

Hanford River Protection Project Enhanced Mission Planning through Innovative Tools: Lifecycle Cost Modeling and Aqueous Thermodynamic Modeling – 12134

Kendra Seniow and Fiona Meinert
Washington River Protection Solutions, LLC, Richland, WA 99352

ABSTRACT

Two notable modeling efforts within the Hanford Tank Waste Operations Simulator (HTWOS) are currently underway to (1) increase the robustness of the underlying chemistry approximations through the development and implementation of an aqueous thermodynamic model, and (2) add enhanced planning capabilities to the HTWOS model through development and incorporation of the lifecycle cost model (LCM). Since even seemingly small changes in apparent waste composition or treatment parameters can result in large changes in quantities of high-level waste (HLW) and low-activity waste (LAW) glass, mission duration or lifecycle cost, a solubility model that more accurately depicts the phases and concentrations of constituents in tank waste is required. The LCM enables evaluation of the interactions of proposed changes on lifecycle mission costs, which is critical for decision makers.

INTRODUCTION

The Department of Energy (DOE) tank farms at Hanford contain approximately 212 million liters of radioactive and chemically hazardous wastes, much of which originated during the reprocessing of spent nuclear fuel to produce plutonium for national defense programs. The mission of the DOE River Protection Project (RPP) is to protect the Columbia River by eliminating the risk to the environment posed by this waste. Successful management of the RPP requires the careful coordination of multiple government contractors that are responsible for the design, construction, operation, and maintenance of facilities and support services. Efforts associated with mission analysis and strategic planning, particularly the development and issuance of the RPP System Plan [1], are essential to this coordination.

The RPP System Plan [1] provides the basis for the alignment of program costs, scope, and schedules from upper-tier contracts to individual operating plans. Updates are made to the RPP System Plan to reflect recent progress, current plans, responses to emergent issues, changes in the regulatory environment, and budgeting constraints. The Hanford Tank Waste Operations Simulator (HTWOS) is the foundation of the RPP system planning process, providing a model that integrates technical parameters with programmatic planning considerations. The HTWOS is a dynamic flowsheet simulator and mass balance model that calculates the flow of both discrete and continuous events occurring during the storage, retrieval, supplemental treatment, pretreatment, and vitrification of Hanford tank waste. By simulating the overall RPP mission, the HTWOS can forecast outcomes of changes to the baseline assumptions, and the sensitivities to alternative retrieval and waste staging strategies, new proposed technologies, and changes to the assumed dates of facility availabilities. The results of HTWOS runs include projections for key mission metrics such as quantities of HLW and LAW glass canisters, total sodium requirements of the system, and dates for completion of retrieval and treatment milestones. These metrics are used in mission analysis applications and are included for the scenarios evaluated in system planning to help guide decisions on how to manage the overall project. Any changes or upgrades made to the HTWOS model that improve the accuracy of the underlying assumptions add fidelity to the model projections, thereby improving its ability to support mission planning. Likewise, any further development to the model that increases the number and kinds of outputs generated provides a broader basis for scenario analysis and gives decision makers a more complete view of mission impacts.

To support enhanced mission planning, two notable modeling efforts within the HTWOS are currently underway to (1) increase the robustness of the underlying chemistry approximations through the development and implementation of an aqueous thermodynamic model, and (2) add enhanced planning capabilities to the HTWOS model through development and incorporation of the Lifecycle Cost Model (LCM). Both tasks are significant undertakings, which will result in incremental changes and additions to the HTWOS model. The two projects were initiated for distinctly different purposes and are being pursued by separate teams of engineers and programmers. However, their integration in the HTWOS will result in improved RPP mission modeling and system planning capabilities. Figure 1 shows the key features and functions of the two tools under development, and their eventual integration with the HTWOS model.

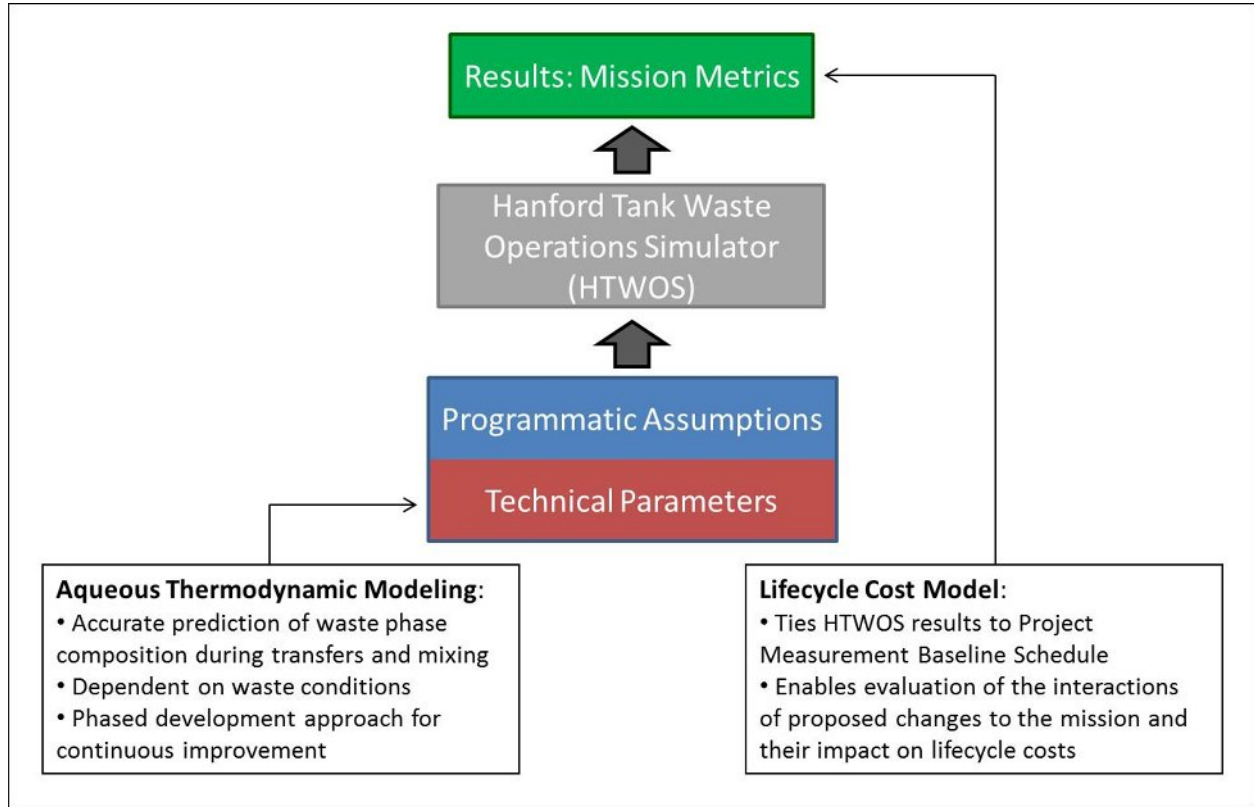


Fig 1. Integration of two modeling tools for enhanced system planning.

