The Consortium for Risk Evaluation with Stakeholder Participation III



Consortium Universities: **Vanderbilt University**, Howard University, Oregon State University, Robert Wood Johnson Medical School, Rutgers University, University of Arizona, University of Pittsburgh

May 8, 2008

Ms. Shirley Olinger, Manager U.S. Department of Energy <u>Office of River Protection</u> P.O. Box 450 MSIN: H6-60 2440 Stevens Center Place Richland, WA 99354

RE: CRESP Review Team Letter Report 4

Dear Ms. Olinger:

This letter report is in follow up to the CRESP ORP Review Team meetings with ORP on February 21 and 22, 2008 and supporting documentation, providing updates on (i) M-12, pretreatment testing and evaluation, including planned pretreatment engineering platform (PEP) testing (Phase I), results of laboratory testing of actual waste samples, simulant development and testing, (ii) M-1, line plugging, and (iii) M-3, vessel mixing. The primary focus of the review was on the draft test plans for the PEP¹.

All CRESP review team members participated; however, David Kosson, Richard Calabrese and Stanley Sandler participated through conference call rather than in person. The agenda for the meeting is provided as Attachment A. Below we provide the CRESP team observations and recommendations regarding each of the review topics.

We would like to compliment ORP on the organization of this review meeting. In particular, the presentations were made by the people who had written the reports and other persons familiar with the processes being discussed were present and directly answered our questions. It also was helpful to have the PowerPoint files of the presentations and other supporting materials provided to us prior to the meeting. The CRESP team appreciates and thanks all of your staff and that of the WTP contractors for their extensive efforts in preparation for and during this review meeting.

Josephson, G., O. Bredt, J. Young and D. Kurath. RPP-WTP Support Program Test Plan: Pretreatment Engineering Platform (PEP) Testing (Phase I), Doc. No. TP-RPP-WTP-506 Rev B, undated.



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¹ Markillie, J.R. Pretreatment Engineering Platform (PEP) Testing (Phase 1), Doc. No. 24590-PTF-TSP-RT-07-001, Rev C, 8 Nov. 2007.

General Comments

The following are general comments on the material reviewed that we believe have substantial, overarching impact to the planned test program and use of the resulting information:

1. **Scope of PEP experiments.** Currently, the PEP test plan covers Phase I testing, which will use a single simulant composition designed to represent a challenging (but not bounding) feed, focusing on leaching process scale-up. The simulant will have a nominal supernate composition with approximately 80% of the tank waste with having less challenging or similar mass loss and aluminum leaching requirements. Carrying out testing with a bounding simulant and test conditions, if selected appropriately, may define some limits of the facility performance (e.g., leaching time cycles, filtration flux rates) but also presents several challenges in using this information for planning WTP operations and program management. The ORP tank wastes to be treated at WTP and to be simulated during PEP testing, are comprised of several different general waste compositions and physical properties arising from the different process chemistries and histories. As a result, the coupled chemistry and physical characteristics of the wastes (including complex waste compositions that may interfere with leaching and other process steps) are likely not to be represented by a single case but rather several limiting cases representing each major waste type. Thus, the relationship of the simulant characteristics (physical and chemical) to the full range of characteristic waste types or envelopes must be clearly defined and understood. ORP has indicated that testing of additional simulants to represent a broader domain of waste characteristics may be explored during Phase II testing, but currently Phase II is largely undefined and not budgeted. It is difficult to know how challenging or representative the Phase I simulant is until additional cases are tested under Phase II are results of actual waste testing are known. We understand that there is additional testing of actual wastes in progress and these tests should provide guidance for the simulants to be used in future PEP testing.

Results from a single challenging case, or even multiple bounding cases, should be used in program management with caution. Estimates of full-scale processing rates solely from a single test condition that was planned to result in relatively slow facility throughput, would likely overestimate the time required to complete the WTP pretreatment mission, with attendant consequences in projections of schedule, budget and supplemental facility needs. It is important the uncertainties in projecting WTP performance that are inherent consequences of the PEP test conditions are recognized and considered in higher level WTP management decisions.

In addition, the overall quantity of hydroxide required to complete the WTP mission, and the resulting quantity of sodium (from sodium hydroxide use) that will have to be processed by the low activity waste (LAW) facility at WTP represents one of the greatest current uncertainties regarding the overall WTP mission. The PEP, coupled with appropriate engineering analysis and bench scale testing, provides an excellent test bed to reduce uncertainty in sodium processing requirements and explore potential process modifications that may reduce sodium use and LAW waste. However, this issue is not explicitly addressed in the current PEP test plan. This testing scope should be considered as plans for Phase 2 testing with the PEP are developed.

