The Process Simulation Revolution: Thermophysical Property Needs and Concerns

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Chemical process simulators have undergone tremendous development in recent years. The new capabilities of these tools have changed the way chemical companies approach many aspects of process design and development, including thermophysical properties. What are the important thermophysical property needs in process simulation remaining to be addressed? What weaknesses in the application of thermophysical properties should users of process simulators be concerned about? Will chemical process simulators become the primary stewards of thermophysical property technology for the chemical industry? How can expertise in the thermophysical property area best be applied to optimize the impact on process design, development, and operation?

Introduction

Over the last decade or so, the chemical process simulator has evolved from many primarily proprietary programs with dedicated development and maintenance staffs at major chemical and petroleum companies to a few commercial products licensed by software companies and accepted nearly universally by industry. During this time, advances in computation technology have greatly expanded the range of applications as well as the ease of use. Where once a few specially trained individuals labored over fixed format input records to simulate a single column or reactor, nearly all process engineers now have the capability to simulate whole chemical processes or plants through a graphical interface on their desktop.

Clearly, the majority of the chemical and petroleum industry has determined that development of process simulation tools is not one of the critical skills which can be cost-effectively maintained within each corporation. Indeed, the continuing rapid development of the commercial simulators seems to confirm the validity of this choice. A number of related skill areas, including the field of thermophysical properties, are now being reevaluated in light of the developments in process simulation. The purpose of this paper is to highlight some of the needs and concerns in the area of thermophysical properties related to the process simulation revolution as viewed from an evolving thermophysical property skill center in the chemical industry.

Another skill area whose evolution has impacted the application of thermophysical properties in process simulators is the collection, evaluation, and compilation of thermophysical property data and prediction methods. Much of this work has been determined to be of common interest to the chemical industry but has been administered through industrial consortia and university-based research efforts, often with some governmental support rather than through direct commercial competition, as in the case of the process simulators. These developments would, themselves, be best addressed as a separate issue, but their impact is coincident with that of the process simulation revolution on thermophysical properties. The product databases of many of these efforts are available directly or as an optional add-on feature of most process simulators. The combined result of these and other effects on thermophysical property skill centers in the chemical industry has been a significant decrease in the number of corporations with dedicated skill groups and a reduction in the staffing of those remaining. A number of companies have recently determined that some of these reductions were overoptimistic and are now reconstituting or "beefing up" such skill groups, but the "steady-state" level is not yet apparent and may well be a characteristic of each corporation's personality based on their product lines and other competitive advantages.

As already implied, developments in process simulation have had a great impact on the thermophysical property skill area. Early process simulators had no built-in databases of pure component data or multicomponent interaction parameters, so that inclusion of such data in the input to each process simulation was a requirement. In this era, it was clear that a staff devoted to collection and development of thermophysical property data was an integral part of any process simulation effort in the chemical industry. In many cases, in fact, it was impossible to get any result from a process simulator without considered thought and some degree of expertise in the area of thermophysical properties. Partly because this level of effort is inconsistent with the vision of plant-scale simulation on every engineer's desktop, all major process simulators now make it possible to get a simulation result with very little or no consideration of the system's thermodynamic or physical properties. While increased user-friendliness is clearly a step in the right direction, it is a two-edged sword which could potentially be combined with clever (or inept) marketing and superficial engineering knowledge to completely discount the truly critical impact of an understanding of thermophysical properties on process simulation and design. No quantity of user-friendly forms and menus can adequately substitute for expertise in the application of thermophysical properties and an understanding of the chemical process being simulated. The questions which users of process simulators must consider include what level of centralized expertise in thermophysical properties is optimal and how is this expertise best used to optimize the impact on process simulation and design.

Process Simulation Tools

Competition between the major vendors of chemical process simulators has resulted in some truly extraordinary tools which are remarkably similar in many respects. This section is devoted to acknowledging the most significant advances in process simulation directly related to thermo-

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physical properties and their application in the chemical industry. The emphasis here is more on trends than on specific features of any of the individual simulators, since they are similar in many ways and appear to be moving in the same direction.

•Pure component databases. The major simulators now have pure component databases with critically reviewed data and parameters for well over 1000 compounds of industrial interest.

•Binary interaction databases. Direct access to binary and multicomponent phase equilibrium data collections is a common add-on option and databases of binary interaction parameters derived from such data are included in some cases. In some cases, separate activity coefficient parameters are provided for each vapor phase model, enhancing the applicability of these models.

•Data regression. Regression of pure component parameters and binary interactions to fit experimental data allows easier incorporation of additional components and binary systems.

