Department of Energy

Washington, DC 20585

November 16, 2011

The Honorable Peter S. Winokur
Chairman
Defense Nuclear Facilities Safety Board
625 Indiana Avenue, NW, Suite 700
Washington, DC 20004

Dear Mr. Chairman:

On August 3, 2011, you transmitted a letter regarding the Defense Nuclear Facilities
Safety Board's (Board) concern related to *"downgraded safety-class mixing controls"* for
nine Pretreatment Facility (PTF) process vessels at the Hanford Tank Waste Treatment
and Immobilization Plant (WTP). Your letter detailed three specific areas where the
Board had concerns with the modeling of heat transfer from the vessels in question, as it
relates to the Hydrogen Generation Rate and the time it takes to approach the Lower
Flammability Limit after a Design Basis Event (DBE).

The WTP Project has reviewed the Board's concerns and concluded the following:

> For all the vessels of interest[1] the classification of the mixing, purge, and vent
> function remained safety class, per the Department of Energy (DOE) approved
> Preliminary Documented Safety Analysis (PDSA) Addendum, section 2.4.1. The
> change to credit a Specific Administrative Control (SAC), rather than an active
> engineered control to accomplish the mixing function post DBE, was made in
> revision 0 of the PTF PDSA Addendum. This change was approved by DOE in
> November 2009, before the Flow, Aerosol, Thermal, and Explosion Model
> (FATE™) model was used. Subsequently, FATE™ was used to more accurately
> estimate hydrogen generation rates for all nine of the vessels.

> The FATE™ model results were used as a basis to change the post DBE safety-
> class mixing controls for only two of the nine vessels from active engineered
> controls to SACs. This is consistent with the Safety Requirements Document
> relating to SACs being acceptable for mitigation of DBE recovery periods greater
> than 1,000 hours.

> In the original PTF PDSA Addendum, the two Feed Evaporation Process vessels
> were shown to be slightly above the 1,000 hour threshold for hydrogen

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[1] (FEP-VSL-00017A/B, FRP-VSL-00002A/B/C/D, PWD-VSL-00033, PWD-VSL-00043, and
PWD-VSL-00044)

buildup, allowing a SAC to be credited. However, because of proximity to the threshold, project engineering judgment determined, and DOE agreed in its Safety Evaluation Report, to credit-active engineering controls. Application of the FATE^{TM} model demonstrated that, for those two vessels, the original estimate was conservative. DOE subsequently approved revision 3 of the PTF PDSA Addendum, in which SACs are credited for these two vessels, vice engineering controls.

The engineered systems that provide mitigation for hydrogen buildup within the vessels have not been removed and the physical design for these vessels is unchanged.
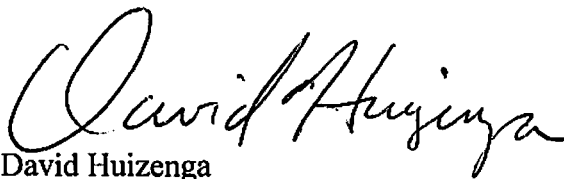
WTP believes conservative assumptions and bounding sensitivity analyses have been utilized in the analysis of heat transfer in application of the FATE^{TM} model for the subject vessels. In determining the inputs to be used in the analysis, conservative values were chosen for the relevant parameters. Where documentation of the justification for maximum values exist, those values were used. Simplifying assumptions were provided, with justification, as to why they are either conservative or have negligible impact on the final temperatures. There are specific assumptions that the Board's staff felt needed more justification, such as saturated conditions in the vessel headspace. Bechtel National Inc., (BNI) has committed to justifying these assumptions, either through technical analysis or sensitivity runs, in the planned revision to the thermal analysis over the next 6 months. The final, confirmed, calculation will be based on verification of these assumptions.

WTP agrees that the description of the model should contain a clearer and more detailed description of conservatisms used. This includes use of additional sensitivity evaluations to clarify the conservatisms used in application of the FATE model. These analyses are planned as part of the update to the FATE model calculation to be completed by BNI by May 31, 2012.

Additional details are provided in the enclosure. WTP believes that based on the results of the FATE model and safety analysis development that redundant, safety class sparging air supply to the two vessels in question (FEP-VSL-00017A and B), is not required. Emergency response procedures, which will be developed to address the SAC in the documented safety analysis, will provide the necessary controls for the post-seismic event hydrogen hazards.

If you have any further questions, please contact me or Mr. Matthew Moury, Deputy Assistant Secretary for Safety and Security, at (202) 586-5151.