AQUEOUS THERMODYNAMIC MODELING

The RPP mission calls for the immobilization of Hanford tank waste in glass at the Hanford Waste Treatment and Immobilization Plant (WTP), which is currently under construction. To minimize the amount of HLW and LAW glass produced, the immobilization process is preceded by a series of pretreatment separation steps, including washing, caustic leaching, filtration, and ion exchange. In addition, tank waste supernatant, water, or caustic solution is added to the waste to facilitate its transfer between storage tanks or retrieval from storage tanks to the WTP. Optimization of these processes requires detailed knowledge of waste properties and anticipated behavior under process conditions. However, Hanford tank waste presents a unique, complex challenge since its composition is not consistent between or precisely characterized for all of the 177 underground storage tanks in which the waste is stored. Generated from various production and separation processes since the early 1940s, the waste consists of over 150 radioactive and nonradioactive species (regulations require the monitoring

of 46 radionuclides and 139 nonradioactive chemical species) in liquid, solid, and slurry phases, often at elevated temperatures. An understanding and means of predicting waste properties is necessary for mission planning, particularly in the HTWOS.

Since the HTWOS is not fundamentally thermodynamic software, waste phase equilibria and reaction extents were initially approximated by extrapolation of limited experimental data and simple split factors known as wash factors. Wash factors are zero-order values (constant and independent of conditions or other variables) that approximate the dissolution of waste components during waste retrieval from tanks. At the time the wash factors were developed (15-20 years ago), computation abilities permitting the use of more sophisticated chemistry correlations in the HTWOS were not readily available and the conditions of the experiments on which the wash factors were based more closely matched the expected operating scenario. Now, wash factors present significant weaknesses in system modeling that must be addressed: (1) since they are zero-order, wash factors cannot account for waste conditions; (2) they assume waste dilution in an excess of water, which may or may not be the case; and (3) they are unidirectional, thereby allowing only for dissolution and not precipitation. The development and inclusion of aqueous thermodynamic modeling in the HTWOS to represent tank waste behavior will address these issues.

Approach

To facilitate solubility modeling, waste constituents have been divided into four categories based on their relative solubility and degree of impact to the retrieval and treatment processes. Table I lists waste constituents tracked by the HTWOS in their respective categories; the Model Development section discusses their handling in the HTWOS. Category 1 contains waste constituents that do not change phase appreciably (i.e., that are highly soluble or highly insoluble). These constituents have been designated as either always in the liquid phase or always in the solid phase for the entire mission in the HTWOS. Simplified correlations have been applied to those constituents of intermediate solubility and low impact, which form Category 2. Those constituents that are both sensitive to waste conditions and have a significant impact on the mission are assigned to Category 3. The thermodynamically based Pitzer ion-interaction model is used to determine aqueous concentrations of these species [2, 3]. Time has been shown to be a significant factor in the effectiveness of caustic leaching in dissolving aluminum solids due to the kinetic limitations in the dissolution of select aluminum compounds. For this reason, Category 4 contains the aluminum compound boehmite (AlOOH), for which a kinetic dissolution model is applied during the caustic leaching operation.

The ability to predict solid-liquid phase distributions is enhanced compared to wash factors for constituents of each category, but by selectively applying models of varying complexity, the complications of such fundamental HTWOS changes are moderated. Furthermore, the programming infrastructure constructed for one category of constituents facilitates development of another category.

Table I. Categorization of Hanford tank waste constituent based on relative solubility and degree of impact to the retrieval and treatment processes.

Approach	Category 1: Highly soluble/insoluble and low impact		Category 2: Intermediate solubility and low impact	Category 3: Intermediate solubility and high impact		Category 4: Kinetic dependent
	Assign to Solid Phase	Assign to Liquid Phase	Simple Equations	Pitzer Model		Kinetic Model
	Very Insoluble	Very Soluble		Ions	Solids	
Components	Sm-151	Sn-126	Pu-238/Pu-239/ Pu-240/ Pu-241/ Pu-242	Al(OH) ₄ ⁻	Al(OH) ₃	AlOOH
	Eu-152/Eu-154/ Eu-155 ^a	C-14		C ₂ O ₄ ²⁻	Na ₂ C ₂ O ₄	
	Pa-231	Ra-226/Ra-228		CO ₃ ²⁻	Na ₂ CO ₃ ·H ₂ O	
	Nb-93m	Ac-227	Ag	F ⁻	Na ₂ SO ₄ ·10H ₂ O	
	Ce	Cm/Cm-242/ Cm-243/Cm-244	Ba	H ₂ O	Na ₃ FSO ₄	
	Co/Co-60	Tc-99	Bi	Na ⁺	Na ₃ PO ₄ ·0.25NaOH ·12H ₂ O	
	La	As	Ca	NO ₂ ⁻	Na ₇ F(PO ₄) ₂ ·19H ₂ O	
	Mg	Be	Cd/Cd-113m	NO ₃ ⁻	NaF	
	Mn	B	Cr	OH ⁻		
	Pr	Be	Fe	PO ₄ ³⁻		
	Rh	CN	Nd	SO ₄ ²⁻		
	Th/Th-229/ Th-232	Cs/Cs-134/ Cs-137	Ni/Ni-63	Cl ⁻		
	Ti	Hg	Sr/Sr-90	HPO ₄ ²⁻		
	Tl	K	Ta	HCO ₃ ⁻		
	Zr/Zr-93	Li	Te			
		Mo	U-232/U-233/U-234			
		Pb	U-235/U-236/U-238			
		Pd	Y			
		Rb				
		Ru/Ru-106				
	Sb/Sb-125					
	Se/Se-79					
	W					
	Zn					

^a All isotopes of an element are treated equivalently.

The development of an enhanced chemistry model for Hanford tank waste and mission planning is a long-term project. The work discussed here represents Phase 1, with subsequent phases to refine and build on that knowledge and the infrastructure developed, in addition to addressing other waste chemistry issues. In this manner, continuous incremental improvements to solubility modeling are achieved in balance with resources. Figure 2 shows how the sequential development of chemistry models for waste categories fosters the evolution of HTWOS modeling.

