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# Selection of Steady-State Process Simulation Software to Optimize Treatment of Radioactive and Hazardous Waste

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# ABSTRACT

The process used for selecting a steady-state process simulator under conditions of high uncertainty and limited time is described. Multiple waste forms, treatment ambiguity, and the uniqueness of both the waste chemistries and alternative treatment technologies result in a large set of potential technical requirements that no commercial simulator can totally satisfy. The aim of the selection process was two-fold. First, determine the steady-state simulation software that best, albeit not completely, satisfies the requirements envelope. And second, determine if the best is good enough to justify the cost. Twelve simulators were investigated with varying degrees of scrutiny. The candidate list was narrowed to three final contenders: ASPEN Plus 10.2, PRO/II 5.11, and CHEMCAD 5.1.0. It was concluded from "road tests" that ASPEN Plus appears to satisfy the project's technical requirements the best and is worth acquiring. The final software decisions provide flexibility: they involve annual rather than multi-year licensing, and they include periodic re-assessment.

# SUMMARY

The process used for selecting a steady-state process simulator for use by the High-Level Waste (HLW) Program at the Idaho National Engineering and Environmental Laboratory (INEEL) is described. The HLW is composed of both radioactive and hazardous constituents, and it involves both solid and liquid waste forms. The treatment technologies for the various waste forms have not yet been officially determined. Multiple waste forms, treatment ambiguity, and the uniqueness of both the waste chemistries and alternative treatment technologies result in a large set of technical requirements that no commercial simulator can totally satisfy.

Consequently, the aim of the selection process was two-fold. First, determine the steady-state simulation software that best, albeit not completely, satisfies the requirements. And second, determine if the best is good enough to justify the cost.

## *The Process*

The decision-making process spanned four and one half months and involved the following five steps, iterated twice: 1) define the requirements; 2) perform an initial screening to determine those commercial offerings with the greatest chance of meeting the requirements; 3) perform a final screening by "road testing" those simulators that pass the initial screening, documenting the results using a requirements matrix; 4) select a "winner" - the simulator with the best qualitative cost/performance ratio; and lastly, 5) determine whether the simulation benefits of the winner justify its cost.

Twelve simulators were investigated. Eight simulators failed to qualify for a "road test": CADSIM Plus Process Simulator, DESIGN II for Windows, HYSYS, Quick Hydraulics Flowsheet Simulator, PD-PLUS Chemical Process Simulator, PROSIM, MASSBAL and SuperPro Designer. Deficiencies with respect to the breadth of unit operation modules, the property/thermodynamic models, and/or the specie set covered by the databases were the main reasons for rejection. The deficiencies appear to be mostly due to market positioning by the software developers that is inconsistent with the project's requirement matrix - a narrow industry focus, for example, such as hydrocarbon processing.

ASPEN Plus 10.2, PRO/II 5.11, and CHEMCAD 5.1.0 were the only products that qualified for "road testing" as stand-alone steady-state process simulators because they were considered to have the best chance of satisfying all the minimum needs of the requirements matrix. ESP 6.2 by OLI Systems, Inc. was investigated further because of the potential of its thermodynamic properties database to add value to any simulator in general and to ASPEN Plus and PRO/II in particular.

## *Decisions*

The final winner of the down-select process based on technical merit was ASPEN Plus. Neither CHEMCAD nor PRO/II outperformed ASPEN Plus in the "road tests." Neither did they satisfy the requirements matrix better.

INEEL currently has two ASPEN Plus licenses, so selecting a different simulator would incur switching costs. Both CHEMCAD and PRO/II have lower acquisition costs (purchasing, licensing, and maintenance fees) than ASPEN Plus, but these potential savings would be more than offset by the switching costs. Consequently, ASPEN Plus is selected as the steady-state process simulator for the project, based on both technical and cost considerations.

It is concluded that the short-term cost/benefit ratio of ASPEN Plus justifies its annual, rather than multi-year term, leasing at this early point of the project's life cycle. ASPEN Plus provides predictive accuracy within 1.5 times standard deviation of measured concentration values for medium-temperature (100 – 150ºC) vapor/liquid equilibrium for critical non-radioactive species. This benefit is felt to be worth the cost associated with two network licenses for

one year. However, the team will re-assess the potential benefit/cost ratio of commercial simulation's contribution to integrated process optimization at year's end after an entire treatment train has been modeled and tested.

It was concluded that the potential benefit of the ASPEN Plus-OLI bridge marketed by ASPEN Technologies is outweighed by its potential drawbacks in the case of this project, so it will not be leased. The benefit of the bridge would be gaining access to property data for several important species not resident in ASPEN Plus for simulating medium-temperature equilibrium. It is not felt at this time, however, that this potential benefit justifies the potential negative consequences. It is recommended that thermodynamic data for key missing species be obtained from literature searches and/or physical experiments and added to ASPEN Plus, as has been done in the past. Such manual database enhancements at this early phase of the project are considered to be more cost effective over a three-year time frame than accruing $60K or so in additional licensing costs, roughly $100K to transport past database enhancements from ASPEN Plus to OLI, and the increased project and integration labor costs from the user-required interventions.

The trade-offs between the pros and the cons of the bridge will be periodically reanalyzed as the properties database needs of the project are clarified and modified over time.

The selection team would have preferred to spend more time on "road testing" and additional iterations of the 5-step process than the schedule permitted. Consequently, the impact of any remaining lack of knowledge perceived by the team was invariably transposed into the strength of the final decisions - the decisions include further testing and re-assessment, and they contain financial commitments for no more than one year. It is felt that these final decisions simultaneously achieve satisfaction of the near-term needs and provide sufficient flexibility to accommodate remaining ambiguities.

## *Recommendations to Other Potential Buyers of Steady-State Process Simulators*

CHEMCAD is worth investigating if the project's physical property needs don't include electrolyte models. It offers steady-state, dynamic, and process control simulation all in one integrated simulation environment. The user interface is easy to use, the price is considerably less than the other two candidates, and the level of customer support from both marketing and the help desk is unmatched.

PRO/II is worth investigating if the project has modest to large physical property needs, a broad process envelope, and ease of use and pricing are primary factors. It costs about 20% less than ASPEN Plus, and the selection team found the user interface to be more intuitive and easier than that of ASPEN Plus.

ASPEN Plus is worth investigating if the project has large physical property needs, a broad process envelope, and there are opportunity/switching costs associated with some of the performance requirements that appreciably lessen the importance of the simulator's acquisition price. Otherwise, its premium pricing will be a deterrent. The appeal of the OLI bridge, also premium priced, may decrease as the number of contributing engineers, the value of any previous database enhancements, and the piecemeal nature of the model development increase.

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## INTRODUCTION

Steady-state simulation of High-Level Waste (HLW) treatment at Idaho National Engineering and Environmental Laboratory (INEEL) will primarily be used to support future process and facility design. This is part of a broader simulation project aimed at the entire process/facility life cycle, beginning at conceptual design and ending with facility closeout.

Integrated steady-state simulation supporting design of future processes and facilities is currently performed using a Visual Basic process simulator linked to EXCEL spreadsheets for input/output. This simulator tracks mass and energy balances, but lacks a physical properties database and significant predictive capability. The unit operations are mathematically represented by mostly "black boxes." More mechanistic modeling based on rigorous representation of critical natural phenomena and thermodynamic equilibrium is required to provide INEEL engineers with the predictive capability necessary for optimization studies. This would allow engineers to assess potential system-wide impacts of proposed changes at individual unit operations.

Such capability will help to reduce the life-cycle schedules and costs of HLW projects, which is imperative given INEEL's legal commitments and shrinking Department of Energy (DOE) budgets. Some waste treatment options currently have no funding planned for integrated pilot plant demonstrations, which increases the role of process simulation.

HLW at INEEL is composed of both radioactive and hazardous constituents, and it involves both solid and liquid waste forms. The treatment technologies for the various waste forms have not yet been officially determined. However, the main treatment alternatives currently involve vitrification, separations, ion exchange, grout, and calcine dissolution. The number and types of unit operations potentially involved with treating the entire waste envelope are large due to multiple waste forms and the treatment ambiguity. It is assumed that no commercial simulation software on the market will completely match the technical needs of the HLW Program because of the uniqueness of both the waste chemistries involved and the alternative process technologies under investigation. Project personnel are not aware of any process simulator, for example, that mechanistically models the vapor/liquid/solid equilibrium of mixtures containing heavy metals and transuranic elements at 650 – 1300ºC. Appreciable additions to the chosen simulator's thermodynamic properties database are expected to be required to fully support optimization and design efforts. It is also possible that some user-defined unit operation models will need to be created.

This report details the relatively quick search for the commercial steady-state simulator that satisfies the simulation project's technical needs the best and will, therefore, minimize the amount of in-house database modification and/or custom coding of unit operation modules required. Simulation results will be used by engineers and scientists to develop higher-level recommendations for DOE and INEEL program managers regarding the treatment of HLW. As such, it is expected that technical personnel will be direct end-users of the simulation results, and program management will be an indirect end-user.

# METHODOLOGY

A systems engineering approach was used to guide the decision-making process. There were five basic subtasks involved: 1) define the requirements; 2) perform an initial screening to determine those commercial offerings with the greatest chance of meeting the requirements; 3) perform a final screening by "road testing" those simulators that pass the initial screening, documenting the results using a requirements matrix; 4) select a "winner" - the simulator with the best qualitative cost/performance ratio; and lastly, 5) determine whether the simulation benefits of the winner justify its cost.

The entire task had to be completed within four and one half months because of a tight schedule dictated by the overall, broader simulation project. Only one team member was assigned to the project full-time, and the time commitment of the other three members ranged between 12% and 75%. The process was front-loaded, i.e., the majority of effort was focused on the earlier steps. The first three and one half months were focused on just step #1 – defining the requirements. This left only one month to complete steps #2 through #5 once and perform a second iteration of steps #1 through #4. The iteration was justified because the cumulative knowledge gained at the completion of step #4 necessitated modification to the requirements matrix. The iteration was fortunately brief because the modifications required were few.

The team members would have preferred to spend more time on "road testing" and additional iterations than the schedule permitted. Consequently, the impact of any remaining lack of knowledge perceived by the team was invariably transposed into the strength of the final decisions, i.e., the decisions contain relatively short-term financial commitments and include periodic re-assessment and review.

A brief description of the team members is presented below to help provide insight into the methodology and potential biases to the reader (as an outsider looking in) that the team members may not be consciously aware of.

## *Team Composition*

The selection team was composed of the four authors, all engineers. One has a Ph.D. in mechanical engineering, one a Ph.D. in chemical engineering, and the remaining two having masters degrees in chemical engineering. Three have worked in industry for over twenty years, and the least experienced engineer has sixteen years in industry. Each has considerable mathematical modeling or simulation experience. Two of the engineers have used ASPEN Plus (from ASPEN Technology) and ESP (from OLI Systems, Inc.) intermittently in the DOE complex over the past decade; and they both used PRO/II (from Simulation Sciences) extensively earlier in their careers, one in the petroleum industry and the other in the chemical industry. The other two engineers have little experience with commercial simulators outside of graduate school, but they have much experience creating mathematical and computer models – process modeling of electrolytic systems such as batteries, plating, and acidic waste treatment, and computational fluid dynamics (CFD) applied to nuclear reactor thermal hydraulics and solid rocket propulsion.

In addition to their graduate engineering degrees, one team member recently completed his MBA, and another is currently pursuing a masters in computer science. None of the team members has ever worked for a software development company or in the simulation industry.

All the developers of the EXCEL-based simulator that is currently being used for design by HLW Program personnel are members of this selection team. These members recognize the limitations of the current "black box" simulator and have advocated for several years that the Program should acquire the predictive and optimization capability that more mechanistic modeling can provide.

# REQUIREMENTS DEFINITION

The technical requirements are presented in terms of four major drivers: 1) the process envelope, 2) functionality and performance, 3) thermodynamic data, and 4) integration with past, present, and future efforts. These four sources are obviously not independent of each other, and how they inter-relate to produce a coherent requirements matrix will quickly become evident. All requirement drivers, except for integration with future scope, are of equally high importance. Concern for future integration has relatively low importance given the scope and schedule uncertainty typical of DOE programs.

## *Process Envelope*

The simulation efforts seek to support the development of treatments for solid calcine, liquid waste, and tank heels, which all contain radioactive and hazardous wastes in various quantities. The main alternatives for treatment of these wastes currently involve vitrification, separations, ion exchange, grout, and calcine dissolution. The chemical and handling processes involved with these technologies are summarized in Table I and constitute the process envelope for the simulation effort. The general type of process is displayed in the first column, with representative unit operations listed in the second column. In some cases specific reference is made to existing or planned operations at INEEL for those familiar with the HLW Program. At this early point in the treatment planning cycle, the process domain shown in Table 1 is assumed to encompass the potential treatment train for all HLW at INEEL. It includes all on-site chemical processing, storage, movement, and handling of all primary and secondary waste streams considered to be reasonably probable at this time.

The primary focus of the simulation efforts will be on the chemical/treatment processes. However, logistical functions such as the storage, movement, and handling of materials will be included to tie processes together and accurately represent inter-process dependencies so that overall system performance can be assessed and optimized. Excluding such logistics would result in a loss of integration and compromise the purpose of this project. As such, models of logistical activities will be of less mathematical rigor than those of chemical processing unit operations, and they will tend to be closer to "black box" models than to models based on first principles.

The simulator needs the capability to model numerous ancillary equipment, such as condensers and heat exchangers because the simulation efforts will support detailed design.

## *Functionality & Performance*

The main use of the steady-state simulator will be to support process and facility design associated with future HLW treatment strategies. Design here refers to process synthesis and configuration, conceptual design, and detailed design. The two questions the simulator will help to answer are: 1) What is the optimum set and sequence of unit operations to implement a given technology alternative? and 2) What is the optimum integrated set of process parameters and equipment specifications?

Answering these questions requires that the simulator have predictive capability and the ability to perform inverse problem solving, i.e. perform optimization. Calculating basic mass and heat balances for a given set of "black boxes" can be performed in the EXCEL-based simulation currently being used by the team. An important reason for pursuing commercial simulators is to obtain the capability to determine optimums and their corresponding mass & heat balances.

# TABLE 1: PROCESS ENVELOPE

(Taken From Table I of Nichols, Taylor, Lauerhass, and Barnes, 2001b)

| Process Type | Process/Operation |
|---|---|
| Drying | Crystallizer |
| | Solids Dryer (Ex. - Rotary Wiped Film, Hollow Flight) |
| | Spray Dryer |
| | Semi-Batch Evaporation<br>• PEWE at INTEC<br>• HLLWE at INTEC |
| Separation (Physical) | HEPA Filtration |
| | Centrifuge |
| | Film Cooler |
| | Sintered Metal Filter |
| | Scrubbers (for particulate removal)<br>• Steam Atomized (Jet Hydrosonic or Free Jet) for very small size<br>• Venturi for small size<br>• Packed bed for coarse size |
| | Sand Filter |
| | Cyclone Separator |
| | Bag House |
| | Settling Tank - Decantation |
| | Liquid Filtration (solids removal)<br>• Diffusion (cartridge-type filters)<br>• Sieve (sintered metal type filters)<br>• Hybrid (cross-flow, spin-jet, etc.) |
| | Grinder |
| Separation (Thermodynamic) | |
| Gas-Solid | Thermal desorption (Hg from GAC/S) |
| | Thermal decomposition (Hg from GAC/S) |
| | Adsorption (silver zeolite trap, silica gel trap) |
| Gas/Solid/Liquid | Spray Quench |
| | Scrubber (venturi, submerged bed) |
| | Mist Eliminator |
| | Knock Out Chiller |
| | Fractional Distillation (LET&D) |
| Ionic Sorption | Ion Exchange |
| Liquid-Liquid | Liquid/Liquid Extraction - Centrifugal Contactors |
| Homogenization (Mixing) | Makeup (blending of liquid/liquid, liquid/solid reagent, solid/solid feed streams) |
| | Suspension (sparging or blending of solids with liquid) |
| Reactors | Direct-Fired Combustion (Noxidizer reduction chamber) |
| | Noxidizer Oxidation Chamber |
| | Dissolution<br>• Calcine<br>• Cesium impregnated AMP from inert PAN substrate |
| | HEDPA Oxidation |
| | Neutralization |
| | Sugar/Nitric Acid (Vitrification Feed Tank) |
| | Aqueous Phase Precipitation of Mercury |

| Process Type | Process/Operation |
|---|---|
| | Dioxin/Furan Formation (can occur in bag house, scrubber, or quench) |
| | Dry Scrubber/Reactor |
| | Calciner/Incinerator |
| | Grouting |
| | Electrochemical Reduction |
| | Melter<br>• Induction<br>• Joule-Heated |
| Handling | Tank System (Liquid)<br>• Storage Tank<br>• Cooling-Jacketed Mixing Tank<br>• INTEC Tank Farm |
| | Calcine (Solid)<br>• Transfer<br>• INTEC Bin Sets |
| | Waste Packaging & Shipping<br>• TRU solids<br>• LLW solids<br>• HLW solids<br>• UDS particulate solids<br>• Spent GAC<br>• Solid Hg<br>• PAN into High Integrity Container (HIC) |
| Heat Exchange | Direct Injection Cooler (denoxidizer cooling chamber) |
| | Heat Exchangers<br>• Condensers<br>• Superheaters |
| Ancillary Equipment | Feed hopper, conveyor, blower, filter, gas mixer, pump |

Acronyms used in table:

AMP – **A**mmonium **M**olybdo**p**hosphate
GAC – **G**ranular **A**ctivated **C**arbon
HEDPA – **H**ydroxy**e**thane **D**i**p**hosphonic **A**cid
Hg – Chemical Symbol for Mercury
HLLW – **H**igh **L**evel **L**iquid **W**aste **E**vaporator
HLW – **H**igh **L**evel **W**aste (high radioactivity)
INTEC – **I**daho **N**uclear **T**echnology & **E**ngineering **C**enter (group of facilities at INEEL where HLW is stored and treated)
LET&D – **L**iquid **E**ffluent **T**reatment & **D**isposal
LLW – **L**ow **L**evel **W**aste (low radioactivity)
PEWE – **P**rocess **E**ffluent **W**aste **E**vaporator
PAN - **P**oly**a**crylo**n**itrile
TRU – **Tr**ans**u**ranic waste
UDS – **U**n**d**issolved **S**olids suspended in liquid waste

Several base requirements flow down from this key capability, among which the most notable are: 1) reliable thermodynamic models for vapor/liquid/solid equilibrium that account for non-ideality, 2) reliable thermodynamic properties database for critical species, 3) ability for a stream to contain solid, liquid, and/or gas phases with multiple chemical species able to exist in all phases present, 4) perform optimization of individual unit operations, 5) capability to perform a multiple case study (automated consecutive running of pre-specified scenarios), and 6) rigorous modules for equilibrium flashes, heat exchangers, distillation columns, and pumps/compressors.

