Excerpted from Chapter 5 "Software Use in Process Design"

AVOIDING PITFALLS IN SOFTWARE USE

Design-related software is an invaluable tool, allowing for design accuracy that could not be imagined 20 or 30 years or even a decade ago. In addition to exponential increases in realism, flexibility, and applicability, design-related software has become much easier to use and understand. The benefits of the ever-increasing trend supporting increasingly easy-to-use software with steep learning curves are many. There are, however, a number of potential design and economic evaluation pitfalls that result from the trend supporting the creation of software that is easy to use and learn. Avoiding potential software use-related errors in the design process therefore becomes as important as the actual software use.

Graphic Interface and Ease of Use

There are four main sources of errors in design and evaluations that stem from attempts to ease software use. The first is due to the practice of embedment, or showing multiple operations as one object on the screen. Many chemical process software packages embed complex operations composed of several pieces of equipment within the larger overall simulation. This reduces the clutter that occurs in compound simulations, thereby providing a clearer view of the process simulation. Embedment can also reduce computational tasks by splitting up large calculation tasks into smaller, more manageable simulation routines. Embedment can, however, be a source of simulation error as it is easy to overlook design and simulation issues in the embedded operations, functions, or procedures. Further, the interface between the embedded and overall simulations in the past has shown errors in transferring information back and forth. The resultant transfer error can then give an impression that the simulation is complete, when in fact only the overall simulation is correct. The obvious example of embedment-related errors is the treatment of distillation columns by many of the off-the-shelf simulation software packages. The simulation scheme displays a single unit, whereas the embedded simulation of the distillation column contains the reboiler and condenser as well as pumps and any number of potential subcomponents. The embedded simulations may also contain entire multiple separation columns even though the simulation flow diagram only graphically displays a single column. Thus, embedment can lead to misleading equipment specifications and resulting incorrect economic evaluations. Further, the overall and embedded simulation interface may not function properly, resulting in false indications of embedded simulation completion or solution.

A second source of design and evaluation error resulting from attempts to make software easier to use is attributed to numerical calculation tolerance levels.[†] The numerical evaluation techniques used in software are very sensitive to convergence criteria specified by the software. These tolerance levels can generally be changed manually and have default values specified by the software programmers. The specified default tolerances are often sufficient for simple calculations. However, default tolerance levels may be inappropriate for delicate, nonlinear, or complex systems. In fact, tolerance levels should be seriously considered and evaluated in any situation where nondestructive error propagation is possible. Automatic use of default tolerances without due consideration can lead to faulty simulations, estimates, and thus incorrect designs. For instance, 0.1 percent mass balance tolerances are quite reasonable for single-unit simulations such as those for heat exchangers. Use of this seemingly

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[†] See general numerical evaluation method texts for more information about the effect of tolerance levels on numerical solutions.

reasonable tolerance in an average refinery simulation containing mass-transfer operations consisting of 6 distillation columns, 15 pumps, and 14 heat exchangers can lead to an unacceptable propagated mass error of 3 percent or more. A good approach to avoid these problems is to begin with larger convergence criteria and reduce them after convergence, until convergence limits are reached.

The third common source of software use error resulting from aesthetic and user-friendliness considerations is the utilization of nonautomatic procedures. In an attempt to ease software use, many packages allow users to employ various degrees of accuracy as well as the complexity associated with this use. This trend can cause users to overlook steps required for accuracy, but not for software operation. For example, many software packages utilize external processing for the completion of such items as separation tray sizing, heat exchanger area sizing, and various equipment pressure drops. Failure to employ and use external software utility functions such as these can be a source of considerable faults.

The final, and perhaps leading, source of software ease-of-use related error is due to built-in default software assumptions. All software packages have default values for the various factors required to operate the software. Most of these are reasonable and appropriate. However, the broad-spectrum use of software does not allow for very accurate defaults. It is therefore up to the software user to determine the correct default values appropriate for the particular circumstance. Ignoring the need to determine and correctly change default values leads to major problems, ranging from simulation error, to economic evaluation error, to reporting grammatical errors. Some of the most common default value types that must be set correctly are provided in Table 5-4.

