub-cellular and cellular systems, to morphology, physiology, to whole organisms. The exploitation of this biological data has become a new challenge and a dramatic opportunity for drug discovery and many other fields. *In-silico* biology (first principles modeling of biological systems) will become a technology driver to transform this biological data into knowledge for drug discovery R&D and personalized medicine.

Among potential benefits from *in-silico* biology are knowledge discovery and management, target validation, and lead optimization. The human genome encodes the complete set of all possible pharmaceutical targets. Virtual cell simulators provide the mathematical modeling framework to capture human knowledge of metabolic and signaling pathways and facilitate biological simulations with predictive power to assist in drug discovery.

Biological cells can be characterized as a living chemical plant, with chemical components, reaction and signal pathways, material and energy flux, etc. Cellular "chemical plant" behaviors are subject to various physiochemical and biological constraints such as material balance, electroneutrality, reaction stoichiometry, thermodynamic constraints, flux capacity constraints, kinetic and regulatory constraints.

Development of virtual cell simulators, as a computational framework for whole cell modeling and simulation, are at its infancy and it promises to be a new world for human imagination and creativity. We expect such a simulator would facilitate modular and iterative development and validation of biological cell models based on a hierarchical assembly of metabolites, proteins, genes, metabolic networks, cellular pathways, enzymatic reaction and transport mechanisms, gene circuit, regulatory networks, intracellular organelles and structures, etc.

Role of Property and Process Models in Product Design

The chemical industry has experienced a rapid shift from commodity chemicals into specialized chemical and biochemical products (Cussler and Wei, 2003). Commodity chemicals are increasingly produced in the developing countries while chemical producers in the developed countries must move to specialized chemical products that compete on performance and quality rather than manufacturing cost.

This shift creates new demands, requirements, and opportunities for process modeling technologies and tools:

- Instead of solving large-scale systems of nonlinear equations for simulating continuous, highly integrated petrochemical plants, specialty chemical producers are interested in quickly and rigorously modeling the dynamic behavior of relatively small batch reactors with overhead condensers.
- Instead of using process models for the purpose of heat and mass balance calculations, polymer producers use models to design new product grades. These models help them understand how polymerization chemistries, process recipes, and equipment design affect the development of polymer molecular structure. Such molecular structure and resulting product properties determine the quality and grades of the product they sell.
- Instead of equation-of-state models for dew point and bubble point calculations, lubricant producers require predictive viscosity models for solvent-polymer additive mixtures as their products are sold based on its impacts on solution viscosity.
- Instead of being concerned with fluid properties such as vapor pressure, heat

capacities and densities, medicinal chemists are interested in solubilities at physiological conditions for millions of drug-like molecules in the compound libraries that they screen in discovery of lead molecules.

However, like chemical process design for large-scale petrochemical plants, the keys to success in chemical product design are: 1) the fundamental understanding of underlying chemical and physical phenomena (molecular structure, chemical reactions, thermophysical properties, mass transfer, etc.) and 2) the molecular insights required to develop first principles models to correlate and predict chemical and physical properties and phenomena. The challenge with product design will be met by coupling past achievements in process modeling with new knowledge that captures the essence of the fundamental driving forces and physical laws that ultimately determine the quality of products we discover and design.

One intriguing area for product design is lead molecule discovery and optimization in drug R&D. As a result of high throughput screening and combinatorial chemistry, a major opportunity emerges with the modeling and predictions of absorption, distribution, metabolism, excretion and toxicity (ADMET) for candidate drug molecules. Current modeling efforts are primarily based on neural networks, empirical rules, or group contributions that offer little fundamental understanding. Models that are based on molecular insights or first principles are desperately needed to advance the state-of-the-art, and they offer a fertile area of activity for chemical engineers.

Computer-Aided Molecular Design (CAMD) (e.g. Ostrovsky et al., 2003) is a promising area which exploits optimization technology (MINLP) similar to that used for process design. However, practical industrial application has yet to be demonstrated.