2. **Planning PEP experiments.** For some cases in the PEP test plans and presentations, precisely what variables or properties are to be measured and how the data obtained will be used to resolve specific issues and improve the WTP design and operations is unclear. In particular, Section 6.4.2 Data Collection and Analyses Matrix provides the data requirements and a general description of the measurements to fill the data requirements, and the Appendices provide details on planned operating conditions (Appendixes A, D) and sampling/analyses (Appendix B). However, there is not a clear mapping of the resulting data and data reduction back to quantification of specific design parameters and constitutive relationships that are needed to meet the specified data requirements (Section 6.4.2.) and allow extrapolating the PEP test conditions to WTP design and operating assumptions. Absent these final steps as part of experimental planning, it is difficult to determine where gaps exist in planned gathering of essential information during the experimental program. In other cases, what exactly is to be measured is not clear.

There also is a need for further justification of the overall test cases. In the integrated PEP testing dealing with caustic and oxidative leaching, there are to be a total of five tests. However, test 2 exactly replicates test 1, and test 5 exactly replicates test 4. Can more useful information, especially with regard to scaling, be obtained by changing at least some of the parameters between tests 1 and 2, and also between tests 4 and 5? There may be other factors driving the experimental design, such as nuclear quality assurance guidelines, but maximum use of test results can be realized by designing each test to complete the spectrum of key variables.

- 3. **PEP testing success criteria.** The criteria for "success" associated with the PEP test program and components of the test plan are not clear. The term to "demonstrate" is used frequently as a testing objective. What are the criteria for the success of a demonstration? Does demonstrate mean that the process being tested works at the design conditions, or that it can be made to work under some conditions though not necessarily the design conditions? Or that the process or component has been operated at specified conditions for a designated time interval or number of cycles? How does the robustness of the process during upsets (e.g., fouling, plugging or less than desired mixing) factor into success criteria? Page 20, Section 4.0 of the test plan contains the only listing of "Success Should be listed for all processes, including leaching, mixing, filtration, mobilization, etc. Demonstration of the ability of the plant to recover from process upsets should be part of testing using the PEP, both during Phase I and Phase II, and with the entire set of simulants being developed.
- 4. **PEP simulant development.** Definition of the primarily chemical aspects of the simulant development program (e.g., choice of minerals as simulant components) appears to be well developed and well managed. The absence of coupling of chemical and physical (rheological) aspects in the simulant development program is a significant concern. Chemistry-rheology phenomena must be fully understood to avoid "surprises"

in the full scale processes. Leaching, settling and filtration processes will be a result of the combination of chemical and physical processes. One example of the need for matching chemical and rheological properties is our concern that the local rheology near a particle will influence the observed leaching reaction rates. Therefore, it is important that rheology of the wastes (as determined in laboratory testing) and their chemistry (aluminum, chromium and other solid phases, as well as solution composition) <u>both</u> be reflected in the simulant characteristics. As indicated earlier, how the simulant properties map onto the domain of actual waste properties should be clearly described. This will be especially important for the integrated Phase 1 testing of the PEP that involves leaching, filtration and slurry mobility issues. Significant effort has been put into simulating the system rheology for the M-1 and M-12 issues (which are solely rheology driven). This experience should be reflected in the PEP testing.

The plan for using a clean or cold CUF (non-radioactive) unit to correlate between the non-radioactive or cold simulant in the PEP and the actual waste results obtained in the hot CUF is well thought out. It would be desirable to run the cold simulant in the hot CUF and the cold CUF to determine experimental uncertainty. This would provide a baseline with a stronger empirical basis for using the cold CUF to look at variations in cold simulant recipes, and to establish experimental relationships between the CUFs, PEP and ultimately the full-scale WTP during systemization.

5. Scaling of Particle Mixing Phenomena. The major focus of the Phase 1 tests, with respect to PJM mixing and mass transfer, is for constant jet discharge velocity (U) on both scales. The length scale (L) ratio is fixed at 4.5 and the time scale (t) is set by the PJM pulsing rate with t ~ L/U. Therefore, when velocities are matched, the WTP time scale is 4.5 times longer than the PEP time scale. Since there is debate about the importance of matching different mixing phenomena, some portions of the tests will be conducted in the PEP at both the PEP and the WTP time scales, and this is certainly worthwhile. We are concerned that these scaling criteria may capture large scale mixing phenomena such as blending of process streams and bulk solids suspension/heat transfer, but may lead to discrepancies in the performance of particle scale processes, since both particle size and chemistry are held constant. With the scaling criteria being used, the PEP is better mixed on the particle scale, leading to faster particle-to-fluid mass transfer rates and higher deposition and resuspension rates of particles from the tank bottom (and filter surfaces). Agitation of particles is better scaled by constant jet power per mass (or volume) of fluid in the tank. Please see Appendix A for further details.

There are further consequences of enhanced mixing on particle scales in the PEP for high solids loading. Fluid stresses acting on particles in the PEP may be greater than in the WTP. When these stresses are less than the yield stress of the simulant, stagnant boundary layers may exist near the surface of particles. Such boundary layers can severely inhibit mass and heat transfer, and are more likely to occur on the WTP scale. While there was mention of performing some tests in Phase 1 that consider scaling on power per volume, they were indicated to be less systematic and of secondary

importance. We believe that tests which demonstrate or reject power per volume as a requisite scaling criterion may be important.