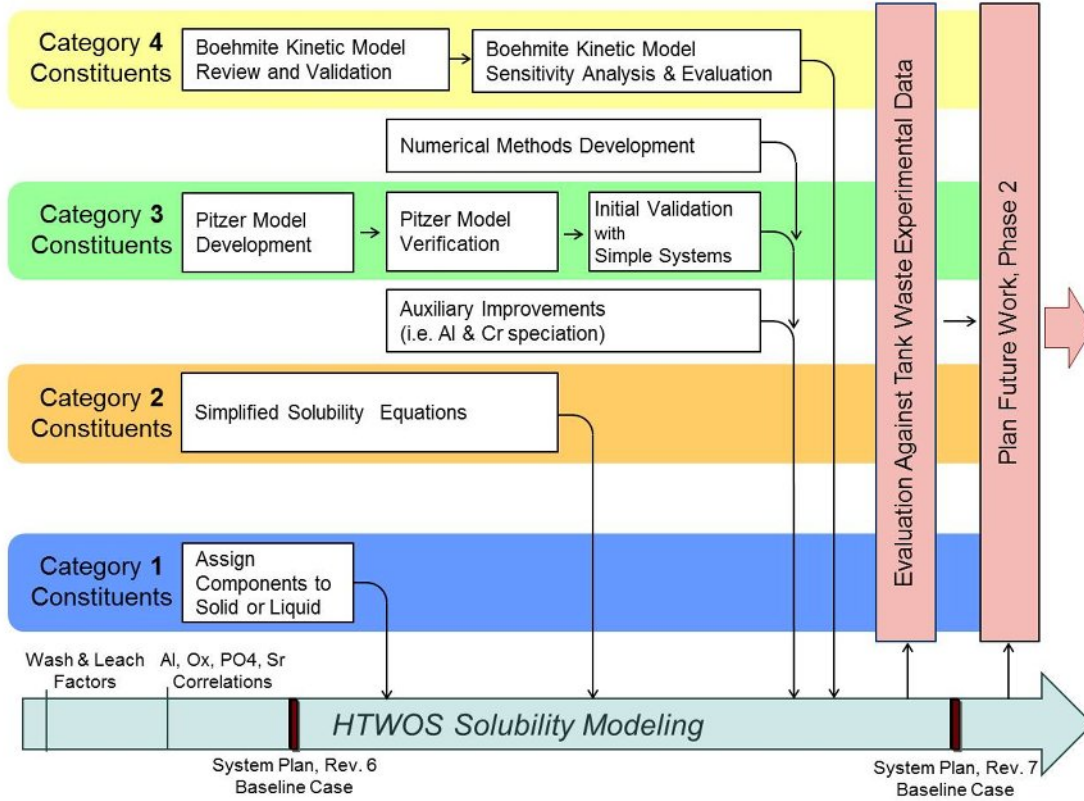


Fig. 2. Phase 1 evolution of HTWOS chemistry modeling.

Model Development

Simplified solubility correlations were developed to provide a better means of predicting solid-liquid phase distribution of Category 2 waste constituents than wash factors, while not demanding significant computation time of the HTWOS model [4]. Information from the thermodynamic simulation software, OLI’s Environmental Simulation Program, provided solubility curves for waste constituents in a range of liquid phase compositions approximating tank waste. Correlations were then fit to these curves, in most cases as a function of ionic strength and hydroxide concentration. Information from prior site studies of selected waste components and solubility data from the literature were also incorporated into the development of the simplified solubility correlations. As an example, the correlation for barium is provided:

$$[Ba^{2+}] = \frac{10^{(a - bX)}}{[OH^-]} \tag{Eq. 1}$$

Where $a = 9.89E-02$ for $X < 0.001$ or $a = 1.98E-01$ for $X \geq 0.001$
 $b = -7.27E-01$ for $X < 0.001$ or $b = -8.47E00$ for $X \geq 0.001$
 $X = [CO_3] + [SO_4] + [PO_4]$.

Because the waste constituents of Category 3 change phase appreciably depending on waste conditions and because they have a significant impact on glass production, a more rigorous model predicting their phase distribution is required for sound system modeling and planning. The Pitzer ion-interaction model is a well-known thermodynamic model for activity coefficients of mixed electrolytes. This model is widely accepted in the scientific community and serves as a foundation to many software programs.

The activity coefficient for each ion is calculated as a function of solution composition, temperature, and as many as six empirical ion-interaction, or Pitzer, parameters. The activity coefficient for each ion is then used in conjunction with the components' chemical potentials to solve for the aqueous concentrations and solid identities and quantities by minimizing the total Gibbs energy of the system. The potential solid identities must be explicitly chosen and their chemical potentials known. Solid compounds were selected by reviewing the solid forms (Table I) of Category 3 constituents most often observed in the waste [5]. While the solids shown in Table I represent the solids expected to be relevant to the use of the model to describe tank waste, all of the solids listed in Table II were included in the development of the Pitzer model for the HTWOS to provide a rigorous chemistry basis over a large range of conditions.

Table II: Solid compounds included in the Pitzer ion-interaction model in the HTWOS based on their potential presence in Hanford tank waste.

Al(OH) ₃	Na ₂ HPO ₄ ·7H ₂ O	Na ₃ PO ₄ ·6H ₂ O
Na ₂ C ₂ O ₄	Na ₂ HPO ₄ ·12H ₂ O	Na ₃ PO ₄ ·8H ₂ O
NaCl	Na ₂ SO ₄	Na ₇ F(PO ₄) ₂ ·19H ₂ O
Na ₂ CO ₃ ·10H ₂ O	Na ₂ SO ₄ ·10H ₂ O	NaF
Na ₂ CO ₃ ·7H ₂ O	Na ₃ FSO ₄	NaHCO ₃
Na ₂ CO ₃ ·H ₂ O	Na ₃ SO ₄ NO ₃ ·1H ₂ O	NaNO ₂
Na ₂ HPO ₄ ·2H ₂ O	Na ₃ PO ₄ ·0.25NaOH·12H ₂ O	NaNO ₃

As an example, Pitzer defined the activity coefficient of an anion, γ_x , as [5]:

$$\ln(\gamma_x) = \left(\frac{z_x^2}{2} + \frac{z_x}{z_c} \right) \left(\frac{2}{z_c} + \frac{z_c}{z_x} \right) + \frac{z_x}{z_c} \left(\frac{2}{z_c} + \frac{z_c}{z_x} \right) + 2\Phi + \frac{z_x}{z_c} \left(\frac{2}{z_c} + \frac{z_c}{z_x} \right) + \frac{z_x}{z_c} \left(\frac{2}{z_c} + \frac{z_c}{z_x} \right) \quad (\text{Eq. 2})$$

