DEFENSE NUCLEAR FACILITIES SAFETY BOARD

Washington, DC 20004-2901

April 3, 2012

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

Dear Mr. Huizenga:

On December 17, 2010, the Board issued Recommendation 2010-2, *Pulse Jet Mixing at the Waste Treatment and Immobilization Plant* [WTP]. The Recommendation states: "Any use of computer simulations must be technically defensible, and the limits of each computational fluid dynamics simulation need to be well understood to prevent potential safety issues from arising during operations." Additionally, Recommendation 2010-2 included a sub-recommendation; "Complete verification and validation of any computational models used by the WTP project team (e.g., Low Order Accumulation Model and FLUENT) based on the results from the large-scale testing." Based on its review of the verification and validation (V&V) plan and associated data gap analysis, the Board is concerned that the project's FLUENT model will not be validated over the complete range of WTP mixing conditions.

The FLUENT model is to be used to confirm that the performance of the WTP mixing systems will meet design requirements. The Board's review of the V&V activities for WTP revealed several deficiencies. For example, the data gap analysis neglected physical parameters that may be necessary to accurately model full-scale mixing behavior in the WTP. As a result, data collected during planned small-scale mixing tests may be insufficient to validate the model adequately. This and other issues are documented in more detail in the enclosed report.

Therefore pursuant to 42 U.S.C. § 2286b(d), the Board requests a report and a briefing within 45 days of receipt of this letter identifying the approach to be used to resolve the issues described in the enclosed report so the FLUENT model will be appropriately validated prior to use for mixing system design confirmation.

Sincerely,

Peter S. Winokur, Ph.D.
Chairman

Enclosure

c: Mr. Dale E. Knutson
Mr. Scott Samuelson
Mrs. Mari-Jo Campagnone

DEFENSE NUCLEAR FACILITIES SAFETY BOARD

Staff Issue Report

February 27, 2011

MEMORANDUM FOR:	T. J. Dwyer, Technical Director
COPIES:	Board Members
FROM:	P. Meyer, A. Poloski
SUBJECT:	Basis for Selection of Validation Data Set, FLUENT Model, Waste Treatment and Immobilization Plant

Background. This report documents issues identified by the staff of the Defense Nuclear Facilities Safety Board (Board) related to verification and validation (V&V) activities for the FLUENT computational fluid dynamics (CFD) model for the Waste Treatment and Immobilization Plant (WTP). The FLUENT model is to be used to confirm that the performance of the plant mixing systems utilizing pulse jet mixers (PJMs) meet design requirements. The WTP V&V plan uses American Society of Mechanical Engineers (ASME) Standard ASME V&V 20-2009, *Standard for Verification and Validation on Computational Fluid Dynamics and Heat Transfer*, which provides a methodology for assessing the accuracy of a given computational simulation.

On December 17, 2010, the Board issued Recommendation 2010-2, *Pulse Jet Mixing at the Waste Treatment and Immobilization Plant*. As part of the continuing review in support of this Recommendation, the Board's staff reviewed the WTP V&V plan and associated gap analysis for experimental data. The purpose of the gap analysis was to identify any additional mixing tests required to complete validation of the FLUENT model. This report focuses on the technical basis used for determining requirements for validation test data.

WTP Project Team's Approach for Determining the Sufficiency of Validation Test Data. The WTP V&V plan specifies test variables that will be used for the validation process. The plan also presents a technical basis for determining the range of experimental conditions (validation points). This basis involves a dimensional analysis of the WTP mixing systems. The resulting set of dimensionless parameters provides the basis for defining the suite of tests required for validation. The dimensional analysis in the V&V plan identifies three dominant parameters important to mixing. The data gap analysis presents a different analysis based on the governing equations in FLUENT, with five dimensionless parameters being identified as important. The recommendation resulting from the data gap analysis is that new mixing tests should be conducted in an 8 ft vessel to obtain data that span the plant-scale parameter ranges, completing a set of experimental data adequate for V&V.

Observations. Based on this review, the Board's staff identified the following issues related to the technical basis for selection of the validation data set.

Consideration of Vessel Length Scales—The dimensionless parameters derived in the V&V plan and the data gap analysis do not incorporate characteristic vessel length scales, such as vessel diameter and fill level. The length scales incorporated in the analysis are limited to the jet nozzle diameter and characteristic particle size. While the choice of dimensionless parameters is not unique, inclusion of the vessel length scales in the analysis results in two additional independent dimensionless parameters. The staff is concerned that by neglecting large vessel scales, the resulting set of dimensionless parameters may not appropriately describe coupling between large-scale and localized mixing phenomena. For example, the transport of solids in large circulatory flow patterns may be coupled to the clearing of solids off the bottom of the vessel during PJM discharge, contributing to the vertical distribution of solids near the suction inlet of the vessel. Tests defined from the limited parameter set that excludes vessel length scales may not capture important mixing phenomena characteristic of plant mixing systems.

