June 7, 2011

The Honorable Inés R. Triay  
Assistant Secretary for Environmental Management  
U.S. Department of Energy  
1000 Independence Avenue, SW  
Washington, DC 20585-0113

Dear Dr. Triay:

The Defense Nuclear Facilities Safety Board (Board) has completed a review of the methodology used by the design authority, Bechtel National, Incorporated (BNI), for the Waste Treatment and Immobilization Plant (WTP) in assessing the accumulation of solids in pulse-jet mixed (PJM) vessels. This methodology utilizes a spreadsheet-based computational model—the Low Order Accumulation Model (LOAM)—to predict accumulation of solids in WTP vessels. The Board does not believe that LOAM is suitable for predicting accumulation of solids in either Newtonian or non-Newtonian full-scale vessels because it under-predicts the accumulation of solids. The Board notes that the Department of Energy (DOE) Office of River Protection used the results from this model as a basis for partial closure of solids accumulation concerns associated with the External Flowsheet Review Team Major Issue 3 (M3), “Inadequate Design of Mixing Systems.” As explained in the Board’s January 6, 2010 letter, accumulation of solids in PJM vessels raises several significant safety-related issues, primarily inadvertent nuclear criticality and the retention and potential release of large quantities of flammable gas.

In the enclosed report, the Board’s staff evaluates the LOAM model and compares model predictions to experimental observations. The experimental data was obtained from tests performed by BNI in a small-scale model of a WTP non-Newtonian process vessel. This report details several deficiencies:

- **Accumulation of solids**—Small-scale test results showed that large particles remained in the test vessel as the pump-out finished and that accumulation of solids over multiple batches should be expected. However, LOAM predicted the opposite behavior. These differences between the predicted behavior and small-scale test results involving the accumulation of large particles can be explained by a fundamental flaw in the mechanics of the LOAM calculations. This modeling flaw artificially influences the predicted removal of rapidly settling particles and makes it impossible to model accumulation of solids in unmixed zones on the vessel bottom.

- **Zone of influence**—Small-scale test results showed that the radius of mobilized solids on the vessel bottom under each pulse jet mixer—the zone of influence—was
significantly smaller than predicted by the LOAM calculations. Thus, LOAM over-predicts the amount of material that is mobilized. The Board has no confidence that LOAM uses a technically valid approach for predicting zone of influence.

• **Cloud height**—The Board’s analysis showed that the equations in LOAM used to predict cloud height (and subsequently the solids concentration at the tank transfer line inlet) are based on a conceptual model that lacks a sound physical basis. LOAM predictions for cloud height do not properly account for increasing energy requirements at increasing tank dimensions. Accordingly, the Board has no confidence that LOAM can reliably predict cloud height and solids concentration at the pump inlet for the actual WTP vessels.

• **Rheological properties**—BNI testing used a Newtonian fluid to assess the performance of process vessels that will contain non-Newtonian fluids. The Board believes that, without definitive supporting test data for PJM vessels at a sufficient scale, this practice is technically unjustified.

Therefore, pursuant to 42 U.S.C. § 2286b(d), the Board requests a report within 60 days of receipt of this letter that (1) states whether DOE will continue to use LOAM as the computational model for accumulation of solids in WTP vessels and for what purpose(s), as well as the technical rationale for each use; (2) provides an approach for formal verification and validation of LOAM (if DOE continues to use it) by employing concepts outlined in Chapter 1 of American Society of Mechanical Engineers V&V 20, *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer*; and (3) explains how the issues identified in the enclosed report will be addressed during large-scale testing for all WTP vessels.

Sincerely,

Peter S. Winokur, Ph.D.
Chairman

Enclosure

c: Mr. Scott L. Samuelson
Mrs. Mari-Jo Campagnone
MEMORANDUM FOR: T. J. Dwyer, Technical Director

COPIES: Board Members

FROM: A. Poloski, S. Stokes, P. Meyer

SUBJECT: Use of Low Order Accumulation Model, Waste Treatment and Immobilization Plant

Background. In a letter dated January 6, 2010, the Defense Nuclear Facilities Safety Board (Board) raised several significant safety-related issues associated with inadequate mixing at the Waste Treatment and Immobilization Plant (WTP), such as inadvertent nuclear criticality and retention and release of large quantities of flammable gas. These issues arise because of the potential for accumulation of solids in pulse-jet mixed (PJM) vessels. The WTP design authority, Bechtel National, Inc. (BNI), utilizes a spreadsheet-based computational model—the Low Order Accumulation Model (LOAM)—to predict accumulation of solids in WTP vessels. The Department of Energy-Office of River Protection (DOE-ORP) used the results from this model as a basis for partial closure of solids accumulation concerns associated with the External Flowsheet Review Team Major Issue 3 (M3), “Inadequate Design of Mixing Systems.” DOE-ORP determined that further testing was needed for PJM vessels that will contain greater concentrations of solids (termed non-Newtonian vessels by BNI). One reason for this decision was that PJM testing and LOAM development prior to June 2010 had focused on designs for Newtonian vessels, which have significantly different internal arrangements from those of non-Newtonian vessels.