Where subscripts refer to all aqueous species, i , anions, a , cations, c , and neutral aqueous species, n , in the system; m is the concentration of a species, i (mol/kg-H₂O), while z_i is its charge and $\sum z_i m_i = 0$. B and C are binary parameters; Ψ , λ , ζ are ternary parameters; Φ is a mixing function; and,

$$= - \frac{\sqrt{I}}{1 + \sqrt{I}} + \frac{2}{I} \ln(1 + \sqrt{I}) + \frac{z_x}{z_c} \left(\frac{2}{z_c} + \frac{z_c}{z_x} \right) + \frac{z_x}{z_c} \left(\frac{2}{z_c} + \frac{z_c}{z_x} \right) \Phi \quad (\text{Eq. 3})$$

where κ is the Debye-Hückel osmotic constant, with a value of 0.3915 kg^{1/2} mol^{-1/2} at 25°C and 1 bar; I is ionic strength; and b is a constant, 1.2.

To determine the composition of the system, the total Gibbs energy is minimized:

$$= \quad (\text{Eq. 4})$$

Where the chemical potential is defined:

$$= \quad + \ln(\gamma_x) = \quad + \quad (\gamma_x) + \ln(\gamma_x) \quad (\text{Eq. 5})$$

The Pitzer parameters account for interaction between two specific analytes (binary parameters) or between three specific analytes (ternary and mixing parameters). Though the Pitzer parameters are available for many components in the literature, it is essential that the set of parameters for a given system be self-consistent. For this reason, the development of the Pitzer model for use in the HTWOS required the collection from literature and reconciliation of Pitzer parameters for all of the Category 3 constituents. A Microsoft Excel¹ workbook was developed to both test the Pitzer model and its calculation of solution compositions and to reconcile parameter and solubility data into a consistent database (referred to as the “HTWOS Pitzer database”) of parameters for the system of Category 3 constituents. The Pitzer model and its development for use with Hanford tank waste is discussed in more detail in “Development of a Thermodynamic Model for the Hanford Tank Waste Operations Simulator” [7, 8]. An example of the model’s prediction of aluminum solubility in NaOH at various temperatures is provided in Figure 3. Data from Wesolowski [9] was used to generate the interaction parameters for $\text{Al}(\text{OH})_4^-$, Na^+ and OH^- . The model prediction is compared to separate data generated by Russell et al. [10].

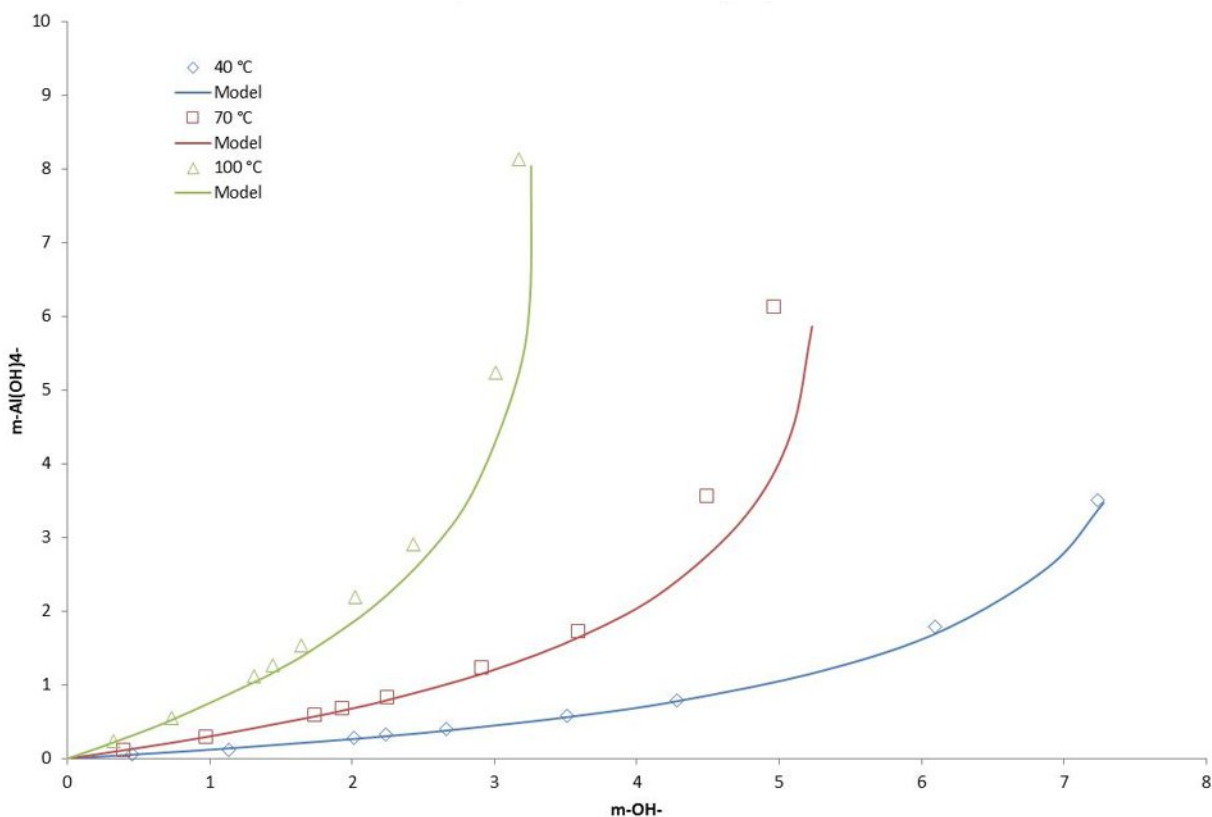


Fig 3. Comparison of solubility isotherms for gibbsite in NaOH at 40, 70, and 100°C generated by the HTWOS Pitzer model and experimentally [10].