Sincerely,

David Huizenga
Acting Assistant Secretary for
  Environmental Management

Enclosure

cc: R. Lagdon, S-5
    M. Campagnone, HS-1.1
    T. Mustin, EM-2
    M. Moury, EM-20
    J. Hutton, EM-20
    K. Picha, EM-21 (Acting)

Additional Detail on the Facility Flow, Aerosol, Thermal, and Explosion (FATE™) Model and Response to Specific Concerns Raised by the Defense Nuclear Facilities Safety Board

Software Description

Because several of the concerns raised in the Defense Nuclear Facilities Safety Board (Board) staff's report are based on the model configuration, a more detailed description of the FATE™ software is warranted. The FATE™ software has been designed for use in modeling operational and accident phenomena in underground storage tanks, nuclear fuel cycle facilities, and chemical processing plants. The original focus of this model application was evaluation of Hanford underground storage tanks. Heat transfer and evaporation/condensation of gases on structures is represented by standard industry correlations for heat transfer. Using an implicit finite-difference formulation, the model estimates heat transfer via conduction, convection, and radiation, subject to the boundary conditions specified for each heat sink surface. For boundary nodes, a heat transfer path is replaced by an appropriate boundary condition (e.g., natural convection).

This application of the model for the Waste Treatment and Immobilization Plant (WTP) was to estimate the temperature profile of the fluid in the black-cell process vessels following a design basis event. The model chosen for this application was taken directly from FATE™ Verification and Validation (V&V) case "tkincell" and only minor modifications were needed for this application. The vessel is modeled as a right-circular cylinder with a sludge layer, liquid layer, and vapor headspace.

The sludge layer in the vessel is modeled as a solid at the bottom of the vessel that is insulated on the sides, but allowed to convect heat to the supernatant layer above it, and to convect and radiate heat to the air in the area below the vessel (skirt and support ring). The sludge layer is modeled as 20 equal sections across the vessel (i.e., flat disks the diameter of the vessel). The temperature is evaluated at each sludge section. Heat can be transferred from the sludge only by conduction to an adjacent sludge section, by radiation and convection from the bottom of the vessel to the black cell, or by convection from the sludge to the liquid above the sludge.

The liquid layer is modeled as a single volume. Evaluation of the heat transfer in this layer concluded that sufficient natural convection exists to effectively mix this region (Reference 2); therefore, the liquid layer is modeled as well mixed with a uniform temperature. Heat is transferred from the liquid layer to the vessel walls by natural convection; through the vessel wall by conduction; and to the black cell by natural convection and radiation. Heat is also transferred from the liquid via evaporation of liquid to the vapor head space.

The vapor head space is modeled as a single volume. Heat is transferred by natural convection from the liquid to the vapor, by natural convection from the vapor to the vessel walls and head, and by radiation from the liquid to the vessel head. The vapor is assumed to enter the vessel at 30 percent relative humidity (RH) at 95° F. With residence times for the purge air between 300 and 600 hours for the 9 vessels of interest, the air leaving the vessel is assumed to be completely saturated.

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The vessel shell (walls, and top and bottom head) is also modeled using an axial conduction network to account for heat transfer from the waste to the submerged wall (by convection), and up and down the vessel shell (by conduction). The non-insulated portions of the vessel wall radiates to the walls of the room and adjacent vessel(s) through a radiation network. Radiation from the top of the vessel is represented by another radiation network to the room ceiling and room walls.

There are two heat sinks to model the room wall, one adjacent to the vessel and a second heat sink for the remaining wall volume. Downward heat transfer from the bottom of vessel is represented by a radiation network to the room floor and convection to the skirt-enclosed volume beneath the vessel. The room walls, ceiling, and floor, face the ambient C5 environment and are cooled by natural convection.

An exhaust fan provides the driving mechanism for the C5 HVAC air flow out of the cell. The active purge forces air into the headspace of the vessel. The vessel headspace vents into the cell. The vessel overflow line is not modeled in these calculations.

FATE™ Software Verification and Validation

WTP procedure *Acquisition and Management of Levels A, B, C, and D Software for EPCC* (Reference 3) implements DOE-O-414.1C for safety software. The WTP designates FATE as Level A Safety Software and follows all requirements prescribed by Reference 4. FATE is supplied by Fauske and Associates, Inc. (FAI), which is a WTP-approved safety software supplier. Therefore, WTP has audited FAI and verified their Quality Assurance A process to perform V&V of the FATE software (Reference 4). The FAI V&V is documented in the FATE/HADCRT manuals. WTP fulfills V&V requirements by running the same test cases as supplied by Fauske and comparing the results. In this case WTP ran 37 cases using 10 modules and verified the results were identical to FAI results. In effect, this validates that the software operates correctly in the WTP computer environment.

