DEFENSE NUCLEAR FACILITIES SAFETY BOARD

Washington, DC 20004-2901

August 3, 2011

Mr. David Huizenga
Acting Assistant Secretary for Environmental
Management
U.S. Department of Energy
1000 Independence Avenue, SW
Washington, DC 20585-0113

Dear Mr. Huizenga:

The Defense Nuclear Facilities Safety Board (Board) reviewed Bechtel National, Incorporated (BNI) calculations of heat transfer from process vessels in the Pretreatment Facility (PTF) at the Waste Treatment and Immobilization Plant (WTP) at the Hanford Site. Based on these calculations, WTP downgraded safety-class mixing controls for nine PTF process vessels. These controls, which were required to prevent flammable conditions potentially resulting in explosions in the vessel headspaces, were changed to a specific administrative control that directs operators to restore mixing within the calculated time following a design basis accident. A small change in temperature (10°F) can result in a major change in hydrogen produced (between 40 and 70 percent) making it vital to have a conservative calculation of maximum temperatures expected in the waste. The Board believes that the analyses performed to date are not reasonably conservative and do not support decisions to downgrade mixing controls.

BNI's calculations determined time-dependent waste temperatures in selected vessels during off-normal conditions following a design basis event. These temperatures were then used to calculate hydrogen generation rates and times to the lower flammability limit for PTF process vessels for post-design basis event conditions. If the time to reach the lower flammability limit is sufficiently long (1,000 hours), the WTP Safety Requirements Document does not require safety-class mixing controls to prevent flammable conditions in the vessel headspaces. The Board's review revealed weakness in the modeling approach, assumptions, and input parameters selected by BNI for heat transfer analyses and raised concerns regarding the suitability of the Facility Flow, Aerosol, Thermal, and Explosion (FATE™) software for accurately modeling heat transfer processes in PTF process vessels. The Board understands that the BNI staff is conducting additional analyses. The Board believes that reasonably conservative finite-element calculations can be performed to better inform a decision about the need for safety-class mixing controls.

Therefore, pursuant to 42 U.S.C. § 2286b(d), the Board requests a report within 60 days of receipt of this letter that addresses the validity of the heat transfer analyses for PTF process vessels at WTP.

Sincerely,

Peter S. Winokur, Ph.D.
Chairman

Enclosure

c: Mr. Scott L. Samuelson
Mrs. Mari-Jo Campagnone

DEFENSE NUCLEAR FACILITIES SAFETY BOARD

Staff Issue Report

May 11, 2011

MEMORANDUM FOR: T. J. Dwyer, Technical Director

COPIES: Board Members

FROM: R. V. Kazban

SUBJECT: Heat Transfer Analyses for Process Vessels in the Pretreatment Facility, Waste Treatment and Immobilization Plant, Hanford Site

This report documents a review by the staff of the Defense Nuclear Facilities Safety Board (Board) of the heat transfer analyses for process vessels in the Pretreatment Facility (PTF) at the Waste Treatment and Immobilization Plant (WTP) at the Hanford Site. The onsite review and follow-up were conducted by members of the Board's staff R. Kazban, P. Meyer, R. Oberreuter, and S. Stokes from November 30 through December 2, 2010, and on December 17, 2010. The staff reviewed the modeling approach and time-dependent temperature results used by Bechtel National, Incorporated (BNI) in calculations of hydrogen generation rates (HGRs) and times to reach the lower flammability limit (LFL) for PTF process vessels. The Board's staff has determined that BNI analysts have not demonstrated that the model results are conservative.

Background. The WTP Safety Requirements Document (SRD) addresses the functional requirement for hydrogen control systems in process vessels to prevent hydrogen accumulation greater than the LFL (i.e., 4 percent by volume) in the vessel headspace. The SRD states that safety-class engineered controls are required for process vessels with a time to reach LFL less than or equal to 1,000 hours. The time to reach LFL depends on the vessel headspace volume, the magnitude of the HGR, and the amount of hydrogen retained in the waste over time. The retained hydrogen is assumed to release instantaneously into the vessel headspace upon resumption of mixing. The amount of hydrogen retained in the waste over a period of time depends on the waste's ability to retain gas and the amount of solids in the process vessel at the start of the accident. Further, the magnitude of the HGR is highly sensitive to even small temperature changes in the waste when organic compounds are present.