To accurately predict aluminum phase distribution during the caustic leaching step of waste pretreatment at the WTP, a kinetic-based model for boehmite dissolution is necessary. Five boehmite dissolution models for caustic leaching published in literature have been examined in addition to the model already included in the HTWOS for this process operation [11]. Of the six models, four were able to be reproduced and validated [12, 13, 14, 15]; whereas, errors were

¹ Excel is a registered trademark of the Microsoft Corporation, Redmond, Washington.

found in the other two. The four models that were reproducible and validated were then tested in their ability to predict caustic leaching results for Hanford tank waste. Each of the models requires the definition of waste parameters; although in many cases, characteristics of the waste (e.g., particle size and density) are difficult to determine and must be estimated. A sensitivity analysis was performed to determine which parameters defining each individual model most impacted its functionality and which model was least sensitive overall to its parameter values. Table III lists the parameters included in the sensitivity study and to which of the four kinetic models they are relevant. The PNNL-20166 model showed greatest sensitivity to temperature and hydroxide concentration, whereas the other three models were most sensitive to at least one of the fit Arrhenius rate constants. Since temperature and hydroxide concentration are more easily measured and controlled than rate constants and because the PNNL-20166 model is least sensitive overall to its parameter values, the PNNL-20166 boehmite kinetic dissolution model may provide more accurate results than the other models available.

Table III. Parameters used in the sensitivity analysis of four boehmite kinetic dissolution models.

Parameter examined in sensitivity analysis	Kinetic model in which sensitivity of the parameter was examined			
	Peterson et al. 2007 [12]	RPP-RPT-45806 [13]	PNNL-20166 [14]	24590-WTP-RPT-PT-02-005 [15]
Arrhenius pre-exponential factor (A)	✓	✓	✓	✓
Arrhenius activation energy (Ea)	✓	✓	✓	✓
Density of the solution (ρ_{soln})	✓	✓	✓	✓
Temperature in degrees C	✓	✓	✓	✓
Fraction of solid aluminum as boehmite (%Boeh)	✓	✓	✓	✓
Fraction of solids in the slurry (Fb)	✓	✓	✓	✓
Concentration of dissolved aluminum in solution at time zero (CAI,0)	✓	✓	✓	✓
Concentration of hydroxide in solution (COH)	✓	✓	✓	✓
Diameter of boehmite particles (dBoeh)	✓	✓	✓	
Percent water		✓		
Fraction of charged surface sites (C)		✓		
Fit exponent (A)			✓	
Fit exponent (B)			✓	
Fit exponent (H)			✓	
Fit exponent (n)				✓

Implementation and Impact

The simplified solubility correlations for Category 2 constituents were recently implemented in the HTWOS. This process required significant rework and reorganization within the HTWOS model to accommodate the added complexity. The overall fraction of solids in the waste processed in the HTWOS model did not change appreciably with the addition of these solubility equations. However, it is difficult to fully analyze their impact to RPP mission duration and other metrics predicted by the HTWOS until the solubility model for Category 3 is implemented.

The implementation of the Pitzer ion-interaction model for Category 3 constituents is in progress. This set of equations is highly complex; however, the programming framework developed for installation of the simplified solubility equations for Category 2 constituents is expected to expedite this work.

Despite the additional computation of the simplified solubility equations for Category 2 constituents, the HTWOS run time did not change. An increase in run time is expected on inclusion of the Pitzer model for Category 3 constituents due its complexity compared to both simple split factors and the simplified equations. To mitigate this effect, substantial focus has been placed on optimizing the calculation of the activity coefficients and the minimum Gibbs energy and final system composition. Multiple methods for solving this system of equations were tested outside of the HTWOS to make the most efficient selection. Though simulated annealing and sequential quadratic programming methods were expected to offer both robustness and speed in calculation, the first was slowed significantly by an excessive number of iterations and the latter was often unable to reach a solution. The most efficient method and the one selected was the SOLGASMIX method [16], which requires an average of ten iterations to reach a solution.

Solubility Model Evaluation

Though the model predictions by the Pitzer model for many simple systems have been compared to experimental data (Figure 3), a rigorous assessment of the solubility model's ability to predict Hanford tank waste phase distribution is necessary for its use in the HTWOS and system planning. The integrated solubility model is designed for complex systems; however, few systems are as complex as Hanford tank waste in terms of its generation, composition, and age. An evaluation is currently underway to:

- Evaluate predictions of the integrated solubility model against experimental data of tank waste and applicable simulants
- Compare the integrated solubility model to other solubility models, including wash factors and the OLI stream analyzer (Environmental Simulation Program).
- Identify strengths and weaknesses of the integrated solubility model to assist in the prioritization of future work in waste chemistry modeling and laboratory research.

Experimental data for comparison includes tank contents characterization data, wash and leach reports summarizing experiments used to develop wash factors, boil-down experiments conducted prior to tank waste volume reduction by evaporation, and other tank waste dissolution studies. Data is first assessed to ensure that all necessary attributes are measured, that experiments were conducted within the design limits of the integrated solubility model, and the accuracy of the measurements made is reasonable.

Model predictions and experimental data will be compared in terms of the relative and percent difference in composition values, the identity of solids predicted, general trends, and other metrics. Figure 4 summarizes the evaluation process.

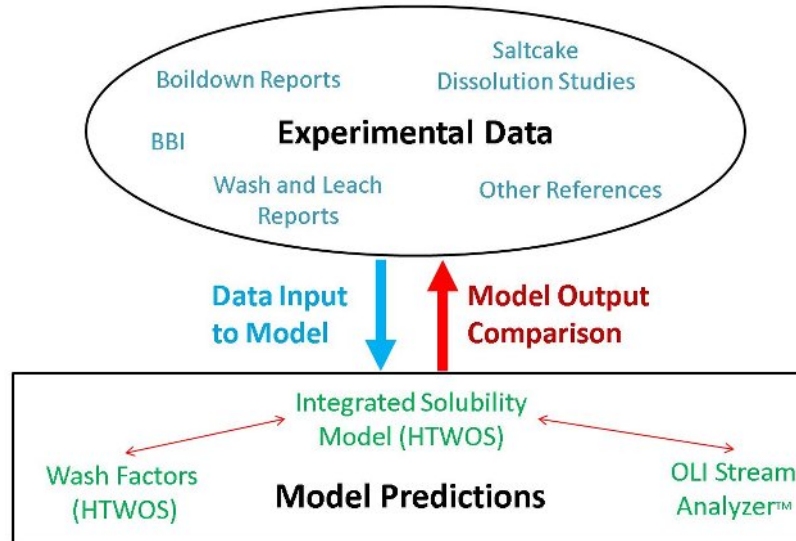


Fig 4. Process planned for the evaluation of integrated solubility model against experimental tank waste data.