On February 11, 2011, the Board’s staff held an on-site review with DOE-ORP and BNI staff to discuss the results of the recently completed small-scale testing with a non-Newtonian vessel PJM configuration using Newtonian simulants.

The purpose of this testing was to compare the predictions of LOAM to the measured concentration of solids remaining in the vessel heel after the vessel contents were pumped out. If LOAM adequately predicted the quantity of solids remaining in the vessel after pump-out, it would be used to predict whether the full-scale, non-Newtonian vessels would accumulate solids during operation.

When calculating the concentration of solids during pump-out, LOAM uses mathematical formulas designed to predict the radius of sediment mobilized on the vessel floor from each individual pulse jet discharge, and the height to which solids are suspended in the vessel (height above the vessel bottom). The BNI staff terms the mobilization radius of a pulse jet the “zone of
influence” (ZOI) and the height of suspended solids the “cloud height” (Hc). The cloud height is important since it contributes to the estimate of concentration of solids at the tank transfer line inlet. LOAM predicts ZOI with several equations, including a radial stress profile, described in the open literature. BNI staff’s use of these predictive equations has been a source of technical controversy with external reviewers, including the Consortium for Risk Evaluation with Stakeholder Participation (CRESP) and Pacific Northwest National Laboratory (see Appendices B and C from “CRESP Review Team Letter Report 7—PJM Vessels,” dated July 1, 2010). CRESP stated in the July 1, 2010, letter report that:

The greatest risk is that the actual ZOI during WTP operations is smaller than predicted by the current design basis and therefore solids accumulation may require more frequent cleanout than predicted. Experimental programs that validate scaling relationships for the ZOI and the integrated vessel performance at full-scale or near full-scale systems are needed.

The small-scale testing consisted of six tests—three tests used water as the interstitial fluid, and three used a mixture of glycerin and water to increase the fluid viscosity. Different solids were used to simulate actual waste solids. These included a two-part simulant of aluminum oxide and 700 µm glass beads (the beads acted as a surrogate for bounding, large particles in the actual waste). Additional tests used a more complex five-part simulant that contained 10 µm tungsten carbide as the bounding plutonium oxide surrogate and 700 µm glass beads. BNI staff performed tests both with and without air spargers, which provide additional mixing energy. During the small-scale testing, BNI staff measured both ZOI and Hc for comparison with the LOAM predictions.

During the on-site review, BNI staff provided the Board’s staff with preliminary data from six small-scale tests and the corresponding LOAM predictions for accumulation of solids, ZOI, and Hc. During this review and in subsequent analysis, the Board’s staff focused on the ability of LOAM to adequately model the accumulation of solids in full-scale Newtonian and non-Newtonian vessels.

**Findings.** According to LOAM predictions for these small-scale tests, nearly all of the large glass beads would be removed during the first half of the pump-out, and there would be no accumulation of solids. Contrary to this prediction, the test data showed that most of the large glass beads remained in the test vessel as the pump-out finished, and accumulation of solids over multiple batches should be expected. The Board’s staff believes the significant differences between the predictions and test results for glass bead accumulation are explained, in part, by a fundamental flaw in the mathematical formulation of the LOAM simulation.

At each time step in the simulation, LOAM calculates the mass of solids removed during pump-out. For rapidly settling particles (those that are minimally suspended off the vessel floor), LOAM calculates the mass of solids removed using the fraction of mobilized solids on the vessel floor. Through this calculation, LOAM implicitly assumes that settled solids have the potential to be remobilized at each time step. LOAM lacks the capability to model “dead zones” (regions on the vessel floor that are completely stagnant). The Board’s staff believes that the inability of LOAM to model dead zones excludes potential accumulation of solids based on slow growth of
dead zones over multiple batches of feed. For a large number of time steps, the calculated concentration of solids during pump-out is driven mathematically to zero by successive multiplication of the fraction of mobilized solids on the vessel floor; hence, LOAM would never predict the accumulation of solids. The Board’s staff discussed these findings with BNI staff, who responded that the current version of the model can indeed model dead zones. BNI staff provided the most recent version of LOAM and a version history to help in investigating differences between model versions. The analysis performed by the Board’s staff revealed that the revised LOAM mathematical formulation also contains this flaw.

The small-scale testing also revealed that the experimentally measured ZOI radii were substantially smaller than predicted by LOAM. Further, LOAM predicts that the ZOI radii would increase with increasing Newtonian viscosity and that there is no influence of solids concentration on ZOI. However, the measured values for ZOI radii in the six tests using fluids with two different Newtonian viscosities sometimes show the opposite of the predicted behavior and indicate that ZOI is a strong function of solids concentration. The Board’s staff believes that the fact that the LOAM model over-predicted the ZOI compared to the small-scale test results is an indicator that the CRESP risk statement cited earlier in this report is a significant concern for full-scale plant operations.