Systems and Architectures for Modeling and Simulation

Historical Perspective

Early development of process simulation started with sequential modular simulation (M.W. Kellog in the late 1950s) and progressed rapidly towards a capability to model complex flowsheets while allowing a significant degree of customization—best exemplified by the FLOWTRAN system developed by Monsanto (Seader et al., 1987). In parallel, an intriguing alternative developed in the form of equation-oriented simulation that originated in mid 1960s from the work by Sargent and Westerberg (1964).

Sequential modular simulation offered the ability to solve the pressing business problem of that era, namely to compute heat and material balances, and matured into the ubiquitous commercial simulators Aspen Plus® and Pro/II®. They offered significant advantages from an end-user viewpoint, such as:

- Rapid modeling of large flowsheets,
- Extensive libraries of physical property models, unit operation models and component databanks,
- Limited need to initialize calculations due to built-in algorithms to select tear stream and initialize models,
- Modular architecture that enabled custom models to be included in the simulation.

Inherent weaknesses have been:

- Slow convergence of recycle systems where recycle to feed ratio is high,
- Systems with complex recycles or high degree of heat integration are slow and difficult to converge and require significant expertise,
- Optimization is limited to a process flowsheets with a very small number of variables and without complex recycles or heat integration.

The desire to optimize a plant design or find the best operating conditions has continued to drive the research in equation oriented simulation until today, resulting in a large body of work by the students of Sargent and Westerberg and in the first equation-oriented simulator, SPEEDUP (Pantelides, 1988). SPEEDUP was a primarily an equation-oriented model writing environment with the ability to solve various types of problems (e.g., steady-state and dynamic simulation, optimization). This direction continued in SPEEDUP's conceptual successors (ASCEND – Carnegie Mellon (Piela et al., 1991), gPROMS – Imperial College and PSE (Barton and Pantelides, 1994), ACM – AspenTech), which, among other things, extended the capabilities to include dynamic optimization and parameter estimation.

In parallel to the "SPEEDUP branch", an effort began at Shell Development in the late 1970s to optimize the real-time operation of large, continuous plants (ethylene plants & refinery units). The business need to implement process optimizers in a profitable manner rapidly oriented this effort towards development of an equation-oriented simulator that was supported by a library of models. Conceptually, this was very similar to the sequential modular simulators of that era, the main difference being the equation-oriented approach to solution. While successful in optimizing plant operation in real time, this effort highlighted the strengths and weaknesses of the equation-oriented approach, such as:

Strengths:

- Ability to converge highly complex flowsheets,
- Rapid convergence from a good starting point,
- Ability to easily solve flowsheets with any set of feasible specifications, not just those on "inputs".

Weaknesses:

- Need for an excellent starting point, which in real-time applications was provided by the plant,
- Initial assembly of a large flowsheet required that each node of the network be initialized separately and that the flowsheet be assembled step-by-step,
- Handling of the phase transitions that take place as operating conditions vary requires techniques vastly different than those used in closed form models for sequential modular simulation,
- Optimization of flowsheets with a large number of degrees of freedom could not be routinely handled by even the most advanced SQP algorithms of the day (Powell, 1978).

The need for cost-effective commercial real-time optimization (RTO) solutions resulted by the early 1990s in DMO from the DMC Corporation, an equation-oriented system that solved the issues of optimization with a large number of degrees of freedom, as well as development of models capable of converging through phase transitions. However, DMO had not solved the issue of initialization and the need to gradually assemble a flowsheet from its converged subflowsheets.

In parallel with the above developments, HyproTech introduced a computational architecture for interactive simulation that combines sequential modular computation with certain elements of the equation oriented approach (Svrcek et al., 1984). This easy to use paradigm, delivered to the user's desktop in early PC and Windows versions, has created a mass market of everyday engineering users.