In response to questions raised by the Board's staff about incorporating characteristic vessel length scales into the dimensional analysis, WTP personnel responded that they addressed the length scales by considering inter-PJM spacing. For example, WTP personnel assert that if the distance between a PJM nozzle and the wall of a test vessel is comparable to the inter-PJM distance in plant vessels, the effects of vessel size are incorporated into the testing. The Board's staff is concerned that this assertion focuses principally on localized jet behavior and discounts any coupling with the larger vessel scales. For example, academic studies of multiphase flow processes have shown that the largest scales are important.[1] Currently, WTP personnel have no plans to obtain the experimental data needed to support their assertions. Further, this approach leads to justifying non-prototypical mixing tests to close perceived gaps in test data.

Physical and Rheological Properties—The WTP V&V plan and gap analysis use highly simplified waste properties as the basis from which to derive dimensionless parameters. The Board's staff is concerned that the selected dimensionless parameters do not reflect more realistic physical and rheological properties important to mixing performance. For example, the dimensional analysis assumes monodispersed particles and neglects consideration of continuous particle size and density distributions. The particle size distribution has been shown to be an important dimensionless parameter for similar multiphase systems.[1] The dimensional analysis does not treat the ratio of solids density to liquid density as an independent dimensionless parameter, but incorporates it into the definition of other parameters. The Board's staff believes that the sufficiency of this approach should be verified. Further, the dimensional analysis does not address the technical complexity of actual waste solids morphology. To account for this complexity, variables describing particle morphology should be included in the dimensional analysis. The dimensionless parameter space also is limited to Newtonian fluids. Recent test results show that yield stress plays an important role in bottom-clearing processes and cannot be ignored. The Board's staff and Department of Energy, Office of River Protection and Bechtel National, Incorporated representatives have discussed these preliminary data and the concerns

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[1] L.R. Glicksman. *Scaling Relationships for Fluidized Beds*. Chem. Eng. Sci. Vol. 39, Issue 9, 1984, 1373-1379.

raised by the results (e.g., bottom clearing is dependent on yield stress). The inclusion of slurry yield stress and settled layer cohesion requires additional dimensionless parameters that imply an expanded technical basis for the V&V program. The Board's staff believe this expanded technical basis is appropriate for non-Newtonian processes vessels as well as any Newtonian process vessels where pulse jet mixing results in localized regions that exhibit non-Newtonian properties.

Completeness of Test Data for Spanning Relevant Parameter Space—The gap analysis uses the absolute minimum and maximum dimensionless parameter values to demonstrate the range of values covered by various tests. However, these ranges neglect the combinatorial set of parameter values required to show that a given test matches relevant plant scale conditions. Further, the analysis does not address or identify the specific combinations of parameter values that represent the most challenging mixing conditions. The Board's staff believes that validating the FLUENT model for the most challenging mixing conditions is necessary to ensure that the performance of the plant mixing systems will meet design requirements.

Non-prototypical Testing—Based on the results of the gap analysis, the WTP project team is planning tests in an 8 ft vessel, which the team argues eliminates remaining gaps in validation test data. Compared to a 38 ft diameter WTP vessel, an 8 ft diameter test vessel represents approximately one-fifth scaling. The recommended tests utilize full-scale jet velocity (12 m/s) and full-scale (4 in) and half-scale (2 in) nozzles to achieve full- and near-full-scale jet behavior. However, the combination of a full-scale jet nozzle and a small-diameter vessel results in non-prototypical test geometries, such as test configurations with only one PJM. Important geometric similarity parameters are not preserved with these configurations. For example, the dimensionless ratio of jet nozzle diameter to vessel diameter for the test geometries is much larger than it is for many of the plant mixing systems. These test geometries, together with the planned operational conditions, are non-prototypical mixing systems with relative power and pulse volumes that are larger than those of some plant geometries. Further, the characteristic settled bed depth for fast settling solids will be much shallower in the test vessels than it will be in the more challenging plant vessels. Consequently, these tests may exhibit more intense, non-prototypical mixing of solids compared with plant designs. To provide data applicable for validation, the staff believes that these tests may need to incorporate reduced jet velocity. However, with reduced jet velocity, any perceived benefit of achieving full-scale jet conditions will be lost.

Conclusions. The Board's staff believes that the FLUENT model will not be validated over the complete range of conditions expected for mixing system operations in WTP. This concern is based on the following observations:

- The dimensionless parameters derived in the V&V plan and the data gap analysis do not involve characteristic vessel length scales such as vessel diameter and fill level. WTP personnel are not planning to obtain additional test data to support their assertion that these large length scales are insignificant.

- The WTP V&V plan and data gap analysis consider simplified waste properties in the development of the dimensionless validation parameter space. The analysis and resulting proposed validation tests exclude particle size and density distributions, particle morphology, and non-Newtonian rheological properties.

- The gap analysis uses the absolute minimum and maximum dimensionless parameter values to demonstrate the range of values covered by various tests. The gap analysis did not consider the combinatorial set of variable values required to show that a given test matches the relevant or the most challenging plant scale conditions in defining the test requirements.

- Planned tests in an 8 ft vessel are non-prototypical and are insufficient to eliminate remaining gaps in validation test data.