FATE is designed as modular software. Test cases are used to test each of the independent modules. Integrated tests are used that test several modules at the same time. One of the integrated tests, "tkincell," was used as the base model for the current vessel temperature model. This test case is nearly identical to the final vessel temperature model, and simultaneously tests all the modules of importance to the vessel temperature model.

The V&V of FATE is covered by the WTP life cycle documentation:
- *Software Life Cycle Documentation for FATE, Volume 1* (Reference 5)
- *Software Life Cycle Documentation for FATE, Volume 2* (Reference 6)
- *Software Life Cycle Documentation for FATE, Volume 3* (Reference 7)

These are supported by the vendor V&V documentation:

Additional Detail on the Facility Flow, Aerosol, Thermal, and Explosion (FATE™) Model and Response to Specific Concerns Raised by the Defense Nuclear Facilities Safety Board

- *Fuel Cycle Facility Source Term Model HADCRT 1.4: Users Manual FAI/02-50* (Reference 8)
- *HADCRT 1.4C: Updates to HADCRT, HANSF MCO, and HANSF SLUDGE Computer Codes* (Reference 9)
- *Specification - HADCRT 1.4 CX Software Change Specification and Validation* (Reference 10)
- *Information - FATE 2.0: Facility Flow, Aerosol, Thermal, and Explosion Model (Improved and Combined HANSF and HADCRT Models)* (Reference 11)
- *Information - FATE 2.058 Software Change Specification and Testing – Generic Models* (Reference 12)

Discussion of Concerns

The Board's staff identified three areas of concern as documented in the Staff Issue Report attached to the Board letter (Reference 1). Specifically, the conclusions were:

A. **Suitability of FATE™** – 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;

B. **Sensitivity Evaluation** – 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 Lower Flammability Limit (LFL) for PTF process vessels; and

C. **Assumptions and Input Parameters** – 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.

The Staff Issue Report contains several specific concerns that are related to each of these three conclusions. The following is a response to each of these concerns.

Additional Detail on the Facility Flow, Aerosol, Thermal, and Explosion (FATE™) Model and Response to Specific Concerns Raised by the Defense Nuclear Facilities Safety Board

A. Suitability of FATE™

Concern A1: 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.

> **Response**: WTP agrees that conservative finite element calculations can be performed for this system; however, the FATE™ software has been determined to be appropriate based on the verification, validation, history of use, software capabilities (e.g., heat transfer), and vendor qualification (see response to Concern A2). Therefore, an additional calculation using finite element analyses such as suggested, is not necessary for the WTP design.

Concern A2: Based on the documentation supplied by FAI 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, Bechtel National Inc., (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[1] or that the FATE™ software was verified to be suitable for modeling heat transfer processes in PTF process vessels.

> **Response**: FATE™ was V&V'd in accordance with the WTP procedure *Acquisition and Management of Levels A, B, C, and D Software for EPCC* (Reference 3), which implements DOE-O-414.1C for safety software.
>
> The project has not evaluated the differences between V&V in accordance with the WTP procedure and ASME V&V20. However, for the reasons noted below, DOE does not believe this is necessary.
>
> The WTP designates FATE™ as Level A Safety Software and follows all requirements prescribed by Reference 4. FATE™ is supplied by FAI, which is a WTP-approved safety software supplier. Therefore, WTP has audited FAI and verified their QA process to perform V&V of the FATE™ software (Reference 4). The FAI V&V is documented in the FATE™/HADCRT manuals. WTP fulfills V&V requirements by running the same test cases as supplied by FAI and comparing the results. WTP ran 37 test cases using 10 modules and compared the results to the FAI work verifying that the same result was obtained. In effect, this validates the software operates correctly in the WTP computer environment. Therefore, the project considers the FATE™ software acceptable for modeling

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

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heat transfer processes in Pretreatment (PTF) process vessels. Additional V&V using ASME V&V20 is not required.

FATE™ is designed as modular software. Test cases are used to test each of the independent modules. Integrated tests are used that test several modules at the same time. One of the integrated tests, "tkincell," was used as the base model for the current vessel temperature model. This test case is nearly identical to the final vessel temperature model, and simultaneously tests all the modules of importance to the vessel temperature model.