Progress to Date

AspenTech has been fortunate to assemble personnel and technologies that represent all three simulation approaches: sequential modular, equation based, and interactive. This has enabled us to combine the strengths of both the sequential modular and equation based approaches (Aspen Plus Version 11):

- Good initialization of a flowsheet is provided by sequential modular iterations through a flowsheet,
- Equation-oriented mode of the models can handle multiple phase transitions, such as vapor/liquid/liquid and liquid/solid systems,
- Physical property models provide analytical derivatives,
- The optimization algorithm has been enhanced to enable solutions of systems with an order of magnitude larger number of degrees of freedom, as well as mixed integer NLP models,
- Architectural ideas from ASCEND have formed a basis for a new generation equation-oriented system architecture, capable of handling engineering simulations, multi-time period models, and mixed integer LP and NLP systems,
- Aspen Custom Modeler® (ACM) can be used to develop equation-oriented models (with model-specific initialization procedures) to run within Aspen Plus or any simulator that supports the CAPE- OPEN standard (Braunschweig et al., 2000),
- Degrees of freedom and structural analysis tools ensure feasible specifications, and
- User specifications are similar to those for sequential modular simulators. The switch between the sequential modular and equation-oriented algorithms is simply a choice of another convergence method.

Therefore, this integrated architecture represents a major step toward the goal of model centricity (consistent models and solutions for all applications). There is only one version of the plant model because sequential modular and equation-oriented models and algorithms are implemented within a single architecture. Any changes to the process flowsheet are applicable to both modes of convergence.

From a plant lifecycle viewpoint, this means that a model that is developed for optimization of plant operating conditions can be readily used for plant revamp design. Changes to the plant optimization model, dictated by the need to accurately represent plant operation, are immediately available for process engineering studies.

Benefits to Process Design and Plant Operation

The integration of the equation-based and sequential modular approaches enables engineers to tackle problems that had been unsolvable in practice. Most importantly, the same model can be used for many different applications, since a user can set specifications on and optimize over any feasible set of variables. Some of the business problems that can be solved through use of the integrated sequential modular / equation-oriented capability are:

- Optimal sizing to meet design targets for a given plant throughput, e.g. size distillation towers so that the tray loading is at a specified value, or size heat exchangers in a network to operate at the target approach temperatures,
- Maintain plant operation at optimum, e.g. optimize reactor conversion and associated plant operation over time to determine the best trade-off between operating and catalyst regeneration costs,
- Prediction of operating conditions at the capacity constraint, e.g. what is the feed rate to a distillation tower when it operates at a tower flooding limit on a given tray, or what is the

feed rate to a furnace at its radiant heat density limit?
- Computation of un-measured equipment performance indicators for use in multivariable control, e.g. downcomer filling and jet flooding for current operating conditions in a distillation tower or radiant heat density in a furnace.

Another model centricity milestone was the integration of steady-state and dynamic simulation in a single, easy to use environment (HYSYS). With this integration, operability, control, and safety studies can be conducted simultaneously with and using the same assumptions as the process design.

Clearly, we could continue by listing many other business problems that now can be solved very successfully in a daily practice of the engineering community. An example of such applications, which exploits the use of equation-oriented modeling for design-type problems, is presented at this conference by Myers and Hanratty (2004),.

Future Direction for Modeling and Applications

The ultimate goal of modeling and simulation is to enable the process industries to make the best decisions in all aspects of enterprise operation (plant design, plant operation, supply chain management, regulatory compliance, etc.). A fundamental requirement is to enable usage of consistent models as decision support tools in all of these areas. This business need dictates our views on future technology directions.

We believe that models will become an even more ubiquitous, fundamental basis for decision making, largely transparent to the user. Better decisions will be enabled by:
- Models being available whenever a decision needs to be made,
- Consideration of the entire solution space and associated uncertainty,
- Ability to routinely solve problems that today require special attention or have no solutions,
- Consistency of all models that support a related set of business processes.

New Types of Solutions

Process Design: Effective methods have been developed for process synthesis in areas where physical characteristics enable special methodology, such as heat exchanger networks (Linnhoff, 1993) or separation systems (Westerberg and Wahnschaft, 1996). Often these methods utilize some simplification of the general MINLP problem. For example, Aspen Water solves the waste-water system design problem by exploring possible topologies using MILP, then using NLP to optimize the detailed conditions within this structure, then iterating to explore other structures.