Knowing beforehand that no commercial simulator will have all the thermodynamic data and unit operation modules corresponding to the process envelope shown in Table 1, the selected simulator must have a high degree of extensibility, i.e., allow easy user customization. The simulator needs to allow the following user interventions: 1) override of default values in the database, 2) additions to the database, and 3) creation of unit operation blocks using a mainstream computer language.

## *Thermodynamic Properties Database*

A set of probable process configurations for HLW treatment that encompasses most of the process envelope described in Table 1 was created, followed by the generation of detailed descriptions for the individual unit operations (Nichols, Taylor, Lauerhass, and Barnes 2001a). Thermodynamic properties needs deduced from the detailed unit operation descriptions are displayed in Table 2. The breadth of both chemical speciation and temperature is very large. The list in Table 2 is not all-inclusive. It is assumed that there are many neutral species and ionic complexes important to the process envelope that are not listed in Table 2, and the selection team expects the simulator's electrolyte thermodynamic models to use the specified ion sets to identify other important complexes and salts.

## *Integration*

ASPEN Plus has a several-year foothold in the HLW Program at INEEL, and another collaborating DOE site selected ASPEN Plus for its steady-state simulation efforts just a few months ago. INEEL's selection team choosing a simulator other than ASPEN Plus would incur appreciable switching costs associated with the inability to fully leverage existing ASPEN Plus licenses, models, database enhancements, and expertise. Consequently, the requirement to integrate with existing simulation efforts, commitments, and experience is considered to be of high importance.

In ASPEN Plus' disfavor, however, is the desire to integrate the steady-state simulation efforts with future simulation scope. ASPEN Plus is strictly a steady-state simulator and isn't integrated with transient, discrete-event, and process control simulation capability as are some other commercial simulators. However, integration with future scope is considered of low importance because present known needs take precedence over future potential needs.

Both integration aspects are discussed in more detail below.

### Present & Past Efforts of Other Groups (i.e., Switching Costs)

A former INEEL scientist worked intermittently for several years gathering, regressing, and validating literature VLE data for acidic nitrate, chloride, and fluoride solutions for use in ASPEN Plus models of Operation's HLW evaporators. These models and database enhancements not only help engineering to support present operational decisions regarding tank blending scenarios, but they could also be part of this project's simulation efforts because all planned future treatment strategies include evaporation to concentrate liquid wastes before primary treatment. It could require considerable effort to transfer the database enhancements to another simulation program because different programs use different electrolyte models, and the exact mathematical and dimensional form of even the same model can differ from one program to another.

# TABLE 2: THERMODYNAMIC PROPERTIES DATABASE NEEDS

| Intra-Phase Chem. Equilibrium | | Inter-Phase Equilibrium | |
|---|---|---|---|
| Vapor | Liquid [1] | Vapor/Liquid | Liquid/Solid [2] |
| *25 - 150°C, 5 - 12 psia*<br>I2, CH3I<br><br>*350 - 1300°C, 5 - 12 psia*<br>Cl2<br>CO, CO2<br>H2, H2O, HCl, HF, H2SO4<br>HgCl, HgCl2, HgO<br>N2, NO, NO2<br>O2<br>SO2, SO3<br>Hydrocarbons [acetone, formaldehyde, butane, butadiene, methane, propane, ethane, dichloroethane, ethylene, benzene, benzaldehyde, monochloroethane, benzo(a)pyrene, chlorobenzene, tetrachlorobiphenyl, toluene, biphenyl, napthalene, and 2-3-7-8 TCDD]<br><br>*650 -1300°C, 5 - 12 psia*<br>Cl species (CaCl2, NaCl, KCl, CsCl, SrCl2)<br><br>Cs species (Cs2O, CsTcO4, CsCl, Cs2CO3, Cs2BO2, CsBO2, CsOH, CsMoO4, CsAlSiO4)<br><br>HNO3, H2S<br><br>Hg species (Hg, Hg2I2)<br><br>I species (I2, AgI, CH3I, CsI, KI, NaI, PdI2)<br><br>Ru species (Ru2, RuO4)<br><br>Tc species (CsTcO4, Tc2O7, HTcO4, TcO2, TcO(OH)2, TcCl4, TcF4, TcF6)<br><br>Species of As, Cd, Pb, Sb, and Sr-90 | *10-150°C, 5 – 12 psia*<br>*(*VLE + LSE)<br>AlF3, Al2O3, Al(PO3)3<br>CaCO3, CaCl2, CaF2, Ca(NO3)2, CaO, Ca(OH)2, Ca0.15Zr0.85O1.85, Ca(PO3)2CaS, CaSO4<br>Cs species (Cs2O, CsTcO4, CsCl, Cs2CO3, Cs2BO2, CsBO2, CsOH, CsMoO4, CsAlSiO4)<br>CO, CO2<br>H2, H2CO3, HCl, HF, HNO3, H2O, H2S, H2SO4, H2SO3<br>Hg species (Hg, HgCl, HgCl2, Hg2Cl2, Hg2I2, HgO, HgS)<br>I2, CH3I, HI, HI3O8<br>NaCl, NaF, NaOH, NaNO3, Na2SO4<br>N2, NO2, N2O4<br>O2<br>Organic phosphates<br>Ru species (Ru2, RuO4)<br>SO2, SO3<br>SiO2<br>Tc species (CsTcO4, Tc2O7, HTcO4, TcO2, TcO(OH)2, TcCl4, TcF4, TcF6)<br>ZrF4, ZrO2, Zr(SO4)2<br><br>Ion Set<br>Cations: Al, Al-F complexes [AlF(+2), AlF2(+1)], As, B, Ba, C, Ca, Cd, Cr, Cs, Fe, H, Hg, Hg-Cl complexes [HgCl(+1)], I, K, Mo, N, Na, Ni, Pb, Pd, Pu, Ru, Se, Si, Sr, Tc, U, Zn, Zr, and Zr-F ionic complexes [ZrF3(+1), ZrF2(+2), ZrF(+3)]<br>Anions: Al-F complexes [AlF4(-1), AlF5(-2)], CO3, Cl, F, Hg-Cl complexes [HgCl3(-1), HgCl4(-2), HgCl5(-3), HgCl6(-4)], I, IO3, NO3, O, OH, PO4, S, SO3, SO4, and Zr-F complexes [ZrF5(-1)]<br><br>(Charged complexes involving F, Cl, and I with Al, Cr, Fe, Zr, and H2BO3 are more crucial than other charged complexes)<br><br>*650 -1300°C, 5 - 12 psia*<br>Glass formers: SiO2, B2O3, Na2O, Li2O, Fe2O3<br><br>Metal oxides (rad and non-rad): Al2O3, CaO, CdO, FeO, K2O, MnO, ZrO2, UO2, and P2O5<br><br>Reductant: C12H22O11 (sucrose)<br><br>Ion Set<br><br>Cations: Al, B, C, Ca, Cd, Fe, H, K, Li, Mn, Na, P, Si, U, and Zr<br>Anions: O | *25-150°C, 5 – 12 psia*<br><br>CaS, CaSO4<br>CO, CO2<br>H2, H2BO3, H2CO3, HCl, HF, HNO3, H2O, H2S, H2SO4, H2SO3<br>NaCl<br>N2, N2O4, NO2<br>O2<br>SO2, SO3<br><br>Cs species (Cs2O, CsTcO4, CsCl, Cs2CO3, Cs2BO2, CsBO2, CsOH, CsMoO4, CsAlSiO4)<br><br>Hg species (Hg, HgO, HgCl2, Hg2I2)<br><br>I2, CH3I<br><br>Ru species (Ru2, RuO4)<br><br>Tc species (CsTcO4, Tc2O7, HTcO4, TcO2, TcO(OH)2, TcCl4, TcF4, TcF6) | *10-100°C, 5 – 12 psia*<br><br>AlF3, Al2O3, Al(PO3)3<br>CaCO3, CaCl2, CaF2, Ca(NO3)2, CaO, Ca(OH)2, Ca0.15Zr0.85O1.85, Ca(PO3)2CaS, CaS, CaSO4<br>Cs species (Cs2O, CsTcO4, CsCl, Cs2CO3, Cs2BO2, CsBO2, CsOH, CsMoO4, CsAlSiO4)<br>HCl, HF, HNO3, H2O, H2S, H2SO4<br>Hg species (Hg, HgO, HgCl2, Hg2Cl2, Hg2I2, HgS)<br>NaCl, NaF, NaOH, NaNO3, Na2SO4<br>Organic phosphates<br>SiO2<br>Tc species (CsTcO4, Tc2O7, HTcO4, TcO2, TcO(OH)2, TcCl4, TcF4, TcF6)<br>Ru species (Ru2, RuO4)<br>ZrF4, ZrO2, Zr(SO4)2<br><br>Ion Set<br>Cations: Al, Al-F complexes [AlF(+2), AlF2(+1)], As, B, Ba, Ca, Cd, Cr, Cs, Fe, H, Hg, Hg-Cl complexes [HgCl(+1)], K, Mo, Na, Ni, Pb, Pd, Pu, Ru, Se, Si, Sr, Tc, U, Zn, Zr, and Zr-F ionic complexes [ZrF3(+1), ZrF2(+2), ZrF(+3)]<br>Anions: Al-F complexes [AlF4(-1), AlF5(-2)], CO3, Cl, F, Hg-Cl complexes [HgCl3(-1), HgCl4(-2), HgCl5(-3), HgCl6(-4)], I, NO3, O, OH, PO4, S, SO4, and Zr-F complexes [ZrF5(-1)] |

Superscripts: [1] Includes all possible dissociation/association from ion set
[2] Includes all salt formation possible from ion set

Besides the simulation engineer supporting Operations, two other HLW engineers, also not part of this simulation project, are currently using ASPEN Plus to assess alternative designs of future off-gas treatment trains. Similar to evaporation, all future treatment strategies require off-gas treatment, so it would be advantageous to be able to incorporate the off-gas models directly into the simulator chosen by the selection team for it's own simulation project. The ability to leverage the simulation expertise of these three other engineers will be proportional to the degree of compatibility of the simulation program selected by the team and ASPEN Plus.

The INEEL currently has two ASPEN Plus licenses – one is a perpetual license, and one is leased on an annual basis. The leased license is used mostly for HLW support by the three engineers mentioned previously. Another Program at the INEEL recently (within the last three months) procured a single-user license for HYSYS, but there is currently little interest in using it by HLW simulation engineers.

This simulation project also has some joint modeling tasks with Savannah River Site (SRS) under a joint Technical Task Plan (TTP ID77WT31, Subtask C). SRS has already chosen ASPEN Plus for their own steady-state simulation efforts. The SRS engineers working on the joint TTP are willing to lease, learn, and use whatever simulator the INEEL selection team chooses. However, SRS's portion of the joint task begins first and may suffer a temporary schedule squeeze because of the learning curve involved with a different program if something other than ASPEN Plus is selected by INEEL's team. SRS also plans to transport its thermodynamic properties database into ASPEN Plus during the next six months. It is not yet clear whether or not SRS' database could fill in any of the gaps in INEEL's thermodynamic data needs. However, the utilization of SRS' data by INEEL if deemed advantageous would be appreciably facilitated if both teams were using the same simulator.

The existence of ASPEN Plus licenses at INEEL and SRS in and of themselves has no financial impact. The fees paid for any current licenses are sunk costs and are therefore irrelevant to the selection team's analysis. Nor are there switching costs directly related to the existing licenses because they appear to be highly utilized by the existing users. Without appreciable underutilization, the licenses do not provide an opportunity for a significant reduction in the incremental costs of this project team using ASPEN Plus. Nor do discounts for additional users provide an opportunity for significant cost reduction because ASPEN Plus' pricing scheme, as communicated to the selection team through the company's sales representatives, offers about $500 - $1,000 discount for an additional user. When commercial simulators lease for annual fees in the mid-to-high $20sK per user, it is unlikely that a relatively small discount will influence the decision-making, especially when the simulation project has a tough set of requirements, as does this project. The influence current ASPEN Plus licenses have upon the decision making comes only from the fact that their existence maintains ASPEN's foothold, thereby causing the significant switching costs related to models, database enhancements, and expertise to accrue.

**Future Scope**

The overall, broader simulation project, of which the steady-state simulation efforts are a subset, will support the entire synthesis/optimization life cycle from process configuration in early design to continuous improvement during operations. This is a broader scope than that of Technology Development's current simulation efforts. In particular, the following activities are being considered for simulation's future role based upon discussions with potential end-users: 1) support process control design; 2) perform concurrent process/cost optimization; 3) provide emissions estimates for permit applications; 4) provide planning basis for trial burns; 5) calculate emissions that are physically unmeasurable on a continuous basis; and 6) support safety analysis by quantifying process/operational variability via dynamic simulation.

The future scope involves process control simulation, transient process simulation, discrete-event simulation, and cost optimization besides steady-state simulation. Obviously, it would be advantageous if the near-term effort put into building the steady-state simulation were extensible to future efforts. Requirements concerning integration with future scope have relatively low importance because the future is inherently ambiguous, with budgets and scope rarely being realized as planned. Consequently, present known needs are considered superordinate to potential future needs.

## *Requirements Matrix*

The aggregate set of requirements that is formed from combining and inter-relating the needs of the process envelope, functionality and performance, the thermodynamic database, and integration is displayed in Table 3. There are two capabilities that lack specific derived requirements: Provide Safety-Related Stream Compositions and Estimate Emissions for Permit Applications. These capabilities will be required in the out-years, and their main impact will be on fidelity constraints for the modeling approaches of individual unit operations. The task of determining desired modeling approaches for individual processes is planned to occur after the software selection has been made because it was assumed that there would not be a large variation in the base set of rigorous (i.e., mechanistic) unit operations offered by the process simulators passing the initial screening. Due to the time constraints on completing the selection process, it was decided to postpone the requirements flow down from such less discriminating factors as modeling approach.

One may notice the absence of specific "ease of use" requirements in the table. This is because of two reasons. First, the process simulation market appears to be relatively stable. It was assumed that most simulators on the market would satisfy a base level of user friendliness. If not, they wouldn't have survived and still be in the market place. Second, it was felt user friendliness could readily be added to the requirement matrix if the "road testing" revealed a disparity in ease of use large enough to cause the selection team to consider it an important discriminating factor.

