Pitfalls in Process Simulation:

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Process simulation is useful and powerful tool to model chemical process flowsheets of varying complexity. Modern day simulators are built with comprehensive pure component databank, exhaustive library of thermodynamic systems and physical property estimation methods, initial estimate generators, in built algorithms for every unit operation in a very user friendly graphical interface manner. These simulators have capability to solve and optimize virtually any flowsheet synthesis problem. Despite such in-built sophisticated and rigorous modelling capabilities, process simulations at times fail to represent real life plant data correctly. In most of such cases, an user exhibits blind faith on simulator's inbuilt capabilities and its default selection of methods which leads to erroneous results.. Since, the simulators can generate multiple and at times, conflicting solutions for same set of input data parameters, it raises doubts about its effectiveness and reliability. There are number of reasons that result in simulation failure. This paper discusses some of the reasons for simulation pitfalls.

Potential issues:

Process simulation allows experimenting with a 'digital twin" of a real-life process plant. Various 'what-if' type scenario analysis and optimization avenues can be tested on the simulation model before implementing in the plant. The success of a simulation model can be measured by the extent it truthfully mimics the real asset or process. This success depends on design techniques applied while modelling the problem. It is a common belief that simulators can provide sophisticated and accurate results in shortest time. However, the truth is that simulations can also fail miserably. It can fail in all the ways that theories can fail, and in all the ways that experiments can fail as well. If process simulation is handled improperly, prospects for simulation failure are high. An understanding of the many ways in which simulations can fail offers a better clarity on reasons for failure and in a way, helps to caution users. Pitfalls of simulation can be categorized as below.

(A) Data entry: This is very common and simplest form of simulation error that can mislead the user. A decimal shift typo error has serious consequences. For example, a decimal level error in specifying wash water flow rate injected on column overhead stream, say inflating it, will result in multiple errors in hardware design including increase in condenser heat duty, increase in cooling media consumption, oversized pipes, oversized efflux drum with boot for water separation, upset in overall water balance, etc....

(B) Incorrect unit of measures (UOM): Again, this is a common data entry type of error. Many times, data available for simulation input is not mentioned in only one single unit of measure for a given parameter. Though simulators have automatic feature of converting units of measure, there is potential for wrong selection of UOMs from the graphic interface menu. As an example, say, entering the feed stream data in molar flows instead of mass flows will lead to erroneous results.

(C) Data reconciliation: Operating plant data obtained from plant DCS system is unlikely to be totally consistent. Depending on relative mode of operation and stability and controllability of the process, there are variations in the parameter values with respect to time. There is no unique, single fixed-point data for any given variable. For example, a simple one feed and two product stream binary distillation column having flow and composition measurement on feed and both products lines will at any given point of time will not satisfy "Feed flow = Products flow" mass balance rule to the perfection. Bigger errors may crop up as feed and product analysis timing may not be consistent with each other or other operating data. Therefore, data reconciliation must be done carefully for obtaining a satisfactory representative data which is consistent and satisfies heat and material balances. Even with correct modelling techniques and appropriate choice of equations to represent the system are used, data reconciliation if not done properly, results in horrendous results.

(D) Ignoring warning messages: A fully converged complex flowsheet using rigorous procedures is no way a guarantee for provides dependable results. Modern day simulators have capability to display the results for selected unit operation or select stream with one single click of the mouse. The detailed simulation text report runs in several pages and most of the times, such detailed report is not generated while converging the simulation model. A detailed text report contains 'warnings and messages" which if ignored can lead to an erroneous simulation. For example, the report may highlight a warning to user about unavailability of binary interaction parameters of certain pairs. Such pairs are defaulted to ideal in absence of any other user supplied data. If a detailed report is not generated and all warnings are not analysed rightly, user can miss such critical warnings leading to simulation failures.

(E) Physical and thermodynamic property model: The user needs to have adequate knowledge of suitability of various thermo methods for various components / situations. The user also needs to be familiar with the specific methods / guidance available from the simulation software guide. Selection of pertinent thermodynamic model and physical property model is most crucial to success of any simulation problem.

Missing, inaccurate or inadequate physical and thermodynamic properties undermine accuracy of results. Most of the in-built properties have a predefined applicability range. The user needs to verify and confirm that the inbuilt databases associated with the selected thermodynamic methods, cover the operating range necessary in the given process. Estimation of missing parameters using various techniques (Example UNIFAC method, or data regression, etc) must be done carefully. Estimated data must be validated before its use in simulation. Describing non-databank components is a real challenge in terms of covering its property estimation range as necessary. It is also precarious to assume that all thermophysical or transport property parameters are available in the simulator database just because the simulator did not flash you an error message.

(F) Too much faith on input data: This is one of the most common reasons of simulation failure. Negligence on mirroring of plant or laboratory data will surely result in an inaccurate simulation model.

(G) Configuration of simulation defaults: Every simulation model has default configuration values of many parameters. These include initial estimation generation methods, selection of minimum tear stream algorithm to decide calculation sequence, flowsheet tolerance values, water decant options, methods for estimating missing data, etc. These defaults need to be reviewed and accepted consciously, they may need to be modified as and if necessary.

(H) Apparent Accuracy: Have you ever noticed a heart-breaking observation of privileged simulation engineers spending a large effort in refining a model with far more precision than the basic data allows for? Sometimes, engineers feel obliged to use simulation tools for optimization issues. There is no point in investing efforts in optimization of a process based on heat exchangers' small-temperature approaches, when the enthalpy model itself is only ±20% accurate. It is extremely important to have cause and effect type of error analysis skills. The user should have a fair understanding of impact of one variable on the entire flowsheet. The process engineering & technology knowledge of an engineer cannot be replaced by a process simulator. In fact, it is a pre-requisite for working on high-end simulators, something akin to requirement of highly skilled driver for a high-end, high-speed car. Failed simulation could be attributed to loss of such skill. Novice users seem to forget that, although simulator can display process parameters, e.g. temperature, apparent accuracy in form of many decimal places, only rarely will more than one decimal make any real difference to hardware selection. For some weird reasons, it is generally believed that the computers can always provide rigorous solutions with quasi-infinite accuracy. In reality, conventional quick estimates, design judgement and sound understanding of engineering principles are necessary while understanding and accepting results. .

Concluding Remarks:

A process simulator is one of the most useful and powerful tools for modelling a process flowsheet. It is very flexible in design and analysis of many simple or complex systems. At the same time, its results can be misleading and prone for generating multiple, conflicting results if proper modelling techniques are not understood and followed. The fundamental understanding of thermodynamics, engineering principles and unit operations, Cause and effect type of error analysis skills, etc play a vital role in successful simulation. It is crucial that the simulation results are not believed blindly. Obtaining just a convergence can never be the assurance of accuracy of simulation. The success depends solely on user's ability to interpret input and output data and onus of accuracy never lies with the simulator.