LIFECYCLE COST MODEL

Analysis of the mission impacts resulting from alternative assumptions is not complete without consideration to the project cost and schedule. Although it is well understood that implementation of a new technology that has the potential to accelerate the treatment duration can create savings in out-year operating costs, predicting the complex interactions of that new technology with the rest of the system and the resulting impacts on lifecycle costs and schedules is much more difficult. The LCM is being developed to link the projected outcomes of alternative scenarios modeled by the HTWOS (which has the ability to predict complex interactions between RPP mission components) to cost and schedule data to automatically generate lifecycle schedules and cost profiles. The HTWOS can be used to evaluate the technical viability of a proposed alternative, while the new LCM will predict the financial merits and feasibility of implementation. Forecasts from the LCM can be compared to the project baseline to help guide decisions and enhance mission planning.

Approach

The initial phase of LCM development involved the creation of the software components that facilitate crosstalk between the HTWOS and the RPP mission cost and schedule data. The two major components that enable the current LCM functionality are the resource-loaded Primavera P6² schedule and the HTWOS database. Currently, the LCM is capable of producing the mission schedule and lifecycle cost profile from a scenario modeled in the HTWOS. Ongoing and future LCM scope involves adding enhanced planning capabilities to the HTWOS model by making use of the newly developed LCM components.

² Primavera is a registered trademark and P6 is a trademark of Primavera Technologies, Inc.

Lifecycle Cost Model Development

Prior to development of the LCM, cost profiles for alternative scenarios were generated by extracting relevant HTWOS data (e.g., predicted dates and durations for key activities) and using them to manually adjust a copy of the performance measurement baseline schedule (also referred to as the baseline schedule). The performance measurement baseline includes all scope, schedule, and budget contained within the approved project baseline, making the baseline schedule a time-phased, logic-driven representation of the detailed RPP work activities. The baseline schedule contains logic ties within individual projects and between projects, including sequences of activities, successor and predecessor dependencies, activity durations, and numerous constraint dates. The widespread use of constraint dates is appropriate for tracking project performance, for which the baseline schedule is intended, but is not suitable for the kind of adjustments and restructuring necessary for alternative scenario analysis. To create a new schedule and associated cost profile based on different assumptions and dates predicted by HTWOS, logic ties had to be broken to move activities as needed, making the manual process time-consuming and prone to errors. The LCM was developed to overcome these issues and to expedite the process for use in mission planning. Two major efforts were involved in creating the current LCM functionality: (1) development of the resource-loaded Primavera P6 schedule, and (2) development of the HTWOS database.

The LCM Primavera P6 schedule incorporates all activities in the baseline schedule (along with their associated budget), with the work breakdown structure³ elements rolled-up to Level 5. This means that all workscope associated with the 16,000 activities (encompassing nearly \$62 billion of workscope) in the performance measurement baseline is included in the LCM; however, the reports are summarized to Level 5 to reduce the number activities to a more manageable 5,800. The LCM schedule accepts HTWOS output data to move activities to the dates predicted by the model. Because not all activities that exist in the schedule are modeled in the HTWOS, significant effort was devoted to establishing logical connections between HTWOS modeled activities (e.g., single-shell tank retrievals, evaporator campaigns, waste feed deliveries to the WTP, etc.) and the remaining RPP mission activities (e.g., construction activities, facility closures, laboratory support, etc.). In contrast to the baseline schedule, activities on the LCM schedule are almost entirely linked by logical connections and not constraint dates, ensuring that all activities can move in time to reflect the assumptions and results of a scenario.

The HTWOS database is an enterprise-level SQL Server⁴ database. All output data generated by an HTWOS run can be stored in the database, and appropriate queries and views can be used to compile and compare the data. The database contains the dates and durations for key mission activities that are used by the LCM to adjust the Primavera P6 schedule.

Figure 5 depicts the integration of the newly developed LCM components with the HTWOS model.

³ The work breakdown structure is a hierarchical, deliverable-oriented grouping of project elements, which organizes and defines the total scope of the project. Each descending level of the work breakdown structure represents an increasingly detailed definition of a project component.

⁴ SQL Server is a registered trademark of Microsoft Corporation, Redmond, Washington.

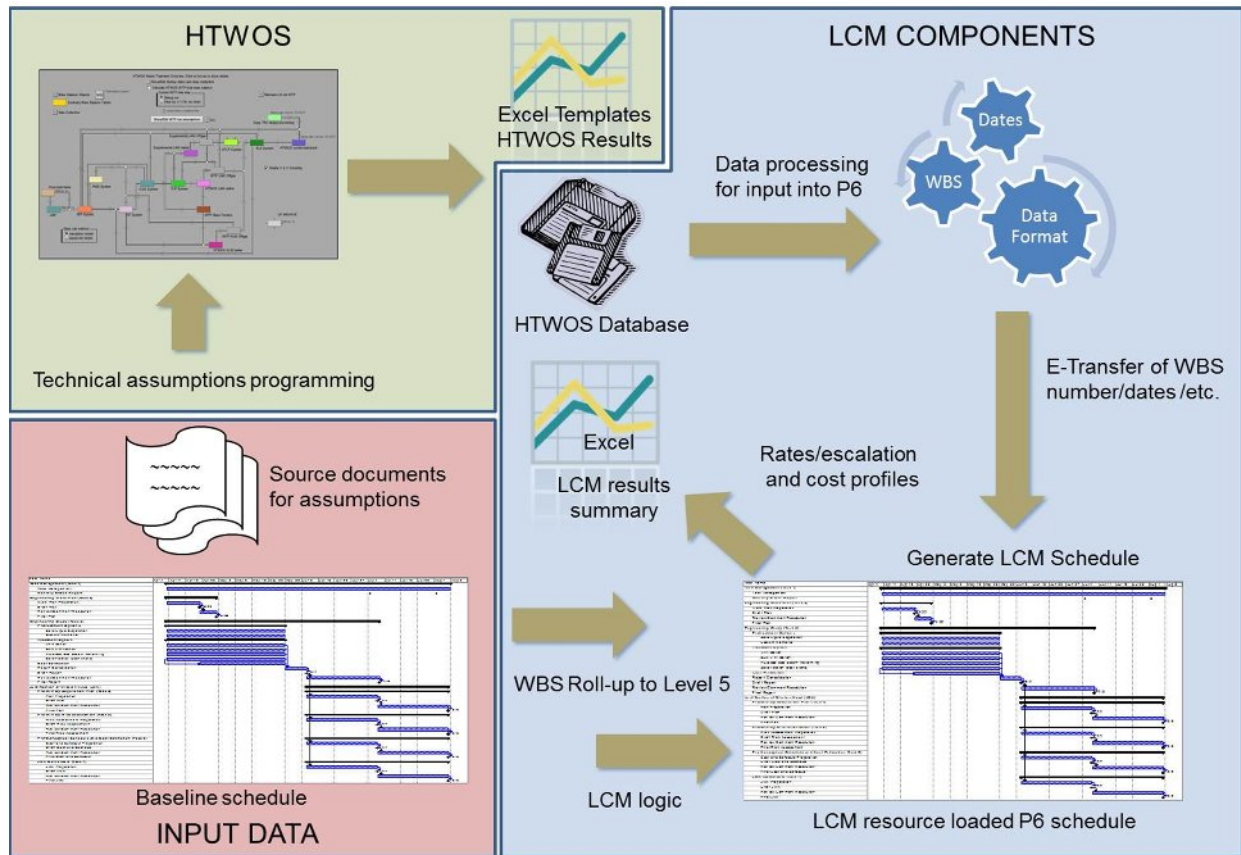


Fig 5. Lifecycle cost model integration with the HTWOS.