# TABLE 3: REQUIREMENTS MATRIX

| Simulation | | Software |
|---|---|---|
| ***Capability*** ***(High-Level Req't)*** | ***Characteristic*** ***(Mid-Level Req't)*** | ***Quantifiable Requirement*** |
| *Current Scope* | | |
| Provide Basic Mass & Heat Balances, Basis for Equipment Sizing, Utilities Req'ts, Consumables Req'ts, etc. for optimums | Can perform predictive steady-state process simulation and optimization | Suite shall have a solver for continuous, steady-state process simulation (with nonrandom inputs) with the following functionality:<br>Best – all functionality listed under Better, plus the following:<br>• Rigorous unit operation models for mixing tank, scrubbers (dust, venturi, ejector fume, and submerged bed), cyclone, packed bed quench, spray quench, ion exchange, grouting, mist eliminator, HEPA filter bank, semi-batch evaporator, catalytic reactor, electrostatic precipitator, gas-phase reactor, and liquid-liquid extraction<br><br>Better - all functionality listed under Worst, plus the following:<br>• Global multi-variable optimization with choice of several optimization methods<br>• Allow user-defined physical properties models/correlations. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density.<br>• Has a batch evaporation module<br><br>Worst:<br>• User selection of units of weight and measure for input/output variables<br>• Pure component physical property database<br>• Standard thermodynamic models for energy balances<br>• Inter-Phase equilibrium is determined by calculating a specie's concentration in both phases by equating its electrochemical potentials, accounting for nonideality<br>• Intra-Phase chemical equilibrium is determined by calculating specie concentrations by minimization of mixture Gibbs free energy, accounting for nonideality and user-imposed stoichiometric constraints<br>• All fundamental thermodynamic data in the physical properties database is referenceable to peer-reviewed literature/databases<br>• Standard non-ideal vapor/liquid/solid thermodynamic models (e.g. NRTL for electrolytes and equations of state for gases) use Binary or Higher-Order Pair interaction parameters that are compiled/validated from experimental data found in peer-reviewed literature<br>• Automatic sequencing of unit operation calculations<br>• Automatic recycle stream identification and flowsheet convergence<br>• Ability for a stream to contain a solid, liquid, and/or gas phase, with multiple chemical species able to exist in all phases present<br>• Optimization of individual unit operations (multiple-design specification capability)<br>• Multiple case study capability (automated consecutive running of pre-specified scenarios)<br>• Black box unit operations: mixer, stream splitter, component separator, stoichiometric reactor<br>• Rigorous unit operations: equilibrium flash calculation, heat exchanger, distillation column, pump/compressor<br>• Allow user-defined unit operation blocks using a mainstream computer language (either FORTRAN, C, or C++) that do not inherently constrain the degree of mechanistic modeling possible (can accept a user's model of nonequilibrium such as finite-rate kinetics, for example)<br>• Allow user-defined physical properties database. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density.<br>• Allow user override of default values of physical properties for individual species<br>• Batch evaporation can be approximated by creating a sequence of repeated flashes |
| | Thermodynamic properties database compares favorably with needs (see Table 2) | Best: steady-state simulator shall have thermodynamic data that satisfies Table 2 completely - i.e., database has data for all neutral compounds and at least one compound of every ionic species specified in Table 2 at the temperature and pressure ranges listed.<br><br>Better: steady-state simulator shall have thermodynamic data for appreciably more species at low temperature than the "Worse" category, or it shall have thermodynamic data for the higher temperatures. The data gathering required to fill in the gaps will be less than in the "Worse" category. |

| Simulation | | Software |
|---|---|---|
| ***Capability*** ***(High-Level Req't)*** | ***Characteristic*** ***(Mid-Level Req't)*** | ***Quantifiable Requirement*** |
| | | Worse: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of many of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. Although data for many species is still lacking, the database provides a solid foundation to build upon and the capability to contribute to design efforts in the short term. Data gathering required to fill in the gaps will be appreciable, but it will be considered practical.<br><br>Worst: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of only a few of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. High-temperature data and/or data for a majority of the species is lacking to such a degree that the simulator as is can not contribute to design efforts in the short-term. Data gathering required to fill in the gaps will be large and a major effort. |
| Integrates With Existing Process Modeling Efforts, Commitments, & Experience | Leverage existing ASPEN Plus models, database enhancements, and expertise | Best: steady-state process simulator shall be able to effortlessly import/export files in ASPEN Plus format. This permits full utilization of SRS and resident ASPEN Plus experience, models, and database enhancements. It offers maximum synergy with other INEEL and SRS HLW simulation efforts.<br><br>Worse: steady-state process simulator can import/export files in ASPEN Plus format, but not all model characteristics are common to both simulation packages (not all unit operation modules are common, conflicts exist between solving algorithms, differing methodologies for handling constraints, etc.), resulting in less-than-complete transportability.<br><br>Worst: steady-state process simulator can not import/export files in ASPEN Plus format. This fails to utilize existing ASPEN Plus models and database enhancements, and ASPEN Plus expertise is utilized only in the broad sense that previous simulation experience will shorten learning curve on new simulator. Redundancy will be the only way to achieve integration between our efforts and those of other resident simulation engineers. This provides almost no synergy with existing simulation capabilities. |
| *Future Scope* | | |
| Provide Safety-Related Stream Compositions | Result fidelity of steady-state simulations is acceptable to Safety Engineers | Fidelity constraints translate into requirements for modeling approaches of individual unit operations (TBD). |
| Estimate Emissions for Permit Applications | Result fidelity of steady-state simulations is acceptable to Idaho DEQ | |
| Perform Concurrent Process/Cost Optimization | Ability to map process design parameters to equipment features to capital costs | Best: The steady-state process simulator shall have the following capabilities:<br>1) perform inverse problem solving regarding cost, i.e., force a manipulated variable's value to optimize a global cost function<br>2) permit value constraints on operating parameters and stream characteristics (composition, temperature, flow rate, etc.)<br>3) determine sizing features related to processing, such as number of trays in a distillation column or length of a plug flow reactor<br>4) permit capital cost functions to be created that depend upon equipment features<br><br>Combined, these abilities will allow the automated optimization of a cost objective function by manipulating process variables while simultaneously enforcing specified waste form required characteristics.<br><br>Better: The steady-state simulator shall have capabilities #3 and #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments."<br><br>Worst: The steady-state simulator shall have capability #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments." Engineers will have to manually perform capability #3, i.e., estimate and input cost-related equipment features to couple with the simulator's cost functions for each run of the optimization "experiment." |

| Simulation | | Software |
|---|---|---|
| ***Capability*** ***(High-Level Req't)*** | ***Characteristic*** ***(Mid-Level Req't)*** | ***Quantifiable Requirement*** |
| Quantify Process Variability (inventories, operating parameters, etc.)<br><br>Project Mass Balances and Effluent Stream Compositions and Flow Rates for Planning Basis of Melter Trial Burn<br><br>Provide Continuous Emissions Estimates of Actual Operations | Have a transient process simulator | Transient simulators are required to provide these future capabilities. Therefore, the choice of steady-state simulator made in the present has to be integrated with the choice of transient simulators to be made in the future if efficiency is to be maximized and work redundancy is to be minimized.<br><br>Best: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are all parts of an integrated simulation package. This option is the most efficient, is the least labor intensive, and it requires the least code maintenance and configuration control overhead because it allows all four distinct simulation objectives to be achieved from one base model build.<br><br>Better: the steady-state process simulator, the transient process simulator, and the transient process control simulator are parts of an integrated simulation package. This option results in only one redundant model build (in the discrete-event simulator).<br><br>Worse: the steady-state process simulator and the transient process simulator are parts of an integrated simulation package. This option results in two redundant model builds (in the process control and discrete-event simulators).<br><br>Worst: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are not parts of an integrated simulation package. This is the most time consuming and labor intensive option because it requires separate model builds of the same system in four distinct simulation packages. |
| Simulate Process Control Schemes | Have constructs amendable to process control simulation | |
| Estimate System-Wide Performance (cap. util., campaign lengths, etc.) | Have a discrete-event, stochastic solver (transient by definition) | |

# INITIAL SCREEN

A summary of the initial screening results for twelve steady-state process simulators is displayed in Table 4. The reasons why a simulator passed or failed the initial screen are briefly listed according to the four main requirement drivers. All the information was obtained from marketing literature (including the Internet) unless otherwise specified. Other possible sources are demos, personal experience, conversations with technical support, and training classes. The simulator, its manufacturer, and additional information sources are listed in the "Software" column. Leasing/purchasing costs for the simulation programs were not known at this stage of the decision making process. Cost was not a factor in the initial screen.

Six simulators failed to pass the initial screen: CADSIM Plus Process Simulator, DESIGN II for Windows, HYSYS, Quick Hydraulics Flowsheet Simulator, PD-PLUS Chemical Process Simulator, and PROSIM. Deficiencies with respect to the breadth of unit operation modules, the property/thermodynamic models, and/or the specie set covered by the databases were the main reasons for rejection. The deficiencies appear to be mostly due to market positioning by the software developers that is inconsistent with the project's requirement matrix - a narrow industry focus, such as processing of hydrocarbons, or too little focus on steady-state simulation.

MASSBAL and SuperPro Designer conditionally passed the screen because they could possibly have acceptable electrolyte models, or have an acceptable set of unit operations and database, respectively. Both simulators offered the possibility of improved integration with future scope. However, the information on MASSBAL and SuperPro Designer was insufficient or too weak for unconditional passing. Consequently, it was decided to "road test" these two simulators only if there was time after testing those that passed the initial screen unconditionally. As it turned out, extra time did not exist to "road test" these two conditional simulators, and they were not given any further consideration.

## *The Short List*

ASPEN Plus 10.2, PRO/II 5.11, and CHEMCAD 5.1.0 were the only three products unconditionally selected to pass on to the next stage, "road testing," as stand-alone steady-state process simulators because they were considered to have the best chance of satisfying all the minimum needs of the requirements matrix. ESP was investigated further because of the potential of its thermodynamic properties database to add value to any simulator in general and to ASPEN Plus and PRO/II in particular.

**Steady-State Simulators**

All three simulators appeared to satisfy the minimal process envelope and functionality/performance requirements, and each seemed to offer an advantage over the other two.

***ASPEN Plus 10.2***

The singular advantage that this widely accepted process simulator appeared to offer was integration with past and present efforts of other simulation engineers. Besides having the potential to appreciably reduce switching costs and lessening schedule constraints, as discussed earlier, using the database enhancements and simulation expertise of others should also improve the accuracy of simulation results.

# TABLE 4: SUMMARY OF RESULTS OF STEADY-STATE PROCESS SIMULATION INITIAL SCREEN

| Software | Process Envelope | Functionality & Performance | Database | Integration | Miscellaneous |
|---|---|---|---|---|---|
| ***Failed Initial Screen (Do Not "Road Test")*** | | | | | |
| *CADSIM Plus*<br><br>Aurel Systems | | 1) Appears to be designed as a dynamic simulator rather than steady state simulation program<br>2) Appears to be more suited to P&ID drawing and process operation simulation, or process control scheme optimization rather than process design/PFD simulation<br>3) Appears to have few property models | 1) Appears to have very little built in chemistry | | |
| *DESIGN II for Windows*<br><br>WinSim Inc.<br><br>(Phone call to tech support on 3-6-01) | | | 1) Database in very limited for inorganic and ionic species | | |
| *HYSIS*<br><br>Hyprotech (AEA)<br><br>[2-Day Training class in March 2001] | | | 1) Database includes only hydrocarbons and gaseous species<br>2) no Hg or Hg compounds, salts, ions, or inorganic solids | | |
| *Quick Hydraulics Flowsheet Simulator*<br><br>Chempute Software | 1) Appears to have limited and perhaps inadequate unit operations | 1) Appears to have limited property models<br>2) Does not appear to have electrolyte models<br>3) Appears more geared for piping systems and hydraulics calculations with limited process simulation | | | |
| *PD-PLUS Chemical Process Simulator*<br><br>Deerhaven Technical Software<br><br>[Demo] | 1) Appears to have limited and perhaps inadequate unit operations | 1) Appears to have limited property models<br>2) Does not appear to have electrolyte models | | | 1) Very awkward user interface (DOS-like) |
| *PROSIM*<br><br>Bryan Research & Engineering | | 1) Appears to be applicable only to hydrocarbon processing | | | |
| ***Conditionally Passed Initial Screen (Evaluate Only If Time Available)*** | | | | | |
| *MASSBAL* | | 1) Vendor data claims use in minerals | | 1) Also has dynamic simulation | |

| Software | Process Envelope | Functionality & Performance | Database | Integration | Miscellaneous |
|---|---|---|---|---|---|
| Open Models, Inc. | | processing industries, so it is assumed to have electrolyte chemistry models. This would need to be confirmed.<br>2) Appears to be easily linked to or embedded in Windows or other programs | | capabilities | |
| *SuperPro Designer*<br><br>Intelligen | 1) The program appears to be the only process simulation program with the primary focus being on waste-processing & environmental impact assessment<br>2) Includes 140 unit operation models<br>3) Batch simulation included | 1) Aqueous chemistry would need to be inputted because limited or no built in electrolyte models | 1) Has a 400 species databank, also access to DIPPR data bank | 1) Process economics included | |
| ***Passed Initial Screen<br>- "Road Test" as Stand-Alone Simulator -*** | | | | | |
| *ASPEN Plus*<br><br>ASPEN Technology<br><br>[Personal experience] | 1) Large set of unit operation modules and broad functionality, presumably why it is so widely used in chemical and nuclear industries | 1) Offers user-defined extensibility with respect to property models, database, and unit operations | 1) Compatibility with OLI may extend electrolyte capability to species not available in ASPEN Plus alone or other programs | 1) Chosen by Savannah River<br>2) Has been used for simulation of evaporation (and in other INEEL programs)<br>3) Properties for some species/complexes have been developed at INEEL | |
| *PRO/II*<br><br>Simulation Sciences | 1) Appears to have complete set of unit operations | 1) Integrated with OLI electrolyte models<br>2) Appears to have complete property models<br>3) Appears to be easily linked to Excel and other Windows programs | 1) Integrated with OLI database | | 1) Appears to be very user friendly<br>2) Available to run on-line with no charge for first two hours, additional time at $250/4 hours<br>3) Downloadable demo also available |
| *CHEMCAD*<br><br>Chemstations | 1) Appears to have complete and diverse set of unit operations<br>2) Has batch simulation capability | 1) Thermodynamic models appears adequate, (at least as good as ASPEN) including electrolyte models<br>2) Appears to have good interface capabilities to Excel and other programs, as well as user-written modules | 1) Includes 1500 component DIPPR data base | 1) Also has transient capabilities - dynamic process simulation and process control simulation<br>2) Module available for dynamic simulation of stirred tank reactors<br>3) Rigorous equipment sizing and cost estimation | 1) Appears to have user friendly graphical interface and good printing capabilities<br>2) Recommended by competitor's tech support (WinSIM) when discussing our application<br>3) 30-day demo |
| ***Database & Model Set Passed Initial Screen<br>- "Road Test" Database/Models -*** | | | | | |
| *ESP*<br><br>OLI Systems, Inc.<br><br>[Personal experience] | 1) Lacking in breadth of unit operation modules | 1) OLI appears to be the most developed and complete electrolyte simulation program, and perhaps the only one able to simulate some of the species in our waste | | | 1) OLI integrated with PRO/II; can be integrated with ASPEN Plus for an additional fee; plans for integration with HYSYS |

***PRO/II 5.11***

The key advantage this simulator appeared to have over the other two is its incorporation of the OLI database and thermodynamic models. Unlike ASPEN Plus that offers a software bridge to OLI software as an add-on for an additional licensing fee, PRO/II appeared to have completely integrated OLI's database/models into its simulation software. This feature could enhance the accuracy of simulation results given OLI's strong focus on electrolyte thermodynamics and speciation for the entire periodic table.

***CHEMCAD 5.1.0***

CHEMCAD offered the potential of being almost the all-in-one simulator, providing steady-state and batch simulation in the short-term and cost optimization, dynamic process simulation, and process control simulation in the future. The only future capability it appeared to lack was discrete-event simulation.

**Thermodynamic Database/Models**

***ESP 6.2***

It was decided to "road test" the OLI database and model set to determine its potential value added since it has a strong electrolyte focus relative to the other commercial offerings, it's integration with two of the winning simulators (ASPEN Plus and PRO/II) has already been automated, and its contents (i.e., value) could theoretically be manually added to any simulator meeting the minimal performance requirements. ESP was not tested further as a stand-alone simulator because the marketing literature and current experience of team members made it clear that its set of unit operation modules was unsatisfactory for the needs of the project. Any references made in the report regarding "road testing" of ESP are made from the perspective of assessing the underlying properties database and thermodynamic models, not from the perspective of a complete simulator.