BNI performed heat transfer analyses for PTF process vessels located in the black cells using the Facility Flow, Aerosol, Thermal, and Explosion (FATE™) software developed by Fauske & Associates, LLC. Using FATE™, BNI calculated time-dependent waste temperatures in selected vessels during off-normal conditions for over 1,000 hours following a design basis event (DBE), assuming a loss of non-safety systems. In this evaluation, BNI analysts took credit for a decrease in the post-accident HGR due to cooling of the waste, which led to an increased time to reach the LFL. For example, the time to reach LFL increased from 735 hours to 3,100 hours for the evaporator feed vessels (FEP-VSL-00017A/B) and from 508 hours to 2,070 hours for the waste feed receipt vessels (FRP-VSL-00002A/B/C/D).[1,2] Based on the results of the HGR and calculations of time to reach LFL, the project determined whether safety-class mixing controls are required in PTF process vessels to prevent flammable conditions in the vessel headspace. In accordance with the addendum to the Preliminary Documented Safety Analysis,[3] WTP personnel changed the requirement for nine PTF process vessels (FEP-VSL-00017A/B, FRP-VSL-00002A/B/C/D, PWD-VSL-00033, PWD-VSL-00043, and PWD-VSL-00044) from engineered safety-class mixing controls to a specific administrative control (SAC) that requires operators to restore mixing within the calculated time to reach the LFL.

The heat transfer processes in PTF process vessels are complex and difficult to model; the calculation depends on the thermal properties of the waste, which vary over time, and the complex nature of the heat transfer networks. HGR is highly sensitive to waste temperature. For example, for a vessel with an operating temperature of 120 °F, a temperature decrease of 10 °F results in a decrease in HGR due to thermolysis of 44 percent and a decrease in HGR due to radiolysis of organics of 25 percent. A change in HGR of this magnitude will significantly reduce the time to reach the LFL.

Observations Resulting from the Staff's Review. The Board's staff evaluated BNI's modeling approach, assumptions, and input parameters and assessed the conservatism of the time-dependent waste temperatures for PTF process vessels. The staff also considered whether additional sensitivity studies would be needed to demonstrate conservatism of the analytical results, and to determine whether the assumptions used in these analyses have safety significance and therefore must be incorporated into the Documented Safety Analysis (DSA). The staff's review resulted in the following observations.

Modeling Approach—BNI analysts developed a set of FATE™ heat transfer models to analyze time-dependent waste temperatures in a primary vessel. These models represent process vessels and other black cell components through a number of geometric and mathematical simplifications (i.e., regions, heat sources, heat sinks, and junctions). The primary vessel is modeled as a cylinder composed of layers to represent different regions within the vessel. A secondary vessel is treated as a single heat source with a constant heat load. For black cells with three or more process vessels, FATE™ heat transfer models represent all secondary vessels as a single composite vessel. Conduction, convection, and radiation networks between heat sinks and heat sources allow for the heat transfer processes between different black cell components. A network of flow paths provides a means of representing air flow in and out of a black cell and an air purge of the primary vessel headspace.

[1] Tsang I. and K. Eager, *Calculation of Hydrogen Generation Rates and Times to Lower Flammability Limits for WTP*, Rev. C, Bechtel National, Inc., 24590-WTP-M4C-V11T-00004, May 17, 2006.
[2] Eager, K., *Revised Calculation of Hydrogen Generation Rates and Times to Lower Flammability Limits for WTP*, Rev. C, Bechtel National, Inc., 24590-WTP-M4C-V11T-00011, May 7, 2010.
[3] Hinckley, J., *Preliminary Documented Safety Analysis: Control Strategy Changes for the PT Facility*, Rev. 3, Bechtel National, Inc., 24590-WTP-PSARA-ENS-09-0001, November 19, 2010.

Geometric and mathematical simplifications and boundary conditions adopted in the FATE™ heat transfer models may have affected the time-dependent waste temperature results for PTF process vessels. For example, the FATE™ heat transfer models represent the sludge layer as a stack of up to 20 sub-layers (also referred to as "slabs") and the supernate layer as a single slab. Therefore, the temperature within the entire sludge layer varies axially, but not radially, and the temperature is uniform within the supernate layer. This approximation is valid for a system in which surface convection governs heat transfer processes, which may not be the case for the given thermal properties of the sludge layer.

For example, for a finite cylinder with internal heat generation and cooling by convection and radiation, the change in temperature over time at the center of the cylinder may differ from the change in temperature over time at its boundaries; the center of the cylinder may undergo heating, whereas the cylinder may exhibit cooling at the boundaries. To account for this modeling artifact, BNI analysts imposed a boundary condition that restricted radial heat transfer from the sides of the sludge layer to the process vessel and to the black cell environment (i.e., insulated boundary condition). However, they did not impose the same boundary condition on the supernate layer. Because the insulated boundary condition did not extend beyond the sludge layer, the assumption of constant radial temperature profiles within the sludge was not valid. Also, non-conservative representation of the supernate layer as a single element with constant temperature would allow higher rates of heat transfer from the sludge layer to the black cell environment by means of the supernate layer. Although the supernate layer can be approximated as perfectly mixed, it would have boundary layers at the sludge and headspace interfaces. Formation of these boundary layers would lead to a lower rate of heat transfer from the sludge to the supernate and from the supernate to the headspace due to lower temperature differences at the interfaces. This in turn would lead to higher temperatures and higher HGRs in the middle of the sludge layer. Thus, the staff believes the representation of the temperature within the sludge slabs and supernate as uniform may not be conservative, while the conservatism of the boundary conditions imposed on the sludge and supernate layers is not evident.