However, design of a general plant structure is a MINLP problem with complex nonlinear subproblems. Widespread adoption of these methods in practice will require a significant investment in software for both problem formulation and solution that can readily be used by design engineers. Recent work on MINLP methods for design (e.g., Lee and Grossman, 2003) shows industrial promise.

Control & Optimization: Current practice employs distinct models and algorithms for advanced process control and for real-time optimization. This division originates in limited capabilities (40 years ago) to develop plant models. Consequently, the control field proceeded with empirical models (linear or nonlinear), while real-time optimization employed steady-state models to optimize large continuous plants. There has been substantial application of non-linear controllers in industry, but still based on empirical models. A promising direction is the combination of empirical and first-principles models, which could lead to a merger of advanced control and real-time optimization into a single discipline and the ability to handle steady-state optimization and dynamic optimization/control problems in a consistent way (e.g., transition to a new steady-state).

Guarantee of optimal results: Global optimization is a tool to improve decision quality (e.g. better gasoline blending) and not just an interesting research topic. Recent developments (Floudas, 2000) offer the potential to solve real-world problems and are being implemented in commercial software. While initial applications may be for specialized problems, we expect their use to be widespread

Uncertainty: Today's modeling and design applications typically provide a single point solution that is based on data and assumptions which will never be exactly correct. We see the potential for a major paradigm shift to solutions which deal with risk and uncertainty—either that provide a better understanding of the solution variability and causal factors, or that provide a solution that explicitly takes uncertainty into account. There has been a great deal of work in this area (see Cheng et al., 2002 for a review), and we feel that it will see industrial application.

Empirical modeling: Data driven statistical techniques such as neural networks, latent variable methods, and image analysis can be used to predict, monitor or control behavior of processes that are difficult to model from first principles or may not even be measurable by traditional instrumentation. We believe that significant benefits can be obtained from using a combination of first-principles models and empirical methods (e.g., Model-based SPC). Such a development is likely to provide a further stimulus for advancements in this arena.

Approximations and extensions of first principles modeling: Advances in computer hardware and modeling software have enabled us to build more and more details into models. This leads to two types of issues in practice: is the model so complex that an average user cannot use it,

and can the available solution methods solve the problem and do so in a reasonable amount of time?

Computational requirements for physical property calculations (particularly for dynamic simulation) have been significantly lowered through use of simplified thermo-physical models that also provide correct derivatives (e.g. Aspen Dynamics®). Recently there have been promising developments that would significantly lower computational requirements for models with a large number of components (Briesen and Marquardt, 2003). These developments have the potential to make accurate results available at an order of magnitude lower cost. There are several potential business uses for such technology, and we expect that it will rapidly develop and become widely available.

An opportunity for more rigorous models is in the area of fluid dynamics. Typically, process models are developed with a detailed treatment of physical properties, phase equilibrium and reaction kinetics but with simplified fluid dynamics, while CFD models treat fluid dynamics rigorously, but with highly simplified or ignored chemistry. There is great benefit from models that treat both chemical and physical phenomena accurately, for example in reactor and design and analysis. Recently, commercial software vendors have begun to tackle this problem (Zitney et al., 2002; Bezzo et al., 2000).

Model Centricity (model consistency)

In addition to process simulation and optimization, the process industries utilize numerous other modeling and optimization tools for specific business problems, such as production planning, scheduling, and distribution. Each application has been approached from a different viewpoint, using the most appropriate technology and devising a user paradigm specific to the business task at hand. As an example, traditionally there are separate modeling / optimization environments used for production planning (simplified models / plan production over multiple time periods) and for plant optimization (rigorous models / optimize for current operating conditions).

Theoretically, one could use rigorous models to compute the operating constraints and then modify the planning model correspondingly. In practice, this happens only as an exception and many planning models do not represent the true capabilities of the plant. If models that are used to make various business decisions are not consistent and accurate, then the business decisions themselves are not consistent and accurate. Significant opportunities will be missed.