# FINAL SCREEN

Two "road tests" were performed to try to get a quick and comprehensive comparison of the three simulators, determine the value added from past database enhancements, determine the potential benefit of access to OLI's databank/model set, and assess the potential benefit that a commercial steady-state process simulator can provide compared to a "black box" approach. One test involved building a simple process model, and the other test involved user-customization exercises. Chemstations and Simulation Sciences provided the team with free, trial, full-strength versions of their simulators for the evaluation. The team used existing licenses for ASPEN Plus 10.2 and ESP 6.2.

CHEMCAD and PRO/II are at a disadvantage in the "road testing" because it is possible that any perceived problems or poor performance with these two simulators could be understood and eliminated with increased understanding of the programs. Unfortunately, the selection schedule doesn't permit the team to gain as much user familiarity with these two programs as it currently has for ASPEN Plus. Nevertheless, a selection decision has to be made despite such ambiguity and disparity. The purpose of the "road testing" is not to eliminate all knowledge gaps, but rather to limit the ambiguity and disparity as much as possible.

## *Process Modeling Test*

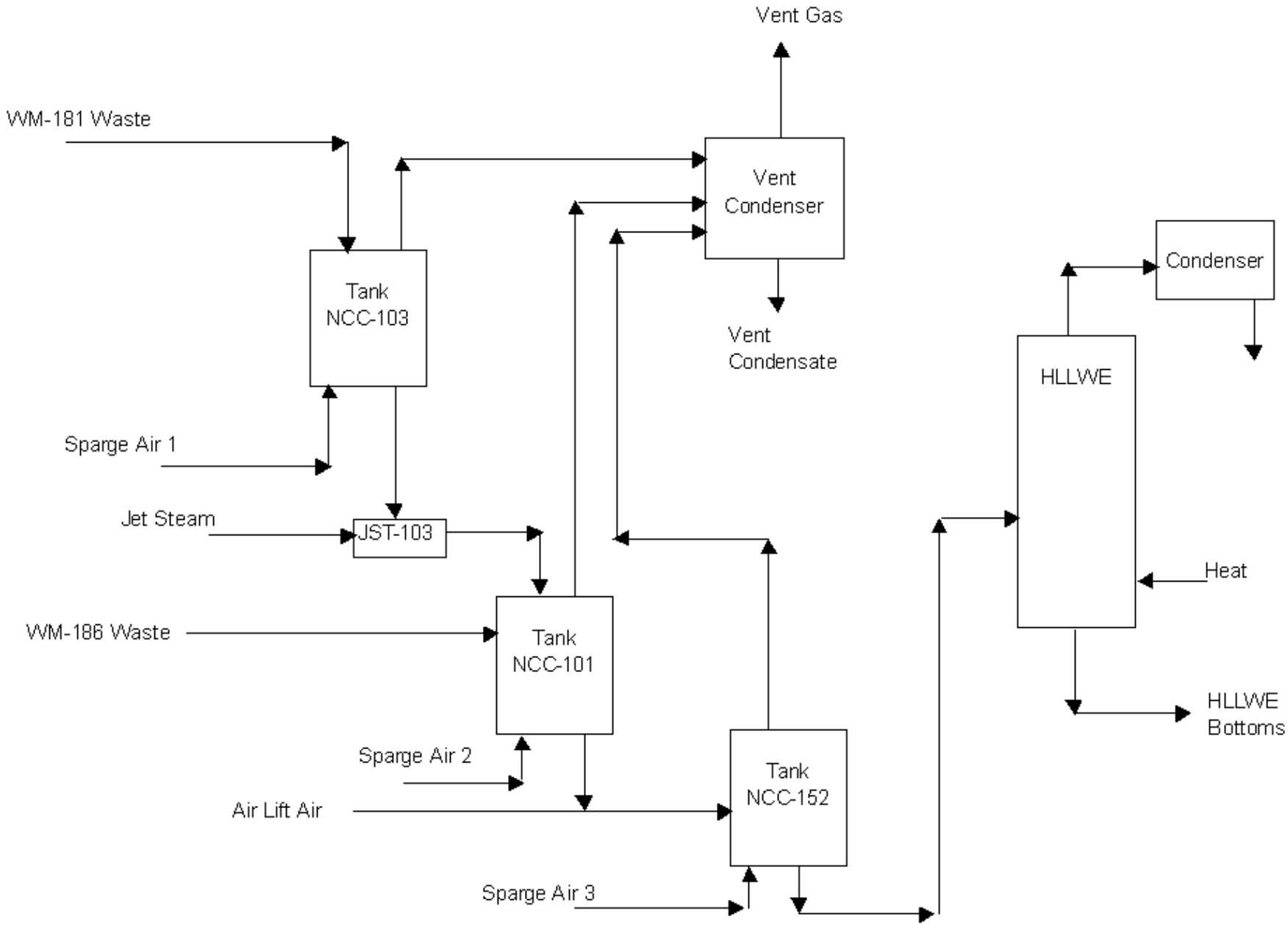
The first "road test" was building and running a simulation of semi-batch evaporation of liquid waste. Its purpose was to test the ability of the simulators to perform medium-temperature vapor/liquid equilibrium (VLE) calculations of critical non-radioactive species. Many of the unit operations in the process envelope involve VLE of these species at 25 – 150ºC.

**Semi-Batch Evaporation**

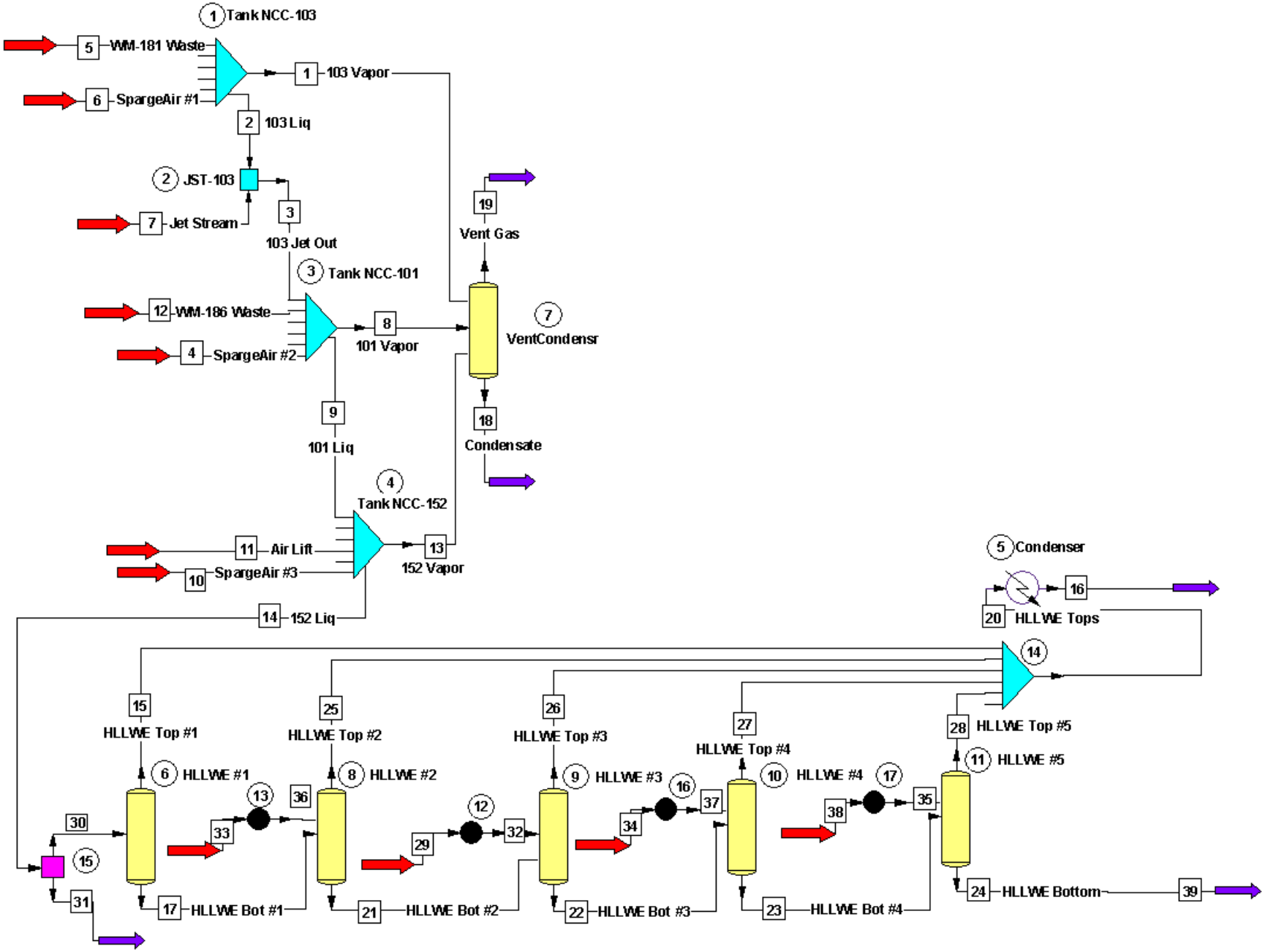
Semi-batch evaporation of dilute waste is currently performed to concentrate liquid waste and reduce its volume by driving off water. This pretreatment will be performed in the future for liquid waste regardless of the final treatment technology selected because of its waste volume reduction. A block flow diagram of the process is displayed in Figure 1. Air and steam jets are used to transfer the liquid waste, so the feed tanks (NCC-103, NCC-101, and NCC-152) are modeled as flashes. The high level liquid waste evaporator (HLLWE) is a semi-batch operation. After an initial charge is given to the evaporator, additional feed is added when the pot volume drops below a thresh-hold value. Enough feed is added in each recharge of the pot to bring the volume up to the initial level. Re-charges are made until the density of the liquid, at the operating temperature of the evaporator, reaches 1.30 g/cm$^3$. Further concentration of the liquid is not desired because of corrosion and operational concerns, so the evaporation process is shut down and the bottoms transferred to a storage tank when the 1.30 density limit is reached.

Usually three to four recharges of the pot are required before the bottoms reach the density limit, so the semi-batch process was modeled as a series of five flashes, one initial charge and four recharges. Even though CHEMCAD has a semi-batch evaporation module, it was not used because PRO/II and ASPEN Plus don't. The five-flash sequence was used to assure a fair comparison between the three simulators. The process flow diagram (PFD) of the simulation model is displayed in Figure 2. The required unit operation data for the simulation is shown in Table 5. The feed fractions shown in the second column of Table 5 for the sequential flashes represent the fraction of the feed stream sent to each flash. 55% of the feed is sent to the first flash, and the remaining 45% is divided equally between the remaining four flashes. It is essentially approximating the initial charge as 55% of the entire feed processed and approximating each of the four recharges as 11.25% of the entire feed processed. These approximations are based upon actual operational data of the HLLWE.

**FIGURE 1: BLOCK DIAGRAM OF PROCESS MODEL TEST - EVAPORATION**



# FIGURE 2: PFD OF SIMULATION MODEL – EVAPORATION



# TABLE 5: UNIT OPERATIONS FOR PROCESS MODEL TEST (EVAPORATION)

| Name | | | Type | Specifications | | |
|---|---|---|---|---|---|---|
| | | | | Temp. (ºC) | Pressure (psia) | Vapor Split |
| Tank NCC-103 | | | 2 phase flash | | 12 | |
| Steam Jet JST-103 | | | | | 17 | |
| Tank NCC-101 | | | 2 phase flash | | 12 | |
| Air lift junction | | | | | | |
| Tank NCC-152 | | | 2 phase flash | | 12 | |
| Vent Condenser | | | 2 phase flash | 28 | 12 | |
| HLLWE | | Feed Fraction | 2 phase flash | | | |
| | Feed Split 1 | 0.55 | 1 | | 12.2 | 0.253 |
| | Feed Split 2 | 0.25 X 0.45 = 0.1125 | 2 | | 12.2 | 0.253 |
| | Feed Split 3 | | 3 | | 12.2 | 0.253 |
| | Feed Split 4 | | 4 | | 12.2 | 0.253 |
| | Feed Split 5 | | 5 | | 12.2 | * |
| HLLWE Condenser | | | | 25 | 12.1 | |
| Tank NCC-122 | | | 2 phase flash | | 12 | |

* Vapor split for last flash was manipulated to control the cumulative flow rate of the tops from all five flashes to a value of 25,533 gmol/hr.

The required feed stream data for the simulation is shown in Tables 6. The composition list is incomplete, but it does contain enough of the critical species to provide a comparative analysis of the three simulators and assess the value of past data enhancements and OLI's database/model set. The compositional data for the liquid waste (WM-181 and WM-186) was obtained from chemical analysis of tank samples and mass balance calculations of previous liquid transfers. The concentration values for the species listed are the same as those used by the current simulation engineer supporting HLLWE operations.

An average flow rate for the evaporator tops during an operational batch run is approximately 25,533 gmol/hr. Because it is difficult to predict density of electrolyte solutions, this overhead flow rate was used as a termination criterion in the simulation "road tests" rather than bottoms density.

This simplified evaporation case is considered a good test case because of the following:

- It is a process that is currently part of Operations, so actual line-data is available for comparison with simulation.
- It is a process that will be part of future treatment, regardless of the eventual treatment alternatives chosen.
- It tests the ability of the simulators to perform VLE, which is a natural phenomena underlying many of the unit operations in the process envelope.
- It tests the simulators' databases/models with respect to many species important to downstream off-gas treatment.
- An ASPEN Plus model already exists, incorporating the database enhancements made over the years.
    - This saves time by not having to create a model in ASPEN Plus.
    - This offers an easy way to assess the value of the database enhancements.
- It is a relatively simple case that would not require the team members to become expert users of the various simulators. The selection schedule did not permit more than a few days for learning curves.

The drawbacks to using evaporation as the main "road test" are:

- There are over twenty different unit operations in the process envelope, of which semi-batch evaporation is only one.
    - It doesn't test the simulators' ability to handle many important radioactive species.
    - It doesn't test the simulators' ability to handle high-temperature processes.
- The process is semi-batch.
    - Being a semi-batch process, error may be introduced into the simulations merely by having to approximate it with a series of steady-state flashes. Even though this may not be a factor in the comparative analysis because the approximation was implemented in the same way in all simulators, it may cloud the assessment of the value of a commercial steady-state simulator compared to the current EXCEL "black box."
    - Being a semi-batch process with inherent variability in the number of recharges and total feed processed per batch, the line data for the bottoms and overheads from Operations may contain much variability.

# TABLE 6: FEED STREAMS FOR PROCESS MODEL TEST (EVAPORATION)

| | WM-181 Waste | WM-186 Waste | Air Sparge 1 | Air Sparge 2 | Air Sparge 3 | Air Lift Air | Jet Steam |
|---|---|---|---|---|---|---|---|
| | | | | | | | |
| Temp. (ºC) | 30 | 25 | 25 | 25 | 25 | 25 | |
| Pressure (psia) | 12.2 | 12.2 | 15 | 32 | 32 | 32 | 112 |
| Vapor Fraction | | | | | | | 1 |
| | | | | | | | |
| Rate | 6.057 | 12.113 | 24.71171 | 1.6 | 0.07 | 0.65 | 100 |
| units | $m^3/d$ | $m^3/d$ | kmol/d | lbmol/hr | lbmol/hr | lbmol/hr | kg/day |
| | | | | | | | |
| Concentration | ***mol/liter*** | ***mol/liter*** | ***mole fraction*** | ***mole fraction*** | ***mole fraction*** | ***mole fraction*** | ***mass fraction*** |
| | | | | | | | |
| O2 | | | 0.21 | 0.21 | 0.21 | 0.21 | |
| N2 | | | 0.79 | 0.79 | 0.79 | 0.79 | |
| H2O | 49.4 | 50.7 | 0.001 | 0.001 | 0.001 | 0.001 | 1 |
| HNO3 | 1.6724 | 1.278 | | | | | |
| NO3- | 0.01832 | 0.04211 | | | | | |
| HCL | 0.01069 | 0.016159 | | | | | |
| HF | 0.089 | 0.0398 | | | | | |
| NANO3 | 0.8751 | 0.811 | | | | | |
| NAHSO4 | 0.0279 | 0.029 | | | | | |
| KNO3 | 0.137 | 0.139 | | | | | |
| H3BO3 | 0.0149 | 0.0126 | | | | | |
| PO4 -3 | | 0.000497 | | | | | |
| AL(NO3)3 | 0.218 | 0.264 | | | | | |
| FE(NO3)3 | 0.012 | 0.0157 | | | | | |
| CD(NO3)2 | 0.00521 | 0.00424 | | | | | |
| CA(NO3)2 | 0.0441 | 0.05 | | | | | |
| PB(NO3)2 | 0.00101 | 0.000418 | | | | | |
| HGCL2 | 0.000453 | 0.000904 | | | | | |
| NI(NO) -1 | 0.00115 | 0.00373 | | | | | |
| CR(NO) -1 | 0.00289 | 0.00413 | | | | | |
| ZR +4 | 0.00458 | 0.0109 | | | | | |

### *ASPEN Plus*

The model for this test case already exists. It was built previously to help Operations determine optimum waste blending strategies for the HLLWE. The database enhancements made over the years, and discussed earlier, were removed so that ASPEN's own databanks would be the source of properties and thermodynamic data/models. The electrolyte NRTL model was selected to represent the aqueous chemistry.