When a scenario is to be analyzed, the technical and programmatic assumptions are implemented in the HTWOS, and the model is run to generate results. Results are electronically transferred to a series of Excel templates, and the enterprise-level SQL Server database. Relevant schedule data is extracted from the database via the Primavera open database connectivity interface and processed for input into P6. Data is then electronically transferred to the LCM P6 file, which has been loaded with the current baseline schedule, cost information, and the LCM logic. The revised time-phased cost information from the resulting schedule is written out to an Excel file, where escalation and a ramp-down pricing algorithm are applied.⁵ The final products of this effort are a series of tables and graphics presenting the technical results from the HTWOS, contained within the automatically populated Excel templates; a Primavera P6 schedule of the activities that make up the lifecycle of the scenario; and tables and graphics presenting the annual cost information, summarized to Level 5 of the work breakdown structure. These products allow subject matter experts to make observations and draw conclusions about the scenario results.

⁵ The ramp-down pricing algorithm is used to simulate the reduction of effort and associated budget for management, operations, and maintenance as each tank farm is closed. The reduction of effort is applied to specific work breakdown structure elements containing those types of costs. The amount of reduction and which work breakdown structures are affected is dependent on the number and the type of tank farm(s) (single-shell tank or double-shell tank) closed in a particular year.

Implementation – Lifecycle Cost Model Results Debut in RPP System Plan (Revision 6)

The initial phase of LCM development was completed in April 2011, and the tool has already played an important role in mission planning. On October 21, 2011, the DOE Office of River Protection submitted Revision 6 of the RPP System Plan [1] to the Washington State Department of Ecology [17], achieving partial completion of milestone M-062-40 of the *Hanford Federal Facility Agreement and Consent Order* [18]. Revision 6 is the first system plan submitted pursuant to the requirements of the milestone, and the newly developed LCM was essential to meeting the requirements.

Schedule and cost information was not previously published in an RPP System Plan; however milestone M-062-40 required that the RPP System Plan (Revision 6) include “estimated schedule impacts of alternative cases relative to the baseline, including cost comparisons.” Ten scenarios were evaluated in RPP System Plan (Revision 6), including the Baseline Case. The unique technical and programmatic assumptions of each scenario (which included new treatment facilities, alternative waste retrieval and staging options, early startup of specified facilities, etc.) were modeled in HTWOS. Scenarios that involved new facilities and scope that is not included in the baseline required supplemental cost estimates and project schedules to be generated for the new scope. That information was loaded into the LCM P6 schedule before inputting the HTWOS results. The ten lifecycle schedules produced by the LCM represented the unique assumptions of the scenarios and the mission impacts of those assumptions as predicted by HTWOS. The additional data provided by the LCM allowed more complete evaluations of the scenarios to be performed and included in the RPP System Plan, increasing the utility of the document as a decision-making tool.

Future Plans for Lifecycle Cost Model

Development of the LCM is ongoing and includes, in addition to the cost and schedule analysis, a fundamental improvement in data collection by the HTWOS. Upgrades are being made to the HTWOS that will allow it to write data to external applications as it is generated, rather than at the end of a run. This has two major benefits. First, the amount of data that can be recorded for a model run is dramatically increased. Second, the use of ancillary software during a model run becomes a possibility for exceedingly complex or computationally demanding simulations. Both enhancements will facilitate implementation of the additional advanced capabilities planned for the HTWOS model.

The enhanced mission planning features that are under development for the HTWOS model make use of the existing LCM components. The HTWOS database is integral to these efforts, with its ability to store large amounts of not only output data (results), but also input parameters for scenario configuration. Technical parameters such as facility capacities, start dates for various activities, and others may be specified through the database via a user interface. The LCM P6 schedule data can also be imported into the database, allowing schedule and cost information to become user-defined parameters via the user interface. This data will be used as constraints to forecast the technical impacts from adding funding restrictions at certain times throughout the mission. The goal is to enhance the model so that optimization objectives (e.g., minimizing HLW canister production versus minimizing overall treatment duration) can be established before a run. The model will self-adjust as it progresses through the simulation to meet the specified targets.

Development of the user interface and all necessary connections for the capabilities described is future scope; however, it is the LCM features and components that have already been

developed that will make those enhanced capabilities a possibility. Figure 6 shows the vision for the future of HTWOS and the LCM.