How can we achieve model consistency throughout the decision making process? With the current disparate application-specific modeling environments, this can be accomplished by adjusting parameters in one model based on predictions from another model ("reference model"). However, this still leaves us with multiple modeling environments, multiple software systems, and multiple interfaces to maintain. Models will be consistent in the vicinity of the operating point where the update was last carried out, but they may not be inherently consistent.

What is needed is software that can model a variety of physical systems and is architected to deliver consistent solutions for a variety of business problems. This will be the subject of the next section.

Future Direction in Software for Modeling

Our goal is to be able to model systems represented by any type of network or flowsheet, where network nodes are modeled at the level of accuracy dictated by the business application. Network models would have node models from different domains. One could configure planning and scheduling models that consist mostly of simplified models, but that model selected nodes by using more accurate models from process simulation, or one could configure plant optimization models that use high accuracy models in critical areas of the plant, while using simpler planning or scheduling models for the remainder of the plant.

Process simulation is a simulation with one set of events. Simulation of a production schedule is a simulation with multiple sets of events. A simulation infrastructure with event management capabilities could handle both types of simulation, as shown in Fig. 8. At the heart of the architecture is the ability to assemble network models consisting of node models that can operate in either sequential modular or equation oriented mode as shown in Fig. 9.

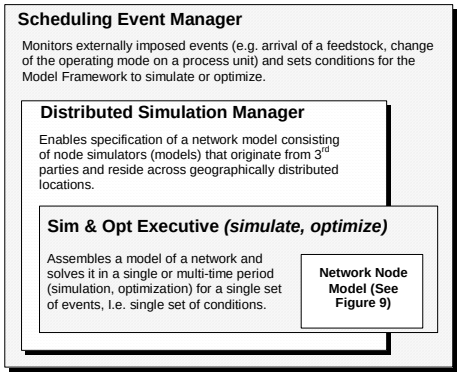

Figure 8. Conceptual Architecture for Generic Simulation Infrastructure.

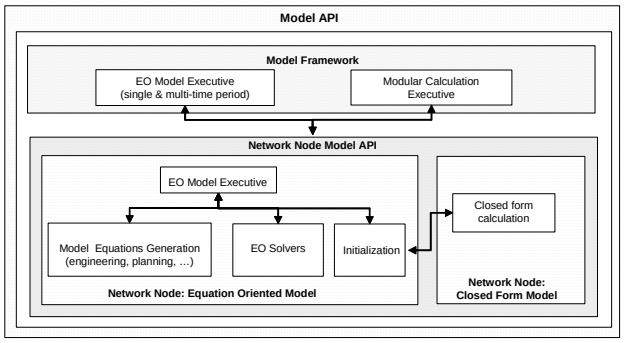

Figure 9. Network Node Model for Generic Simulation Infrastructure.

In order to facilitate deployment of models within any business application, the entire model behaves as a software service, communicating though a defined API (data and methods). The model framework, which has some similarities to the "model server" described by Pantelides and Britt (1995), generates either single or multi-time period models, while each network node is represented by a model that can operate as an equation-oriented model or as a closed form model. Let us consider how this architecture can create various types of simulation and optimization systems:

- *Simulation for process design & optimization:* Node models are typical engineering models of today. In addition, each model can operate as a steady-state or as a dynamic model, thereby enabling seamless transition between steady-state and dynamic simulation, and it can be solved through sequential-modular or equation-oriented methods.
- *Production planning:* Any node that can operate under several different operating modes (as in refinery planning) is replicated into a corresponding number of nodes. Each node model can be a simplified, linear model (as is the case in most planning systems today) or by more accurate non-linear models that could be either approximate non-linear models or rigorous nonlinear models.
- *Multivariable process control:* The entire process unit could be represented by a single empirical model (as it is common today) or by a network of empirical and first principles models.
- *Simulation of a schedule:* The Scheduling Event Manager shown in Fig. 8 interprets a schedule generated through additional methods. The architecture enables, for instance, a dynamic tank model to be a part of the plant model.

The described architecture also streamlines a number of model management issues (case management, library management, implementation in a plant environment, and imbedding within decision making tools, etc.).