•Expanded suite of thermodynamic options. Inclusion of additional and more flexible thermodynamic options has made it easier to adapt thermodynamic models developed for other simulators. Inclusion of the latest equation of state options including extended α functions, asymmetric interactions, etc. has made it easier to model many systems with greater accuracy.

•Flexible combination of thermodynamic options. The ability to mix and match parts of various thermodynamic options into a customized model allows the design of a thermodynamic model based on the data available and calculations desired for a given system.

•Pure component property estimation. In cases where only rough estimates of certain properties are required, the ability to easily obtain estimated parameters from structure is a useful tool.

•Binary interactions from structure. Inclusion of prediction methods such as UNIFAC have made it easier to do preliminary screening studies for some systems. In some cases, UNIFAC estimates can be used to fill in gaps in the interaction matrices of other activity coefficient models automatically!

•Electrolyte equilibria. All of the major simulators now include methods to model the complex interactions in electrolyte systems. Additional automated features and inclusion of interaction databases are making these systems easier to model.

•Reactive distillation. There is no way to adjust a traditional thermodynamic model to properly account for a column which does not maintain a component mass balance. The ability to model reactions and phase equilibria simultaneously has extended the use of thermodynamic models to new types of systems.

•Mass-transfer limited distillation. A more rigorous approach to tray efficiencies makes the underlying thermodynamic model more useful and extends the understanding of how many systems work. It also requires a better understanding of some other physical properties, however, placing new emphasis on the estimation and correlation of transport properties.

•Property table and plot generation. The ability to generate tables and plots of thermophysical property data makes it easier to understand and to debug as well as to take advantage of unique features in some systems.

•Data visualization. Binary and ternary equilibrium plots make it easier to prepare, analyze, and evaluate thermodynamic models. Newer data visualization tools such as residue curve maps make it possible to understand the thermodynamic implications of azeotropic systems.

•Incorporation of alternate property options. For those corporations with thermodynamic models from older simulators or who wish to use methods not yet incorporated in the simulator, the ability to incorporate alternate methods to calculate individual thermophysical properties is an invaluable tool.

Development Needs

Here are some areas in which additional development work could significantly aid users in the application of thermophysical properties in process simulators:

•Incorporate new thermodynamic model developments. As new methods are developed, tested, and accepted, they must continue to be incorporated into the simulators.

•Make prediction more flexible (controllable). In cases where additional knowledge of the compounds or conditions of interest could be used to guide the estimation process, a flexible framework allowing easier user-guidance would be helpful. One possible step would be an optional "expert prediction mode" which interacts with the user in the selection and application of prediction methods. This would make the options more obvious and allow for user override where appropriate.

•Ease access and archival of property parameters. Parameters estimated or extracted from databases should be available for inspection (optionally) along with details of the estimation procedure where appropriate. In addition, the ability to archive all thermophysical property parameters used in a simulation for future use ensures reproducibility (especially when databases change from version to version of the simulator).

•Simulate polymer systems. There is currently a lot of development work in this area, but little consensus on the best models. As the best models are identified, thermodynamic methods and unit operations for polymer systems should become more readily available in process simulators.

•Do more data visualization. These tools are useful for analysis by thermophysical property experts and instruction of other simulator users. Development and inclusion of more such tools is an important goal.

•Help gauge the impact of thermophysical property choices. The impact of the thermophysical property options and parameters needs to be made more visible to users. Perhaps this could be done through multiple simulations with different options and/or some random perturbation of property parameters to indicate the true range of variability.

Concerns

Many of the drawbacks of the process simulators with respect to thermophysical properties are direct results of the advances. Some could be addressed (at least partially) through modified implementation, while others can only be addressed through education of the user community. It is much too easy to blame the tool rather than the uninformed or naive user, but increasing the level of user sophistication should be a goal of the vendor and the licensee. Here are some concerns about the application of thermophysical properties in current and future process simulators. Efforts to alleviate and/or avoid these problems would do a service to the process simulation community and the chemical process industry.

•Can simulation be too easy? When a process can be simulated by graphically placing and connecting process units and responding to a small number of forms windows, the number of assumptions and simplifications made along the way is less obvious than when the user was forced to think about each of these individually. This can easily result in overconfidence in the validity of the default assumptions and in the quality of the simulation results.

•A bad answer can be worse than no answer at all! There seems to have been a lot of effort put into maximizing the likelihood of arriving at a converged simulation result while minimizing the user interaction. Simulator users and developers alike need to be more aware that it is not obtaining *an* answer which is important but obtaining *the* correct answer (or a close approximation). For example, no simulator should give a converged solution for a liquid/liquid extractor modeled with the Wilson activity coefficient model (which does not allow the coexistence of two liquid phases). False solutions and misidentified phases in high-temperature, high-pressure flashes using the equation of state are also problematic.