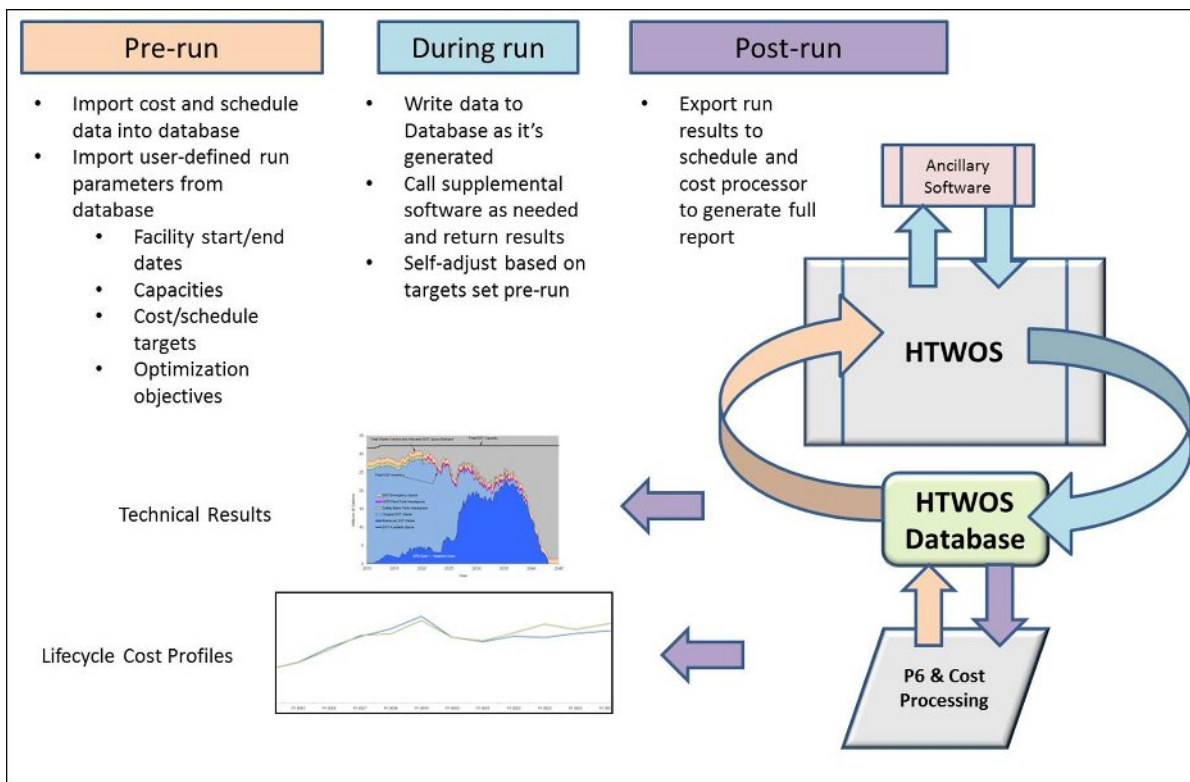


Fig 6. Future enhancements for HTWOS.

CONCLUSION

The HTWOS is an essential tool for RPP mission planning. The two major modeling efforts currently underway, to develop aqueous thermodynamic models and the LCM, are being pursued to enhance the utility of the HTWOS by improving the underlying chemistry and providing the capability to automatically produce a more complete set of mission metrics, including cost and schedule information.

The two innovative tools are under development separately, with independent project scopes and schedules. The model changes necessary for the improvements are incrementally implemented into HTWOS and significant future work is planned for both. Independently, both model tools enhance the fidelity of HTWOS results. Together, the solubility model and LCM complement one another as an integrated improvement to the HTWOS model. Enhanced validity of technical assumptions provides more reliable model projections, improving the basis for schedule and costs generated by the LCM.

REFERENCES

1. Certa et al, 2011, *River Protection Project System Plan*, Rev. 6, ORP-11242, Washington River Protection Solutions, LLC, Richland, Washington.
2. Pitzer, K.S., 1973, "Thermodynamics of Electrolytes. I. Theoretical Basis and General Equations," *Journal of Physical Chemistry*, Vol. 77, Issue 2, pp. 268-277.

3. Pitzer, K.S., and Kim, J.J., 1974, "Thermodynamics of Electrolytes: IV. Activity and Osmotic Coefficients for Mixed Electrolytes," *Journal of the American Chemical Society*, Vol. 96, Issue 18.
4. Disselkamp, 2010, *Simplified Solubility Estimates for Selected Waste Compounds*, RPP-RPT-47542, Washington River Protection Solutions, LLC, Richland, Washington.
5. Reynolds, 2010, *Wash and Leach Factor Work Plan*, RPP-PLAN-46002, Washington River Protection Solutions, LLC, Richland, Washington.
6. Moffat, H.K., and Colon, C.F.J., 2009, SAND2009-3115, *Implementation of Equilibrium Aqueous Speciation and Solubility (EQ3 type) Calculations into Cantera for Electrolyte Solutions*, Sandia National Laboratories, Albuquerque, New Mexico.
7. Carter, R., 2011, "Development of a Thermodynamic Model for the Hanford Tank Waste Operations Simulator," Waste Management Symposium 2012, Phoenix, Arizona.
8. Carter, 2011, *Development of a Thermodynamic Model for the Hanford Tank Waste Operations Simulator (HTWOS)*, RPP-RPT-50703, Washington River Protection Solutions, LLC, Richland, Washington.
9. Wesolowski, D., 1992, "Aluminum speciation and equilibria in aqueous solution: I. The solubility of gibbsite in the system Na-K-Cl-OH-Al(OH)₃ from 0 to 100 °C," *Geochimica et Cosmochimica Acta*, Vol. 56, pp. 1065-1091.
10. Russell, A.S., Edwards, J.D., and Taylor, C.S., 1955, "Solubility and density of hydrated alumina in NaOH solutions," *Journal of Metals*, Vol. 7, pp. 1123-1128.
11. Harrington, 2011, *Comparison of Boehmite Caustic Leach Models from Literature*, RPP-RPT-49389, Washington River Protection Solutions, LLC, Richland, Washington.
12. Peterson, R.A., Lumetta, G.J., Rapko, B.M., and Poloski, A.P., 2007, "Modeling of Boehmite Leaching from Actual Hanford High-Level Waste Samples," *Separation Science and Technology*, Vol. 42, Issue 8, pp. 1719-1730.
13. Disselkamp, 2011, *Development of a Kinetic Model of Boehmite Dissolution in Caustic Solutions Applied to Optimize Hanford Waste Processing*, Rev. 1, RPP-RPT-45806, Washington River Protection Solutions, LLC, Richland, Washington.
14. Mahoney et al, 2011, *Alternative Sodium Recovery Technology – High Hydroxide Leaching: FY10 Status Report*, PNNL-20166 (EMSP-RPT-002), Pacific Northwest National Laboratory, Richland, Washington.
15. Stone, 2011, *Flowsheet Bases, Assumptions, and Requirements*, Rev. 6, 24590-WTP-RPT-PT-02-005, Bechtel National, Inc., Richland, Washington.
16. Weber, C.F., 1998, "Convergence of the Equilibrium Code SOLGASMIX," *Journal of Computational Physics*, Vol. 145, pp. 655-670.
17. Fletcher, T. W., 2011, "Submittal of River Protection Project System Plan Revision 6 in Partial Completion of Hanford Federal Facility Agreement and Consent Order (HFFACO) Interim Milestone M-062-40," (Letter 11-TDP-086 to J. A. Hedges, Program Manager, Nuclear Waste Program, State of Washington, Department of Ecology, October 21), U.S. Department of Energy, Office of River Protection, Richland, Washington.
18. Ecology, EPA, and DOE, 1989, *Hanford Federal Facility Agreement and Consent Order--Tri-Party Agreement*, as amended, Washington State Department of Ecology, U.S. Environmental Protection Agency, and U.S. Department of Energy, Olympia, Washington.