Collaborative Process Design Environments

Process and product design involves many disciplines and is highly collaborative. Models and data are shared among users and disciplines both informally and in a formal process of approval and issuing. It is estimated that engineers spend 60% of their time searching for data from disparate sources, collating and transcribing the data, and filing the results. While we have no quantitative data, the time spent duplicating models for different purposes and in reconciling their differences is certainly also significant. The opportunity cost is high. The construction industry consortium FIATECH (www.fiatech.org) has estimated that improved collaborative design processes have the potential to reduce time to plan and implement a capital project by 20-50%, reduce capital costs by 15% and reduce operating costs by 2%, which typically would yield a 2 point increase in Operating Return on Net Assets.

However, it is not meaningful to converge all applications used across the design life-cycle into a single integrated system; each discipline has unique objectives and workflow, places different requirements on process and data models, and requires specialized functionality in their tools and applications.

A number of software architectures have been proposed that attempt to minimize data transcription time and cost and reduce the opportunity for error. In the simplest form, tools are connected directly by interfaces (Fig. 10). This approach can offer a simple and easy-to-implement solution for data exchange between a few tools. However, the cost becomes prohibitive in anything other than simple cases—if we have N tools in a system, we must construct N*(N-1) interfaces.

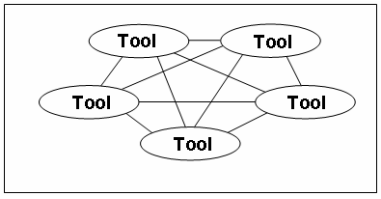

Figure 10. Point to Point Integration.

If a standard interface that translates the internal data to a standard neutral exchange format is provided for each application, only N interfaces are required. This simplification demonstrates the power of data exchange standards (which applies equally to any of the other architectures discussed here). Unfortunately, despite enormous effort and available data modeling technology, efforts to develop successful public standards for design data exchange have not been successful. The most relevant

example is pdXi (Motard et al., 1995), but the same is also true for the much more data intensive detailed design and engineering disciplines.

The architecture in Fig. 10 facilitates data exchange but does not provide management or security of the data exchange or work flow. Thus, this approach is best suited to a single-user performing a set of closely coupled analyses, such as simulation and heat exchanger design. AspenTech has directly interfaced its major design tools with Aspen Plus and HYSYS to support this workflow.

The so-called "hub and spoke" architecture (Fig. 11) does provide workflow management and security of data exchange. In a hub and spoke implementation, tools are located among their respective users, and each is connected to a central database. Data are exchanged by being stored in the database then retrieved by tools used later in the design life-cycle. This approach suffers two distinct limitations. Firstly, any data that must be transferred between tools must be represented in the schema (ideally, an industry standard) of the central database. As new tools are integrated, the schema must be extended. In practice, schemas cannot be extended arbitrarily; at some point they must be re-engineered. This is a major task, and data migration is a serious problem. Secondly, the central database is a common failure point.

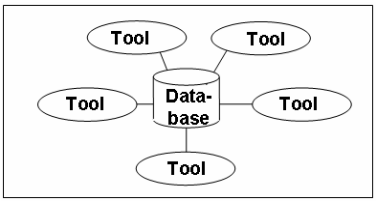

Figure 11. Hub and Spoke Architecture.

The hub and spoke architecture does provide a highly flexible, dynamic and concurrent environment. In the special case of a team of engineers of the same discipline, collaborating on the same design (for example, a lead engineer and one or more process engineers designing a single process unit), this advantage far outweighs the disadvantages of hub and spoke, and this architecture is close to ideal. Aspen Zyqad™ exemplifies this approach.

The limitations of hub and spoke for disparate workgroups and disciplines are overcome in the so-called "publish and subscribe" architecture (Fig. 12). Again the tools are located among their respective users, but they are connected to a data transport bus. Data are exchanged by being "published" by the authoring application; all applications "subscribe" to receive any classes of messages that might contain data that they might use. The data transport bus delivers published data to each of the applications subscribed to a particular message class. This architecture can be built with a high degree of redundancy, and information buses feature guaranteed delivery of messages – should the bus fail, the messages will not be lost but will be delivered from a cache once the bus is re-started.