Further, the method used for the FATE™ models' discretization of the sludge layer and imposed boundary conditions may have affected the calculations of time to reach LFL for PTF process vessels. BNI analysts calculated the total hydrogen generation within the entire sludge layer as a sum of the hydrogen generation in each slab. Because the FATE™ model's discretization does not allow for axial and radial temperature variations within a slab, this calculation was based on a single temperature for each slab. The Board's staff determined that, given the nonlinear nature of the HGR as a function of temperature, estimating the total hydrogen generation in a sludge layer based on an average temperature can lead to a non-conservative result. Hydrogen generation calculations based on a discretized sludge layer and temperature distributions that vary spatially within the sludge layer could produce acceptable results with negligible error if the sludge layer were discretized into a sufficiently large population of control volumes. Alternatively, hydrogen generation calculations based on a single temperature value could produce conservative results if this temperature value were selected to capture the nonlinear nature of the HGR function and, in general, were higher than the average temperature of the sludge layer.

Based on the documentation supplied by Fauske & Associates, LLC, the FATE™ software has undergone a verification and validation process. The vendor performed verification and validation by executing, in general, one simplified test case for each software module and comparing FATE™ results with either experimental data published in the open literature or a closed-form solution. However, in discussions with the Board's staff, BNI analysts have not been able to demonstrate that this verification and validation process meets the requirements of the methodology outlined in American Society of Mechanical Engineers (ASME) V&V 20[4] or that the FATE™ software was verified to be suitable for modeling heat transfer processes in PTF process vessels.

The Board's staff believes it is necessary to determine the effect of each geometric and mathematical simplification and imposed boundary condition on the time-dependent temperature, HGR, and time to reach LFL for each PTF process vessel to ensure that safety-class mixing controls are conservatively identified. Further, it would be advisable to evaluate the suitability of the FATE™ software for modeling heat transfer processes in PTF process vessels by performing software verification and validation consistent with ASME V&V 20.

Assumptions and Input Parameters—In calculating time-dependent vessel temperatures and HGRs, BNI analysts used a number of design input parameters and assumptions, such as vessel maximum operating temperatures; heat generation rates; maximum normal operating temperatures for confinement heating, ventilation, and air conditioning (HVAC) systems; and thermal properties of the waste. While some of these assumptions have adequate technical justification, others require additional justification to be technically acceptable. Moreover, several of the assumptions that require additional justification can have a considerable impact on the time-dependent temperature results leading to reduced time to LFL.

For example, BNI's calculations show that for some process vessels evaporative cooling in the vessel headspace accounts for about 20 percent of the total heat removal. To derive this result, BNI analysts assumed that purge air enters the vessel headspace at low humidity and exits the vessel fully saturated. BNI analysts also assumed that the waste has the same material properties as water; for example, they assumed that the vapor pressure of liquid high-level waste is the same as that of water. However, the presence of sodium and other dissolved solids in Hanford's liquid tank waste reduces the waste's vapor pressure relative to that of water, and a reduction in the liquid vapor pressure directly translates into a reduction in the evaporation rate. Further, the presence of fine particles resting on the liquid's surface (surface scum) or foaming of the waste could reduce the wetted contact area and diminish mass transfer rates. These two conditions could contribute to incomplete headspace saturation—that is, less evaporation and evaporative cooling than is assumed in the FATE™ heat transfer models. Therefore, the conservatism of BNI analysts' assumption that air leaving the vessel headspace is fully saturated is not evident.

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[4] ASME V&V 20, *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer*, American Society of Mechanical Engineers, 2009.