Calculation of cloud height is important in estimating the concentration of solids at the transfer line inlet. LOAM determines cloud height by modeling the “up-wash” flow field independently of the solid phase, and then balances the vertical velocity component against the settling velocity of individual particles. This approach results in the predicted cloud height being linearly proportional to the vessel scale. However, data from tests conducted at Pacific Northwest National Laboratory show that cloud height is nearly independent of vessel scale (see Appendix C of PNNL-19085, Assessment of Differences in Phase 1 and Phase 2 Test Observations for Waste Treatment Plant Pulse Jet Mixer Test with Non-Cohesive Solids, October 2010). The LOAM cloud height equations neglect the fact that the up-wash occurs in density-stratified conditions, where gravitational forces act to retard the bulk-fluid motion. Consequently, LOAM predicts non-physical results for cloud height scale-up that do not properly account for increasing potential energy requirements at increasing scale. For this reason, the Board’s staff believes it is inadvisable to rely on LOAM to predict cloud height (and subsequent concentration of solids at the tank transfer line inlet) in PJM vessels at full scale.

During the on-site review, the Board’s staff questioned the technical basis for the use of Newtonian fluids, such as water and the glycerin/water mixture, to assess the performance of non-Newtonian process vessels. BNI staff stated that the high-shear environment produced by PJMs makes a non-Newtonian fluid behave essentially as a Newtonian fluid. In this case, the motion of rapidly settling particles is greatest at the infinite shear viscosity of the non-Newtonian fluid. On this basis, BNI staff considered tests with a Newtonian fluid having a viscosity equivalent to the infinite shear viscosity to be conservative. BNI staff described this as an “informed assumption.” They stated that they are currently writing a white paper validating the assumption that testing non-Newtonian vessels with Newtonian fluids is acceptable. In addition, they acknowledged that LOAM lacks the capability to model non-Newtonian fluids.
The Board’s staff believes that, in the absence of definitive supporting PJM test data at a sufficient scale, the practice of using a Newtonian fluid to assess the performance of PJM vessels designed for non-Newtonian fluids is not technically justified. Specifically, the Board’s staff is concerned that a Newtonian simulant does not mimic the increased rate of jet velocity decay observed in non-Newtonian fluids. For example, increased energy dissipation in non-Newtonian fluids could produce smaller zones of turbulence and larger laminar flow zones that would greatly reduce the ability of the PJMs to suspend and mobilize solids. Moreover, BNI staff’s assumption fails to address the expected range of spatially and temporally dependent apparent viscosities resulting from the periodic nature of PJM operations.

The Board’s staff questioned whether LOAM had been formally verified and validated using the concepts outlined in Chapter 1 of American Society of Mechanical Engineers (ASME) V&V 20, Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer. BNI staff responded that LOAM was a tool for risk reduction and that such a high degree of technical rigor was unwarranted. However, BNI management committed to the Newtonian vessel designs and has continued with fabrication and installation of these vessels based on BNI assessments that included LOAM predictions for the accumulation of solids. BNI staff stated a new model that will use the commercial computational fluid dynamics code FLUENT would be developed for confirmation of the final vessel designs. The FLUENT model would be verified and validated using ASME V&V 20. BNI staff also stated that significant technical challenges arise in using FLUENT to model PJM process vessels. Because of these challenges, they are considering pursuing a formal verification and validation of LOAM using ASME V&V 20. Under this scenario, LOAM would be used to confirm the final vessel designs prior to commissioning.

The Board’s staff believes that LOAM’s deficiencies would have been identified before the Newtonian vessel designs were confirmation ready if the model had been properly verified and validated using the concepts outlined in Chapter 1 of ASME V&V 20.

Conclusions. The Board’s staff does not believe LOAM is suitable for predicting the potential for accumulation of solids in full-scale vessels for the following reasons:

• Accumulation of solids—The preliminary small-scale test results showed that large particles remained in the test vessel as the pump-out finished and that accumulation of solids over multiple batches should be expected. However, LOAM predicted the opposite behavior. These differences between experimental and predicted results involving the accumulation of large particles can be explained by a fundamental flaw in the mechanics of the LOAM calculations. This modeling flaw artificially influences the predicted removal of rapidly settling particles and makes it impossible to model accumulation of solids in dead zones on the vessel bottom.

• Zone of influence—Test results showed that the radius of mobilized solids around each pulse jet mixer—the ZOI—was significantly smaller than predicted by the LOAM calculations. The staff is not confident that LOAM uses a technically valid approach for predicting ZOI.
• **Cloud height**—The analysis by the Board’s staff showed that the equations in LOAM used to predict cloud height (and subsequently the solids concentration at the pump inlet) are based on a conceptual model that lacks a sound physical basis. LOAM predictions for cloud height scale-up do not properly account for increasing potential energy requirements at increasing scale. Accordingly, the staff is not confident that LOAM can reliably predict cloud height and concentration of solids at the pump inlet for the actual WTP vessels.

• **Rheological properties**—BNI testing used a Newtonian fluid to assess the performance of process vessels that will contain non-Newtonian fluids. The Board’s staff believes that without definitive supporting test data for PJM vessels at a sufficient scale, this practice is technically unjustified.