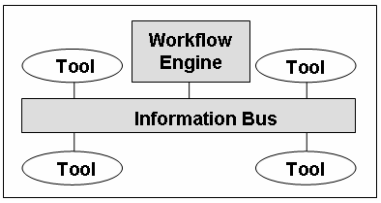

Figure 12. Publish and Subscribe Architecture.

During a plant's operational life-cycle, design is ongoing (e.g., during revamps and debottlenecking). Equally, the data derived during design can be highly valuable to support day-to-day operations such as RTO, maintenance, troubleshooting and equipment substitution. The design data, if available, are an asset in their own right throughout the plant's life. In addition to facilitating data exchange and work flow integration, successful infrastructures will also support creation of the information asset as the design progresses. A life-cycle database might be one application connected to the information bus to collect messages and build the information asset as the design progresses (Fig. 13).

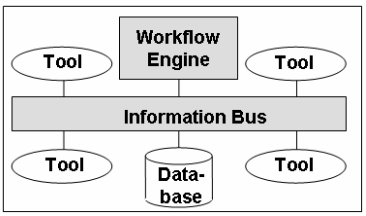

Figure 13. Publish and Subscribe Architecture with Information Asset Database.

Collaborative design is an emerging field, and although most of the difficulties are practical, they have proven to be resistant to progress. Today, each owner company and engineering contractor has its own work processes. The work process has a significant impact on what data must be exchanged in an information package (including how the data must be structured). Until work processes are aligned, each client/contractor pairing will require a bespoke implementation of the infrastructure. Conversely, competitive differentiation between contractors arises in part from their work processes. Equally, today's bidding environment disincentivises data exchange. Our conclusion, after having been actively involved in several public and proprietary efforts to develop collaborative systems and standards, is that business goals will need to be aligned if the potential savings from collaborative design are to be achieved.

Conclusions

As we have seen, significant advances in technology have been made over the past few years in each of the three areas covered in this paper: physical property modeling, simulation and optimization, and collaborative design. Notably though, only steady-state simulation and related physical property modeling have achieved universal adoption. To cite just a few remaining "gaps":

- Many seemingly mature technologies such as dynamic simulation and synthesis methods remain the domain of specialists,
- Mature, generic tools for design optimization and for handling uncertainty are not available,
- Industry standard data models for process design and plant asset data have not been widely adopted.

Thus, there remain huge opportunities for both the wider industrial application of mature technologies and continued technology development. However, with some exceptions, the gaps are not a result of inadequacies in the underlying math and chemical science technologies. Rather, they result from a combination of factors, such as:

- Absence of proven, repeatable, broad-based economic return
- Immature understanding of how to formulate problems and package available technology for practical solutions to real problems of industrial interest.
- Shortcomings in usability (by non-experts) and sustainability in available software, both in engineering and online applications.
- Difficulties in finding a successful model for how to develop standards for data, models, and workflow, and ensure that they are adopted. With the exception of CAPE-OPEN, such success as there has been has arisen when a vendor has worked with its own customer base to develop a *de facto* standard.

As we have seen in this paper, application development has largely proceeded along two tracks—model/simulation-centric and design/data-centric—while properties represent a third, more or less independent, area. While it is important to maintain a focus in each of these three areas in order to successfully address the gaps discussed above, their convergence is also necessary to realize the full promise of CAPD. Thus, we foresee:

- The development of product design software with built-in engineering and mathematics analogous to that available today for process design, as well as support for integrated product and process design.
- Emergence of matched modeling and optimization approaches that enable true model centricity and global optimization. For example, cost models that are compatible with design optimization solutions.
- Software architectures that combine the model/simulation-centric and design/data-centric tracks, largely achieved by treating models as another form of information asset in Fig. 13, separate from specific applications.

Progress will result from the continued partnership of academia, manufacturers, and software vendors.

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