Thermodynamic Property Packages

As discussed in greater detail earlier in the chapter, correct selection of thermodynamic property packages is critical to accurate, worthwhile simulations. However, the validity of a simulation that only works under one set of thermodynamic property estimation methods is questionable as thermodynamic property packages are estimates. Therefore, use of multiple property packages to simulate a process is recommended. The benefits of evaluating designs under various assumptions upon which a number of thermodynamic packages are based yields a more robust design. Furthermore, it is easy to perform in almost all simulators available today. Any associated design changes required for accommodating multiple thermodynamic packages are reflective of the need for process design robustness required for real-world situations, and equipment specifications that meet these requirements yield a correspondingly more realistic process. Thus, utilization of multiple thermodynamic packages in simulating a design gives an added degree of realism, robustness, and acceptability while requiring relatively little effort.

Simulation Realism

Perhaps the most serious source of software use errors arises from unrealistic use of simulation software. Many, if not all, current simulation software programs can

Table 5-4 Commonly defaulted software parameters

Application	Commonly defaulted parameters
Simulators	
Thermodynamic property package	Binary coefficient types Possible phases
Equipment	
Pumps and compressors	Efficiencies Values and types
Liquid storage vessels	Liquid level
Vapor storage vessels	Pressure
Separation columns	Tray/packing efficiencies Subcomponent equipment types Specification types Reflux ratios Draw types Tray performance
Heat exchangers	Type Pressure drop Heat-transfer efficiency
Economic evaluators	Utility availability Utility costs Tax rates Local economic factors Salaries Construction costs

function in an unrealistic manner. It is therefore critical that the software user employ sound engineering judgment when employing software capable of unrealistic behavior, as the point of simulation is to approximate reality. Simulator unreal behavior extends into a number of areas. First, simulators allow unrealistic parameters to be used, generally without warning of the improbable scale of parameters used. These generally apply to such factors as efficiencies, sizing of units, recycle ratios, and other such criteria. Table 5-5 displays some of the most commonly encountered unreal simulation parameters and an explanation of their effect.

Use of inappropriate parameter scales can be prevented to a certain extent by understanding the various levels of detail provided by the software, especially simulations. The utilization of dynamic simulations, which emulate material and energy flow more accurately, gives a much more realistic behavior picture for the design. Because dynamic simulations are more realistic in their treatment of material and energy flow, they will generally not work very well for unrealistic parameters and will often indicate that unrealistic parameters are specified.

Another major potential source of error is due to the utilization of logical operations in simulators. Many simulators allow the use of logical operations. These commonly include recycle, splitters, mixers, and theoretical heat-transfer equipment. While these logical operations are useful, care must be taken when they are employed since

Table 5-5 Examples of commonly encountered unreal simulation parameters

Operation	Parameter	Error	Explanation
Distillation columns	Reflux ratio/ reboil ratio	High reflux/reboil ratios are attractive to use since they allow easy control and good performance	High reflux and reboil ratios, compared to their minimum, results in poor economics.
	Pressure drop	No pressure gradient across the tray/packed section	Lack of a pressure gradient affects vapor flow
Extraction columns	Pressure drop	No pressure gradient across the tray/packed section	Lack of a pressure gradient can result in anomalous numerical solutions and similar simulation results
All operations	Pressure drop	No frictional pressure losses	Avoiding frictional losses does not give an accurate picture of necessary pressurizing equipment
Pressurization units	Efficiency	Unrealistically high efficiencies	Does not portray real equipment requirements and possibly allows physically impossible processing

enacting similar processing with real equipment can be difficult, if not impossible. For instance, a two-vapor-stream mixing operation can be as simple as connecting two pipes to a third through two one-way valves. On the other hand, a liquid stream splitter requiring one logical operation may require a series of distillation and extraction columns, with all their associated auxiliaries. Of course, some processes carried out by logical operations are impossible.