### *PRO/II*

This program has an intuitive user-interface and is easier to use than ASPEN Plus. The simulation engineer testing it was able to quickly build and run the test model. The OLI databank/models option was selected to represent the aqueous electrolyte chemistry rather than NRTL in order to better compare PRO/II with ESP. ESP's online help explains that the OLI thermodynamic framework for aqueous electrolyte chemistry is based upon the Revised Helgeson Equation of State and the Bromley-Zemaitis and Pitzer formulations. It is assumed that the OLI databank/models option in PRO/II uses the same thermodynamic framework as ESP.

The only surprise for the team concerned the database. It was assumed that the simulator's database would be the same as OLI's ESP simulator since PRO/II claims to have OLI's database as an integrated databank. It was a surprise, then, to find that mercury-chloride species didn't exist in PRO/II's database, given that the current version of OLI has them. A call to Simulation Sciences' technical support revealed that the current and four-year-old version of OLI (6.2) isn't integrated into PRO/II, but rather the previous version (6.0) is. Consequently, either mercury-chloride species weren't included in version 6.0, or the integration is not as complete as claimed. This situation causes one to question Simulation Sciences' continued commitment to the integration of OLI when version 6.2 is four or more years old and it has yet to be incorporated into PRO/II.

The absence of mercury-chloride species in the database was disappointing because the treatment of mercury in the off-gas is expected to be an important technological hurdle, and the capability to predict partitioning of mercury from evaporative pretreatment would help process and equipment design of downstream unit operations.

### *CHEMCAD*

The program is also very user-friendly, and it was relatively easy for the simulation engineer to quickly assimilate enough to navigate in the program, build the model, and run the simulation. Chemstation's technical support was extremely responsive. The electrolyte NRTL model was selected to represent the aqueous chemistry.

The big deficiency in CHEMCAD that was revealed by this test case was the program's lack of critical species in its database. None of the species listed after $PO4^{-3}$ in Table 6 existed in CHEMCAD's database. It was felt that the absence of these species would cause appreciable error in the results. The lack of several nitrates (aluminum, iron, cadmium, calcium, and lead) would impact the predicted partitioning of nitric acid and the potassium and sodium nitrates. Not having Al(NO3)3 would overestimate the volatility of HF because aluminum and fluoride are known to form ionic complexes in aqueous solutions. As with PRO/II, the absence of mercury-chloride species in the database was disappointing.

### *Results*

Comparison of Base Simulators

The results of the test simulations are shown in Table 7. The "Operations' Data" columns refer to actual data from five batches run by Operations for the feed blend of WM-181 and WM-186 waste tanks shown in Table 6. It can be seen that there is large inter-batch variation for the ionic composition of the condensed overhead (Condensate). The value of the standard deviation is approximately half of the average for most species.

# TABLE 7: SIMULATION RESULTS FOR PROCESS MODEL TEST (EVAPORATION)

| | OPERATIONS' DATA | | | | SIMULATION RESULTS | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Average | Standard Deviation | 1 Std Dev Range Around Ave | | ASPEN w/o Data Enhancements | PRO/II | CHEMCAD | ESP | ASPEN w/INEEL Data Enhancements |
| | | | - Std Dev | + Std Dev | | | | | |
| **Intermediate Stream** | | | | | | | | | |
| Total HLLWE Feed, Mol/hr | | | | | 41,434 | 40,564 | 40,559 | 41,526 | 41,548 |
| | | | | | | | | | |
| **Products** | | | | | | | | | |
| | | | | | | | | | |
| Bottoms rate, mol/hr | | | | | 15,944 | 15,031 | 14,890 | 15,688 | 16,015 |
| Bottoms rate, L/hr | | | | | 315.8 | 309.8 | 298.8 | 299.3 | 322.7 |
| Bottoms density, kg/liter | | | | | 1.292 | 1.257 | 1.143 | 1.162 | 1.248 |
| Bottoms density at 25 C, kg/liter | | | | | 1.383 | 1.279 | | 1.266 | 1.329 |
| Bottoms temperature, C | | | | | 103.8 | 102.8 | 99.5 | 103.5 | 104.6 |
| | | | | | | | | | |
| Condensate rate, mol/hr | | | | | 25,533 | 25,533 | 25,533 | 25,541 | 25,533 |
| Condensate rate, L/hr | | | | | | | | | |
| Condensate composition | | | | | 461.7 | 463.2 | 467.2 | 459.9 | 462.5 |
| H2O, mol/liter | | | | | 5.49E+01 | 5.47E+01 | 5.09E+01 | 5.41E+01 | 5.41E+01 |
| H+, normal | 3.85E-01 | 2.01E-01 | 1.84E-01 | 5.85E-01 | 1.85E-01 | 4.04E-01 | 1.68E+00 | 7.37E-01 | 5.40E-01 |
| Cl-, mg/liter | 8.95E+01 | 3.49E+01 | 5.46E+01 | 1.24E+02 | 5.12E+01 | 5.70E+01 | 1.86E+00 | 2.44E+01 | 1.42E+02 |
| F-, mg/liter | 2.32E+01 | 1.47E+01 | 8.51E+00 | 3.79E+01 | 3.45E+00 | 4.94E+02 | 1.02E+03 | 4.74E-03 | 7.58E+00 |
| Hg+2, mg/liter | 1.17E+01 | 5.09E+00 | 6.64E+00 | 1.68E+01 | 2.68E-01 | NA | NA | 4.60E+00 | 5.93E+00 |
| O2, mol fraction | | | | | 3.02E-06 | 5.66E-06 | 3.00E-06 | 5.31E-06 | 2.59E-06 |
| N2, mol fraction | | | | | 5.87E-06 | 1.11E-05 | 6.00E-06 | 9.17E-06 | 5.06E-06 |
| HgCl+, mol fraction | | | | | 2.08E-14 | NA | NA | 2.50E-10 | 2.71E-11 |
| HgCl3-, mol fraction | | | | | 3.11E-13 | NA | NA | 3.21E-09 | 4.66E-09 |
| HgCl4-2, mol fraction | | | | | 1.07E-14 | NA | NA | 3.49E-11 | 1.09E-09 |
| H3BO3, mol fraction | | | | | 0 | NA | 8.40E-05 | 0 | 0 |
| | | | | | | | | | |
| Split: Cond/(Cond + Bottoms) | 0.59 | 0.02 | 0.57 | 0.61 | 0.59 | 0.60 | 0.61 | 0.61 | 0.59 |
| | | | | | | | | | |
| | | | | | | | | | |
| ***ACCURACY METRIC - Distance From Average ([sim - ave]/std dev)*** | | | | | | | | | |
| H+ in condensate | | | | | -0.99 | 0.10 | 6.43 | 1.75 | 0.78 |
| Cl- in condensate | | | | | -1.10 | -0.93 | -2.51 | -1.86 | 1.50 |
| F- in condensate | | | | | -1.34 | 32.01 | 67.51 | -1.58 | -1.06 |
| Hg in condensate | | | | | -2.25 | | | -1.40 | -1.14 |
| Average Absolute Distance | | | | | 1.42 | 8.26 | 25.49 | 1.65 | 1.12 |

The accuracy metric, the distance from the average, is the difference between the predicted concentration and operations' average, normalized by operations' standard deviation. The smaller the absolute value of the metric, the more accurate (i.e., closer to operations' average) the prediction. CHEMCAD considerably overestimates the amount of hydrogen and fluoride in the overheads, most likely due to the lack of accounting for aluminum-fluoride complexing as anticipated. It is unclear why PRO/II estimated such a greater presence of fluoride in the overheads than ASPEN Plus. It might be due to differences in the thermodynamic models used by the two programs. It is interesting to note that ASPEN Plus underestimated the presence of all four species in the overheads.

If all species have equal importance, then the average absolute distance can be used to rank the accuracy of the three simulators. In this case, ASPEN Plus is clearly the most accurate, and CHEMCAD is clearly the least accurate. With respect to individual species, however, PRO/II predicted best hydrogen and chloride volatility, and ASPEN Plus was the most accurate for fluoride and mercury. PRO/II and CHEMCAD, of course could not predict mercury volatility because of mercury's noticeable absence from their databases.

## Added Value of Past Data Enhancements

One can see that the past database enhancements are beneficial by comparing results for base ASPEN Plus and ASPEN Plus W/Enhancements shown in Table 7. The absolute average distance is smaller by about 1/3 of a standard deviation with the enhancements, and accuracy for three of the four species is improved.

Improvement in accuracy is expected given the fact that the database enhancements were specifically focused on HLLWE to support Operations. Some of the engineers that support Operations express strong, positive feelings regarding the enhancements and the need to keep them. The VLE of species for which the data enhancements were made is also involved in several off-gas unit operations. Consequently, it is assumed that these data enhancements will improve the model fidelity of several other unit operations in similar fashion and are worth keeping.

## Benefit of Tie to OLI Databank/Model Set

### *From PRO/II and CHEMCAD*

The big difference between the results of PRO/II and ESP shown in Table 7 is surprising and causes the selection team to again question the completeness of PRO/II's incorporation of OLI's databank/model set. Is the difference in results solely because of database differences between ESP 6.0 and ESP 6.2? The selection team requested a trial version of ESP 6.0 to assess the differences in the databases in an attempt to answer this question, but OLI Systems, Inc. refused, saying that it doesn't pass out old versions for which it no longer provides technical support. So the exact reason(s) for PRO/II's poorer performance relative to ESP remains unanswered. Regardless, the simulation results suggest that complete incorporation of OLI's current 6.2 database would be beneficial to PRO/II. It is also obvious that a tie to OLI would be very beneficial for CHEMCAD, but one does not currently exist.

### *From ASPEN Plus*

Table 7 shows that ESP has worse accuracy metrics than ASPEN Plus with or without the data enhancements, with one exception - the base ASPEN Plus' prediction of mercury concentration is less accurate than that of ESP. This suggests that a tie to OLI's database from ASPEN Plus would provide little, if any, benefit to the predicting of phase partitioning of key nonradioactive species during HLLWE operations. However, this doesn't mean that the OLI database would not provide any simulation benefits. To the contrary, the OLI database includes several species important to many unit operations, such as radioactive compounds, that are not found in ASPEN Plus' own databanks.

ASPEN Plus has an add-on, for an additional fee, that allows it to tie into OLI's physical properties database and models. The add-on appears to include a portion of ESP (the OLI databank/model set and some unit operation algorithms) and a software bridge that links it to the ASPEN Plus software.

The team performed a one-salt aqueous flash test case using a trial version of the bridge provided free of charge by ASPEN Technologies. This hands-on experience raised some concerns. It was hoped that the bridge would treat the OLI databank/model set just like any other databank internal to ASPEN Plus. However, such complete transparency to the user is not provided by the bridge. Instead, the bridge requires user intervention that is not necessary when switching between ASPEN's internal databababanks. The user has to manually compare the chemistry files of the two simulators generated by the bridge software and modify the species' names in the ASPEN Plus file (which has a "bkp" extension) to be consistent with those in the OLI file. One has to repeat this process every time species are added to the solution chemistry. This part of the model creation was performed for the relatively simple HLLWE test case. The result was a list of over 200 specie names in each of the simulators' chemistry files, each name requiring manual comparison and reconciliation between the two files. An entire treatment train will contain over twenty unit operations and will have many more species than just the few included in the HLLWE test case. The models will be built gradually, expanding the solution chemistry and number of processing units with time, so this labor-intensive step will have to be repeated many times during a model's life cycle.

The bridge appears to increase the difficulty of using a "divide and conquer" strategy for model development - parceling out portions of the model to project personnel and maintaining an integrated model by periodically merging updates of the submodels. Optimization runs and design efforts using individual submodels would have little value for integrated design unless they were performed with the same property models used by the bridge-based integrated model. Consequently, contributing simulation engineers whose submodels were required to use OLI to support integrated optimization would have to use the bridge for their own design studies in order to maintain consistency in the design decisions. It is not known how much labor will be required to maintain consistency in the bride-generated chemistry files between the integrated model and the individual submodels.

The bridge also may increase the difficulty of integrating with the simulation efforts of groups outside of the project that use ASPEN Plus. The creation and maintenance of some of the potential submodels are, and will probably continue to be, supported by other departments to solve specific problems of a narrower scope, such as the HLLWE model that currently supports Operations. These models could be merged into the integrated model to save development efforts, but they were not made for that intent, nor were they built using the bridge. In some cases, the original aim of the models may have little need for the use of the OLI database. The simulation engineers responsible for such potential submodels may resist using the bridge merely to support the objectives of this project when the increased labor from the bridge-required user interventions doesn't benefit their own work.

According to literature from ASPEN Technologies and Simulation Sciences, the strength of OLI's databank is its breadth of speciation at lower temperatures, and the strength of ASPEN Plus' databanks is its large temperature range. OLI has more species but a restriced temperature range. ASPEN has fewer species but a bigger temperature range. This provides both an advantage and a disadvantage.

The advantage is that the bridge will allow a simulation engineer to use OLI's databank/model set for those unit operations requiring medium-temperature equilibrium and ASPEN's databanks for those unit operations involving high temperature gas. The entire treatment process envelope involves both types of unit operations, so it appears that the bridge would appreciably increase the functionality of ASPEN Plus for this project.

The disadvantage, however, is that OLI's temperature range of focus is the same as that of the past database enhancements made by INEEL engineers over the years. Only one databank can be assigned to a unit operation. In order to use these database enhancements and OLI in a complementary manner, i.e., use them simultaneously for a unit operation involving medium-temperature equilibrium, would require transporting the enhancements to OLI so that the bridge would consider them part of the OLI databank.

Ironically, the disadvantages of the bridge with respect to integration with other simulation groups and past database enhancments are such that the ASPEN Plus-OLI combination via the bridge has some of the same drawbacks

as any non-ASPEN candidate and attacks the "Best" categorization ASPEN Plus received for integration in the requirements matrix assessment. "Switching" costs would essentially be incurred, similar to the case of CHEMCAD or PRO/II being chosen.

The single-user annual license fee for the bridge add-on is around $20K, close to the fee for ESP itself. In the case of an annually-renewable two-user network license, the annual incremental cost for the bridge is roughly $23.5K, so the incremental cost per user decreases considerably as the number of users increases. Regardless of the number of user licenses leased, it appears that using the bridge would increase annual licensing costs by $20K or more.

***Conclusions***

The following conclusions are made from the semi-batch evaporation "road test:"

- Both CHEMCAD and PRO/II have an easier user-interface, and are noticeably less difficult to learn how to use, than ASPEN Plus. However, the difference in ease-of-use is not large enough to be a discriminating factor against ASPEN Plus.
- CHEMCAD has a relatively poor database that results in unacceptably low accuracy. The only way to overcome this deficiency would be to manually enter database enhancements for the many species excluded from its database.
- PRO/II's accuracy is mixed. It is the most accurate for some species, and inaccurate for others. This product's database also lacks some critical species for which data would need to be manually entered.
  - Whether or not its database includes those species assumed to be unique to OLI's database (such as radioactive species) is still unclear given its comparison with ESP 6.2's performance and mercury-chloride data.
- ASPEN Plus has the best all around accuracy for medium-temperature (low 100s$^{o}$C) VLE for critical non-radioactive species.
  - The database enhancements made by INEEL engineers over the years do improve the accuracy of HLLWE simulations. It is assumed that they will also improve model accuracy of several off-gas treatment unit operations.
    - The data enhancements are worth keeping. They should be ported if a simulator other than ASPEN Plus is selected.
- Procurement of a commercial steady-state process simulator is worth pursuing for this project.
  - An accuracy level within 1.5 times actual standard deviations can be achieved for predicted concentrations of many species deemed critical to several unit operations by mechanistic modeling of medium-temperature VLE.
- Appreciable database enhancement will be required regardless of which simulator is selected.
  - CHEMCAD lacks much, PRO/II lacks some, ASPEN Plus lacks radioactive species, and ESP lacks high-temperature content
  - Reinforces the need for "Road testing" of simulators' user customization capabilities.
- The consequences of using the ASPEN Plus-OLI bridge add-on are mixed.
  - Doesn't provide increased overall accuracy for medium-temperature equilibrium of critical non-radioactive species.
  - Pros
  - OLI may have largest number of species at lower temperatures of any simulation database
    - Gain access to critical radioactive species not available in other simulators for medium-temperature equilibrium while maintaining access to ASPEN's high temperature data.
      - Increased functionality for a process envelope that spans both temperature regimes.
  - Cons
    - Increases annual licensing costs by $20K or more
      - Amounts to $60K or more over three years.
    - Increases labor cost
      - User intervention is required when making/changing solution chemistry.
      - May be laborious to maintain consistency between bridge-generated chemistry files of specialized submodels and the integrated model.