•Beware of limitations. Commercial chemical process simulators are powerful tools with many capabilities, but there are limitations. The developers at all the major simulator companies agree that neither their product or their help line is an adequate substitute for expertise in thermophysical properties or a number of other skill areas. Somewhere in marketing–management interchange and/or user training, this is too often de-emphasized. We must all work to make sure expectations are more in line with the capabilities of the tools.

•Application must remain a responsibility of the user. Keep in mind that the goal of the simulator vendor is to develop and market simulation tools, while the goal of a chemical company is to develop and market chemical products. Since the ultimate responsibility for operation of the chemical plant lies with the chemical company, it must ensure that both thermophysical properties and the simulation tool are properly applied toward this end. In addition, experience gained through application of thermophysical properties and simulation tools becomes a corporate asset which can enhance the quality and efficiency of future applications.

•Think about it! There is no substitute for a skeptical user. A user who spent days or weeks putting together a model of a process perhaps felt obligated to spend at least a few minutes thinking about the results to see if they made sense, but this effort may seem less justifiable when the model is put together in minutes or hours. If anything, the opposite should be true, since the user has spent less time developing an understanding of the system in the latter case. Users should be encouraged to review all simulation results with a skeptical eye and get a second opinion when there is any doubt.

The Role of the Thermodynamicist

Until there are no new chemical processes and products or all pure component and mixture properties can be accurately determined from chemical structure alone, there will be some need for engineers skilled in the thermophysical property area. The availability of pure component and binary phase equilibrium databases does not invalidate the role of the experimental thermodynamicist. In some respects, this job becomes more difficult as the "easy" measurements are made and those which were previously difficult or impossible remain. Similarly, the role of the thermophysical property specialist in process simulation applications is becoming less routine. While it may have been common in the past to spend weeks or months collecting data and regressing parameters for each process thermodynamic model, this is now rarely necessary and justifiable. In the future, the primary role will be that of a problem solver/consultant/skill resource.

In order to maximize the value of the thermophysical property skill area as a corporate asset, application thermodynamicists will have to spend a higher percentage of time on

•educating the process simulator user community on the usage and limitations of the thermophysical options present in the simulators,

•working with the skeptical to resolve questions about simulation results,

•developing thermodynamic models which take advantage of the built-in options of the simulators and incorporate additional knowledge required for specific applications,

•evaluating new thermodynamic models, correlations, and prediction methods in the role of corporate technology steward,

•working with experimental thermodynamicists to ensure that experiments are designed to yield the optimal amount of additional information required for process simulation applications,

•cooperating with universities, government agencies, and industrial partners in consortia organized to pursue the more general common interests which are most cost-effectively addressed through mutual effort,

•determining the level of complexity and effort required for each model based on the intended application, and

•consulting directly with users to solve problems and answer questions which require detailed understanding of thermophysical properties and their application.

Correspondingly, less time will be spent on

•searching literature for experimental data of all types,

•regressing pure component correlation parameters and binary interactions,

•estimating thermophysical property data and parameters,

•compiling data and correlation parameters,

•preparing tables and plots of thermophysical properties for users, and

•programming new thermodynamic models for use in process simulators.

While all of the items on the latter list remain important, more responsibility for some must be transferred to users, simulator vendors, and consortia, while others will be made more efficient through more advanced tools. The net result is that the thermophysical property skill area will be much more interactive with process engineers and others inside and outside the corporation. Because of this, the duties will be more diverse, less routine or predictable, and even more challenging. The process simulation revolution has helped to make thermophysical properties more accessible to everyone and irreversibly changed the role of the thermophysical property specialist.

Conclusions

Many developments in chemical process simulators have made it easier to apply thermophysical properties to process design, development, and operation. There are still, however, a number of development needs and areas of concern which have been identified. One of the continuing roles of thermodynamicists will be to address these needs and concerns within the process simulator vendors.

Collection and evaluation of thermophysical property data are increasingly becoming centralized as part of large cooperative efforts with industrial sponsorship. Thermodynamicists will continue to play primary roles in these important efforts as well as experimental measurement and the development and evaluation of prediction methods.

With better thermophysical property data and methods more accessible to process engineers through chemical process simulators, the role of thermophysical property specialists in the chemical industry will be more focused on experimental measurement and applications specific to the needs of the individual chemical company. Accordingly, support and education of the user community as well as oversight of consortia and communication with simulator vendors are increasingly important.

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