The V&V of FATE™ is covered by the WTP life cycle documentation:
- *Software Life Cycle Documentation for FATE, Volume 1* (Reference 5)
- *Software Life Cycle Documentation for FATE, Volume 2* (Reference 6)
- *Software Life Cycle Documentation for FATE, Volume 3* (Reference 7)

These are supported by the vendor V&V documentation:
- *Fuel Cycle Facility Source Term Model HADCRT 1.4: Users Manual FAI/02-50* (Reference 8)
- *HADCRT 1.4C: Updates to HADCRT, HANSF MCO, and HANSF SLUDGE Computer Codes* (Reference 9)
- *Specification - HADCRT 1.4 CX Software Change Specification and Validation* (Reference 10)
- *Information - FATE 2.0: Facility Flow, Aerosol, Thermal, and Explosion Model (Improved and Combined HANSF and HADCRT Models)* (Reference 11)
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B. Sensitivity Evaluation

Concern B1: 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.

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.

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Response: The assumptions used in FATE^{TM} were developed to provide model outputs (e.g., temperatures) that would result in upper bounds for HGRs and times to LFL. When determining the inputs to be used in the analysis, values were chosen that would provide high temperatures while still representing the physical problem being solved. When a credible maximum value existed, those were used.

For example, the vessel initial conditions are the maximum vessel temperature and maximum vessel volume. Simplifying assumptions were provided with justification why they are either conservative or have negligible impact on the final temperatures. As examples: 1) it is conservative to insulate the sides of the sludge layer; and 2) the liquid layer can be modeled as a uniform temperature because heat generating liquids above a hotter surface will have significant internal convection currents. When it was not clear what affect an input or assumption had on the final liquid or sludge temperature, sensitivity cases were performed. For example, sensitivity cases were modeled in FATE^{TM} when it was not clear what would lead to high sludge layer temperatures; a sludge layer with 55% liquid by volume, or a sludge layer with 76 percent liquid by volume. Additional discussion is provided in response to Concern C1 below.

Concern B2: In response to inquiries by the Board's staff during its on-site review, BNI analysts performed additional informal sensitivity studies. One such study used a lower value of thermal conductivity, while another used a lower value of heat capacity for the sludge layer than had previously been used in the FATE^{TM} 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 supernatant layers, and the settling rate of solids.

Response: The values for heat capacity and thermal conductivity currently used in the heat transfer analysis are based on values that result in higher sludge temperatures than those anticipated and in higher hydrogen generation rates. Sludge and material properties are provided in 24590-WTP-M4C-V11T-00011, Rev C, Assumption 6.2.2. The Board staff asked for "what if" runs to be performed for vessels FEP-00017A/B; one run where the heat capacity of the sludge was reduced from 0.6 W/m-K to 0.5 W/m-K (about 20 percent reduction in conductivity), and one run where the heat capacity was reduced from 2.4 kJ/kg-K to 1.8 kJ/kg-K (50 percent reduction in heat capacity). As expected, reducing these values increased the calculated temperature. In addition, the stainless steel emmisivity was chosen to be 0.81, which is representative of oxidized steel, rather

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than a value of 0.2, which is typical for cleaned or polished steel. A higher stainless steel emmisivity used on the vessel shell means that the vessel will absorb more radiant heat transferred from the room, and reflect very little, leading to higher liquid and sludge temperatures in the vessel. Similarly, the air temperature of the vessel headspace purge was conservatively chosen as 95° F, which is over 10° F higher than the highest monthly average ambient temperature at the Hanford site from the last approximately 50 years (24590-WTP-U0C-50-00002, Rev D, Assumption 1). This maximum average air temperature is appropriately bounding given the fact that the vessel temperatures are calculated over 1000 hours (about 42 days) and this is a post-DBE loss of power scenario. Similarly, the sludge layer has conservatively been given an insulated boundary condition on the sides of the sludge. Heat transfer within the sludge layer is governed by the conservative low thermal conductivity, high density, low heat capacity, and high heat generation rate. The temperature of the supernatant layer is treated as uniform, based on the internal buoyancy and density driven natural convection currents within the waste (24590-WTP-U0C-50-00002, Rev D, Assumption 9). The settling rate of solids is assumed to be instantaneous for the thermal analysis. Instantaneous settling concentrates the heat emitting isotopes in the sludge layer, which increases the sludge temperature compared to a slower (finite) settling rate. This result decreases the time to LFL.

Concern B3: 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.