- "Switching costs" incurred if integration capability is to be maintained.
  - Increased difficulty integrating with simulation efforts of other groups.
  - Transporting past ASPEN Plus database enhancements to OLI.

## *User-Supplied Database Enhancements*

The process model "road test" reinforced to the team the reality that database enhancements would be required regardless of what simulator is chosen. Consequently, attempts were made to add species to the simulators' databases. This exercise was not performed on ASPEN Plus because it is already known that satisfactory capability for user-supplied database enhancements exists through personal experience of team members.

### *PRO/II*

Creating new species was easy and no problems were encountered, but data regression gave mixed results. PRO/II will only regress data to NRTL, not OLI's model. That brings up the question of whether or not a user can simultaneously use OLI and NRTL models, each for a different set of species, in the same simulation. The team doesn't know the answer to that question.

Regressing VLE data was easy to perform, but the thermodynamic correlation created had poor accuracy. H2O-HCl vapor liquid equilibrium data that was part of past database enhancements to the ASPEN Plus HLLWE simulation was entered into PRO/II and regressed. Below is the output from the 8-parameter NRTL regression exercise:

## TABLE 8: ACCURACY OF PRO/II VLE DATA REGRESSION

| Point | EXP | CALCULATED | CALC-EXP DEVIATION | PERCENT DEVIATION |
|---|---|---|---|---|
| 1 | 4.20000E-10 | 4.84075E-08 | 4.79875E-08 | 11425.5875 |
| 2 | 9.20000E-09 | 2.47446E-07 | 2.38246E-07 | 2589.6354 |
| 3 | 2.00000E-08 | 4.95670E-07 | 4.75670E-07 | 2378.3506 |
| 4 | 1.20000E-07 | 9.93296E-07 | 8.73296E-07 | 727.7471 |
| 5 | 7.10000E-07 | 2.49689E-06 | 1.78689E-06 | 251.6740 |
| 6 | 3.30000E-06 | 5.03956E-06 | 1.73956E-06 | 52.7139 |
| 7 | 2.00000E-05 | 1.02673E-05 | -9.73272E-06 | -48.6636 |
| 8 | 6.60000E-05 | 1.50808E-05 | -5.09192E-05 | -77.1504 |

INEEL internal reports of past ASPEN Plus database enhancements reveal that ASPEN Plus' regression of the same data compared well to the experimental values. The explanations for the discrepancy between the two regressions are unknown.

### *CHEMCAD*

The simulation engineer tried to enter several new species and their corresponding equilibrium equations and standard Gibbs free energy, enthalpy, and entropy of formation. Although the overall process of entering the data was relatively straight, several inconveniences and problems were noted.

Inconveniences

The simulation engineer quickly became aware that the user has to page through the entire equilibrium equations set in order to view, edit, or add a single equation. It only takes a few electrolytic species before one ends up with quantities of equilibrium equations in the double digits. It was annoying to have to page through the entire set every time the program required the user to enter the equation screen.

There are three or four screens that require the user to enter the molecular weight of a new species being entered into the database. If the MW isn't manually entered in all the various screens, a mass balance error statement will be received when trying to run the simulation. Requiring the user to go to several different screens to enter the same piece of data is a waste of the user's time.

CHEMCAD has a components list (electrically neutral compounds) and electrolyte set. The electrolyte set consists of an ionic specie list and equilibrium equations corresponding to members of the components. Every time it is desired to automatically update the electrolyte list and equations (when a salt in the installed database is added to the component list, for example), the user has to erase the current electrolyte list and equations and rerun the electrolyte generation routine. However, user-defined ionic species and equations are not automatically added to the electrolyte set by the electrolyte generation routine even though the data was previously entered. Consequently, all user-specified equilibrium equations and ionic species are required to be manually entered into the electrolyte set every time the user runs the electrolyte generation routine.

The process required to delete a species from the electrolyte set is not forgiving. The user has to first set the species' concentration in all the individual stream definitions to zero and delete it from the components list before trying to delete it from the electrolyte set. Failure to follow that sequence causes the program to crash.

Problems

Two serious problems were encountered. The addition of the first few species to the electrolyte set was successful (Al(NO3)3, Al(NO3)3*9H2O, and AlF3), but the program had problems handling the inclusion of HgCl2. The program crashed every time the engineer selected the "Run" menu item. It wouldn't crash, however, if the engineer manually sequenced the simulation through each successive unit operation twice. Convergence of the individual unit operations was not obtained until the second attempt.

The second problem encountered was the inability to copy a data set from one model to another. Although the component list completely transfers over, the electrolyte set does not. Thermodynamic property data for new species does transfer, and new neutral species will show up in the components list of the target file. However, membership in the electrolyte set is lost and has to be manually re-entered. Consequently, it appears that the copying of electrolyte chemistry (the data set comprised of ionic species and equilibrium equations) from one CHEMCAD file to another is not automated.

These inconveniences and problems are disappointing in light of the large amount of database enhancements CHEMCAD will require to achieve acceptable predictive accuracy.

***Conclusions***

There are three main conclusions from this test of user-customization:

- Database enhancements can be made in PRO/II very easily.

- The exercises raised more questions regarding PRO/II than it answered – can database enhancements be made and still use the OLI databank/model set for program-resident species, and can accurate regressions consistently be performed?

- CHEMCAD would require much more effort to make the necessary database enhancements than would ASPEN Plus or PRO/II. It would be very time consuming and inefficient to try to add all the species that CHEMCAD's database lacks.

## *Satisfying The Requirements Matrix*

Tables 9, 10, and 11 show the team's assessment of the ability of ASPEN Plus 10.2, PRO/II 5.11, and CHEMCAD 5.1.0, respectively, to satisfy the entire requirements matrix. The knowledge of the programs expressed in the assessment column, the last column, came from user manuals, calls to technical support, and explorations during the "road testing." Both ASPEN Plus and PRO/II fail to satisfy the bare requirements regarding cost optimization, and CHEMCAD barely satisfies the minimum requirements for predictive steady-state simulation and the thermodynamic properties database. Such major deficiencies are shaded gray in Tables 9-11. The strongest factor in favor of ASPEN Plus is its integration with the simulation efforts of other groups and past database enhancements. PRO/II is deemed to have the greatest potential for a favorable thermodynamic properties database for the project's entire process envelope because of its integrated tie to OLI. CHEMCAD's strong point, on the other hand, is its ability to satisfy the requirements regarding integration with future scope, which is the least important factor.

# TABLE 9: REQUIREMENTS MATRIX FOR ASPEN PLUS

(√: meets requirement)

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| *Current Scope* | | | |
| Provide Basic Mass & Heat Balances, Basis for Equipment Sizing, Utilities Req'ts, Consumables Req'ts, etc. for optimums | Can perform predictive steady-state process simulation and optimization | Suite shall have a solver for continuous, steady-state process simulation (with nonrandom inputs) with the following functionality: | **Satisfies Worst and Has Some of Better & Best** |
| | | Best – all functionality listed under Better, plus the following: | |
| | | • Rigorous unit operation models for mixing tank, scrubbers (dust, venturi, ejector fume, and submerged bed), cyclone, packed bed quench, spray quench, ion exchange, grouting, mist eliminator, HEPA filter bank, semi-batch evaporator, catalytic reactor, electrostatic precipitator, gas-phase reactor, and liquid-liquid extraction | Has cyclone, venturi scrubber, batch & semi-batch reactor, electrostatic precipitator, liquid-liquid extraction, plug flow reactor, CSTR reactor, equilibrium reactor (all reactors can be gas/liquid but no solid). Ion exchange module available at additional cost. |
| | | Better - all functionality listed under Worst, plus the following: | |
| | | • Global multi-variable optimization with choice of several optimization methods | √ |
| | | • Allow user-defined physical properties models/correlations. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density. | √ |
| | | • Has a batch evaporation module | No - Batch distillation module is available for additional cost. |
| | | Worst: | |
| | | • User selection of units of weight and measure for input/output variables | √ |
| | | • Pure component physical property database | √ |
| | | • Standard thermodynamic models for energy balances | √ |
| | | • Inter-Phase equilibrium is determined by calculating a specie's concentration in both phases by equating its electrochemical potentials, accounting for nonideality | √ |
| | | • Intra-Phase chemical equilibrium is determined by calculating specie concentrations by minimization of mixture Gibbs free energy, accounting for nonideality and user-imposed stoichiometric constraints | √ |
| | | • All fundamental thermodynamic data in the physical properties database is referenceable to peer-reviewed literature/databases | √ - Assume sources are referenceable |
| | | • Standard non-ideal vapor/liquid/solid thermodynamic models (e.g. NRTL for electrolytes and equations of state for gases) use Binary or Higher-Order Pair interaction parameters that are compiled/validated from experimental data found in peer-reviewed literature | √ - Assume sources are referenceable |
| | | • Automatic sequencing of unit operation calculations | √ |
| | | • Automatic recycle stream identification and flowsheet convergence | √ |
| | | • Ability for a stream to contain a solid, liquid, and/or gas phase, with multiple chemical species able to exist in all phases present | √(only some unit operations allow solid) |
| | | • Optimization of individual unit operations (multiple-design specification capability) | √ |
| | | • Multiple case study capability (automated consecutive running of pre-specified scenarios) | √ |
| | | • Black box unit operations: mixer, stream splitter, component separator, stoichiometric reactor | √ |
| | | • Rigorous unit operations: equilibrium flash calculation, heat exchanger, distillation column, | √ |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| | | pump/compressor<br>• Allow user-defined unit operation blocks using a mainstream computer language (either FORTRAN, C, or C++) that do not inherently constrain the degree of mechanistic modeling possible (can accept a user's model of nonequilibrium such as finite-rate kinetics, for example)<br>• Allow user-defined physical properties database. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density.<br>• Allow user override of default values of physical properties for individual species<br>• Batch evaporation can be approximated by creating a sequence of repeated flashes | √ FORTRAN and probably C, C++<br>√<br>√<br>√ |
| | Thermodynamic properties database compares favorably with needs (see Table 2) | Best: steady-state simulator shall have thermodynamic data that satisfies Table 2 completely - i.e., database has data for all neutral compounds and at least one compound of every ionic species specified in Table 2 at the temperature and pressure ranges listed.<br><br>Better: steady-state simulator shall have thermodynamic data for appreciably more species at low temperature than the "Worse" category, or it shall have thermodynamic data for the higher temperatures. The data gathering required to fill in the gaps will be less than in the "Worse" category.<br><br>Worse: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of many of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. Although data for many species is still lacking, the database provides a solid foundation to build upon and the capability to contribute to design efforts in the short term. Data gathering required to fill in the gaps will be appreciable, but it will be considered practical.<br><br>Worst: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of only a few of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. High-temperature data and/or data for a majority of the species is lacking to such a degree that the simulator as is can not contribute to design efforts in the short-term. Data gathering required to fill in the gaps will be large and a major effort. | **Satisfies Worse**<br><br>Incorporating past INTEC VLE regression efforts addresses deficiencies cited below and may bring performance up to "Better" category.<br><br>√ - Lacks binary pair data for Al-F complexes; poorly represents HNO3/water system for dilute concentrations of interest; lacks interactions between HNO3 and nitrate salts; gives poor HCl/water results for >0.5M HCl solutions. |
| Integrates With Existing Process Modeling Efforts, Commitments, & Experience | Leverage existing ASPEN Plus models, database enhancements, and expertise | Best: steady-state process simulator shall be able to effortlessly import/export files in ASPEN Plus format. This permits full utilization of SRS and resident ASPEN Plus experience, models, and database enhancements. It offers maximum synergy with other INEEL and SRS HLW simulation efforts.<br><br>Worse: steady-state process simulator can import/export files in ASPEN Plus format, but not all model characteristics are common to both simulation packages (not all unit operation modules are common, conflicts exist between solving algorithms, differing methodologies for handling constraints, etc.), resulting in less-than-complete transportability.<br><br>Worst: steady-state process simulator can not import/export files in ASPEN Plus format. This fails to utilize existing ASPEN Plus models and database enhancements, and ASPEN Plus expertise is utilized only in the broad sense that previous simulation experience will shorten learning curve on new simulator. Redundancy will be the only way to achieve integration between our efforts and those of other resident simulation engineers. This provides almost no synergy with existing simulation capabilities. | **Satisfies Best**<br><br>√ - Permits direct use of previous in-house ASPEN Plus data regressions of electrolyte thermodynamic models, filling in important data gaps and increasing accuracy of results |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| *Future Scope* | | | |
| Provide Safety-Related Stream Compositions | Result fidelity of steady-state simulations is acceptable to Safety Engineers | Fidelity constraints translate into requirements for modeling approaches of individual unit operations (TBD). | N/A |
| Estimate Emissions for Permit Applications | Result fidelity of steady-state simulations is acceptable to Idaho DEQ | | |
| Perform Concurrent Process/Cost Optimization | Ability to map process design parameters to equipment features to capital costs | Best: The steady-state process simulator shall have the following capabilities:<br>1) perform inverse problem solving regarding cost, i.e., force a manipulated variable's value to optimize a global cost function<br>2) permit value constraints on operating parameters and stream characteristics (composition, temperature, flow rate, etc.)<br>3) determine sizing features related to processing, such as number of trays in a distillation column or length of a plug flow reactor<br>4) permit capital cost functions to be created that depend upon equipment features<br><br>Combined, these abilities will allow the automated optimization of a cost objective function by manipulating process variables while simultaneously enforcing specified waste form required characteristics.<br><br>Better: The steady-state simulator shall have capabilities #3 and #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments."<br><br>Worst: The steady-state simulator shall have capability #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments." Engineers will have to manually perform capability #3, i.e., estimate and input cost-related equipment features to couple with the simulator's cost functions for each run of the optimization "experiment." | **Not Acceptable**<br><br>√ - User defined cost function can be objective function<br>√<br><br>No - Sizing not available for many modules, but is available for some<br>No - User can create any function based on available parameters, but sizing parameters not available for many pieces of equipment.<br><br>No - Combination of features doesn't adequately facilitate cost optimization |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| Quantify Process Variability (inventories, operating parameters, etc.)<br><br>Project Mass Balances and Effluent Stream Compositions and Flow Rates for Planning Basis of Melter Trial Burn<br><br>Provide Continuous Emissions Estimates of Actual Operations | Have a transient process simulator | Transient simulators are required to provide these future capabilities. Therefore, the choice of steady-state simulator made in the present has to be integrated with the choice of transient simulators to be made in the future if efficiency is to be maximized and work redundancy is to be minimized.<br><br>Best: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are all parts of an integrated simulation package. This option is the most efficient, is the least labor intensive, and it requires the least code maintenance and configuration control overhead because it allows all four distinct simulation objectives to be achieved from one base model build.<br><br>Better: the steady-state process simulator, the transient process simulator, and the transient process control simulator are parts of an integrated simulation package. This option results in only one redundant model build (in the discrete-event simulator).<br><br>Worse: the steady-state process simulator and the transient process simulator are parts of an integrated simulation package. This option results in two redundant model builds (in the process control and discrete-event simulators).<br><br>Worst: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are not parts of an integrated simulation package. This is the most time consuming and labor intensive option because it requires separate model builds of the same system in four distinct simulation packages. | **Satisfies Worst**<br><br>√- ASPEN Plus is a steady-state simulator |
| Simulate Process Control Schemes | Have constructs amendable to process control simulation | | |
| Estimate System-Wide Performance (cap. util., campaign lengths, etc.) | Have a discrete-event, stochastic solver (transient by definition) | | |

# TABLE 10: REQUIREMENTS MATRIX FOR PRO/II

(√: meets requirement)