Another assumption made by BNI analysts in the FATE™ heat transfer models is immediate waste settling after loss of mixing—that is, solids immediately settle into a sludge layer at the bottom of the vessel with a 76 percent volume fraction of liquid. This assumption does not account for the waste having a finite settling time (i.e., gradual change in the volume fraction of liquid in the sludge layer) or for the potential for hydrogen to begin accumulating in the slurry layer before the waste is fully settled. For example, in response to inquiries by Board's staff, BNI analysts demonstrated that for waste with a 120-hour settling time and 100 percent gas retention in the sludge layer during settling, the time to reach LFL would decrease on the order of 10 percent[5] relative to a case with immediate waste settling. Also, the rate of waste settling will vary depending on the physiochemical properties of the waste, the concentration of solids, and the vessel geometry (i.e., height, diameter, and configuration of vessel internals). Compressive settling would lead to transient concentrations of solids and the retention of gas bubbles. This would alter the heat capacity and thermal conductivity of the sludge. Therefore, the Board's staff expects that the heat capacity and thermal conductivity of the sludge will vary with time and position in the vessel; neither of these factors is reflected in the FATE™ models used by BNI analysts. The Board's staff believes that BNI analysts' assumption of immediate waste settling with instantaneous change in the liquid volume fraction and constant thermal properties is not always conservative.

BNI analysts' selection of assumptions and input parameters directly impacts the results of the FATE™ heat transfer models for PTF process vessels. The Board's staff therefore believes BNI analysts should determine (e.g., through sensitivity analyses) whether each assumption and input parameter is conservative and to what extent it will impact vessel temperatures, HGRs, and times to reach LFL. Additionally, because the project uses these calculations to determine whether safety-class mixing controls are required, it is appropriate to determine which assumptions and input parameters must be monitored during operations and whether they warrant control in the safety basis. For example, if the assumptions regarding evaporative cooling (i.e., supernate vapor pressure) impact the final determination of controls, a safety basis control on supernate vapor pressure may be required (e.g., a maximum limit on sodium concentration). BNI analysts have not performed sufficient sensitivity analyses to make it clear to the Board's staff which, if any, assumptions and input parameters require protection.

Sensitivity Studies—BNI analysts performed limited sensitivity studies to investigate the effects of variations in thermal conductivity, the specific heat capacity of sludge, and the depth of the slurry layer. BNI analysts determined that lower values for thermal conductivity and the specific heat capacity of sludge would result in higher sludge temperatures and reduced time to LFL. BNI analysts also established that a more compact slurry layer (i.e., a slurry layer with smaller liquid volume fraction) would result in a longer time to reach LFL. These conclusions confirm the Board's staff concerns on the significance of the selection of proper thermal properties.

In response to inquiries by Board's staff during its on-site review, BNI analysts performed additional informal sensitivity studies. One such study used a lower value of thermal

[5] Meehan J.L., *Response to Defense Nuclear Facilities Safety Board Request to Provide Basis for Concluding that Gas is Released from the Waste while Solids are Settling*, RPP-WTP, CCN 234709, May 18, 2011.

conductivity, while another used a lower value of heat capacity for the sludge layer than had previously been used in the FATE™ heat transfer models. Both studies yielded higher post-accident temperature profiles for PTF process vessels and reduced the time to LFL on the order of 10 percent, which would not require the addition of safety-class mixing controls. However, BNI analysts have not yet determined the sensitivity of the results to other assumptions and input parameters, such as the emissivity of the stainless steel vessels, the air temperature of the vessel headspace purge, the temperature distribution of the sludge and supernate layers, and the settling rate of solids.

The Board's staff believes these limited studies did not demonstrate that BNI analysts have conservatively modeled post-accident waste temperatures in the PTF process vessels over time. The staff believes a comprehensive sensitivity study to determine the effects of modeling simplifications, assumptions, and input parameters on the results derived for time-dependent temperatures, HGRs, and times to reach LFL for PTF process vessels is warranted.

Conclusions. BNI analysts have not demonstrated that the accuracy of the FATE™ heat transfer analyses and the conservatism of their modeling approach, assumptions, and input parameters are sufficient to provide a robust basis for downgrading the safety classification of mixing controls for WTP process vessels. BNI analysts also have not evaluated whether safety-related controls are necessary to ensure that critical assumptions and/or input parameters are maintained during plant operations so that actual waste temperatures and consequently HGRs will not exceed calculated estimates. The Board's staff believes it would be advisable for the Department of Energy to ensure that BNI analysts (1) establish the suitability of the FATE™ software for modeling heat transfer processes in PTF process vessels by performing software verification and validation consistent with ASME V&V 20 or, alternatively, reevaluating heat transfer processes in PTF process vessels using suitable engineering methods; (2) perform a comprehensive sensitivity study to determine the cumulative effect of the modeling approach, assumptions, and input parameters on the conservatism in the time-dependent temperature results, HGRs, and times to reach LFL for PTF process vessels; and (3) determine which assumptions and input parameters have an important impact on the results of heat transfer calculations, and evaluate the need and ability to control these assumptions and input parameters during plant operations.