> **Response:** The concerns raised by the Board's staff all relate to potential non-conservatisms in transient conditions. The WTP project believes that the selected inputs used in the analysis are conservative values for the parameters for the physical problem being solved. When a credible maximum value existed, those were used. For example, the vessels are initialized at the maximum vessel temperature and maximum vessel volume; however, simplifying assumptions are made with justification why they are either conservative or have negligible impact on the final temperatures. As an example, it is conservative to insulate the sides of the sludge layer, while the liquid layer can be modeled as a uniform temperature because heat generating liquids above a hotter surface will have significant internal convection currents (24590-WTP-U0C-50-00002, Rev D, Assumption 9). When it was not clear what affect an input or assumption has on the final liquid or sludge temperature, sensitivity cases were performed. For example, sensitivity cases were modeled in FATE^{TM} when it was not clear what would lead to higher sludge layer temperatures; a sludge layer with 55 percent

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liquid by volume, or a sludge layer with 76 percent liquid by volume. This sensitivity case determined that the deepest credible settle layer (76 percent liquid by volume) will lead to higher sludge layer temperatures.

C. Assumptions and Input Parameters

Concern C1: 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., supernatant vapor pressure) impact the final determination of controls, a safety basis control on supernatant 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.

> **Response**: WTP agrees that the description of the model should contain a clearer and more detailed description of conservatisms used. This includes use of additional sensitivity evaluations to clarify the conservatism used in the FATE model, which have already been planned based on the Board staff's reviews in December 2010 and April 2011. Evaluation of design assumptions to determine which are required to be protected to maintain the safety barriers at the WTP is an ongoing activity performed as part of the safety analysis process, which will identify those assumptions that need to be protected in the further development of the Documented Safety Analysis per the project baseline schedule.
>
> The requirements for documenting and tracking assumptions requiring verification are provided in WTP Procedure, 24590-WTP-3DP-G04B-00037, *Engineering Calculations*.

Concern C2: 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 supernatant 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 supernatant 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.

> **Response**: Modeling simplifications were made to ensure conservative (higher) sludge temperature. The sludge layer is modeled as insulated on the sides, such that the sludge can only transfer heat through convection to the liquid above, or through convection and radiation off the bottom surface of the vessel. Assuming

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> heat losses from the sides of the sludge layer would lead to lower sludge temperatures in all cases.

Concern C3: 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 supernatant 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 supernatant 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 supernatant layer. Although the supernatant 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 supernatant and from the supernatant to the headspace due to lower temperature differences at the interfaces. This in turn would lead to higher temperatures and higher Hydrogen Generation Rate in the middle of the sludge layer. Thus, the staff believes the representation of the temperature within the sludge slabs and supernatant as uniform may not be conservative, while the conservatism of the boundary conditions imposed on the sludge and supernatant layers is not evident.

> **Response:** Ignoring heat losses from the sides of the sludge (i.e., insulated) will result in higher sludge temperatures in all cases because heat is only lost by convection to the liquid above, or by conduction through the bottom of the vessel. While this does not accurately reflect the vessel design performance, it yields conservatively higher sludge temperatures and correspondingly higher hydrogen generation rates. The liquid layer is assumed to have a uniform temperature because heat generating liquids above a hotter surface will have significant internal convection currents (24590-WTP-U0C-50-00002, Rev D, Assumption 9). Heat transfer between the supernatant layer and the sludge is calculated using standard convective heat transfer correlations, which are adjusted for the fluid properties in the vessel. Using an implicit finite-difference formulation, the model estimates heat transfer via conduction, convection, and radiation from the liquid layer subject to the boundary conditions specified. For boundary nodes, a heat transfer path is replaced by an appropriate boundary condition (e.g., natural convection).

Concern C4: Further, the method used for the FATE™ models' discretization of the sludge layer and imposed boundary conditions may have affected the calculations of time

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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.

> **Response:** The sludge layer is modeled as 20 discrete slabs and sludge has 20
> axial data points. The temperature does not vary radially because of the insulated
> boundary condition on the sides of the sludge slab. In the 9 vessels of concern,
> the individual slab thickness is relatively thin, between 0.75 inches (PWD-VSL-
> 00033) and 3.5 inches (FRP-VSL-00002A) and the vessel diameters are large,
> between 22 feet and 47 feet respectively. Because of the relatively small
> sediment depths the sludge layer slab is a thin disk of material. The number of
> slabs can be increased to increase the resolution of the temperature profile.
> However, the resulting HGR time to LFL calculation will not be significantly
> refined by increasing the resolution of the temperature profile.