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| *Current Scope* | | | |
| Provide Basic Mass & Heat Balances, Basis for Equipment Sizing, Utilities Req'ts, Consumables Req'ts, etc. for optimums | Can perform predictive steady-state process simulation and optimization | Suite shall have a solver for continuous, steady-state process simulation (with nonrandom inputs) with the following functionality:<br>Best – all functionality listed under Better, plus the following:<br>• Rigorous unit operation models for mixing tank, scrubbers (dust, venturi, ejector fume, and submerged bed), cyclone, packed bed quench, spray quench, ion exchange, grouting, mist eliminator, HEPA filter bank, semi-batch evaporator, catalytic reactor, electrostatic precipitator, gas-phase reactor, and liquid-liquid extraction<br><br>Better - all functionality listed under Worst, plus the following:<br>• Global multi-variable optimization with choice of several optimization methods<br><br>• Allow user-defined physical properties models/correlations. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density.<br><br>• Has a batch evaporation module<br><br>Worst:<br>• User selection of units of weight and measure for input/output variables<br>• Pure component physical property database<br>• Standard thermodynamic models for energy balances<br>• Inter-Phase equilibrium is determined by calculating a specie's concentration in both phases by equating its electrochemical potentials, accounting for nonideality<br>• Intra-Phase chemical equilibrium is determined by calculating specie concentrations by minimization of mixture Gibbs free energy, accounting for nonideality and user-imposed stoichiometric constraints<br>• All fundamental thermodynamic data in the physical properties database is referenceable to peer-reviewed literature/databases<br>• Standard non-ideal vapor/liquid/solid thermodynamic models (e.g. NRTL for electrolytes and equations of state for gases) use Binary or Higher-Order Pair interaction parameters that are compiled/validated from experimental data found in peer-reviewed literature<br>• Automatic sequencing of unit operation calculations<br>• Automatic recycle stream identification and flowsheet convergence<br>• Ability for a stream to contain a solid, liquid, and/or gas phase, with multiple chemical species able to exist in all phases present<br>• Optimization of individual unit operations (multiple-design specification capability)<br>• Multiple case study capability (automated consecutive running of pre-specified scenarios)<br>• Black box unit operations: mixer, stream splitter, component separator, stoichiometric reactor<br>• Rigorous unit operations: equilibrium flash calculation, heat exchanger, distillation column, pump/compressor | **Satisfies Worst & Has Some of Better and Best**<br><br>Has cyclone, dissolver, crystallizer and wiped film evaporator. Does not have unique modules for scrubbers, quench columns or ion exchange.<br><br>No<br><br>√ - Up to 15 user added "method sets" can be added and any of the predefined thermodynamic property models can be modified.<br>√ - Has batch distillation; also has batch reactor<br><br>√<br>√<br>√<br>√<br><br>√<br><br>√ - Electrolyte chemistry uses a version of OLI, which is referenceable<br><br>√ - Electrolyte chemistry uses a version of OLI, which is referenceable<br><br>√<br>√<br>√<br><br>√<br>√<br>√<br><br>√ - 3 heat exchanger unit operations, including rigorous sizing, several types of |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| | | • Allow user-defined unit operation blocks using a mainstream computer language (either FORTRAN, C, or C++) that do not inherently constrain the degree of mechanistic modeling possible (can accept a user's model of nonequilibrium such as finite-rate kinetics, for example)<br>• Allow user-defined physical properties database. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density.<br>• Allow user override of default values of physical properties for individual species<br>• Batch evaporation can be approximated by creating a sequence of repeated flashes | distillation<br>√ - Fortran<br><br>√ - User supplied physical properties and databases can be easily added<br><br>√<br>√ |
| | Thermodynamic properties database compares favorably with needs (see Table 2) | Best: steady-state simulator shall have thermodynamic data that satisfies Table 2 completely - i.e., database has data for all neutral compounds and at least one compound of every ionic species specified in Table 2 at the temperature and pressure ranges listed.<br><br>Better: steady-state simulator shall have thermodynamic data for appreciably more species at low temperature than the "Worse" category, or it shall have thermodynamic data for the higher temperatures. The data gathering required to fill in the gaps will be less than in the "Worse" category.<br><br>Worse: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of many of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. Although data for many species is still lacking, the database provides a solid foundation to build upon and the capability to contribute to design efforts in the short term. Data gathering required to fill in the gaps will be appreciable, but it will be considered practical.<br><br>Worst: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of only a few of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. High-temperature data and/or data for a majority of the species is lacking to such a degree that the simulator as is can not contribute to design efforts in the short-term. Data gathering required to fill in the gaps will be large and a major effort. | **Satisfies Between Worse & Better**<br><br>The claim to have OLI's database integrated within the software pushes it towards "Better." However, being a version behind (OLI 6.0 rather than 6.2), lacking data for mercury-chloride species, and not being able to regress data to OLI's model lessen confidence in the claim and pushes it towards "Worse." |
| Integrates With Existing Process Modeling Efforts, Commitments, & Experience | Leverage existing ASPEN Plus models, database enhancements, and expertise | Best: steady-state process simulator shall be able to effortlessly import/export files in ASPEN Plus format. This permits full utilization of SRS and resident ASPEN Plus experience, models, and database enhancements. It offers maximum synergy with other INEEL and SRS HLW simulation efforts.<br><br>Worse: steady-state process simulator can import/export files in ASPEN Plus format, but not all model characteristics are common to both simulation packages (not all unit operation modules are common, conflicts exist between solving algorithms, differing methodologies for handling constraints, etc.), resulting in less-than-complete transportability.<br><br>Worst: steady-state process simulator can not import/export files in ASPEN Plus format. This fails to utilize existing ASPEN Plus and models and database enhancements, and ASPEN Plus expertise is utilized only in the broad sense that previous simulation experience will shorten learning curve on new simulator. Redundancy will be the only way to achieve integration between our efforts and those of other resident simulation engineers. This provides almost no synergy with existing simulation capabilities. | **Satisfies Worst**<br><br>√ |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| *Future Scope* | | | |
| Provide Safety-Related Stream Compositions | Result fidelity of steady-state simulations is acceptable to Safety Engineers | Fidelity constraints translate into requirements for modeling approaches of individual unit operations (TBD). | N/A |
| Estimate Emissions for Permit Applications | Result fidelity of steady-state simulations is acceptable to Idaho DEQ | | |
| Perform Concurrent Process/Cost Optimization | Ability to map process design parameters to equipment features to life-cycle costs | Best: The steady-state process simulator shall have the following capabilities:<br>1) perform inverse problem solving regarding cost, i.e., force a manipulated variable's value to optimize a cost function<br>2) permit value constraints on operating parameters and stream characteristics (composition, temperature, flow rate, etc.)<br>3) determine sizing features related to processing, such as number of trays in a distillation column or length of a plug flow reactor<br>4) permit capital cost functions to be created that depend upon equipment features<br>Combined, these abilities will allow the automated optimization of a cost objective function by manipulating process variables while simultaneously enforcing specified waste form required characteristics.<br>Better: The steady-state simulator shall have capabilities #3 and #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments."<br>Worst: The steady-state simulator shall have capability #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments." Engineers will have to manually perform capability #3, i.e., estimate and input cost-related equipment features to couple with the simulator's cost functions for each run of the optimization "experiment." | **Not Acceptable**<br>No<br>√ - Has multivariable controller that can adjust an unlimited number of variables to meet the same number of specifications<br>No - for a very limited number of unit operations (rigorous capability for heat exchangers )<br>No – But probably could with much effort<br>No - Combination of features doesn't adequately facilitate cost optimization |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| Quantify Process Variability (inventories, operating parameters, etc.)<br><br>Project Mass Balances and Effluent Stream Compositions and Flow Rates for Planning Basis of Melter Trial Burn<br><br>Provide Continuous Emissions Estimates of Actual Operations | Have a transient process simulator | Transient simulators are required to provide these future capabilities. Therefore, the choice of steady-state simulator made in the present has to be integrated with the choice of transient simulators to be made in the future if efficiency is to be maximized and work redundancy is to be minimized.<br><br>Best: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are all parts of an integrated simulation package. This option is the most efficient, is the least labor intensive, and it requires the least code maintenance and configuration control overhead because it allows all four distinct simulation objectives to be achieved from one base model build.<br><br>Better: the steady-state process simulator, the transient process simulator, and the transient process control simulator are parts of an integrated simulation package. This option results in only one redundant model build (in the discrete-event simulator).<br><br>Worse: the steady-state process simulator and the transient process simulator are parts of an integrated simulation package. This option results in two redundant model builds (in the process control and discrete-event simulators).<br><br>Worst: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are not parts of an integrated simulation package. This is the most time consuming and labor intensive option because it requires separate model builds of the same system in four distinct simulation packages. | **Satisfies Worst**<br><br>√ - PRO/II is a steady-state simulator |
| Simulate Process Control Schemes | Have constructs amendable to process control simulation | | |
| Estimate System-Wide Performance (cap. util., campaign lengths, etc.) | Have a discrete-event, stochastic solver (transient by definition) | | |

# TABLE 11: REQUIREMENTS MATRIX FOR CHEMCAD

(√: meets requirement)

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| *Current Scope* | | | |
| Provide Basic Mass & Heat Balances, Basis for Equipment Sizing, Utilities Req'ts, Consumables Req'ts, etc. for optimums | Can perform predictive steady-state process simulation and simulation | Suite shall have a solver for continuous, steady-state process simulation (with nonrandom inputs) with the following functionality:<br>Best – all functionality listed under Better, plus the following:<br>• Rigorous unit operation models for mixing tank, scrubbers (dust, venturi, ejector fume, and submerged bed), cyclone, packed bed quench, spray quench, ion exchange, grouting, mist eliminator, HEPA filter bank, semi-batch evaporator, catalytic reactor, electrostatic precipitator, gas-phase reactor, and liquid-liquid extraction<br><br>Better - all functionality listed under Worst, plus the following:<br>• Global multi-variable optimization with choice of several optimization methods<br><br>• Allow user-defined physical properties models/correlations. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density.<br>• Has a batch evaporation module<br><br>Worst:<br>• User selection of units of weight and measure for input/output variables<br>• Pure component physical property database<br>• Standard thermodynamic models for energy balances<br>• Inter-Phase equilibrium is determined by calculating a specie's concentration in both phases by equating its electrochemical potentials, accounting for nonideality<br><br>• Intra-Phase chemical equilibrium is determined by calculating specie concentrations by minimization of mixture Gibbs free energy, accounting for nonideality and user-imposed stoichiometric constraints<br>• All fundamental thermodynamic data in the physical properties database is referenceable to peer-reviewed literature/databases<br><br>• Standard non-ideal vapor/liquid/solid thermodynamic models (e.g. NRTL for electrolytes and equations of state for gases) use Binary or Higher-Order Pair interaction parameters that are compiled/validated from experimental data found in peer-reviewed literature<br>• Automatic sequencing of unit operation calculations<br>• Automatic recycle stream identification and flowsheet convergence | **Barely Satisfies Worst, But Has Some of Better and Best**<br><br>Has venture scrubber, cyclone, filter bank, semi-batch evaporator, electrostatic precipitator, and liquid-liquid extraction<br><br>No – single objective function & one optimization method<br><br>No - but tech support claims it can be done with much effort<br><br>√ - Also has batch distillation and batch reactor<br><br>√<br>√<br>√<br><br>√- However, liquid/solid equilibrium is limited to a maximum of ten solid species that user determines apriori. Doesn't predict what species of the entire mixture are thermodynamically possible in solid phase, but rather predicts solubility of only the 10 user-specified species.<br><br>√<br><br>√ - Uses publicly available journals, DIPR (physical properties), and Dechema (binary interaction parameters)<br><br>√ Data Sources: Uses Dechema database and regressions performed on data from publicly available journals<br>√<br>√ |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| | | • Ability for a stream to contain a solid, liquid, and/or gas phase, with multiple chemical species able to exist in all phases present | √ |
| | | • Optimization of individual unit operations (multiple-design specification capability) | √ |
| | | • Multiple case study capability (automated consecutive running of pre-specified scenarios) | √ - 2 independent, 12 dependent variables |
| | | • Black box unit operations: mixer, stream splitter, component separator, stoichiometric reactor | √ |
| | | • Rigorous unit operations: equilibrium flash calculation, heat exchanger, distillation column, pump/compressor | √ - Also has reactive distillation |
| | | • Allow user-defined unit operation blocks using a mainstream computer language (either FORTRAN, C, or C++) that do not inherently constrain the degree of mechanistic modeling possible (can accept a user's model of nonequilibrium such as finite-rate kinetics, for example) | √ - Visual Basic for EXCEL interface; Visual C for subroutines |
| | | • Allow user-defined physical properties database. Physical properties used here in this table is a global term including thermodynamic properties, kinetic properties such as reaction rates, and transport properties such as viscosity and density. | √ - But inefficient and glitchy |
| | | • Allow user override of default values of physical properties for individual species | √ - Done by creating redundant component |
| | | • Batch evaporation can be approximated by creating a sequence of repeated flashes | √ |
| | Thermodynamic properties database compares favorably with needs (see Table 2) | Best: steady-state simulator shall have thermodynamic data that satisfies Table 2 completely - i.e., database has data for all neutral compounds and at least one compound of every ionic species specified in Table 2 at the temperature and pressure ranges listed.<br><br>Better: steady-state simulator shall have thermodynamic data for appreciably more species at low temperature than the "Worse" category, or it shall have thermodynamic data for the higher temperatures. The data gathering required to fill in the gaps will be less than in the "Worse" category.<br><br>Worse: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of many of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. Although data for many species is still lacking, the database provides a solid foundation to build upon and the capability to contribute to design efforts in the short term. Data gathering required to fill in the gaps will be appreciable, but it will be considered practical.<br><br>Worst: steady-state simulator shall have thermodynamic data for V/L/S equilibrium of only a few of the species listed in Table 2 at 10-150ºC and 5 – 12 psia. High-temperature data and/or data for a majority of the species is lacking to such a degree that the simulator as is can not contribute to design efforts in the short-term. Data gathering required to fill in the gaps will be large and a major effort. | **Satisfies Worst**<br><br>√ - Lacks radioactive species, most heavy metals, and several important compounds such as nitrates and aluminum complexes |
| Integrates With Existing Process Modeling Efforts & Experience | Leverage existing ASPEN Plus models, database enhancements, and expertise | Best: steady-state process simulator shall be able to effortlessly import/export files in ASPEN+ format. This permits full utilization of SRS and resident ASPEN Plus experience, models, and database enhancements. It offers maximum synergy with other INEEL and SRS HLW simulation efforts.<br><br>Worse: steady-state process simulator can import/export files in ASPEN Plus format, but not all model characteristics are common to both simulation packages (not all unit operation modules are common, conflicts exist between solving algorithms, differing methodologies for handling constraints, etc.), resulting in less-than-complete transportability.<br><br>Worst: steady-state process simulator can not import/export files in ASPEN Plus format. This fails to utilize existing ASPEN Plus models and database enhancements, and ASPEN Plus expertise is utilized only in the broad sense that previous simulation experience will shorten learning curve on | **Satisfies Worst**<br><br>√ |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| | | new simulator. Redundancy will be the only way to achieve integration between our efforts and those of other resident simulation engineers. This provides almost no synergy with existing simulation capabilities. | |
| *Future Scope* | | | |
| Provide Safety-Related Stream Compositions | Result fidelity of steady-state simulations is acceptable to Safety Engineers | Fidelity constraints translate into requirements for modeling approaches of individual unit operations (TBD). | N/A |
| Estimate Emissions for Permit Applications | Result fidelity of steady-state simulations is acceptable to Idaho DEQ | | |
| Perform Concurrent Process/Cost Optimization | Ability to map process design parameters to equipment features to capital costs | Best: The steady-state process simulator shall have the following capabilities:<br>5) perform inverse problem solving regarding cost, i.e., force a manipulated variable's value to optimize a global cost function<br>6) permit value constraints on operating parameters and stream characteristics (composition, temperature, flow rate, etc.)<br>7) determine sizing features related to processing, such as number of trays in a distillation column or length of a plug flow reactor<br>8) permit capital cost functions to be created that depend upon equipment features<br>Combined, these abilities will allow the automated optimization of a cost objective function by manipulating process variables while simultaneously enforcing specified waste form required characteristics.<br>Better: The steady-state simulator shall have capabilities #3 and #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments."<br>Worst: The steady-state simulator shall have capability #4. Automated optimization will not be achieved, but simulation engineers could manually perform the optimization through statistically designed simulation "experiments." Engineers will have to manually perform capability #3, i.e., estimate and input cost-related equipment features to couple with the simulator's cost functions for each run of the optimization "experiment." | **Satisfies Better**<br>No - Capital costs of single unit operation can be optimized, but global cost can't be objective function<br>√<br>√<br>√<br>√ |

| Simulation | | Software Suite | |
|---|---|---|---|
| ***Capability (High-Level Req't)*** | ***Characteristic (Mid-Level Req't)*** | ***Quantifiable Requirement*** | ***Vendor Capability to Meet Req't*** |
| Quantify Process Variability (inventories, operating parameters, etc.)<br><br>Project Mass Balances and Effluent Stream Compositions and Flow Rates for Planning Basis of Melter Trial Burn<br><br>Provide Continuous Emissions Estimates of Actual Operations | Have a transient process simulator | Transient simulators are required to provide these future capabilities. Therefore, the choice of steady-state simulator made in the present has to be integrated with the choice of transient simulators to be made in the future if efficiency is to be maximized and work redundancy is to be minimized.<br><br>Best: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are all parts of an integrated simulation package. This option is the most efficient, is the least labor intensive, and it requires the least code maintenance and configuration control overhead because it allows all four distinct simulation objectives to be achieved from one base model build.<br><br>Better: the steady-state process simulator, the transient process simulator, and the transient process control simulator are parts of an integrated simulation package. This option results in only one redundant model build (in the discrete-event simulator).<br><br>Worse: the steady-state process simulator and the transient process simulator are parts of an integrated simulation package. This option results in two redundant model builds (in the process control and discrete-event simulators).<br><br>Worst: the steady-state process simulator, the transient process simulator, the transient process control simulator, and the transient discrete-event simulator are not parts of an integrated simulation package. This is the most time consuming and labor intensive option because it requires separate model builds of the same system in four distinct simulation packages. | **Satisfies Better**<br><br>√- Has dynamic column, dynamic vessel, PID controller, control valve, stream time delay, outlet stream time switch, ramp controller or discrete event manager. Can run steady-state unit ops concurrently with transient unit ops. |
| Simulate Process Control Schemes | Have constructs amendable to process control simulation | | |
| Estimate System-Wide Performance (cap. util., campaign lengths, etc.) | Have a discrete-event, stochastic solver (transient by definition) | | |

# BEST SIMULATOR BASED ON TECHNICAL MERIT

A summary scorecard is displayed in Table 12 that condenses the results from the all-inclusive requirements matrix regarding the entire scope and process envelope, the more singular-focused evaporator and database enhancement "road tests," and cost information.

CHEMCAD receives a "Worst –" for predictive steady-state process simulation because of its limit of ten solid species and its requirement that the user specify them apriori, barely meeting the requirement to predict liquid/solid equilibrium. CHEMCAD has the highest performance, and ASPEN Plus and PRO/II unacceptable performance, in the least important area of future integration. Consequently, CHEMCAD receives the lowest overall categorization of the three simulators. Both ASPEN Plus and PRO/II receive higher performance ratings than CHEMCAD because of their superior performance regarding the high-importance requirements.

ASPEN Plus edges out PRO/II for the highest overall categorization mostly because of its superior ability to integrate with the simulation efforts of other groups. However, ASPEN Plus would still edge out PRO/II without a higher rating for integration because of the ambiguity surrounding PRO/II's higher rating for thermodynamic properties database. This ambiguity concerns the content level of PRO/II's database given the discrepancy in predictive accuracy and included species between ESP and PRO/II in the semi-batch evaporation "road test."

CHEMCAD receives the lowest grade of "Unacceptable" for the semi-batch evaporation "road test" due to the lack of key complexing ions in its database. It also receives the lowest grade for implementing database enhancements because adding species to the electrolyte database was found to be laborious and possibly problematic. PRO/II's ability to satisfactorily provide for database enhancements is questionable because of its poor regression of H2O-HCl VLE data. Both the requirements matrix assessment and "road tests" place ASPEN Plus as the front runner, PRO/II a close second, and CHEMCAD a distant last. Consequently, ASPEN Plus is considered to be the steady-state simulator that best meets the project's technical needs.

# TABLE 12: SCORECARD SUMMARY

| | | | CHEMCAD 5.1.0 | PRO/II 5.11 | ASPEN Plus 10.2 |
|---|---|---|---|---|---|
| **Requirements Matrix** | | | | | |
| **Capability (High-Level Requirement)** | **Characteristic (Mid-Level Requirement)** | **Importance of Requirement** | **Performance Categorization** (Highest Performance Shaded Gray) | | |
| Provide Basic Mass & Heat Balances, Basis for Equipment Sizing, Utilities Req'ts, Consumables Req'ts, etc | Can perform basic steady-state process simulation | High | Worst - | Worst + | Worst + |
| | Thermodynamic properties database compares favorably with needs (see Table 2) | High | Worst | Worse + | Worse |
| Integrate With Existing Process Modeling Efforts, Commitments, & Experience | Leverage existing ASPEN Plus models, database enhancements, and expertise | High | Worst | Worst | Best |
| Integrate With Future Simulation Scope | Perform cost optimization | Low | Better | Not Acceptable | Not Acceptable |
| | Perform dynamic process simulation, process control simulation, and discrete-event simulation) | | Better | Worst | Worst |
| | | ***Overall Categorization:*** | Worst | Worse | Worse + |
| **"Road Testing"** | | | | | |
| Process Model: Semi-Batch Evaporation | | Predictive Accuracy: | Unacceptable | Acceptable | Acceptable |
| User-Customized Database Enhancements | | Ease of Adding New Species: | Laborious | Acceptable | Acceptable |
| | | Regression Accuracy: | N/A | Questionable | Acceptable |
| **Some Applicable Cost Data** | | | | | |
| Annual Cost Per User * | | | $12.8K | $22.3K | $28.2K |
| Cost Saving Per User (APEN Plus – Selection) | | | $15.4K | $5.9K | $0 |
| Three-Year Cost Savings For Two Users | | | $92.4K | $35.4K | $0 |
| Cost of Transporting Past ASPEN Plus Database Enhancements ** | | | $100K | $100K | $0 |

* Based on two network licenses for three years. Future lease and maintenance fees assumed to have same present value as current fees.

** Literature search, data regression, and validation estimated to take 3 person-weeks of an engineer/scientist highly skilled in thermodynamic theory for every distinct aqueous binary system investigated, resulting in a burden rate of approximately $10K for each binary system. Transporting enhancements from one simulator to another is assumed to cost only half as much since the literature search has already been done. Past database enhancement efforts involved approximately twenty binary systems, resulting in a transporting cost of (20 systems * 10 $K/system *0.5=) $100K, assuming that the data entry and regression could be done as easily in the target simulator as in ASPEN Plus, which might be true for PRO/II but is definitely not true for CHEMCAD.

# FINAL DECISIONS

There is much consistency between the different sources of data. In descending order of meeting the technical needs of the project the best, both the requirements matrix and "road testing" result in ASPEN Plus, PRO/II, and then CHEMCAD. However, all the pertinent decisions cannot be made until three issues are addressed: the cost factor, the benefit of a commercial simulator versus the status quo "black box," and the ASPEN Plus–OLI bridge add-on.

## *Financial Analysis*

The acquisition cost of each of the three simulators, as one might expect, is inversely proportional to the simulator's "road test" performance and its ability to satisfy the technical requirements. So the first question that has to be answered is, "Is the higher price of ASPEN Plus justified by its perceived higher technical merit?" Some pertinent cost data is displayed in Table 12. The estimated annual costs per user shown are based upon using two network licenses for three years. Three years was considered a good time-frame for the cost analysis, and annual licensing was considered more practical than term licensing, because of the potential for future changes in the projects' work scope. Annually-renewable licenses are leased in the case of ASPEN Plus and PRO/II. CHEMCAD, on the other hand, is purchased rather than leased, so its three-year cost involves the purchase price in year one, and only a maintenance fee in years two and three. Future lease and maintenance fees are assumed to have the same present value as the fees in this current year.

It can be seen that choosing CHEMCAD rather than ASPEN Plus could save approximately $92K in leasing fees over three years, and PRO/II could save $34K. It is assumed for the time being that past database enhancements made for ASPEN Plus will improve the predictive accuracy of the integrated model and are worth utilizing. Table 12 shows that just the switching costs associated with transporting past database enhancements from ASPEN Plus to either of the other two candidate simulators is estimated at $100K and is larger than the potential 3-year savings arising from smaller purchasing/licensing costs of the other two candidate simulators. Consequently, there is no reason to justify purchasing either CHEMCAD or PRO/II since they do not score higher in the requirements matrix or road tests, and their acquisition cost savings are more than offset by just one of the switching costs. Therefore, the higher price of ASPEN Plus carries a higher benefit/cost ratio than the other two candidates and its higher three-year price is justified for the needs of this project.

## *Versus the Status Quo*

The next question that has to be answered is, "Is the difference in the predictive and optimization capability between ASPEN Plus and the current EXCEL-based simulator worth the incremental cost?" The qualitative answer to that question is assumed to be "Yes." Achieving the proper level of simulation that can more than pay for itself by reducing process and facility design costs is the goal. It is assumed that predictive accuracy between 1 and 1.5 times standard deviation will facilitate design enough to be worth the costs of the simulation efforts associated with two network licenses, one for the engineers at SRS and one for the INEEL team.

Total costs of the simulation effort and total benefits will be monitored over time to continually assure that the value added exceeds the cost. The benefit/cost ratio will be reassessed annually and the number of licenses and engineers will be adjusted accordingly. The team will be better able to assess the benefit/cost ratio of simulation's potential contribution to integrated process optimization once an entire treatment train is modeled in the selected commercial simulator and comparisons are made between simulator predictions and measured data. Consequently, the two network licenses will be leased on an annual basis until the expected benefit/cost ratio can justify longer-term financial commitments.

## *ASPEN Plus – OLI Bridge Add-On*

The last question to answer is, "Is the ASPEN Plus-OLI bridge add-on worth leasing?" The answer is "No" because of the bridge's lack of complete transparency to the user and concerns regarding integration. There are three main negative consequences of the bridge: 1) it requires appreciable user intervention when making/changing solution chemistry, which will be happening continually throughout the project's life because of the model's piecemeal development, 2) it increases annual licensing costs by approximately $20K, and 3) it incurs either a cost of roughly $100K to transport past database enhancements to OLI or the loss of the improved accuracy derived from such enhancements.

The benefit of the bridge would be to gain access to property data for several important species for simulating medium-temperature equilibrium. It is not felt at this time, however, that the potential benefit of the bridge outweighs its potential negatives. It is recommended that thermodynamic data for key missing species be obtained from literature searches and/or physical experiments and added to ASPEN Plus, as has been done in the past. Such manual database enhancements at this early phase of the project are considered to be more cost effective over a three-year time frame than accruing $60K or so in additional licensing costs, roughly $100K to transport past database enhancements from ASPEN Plus to OLI, and the increased project and integration labor costs from the user-required interventions.

The trade-offs between the pros and the cons of the bridge will be periodically reanalyzed as the properties database needs of the project are clarified and modified with time.

## *Remaining Ambiguities*

The main remaining knowledge gaps concern the performance of PRO/II, the value of past database enhancements, and the value added by the ASPEN Plus-OLI bridge.

**Performance of PRO/II**

Both the requirements matrix assessment and the "road testing" raised important questions regarding PRO/II that time did not allow to be answered. For example, exactly how much of OLI is incorporated into PRO/II? Simulation Sciences has told the team that it plans on integrating the future version of OLI (v. 6.5) into the next version of PRO/II; but given the fact that the current integration is outdated by several years and appears to be incomplete, one may not be convinced of the commitment of Simulation Sciences to continue integrating future OLI releases into its simulator. And, what effort is required to accurately regress thermodynamic data in PRO/II?

**Value of Past ASPEN Plus Database Enhancements**

The potential impact of the past ASPEN Plus database enhancements on the predictive accuracy of the integrated model is assumed to be worth the estimated $100K switching cost. This assumption, however, is based solely on the strong feelings of the engineers that use the enhancements in their HLLWE simulations supporting Operations and on the comparison of Operations data with base ASPEN Plus results in the "road test." What is the exact monetary value of increasing predictive accuracy by one third of a standard deviation? And what will the aggregate impact of the enhancements be in the integrated model?

**Value of the OLI Bridge**

Much ambiguity still remains regarding the specie set and temperature range of OLI's properties database compared to that of ASPEN Plus, INEEL's past database enhancements, and the needs of the project. Is the potential value added from the bridge worth the higher acquisition price and the cost of transporting past database enhancements?

**Dealing With The Knowledge Gaps**

The selection team would have preferred to spend more time on "road testing" and additional iterations of the 5-step decision making process to fill in these knowledge gaps. However, the selection schedule did not permit it. Consequently, the impact of any remaining lack of knowledge perceived by the team was invariably transposed into the strength of the final decisions - the decisions include further testing and re-assessment, and they contain financial commitments for no more than one year.

As the treatment train model is built, as insights are gained into the optimum level of mechanistic modeling, as the properties database needs become clearer, as the dialogue increases with simulation engineers of other groups that can be potential contributors to the integrated model, and as time unfolds these ambiguities will be eliminated and decisions will be modified accordingly.

## *Recommendations to Other Potential Buyers of Steady-State Process Simulators*

**CHEMCAD**

Evaluating CHEMCAD was like finding a high-quality shoe at a rock-bottom price at a shoe store, only to find out from the sales clerk that the manufacturer doesn't make the shoe in a foot size as large as yours. Maybe the leather will stretch with time and become comfortable? - you propose to yourself. So you try on the largest size the manufacturer does make. Despite badly wanting the shoe to fit, it quickly becomes evident that the undersized shoe will never comfortably fit. Sadly, you return the shoes in the box to the sales clerk and keep on looking.

CHEMCAD is worth investigating if the project's physical property needs don't include electrolyte models. It offers steady-state, dynamic, and process control simulation all in one integrated simulation environment. The user interface is easy to use, the price is considerably less than the other two candidates, and the level of customer support from both marketing and the technical help desk is unmatched.

**PRO/II**

Evaluating PRO/II was like finding what appears to be a good bargain - high functionality at modest cost. After getting a pair your size from the sales clerk, you become slightly confused. The manufacturer claims the shoes are waterproof and that the soles can last up to five years. You look at what appears to be untreated leather and ask yourself, "Can this really be water proof? Maybe it's just water resistant?" You look at the thin sole and wonder to yourself how it could ever last five years of daily use. You acknowledge that the manufacturer's claims can be true – you just might be too unfamiliar with the material makeup of the leather and sole – but you don't have time to do what is necessary to reconcile your expectations with your brief personal experience, after all, the store closes in fifteen minutes. You return the pair of shoes to the clerk and keep looking.

PRO/II is worth investigating if the project has modest to large physical property needs, a broad process envelope, and ease of use and pricing are primary factors. It costs about 20% less than ASPEN Plus, and the selection team found the user interface to be more intuitive and easier than that of ASPEN Plus.

**ASPEN Plus**

Evaluating ASPEN Plus was like searching for a new shoe for your musical band. After hours of shoe shopping, you realize that none of the other shoes you have looked at fit your feet as well as your current band shoe. Even though it is the highest priced dress shoe on the market, none of the other shoes you have tried have offered a compelling reason to switch. So you go over to the rack displaying models from the manufacturer of your current shoe, and you realize that they also make another shoe with more functionality.

This new style is waterproof and has a tread that offers more traction, and it costs about 50% more than the old style. Your band does several outdoor shows a year, and the waterproofing and better traction would be welcomed features during those unlucky times when your show is caught in the middle of a storm, and you are disassembling your equipment in the rain and mud. The display shoe is brown, so you ask the clerk for a black pair. He comes back and tells you that the style has limited distribution so the manufacturer only makes it in one color –brown. This is not good because the color of the current shoe your band wears is black, and the band's wardrobe matches nicely with the color black but not with the color brown. The other band members like the current style shoe, so you know that purchasing the old style is a safe bet. But you think that they may also see the wisdom of the functionality the new style offers.

You quickly do some rough math, and you are not convinced that the increased functionality of the shoe is worth the higher purchase cost and the secondary costs associated with procuring a compatible wardrobe. You really become uneasy when you realize that the cost of switching shoe styles is exacerbated by the number of people involved – all the band members and attire have to be compatible and complementary. So instead of buying the new style shoe today, you decide to buy the old style and see if you can manually add the increased functionality yourself.

You buy a pair of the old shoes. You make a note in your planner for tomorrow to purchase a waterproofing solution for leather and to make an appointment with a cobbler to discuss attaching an additional tread to the soles. Your aren't sure, but you think that your planned customization will provide the increased functionality at lower cost and less inconvenience to the other band members.

ASPEN Plus is worth investigating if the project has large physical property needs, a broad process envelope, and there are opportunity or switching costs associated with some of the performance requirements that appreciably lessen the importance of the simulator's acquisition price. Otherwise, its premium pricing will be a deterrent. The appeal of the OLI bridge, also premium priced, may decrease as the number of contributing engineers, the value of any previous database enhancements, and the piecemeal nature of the model development increase.

# REFERENCES

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