Concern C5: 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.

> **Response:** When determining the inputs to be used in the analysis, conservative
> values were chosen for the relevant parameters. Where credible maximum values
> exists, those were used. Simplifying assumptions were provided with justification
> why they are either conservative or have negligible impact on the final
> temperatures. There are specific assumptions that the Board's staff felt need more
> justification, such as saturated conditions in the vessel headspace. BNI has
> committed to justifying these assumptions, either through technical justification or
> sensitivity runs, in the planned revision to the thermal analysis over the next six
> months. The final, confirmed, calculation will be based on verified assumptions.

Concern C6: 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

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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.

> **Response:** The thermal analysis assumes that the air purge enters the headspace at the *maximum* credible post-compressor humidity and maximum credible long-term average post-DBE temperature. As a modeling simplification, the supernatant was treated as water for the purposes of evaporation. As indicated in the discussion above the actual waste will have a lower vapor pressure when compared to water because of the presence of dissolved salts. In addition, the residence time of the purge air in the vessel headspace is between 300 and 600 hours for the nine vessels of concern. This condition will allow the water vapor in the head space to reach equilibrium.
>
> The planned revision of the thermal analysis will be documented in a formal engineering calculation. The assumption for headspace air saturation will be evaluated at that time, considering actual vapor pressure and the purge residence time. The 9 vessels of concern are not mixed for the duration of the scenario, and each vessel is treated with anti-foam.

Concern C7: 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 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

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sludge will vary with time and position in the vessel; neither of these factors is reflected in the FATE^{TM} 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.

Response: The choice of immediate settling of the waste was made because it is a conservative assumption for thermal analysis of the vessels as follows:

1. The settling rate of solids is assumed to be instantaneous for the thermal analysis. Instantaneous settling concentrates the heat emitting isotopes in the sludge layer, which increases the sludge temperature compared to a slower (finite) settling rate. This result decreases the time to LFL.
2. Immediate settling starts the scenario for post-DBE events with a sludge layer at the maximum temperature (the vessels of concern cool over time) rather than allowing the solids to cool while settling.
3. As shown in CCN 234709, the temperature of the vessel is not strongly dependent on gas retention.
4. It is agreed that the thermal conductivity and heat capacity of the waste will vary as the solids settle. However, the settled solids condition, which is assumed in the FATE model, will result in higher hydrogen generation rates for the vessel compared to well mixed or partially mixed solids and liquids.

References

1) Letter from Peter S. Winokur, Ph.D., Board Chairman to David Huizenga, U.S, Department of Energy, August 3rd, 2011.
2) Memorandum CCN 119059, Turbulent Mixing Due to Natural Convection in Newtonian Vessels with Low Solids, Roger Lanning to Andy Larson, April 18, 2005.
3) 24590-WTP-GPP-SQP-100 ACQUISITION and MANAGEMENT of LEVELS A, B, C and D SOFTWARE for EPCC
4) 24590-WTP-AR-QA-10-014, Supplier Audit Report - Fauske and Associates, LLC - Burr Ridge, Illinois
5) 24590-WTP-AR-QA-10-014, Supplier Audit Report - Fauske and Associates, LLC - Burr Ridge, Illinois
6) 24590-WTP-SWLCD-ENS-09-0001-01, Rev 1, Software Life Cycle Documentation for FATE, Volume 1
7) 24590-WTP-SWLCD-ENS-09-0001-02, Rev 2, Software Life Cycle Documentation for FATE, Volume 2
8) 24590-WTP-SWLCD-ENS-09-0001-03, Rev 1, Software Life Cycle Documentation for FATE, Volume 3
9) 24590-SC-HXYG-0055-02-02, Fuel Cycle Facility Source Term Model HADCRT 1.4: Users Manual FAI/02-50

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10) 24590-SC-HXYG-0055-03-05, HADCRT 1.4C: Updates to HADCRT, HANSF MCO, and HANSF SLUDGE Computer Codes

11) 24590-SC-HXYG-0055-05-00001, Specification - HADCRT 1.4 CX Software Change Specification and Validation

12) 24590-SC-HXYG-0055-06-00001, Rev A, Information - FATE 2.0: Facility Flow, Aerosol, Thermal, and Explosion Model (Improved and Combined HANSF and HADCRT Models)

13) 24590-SC-HXYG-0055-06-00002, Rev A, Information - FATE 2.058 Software Change Specification and Testing – Generic Models