The scaling of particle settling and mixing by the gas spargers also should be further considered. While one can scale flows for turbulence, the force of gravity cannot be scaled in the equipment. Since gravitational force is the cause of particle settling and mixing by buoyant bubble plumes, and since it cannot scaled as can other parameters, will there be a scaling inconsistency here? Scaling of the effects of gas sparging was not discussed in the presentations, and is given much less emphasis in the documents given for review than PJM scaling.

In summary, verification of correct scaling of particle agitation should be an important Phase 1 focus, emphasizing effects at the particle length scale.

- 6. **Data archiving.** The raw, qualified data that are being generated in this program need to be archived in a way that allows their rapid retrieval together with as much background information as possible. "Data" should not simply be archived in the form of correlations, regardless of how robust these are. It is not evident that qualified archiving was being planned for the PEP results. During the development and lifetime of the PEP, and the longer lifetime of the WPT, all qualified data and calculations obtained over the history of the project should be readily available. This would allow engineers in the future to understand the basis for design changes and likely will be valuable in diagnosing unforeseen problems. Especially important would be archiving PEP (and later WTP) operating data from different types of simulants (in PEP testing) and different wastes (WTP operations).
- 7. Integration of M-1, M-3 and M-12 Results into PEP Phase 1 Testing Program. There appears to be a need for greater integration and coordination among the M-1, M-3 and M-12 testing procedures and programs. In many of the documents and presentations reviewed, there are quite useful diagrams and flow charts that relate various sub-tasks to the overall objectives, and that provide insight as to how information flows within a specific issue response. Yet, there are no such diagrams, flow charts or tables that show the interrelation among the various tasks and programs that clearly have interrelationships. Information flow diagrams should be developed that show the interrelationship and flow of critical information among the various tasks and project phases that are essential to the success of the WTP test programs. Similarly, management processes should be in place to ensure that the needed information flows do occur. Without this sort of management of testing and data analysis some of the tests and analysis efforts could be of limited value since they may be redundant by overlapping with other tests being conducted concurrently or by not using relevant information being developed in other parts of the project. This observation is also applicable to issues M-4, M-5, M-6, M-8, M-9, M-13, and possibly M-15. These include addressing:
 - a. the connection/interrelationship among the various issue response plan tasks that are currently underway;

- b. the mechanism by which current findings from one issue response task can immediately impact or change the direction of tasks from related issue response programs; and,
- c. how Phase 1 PEP test results will impact the development of the Phase 2 PEP test program (and beyond).

The importance of such synergy can be illustrated by the following example. Currently, M-3 tests of PJM mixing capabilities with respect to solids suspension in water are underway on various scales (3 different tank sizes), and will be completed within the next 3 months. Understanding suspension stability and sedimentation are most critical in water where the amount of solids is small and the settling velocity is high. PEP tests will be carried out for at least the next 9 months. It would seem reasonable that some of the M-3 tests focus on the adequacy of the current PEP scaling criteria versus criteria based on jet power per volume to predict how well the solids will be suspended on the three M-3 test scales. These results could have immediate impact on the PEP Phase 1 test matrix, and should be used to guide future PEP studies. Similar interrelationships exist between the M-1 and PEP/M-12 test programs.

- 8. Advantages of Pilot-scale Testing. Several comments during the review meeting indicated that the design and fabrication of the PEP has been a good learning experience and provided feedback to the PTF designers. It is important to document the lessons learned and the value of the PEP system development and subsequent pilot testing, both to capture the new knowledge and to provide a basis to support the value of future process piloting efforts by DOE-EM. For example, what lessons were learned that were that valuable? What equipment redesigns were required? Did any of these lessons learned resolve EFRT issues? Were any new issues identified? Can the cost savings as a consequence of the pilot experience be quantified?
- 9. Testing in Support of M-1, Plugging in Process Piping. Issue M-1, Plugging in Process Piping, has been focused on providing an engineering basis to preclude processing interruptions from pipe plugging caused by settling solids. A draft design guide was issued based on recognized mineral industry transport correlations to establish critical velocities to maintain slurry stability and avoid plugging. Confirmation that these industry-accepted correlations are adequate for WTP design is being tested, given that Hanford tank waste contains significantly more 10-to-100 micrometer particles than were used to develop the correlations,. The approach being used is to prepare slurries using single size/density particles (stainless steel powder, alumina particles, and glass beads with kaolin additions to attain 3 and 6 Pa shear stress) to directly compare experimental results to the correlations. It may be useful instead to formulate particle size and density distributions similar to those that have been determined in testing of planned WTP waste feeds. The planned particle size simulants may not properly reflect the whole range of slurry rheology and potential cohesion resulting from chemistry-particle interactions. It is unclear that this approach will provide complete confirmation of the draft design guides that are relevant to avoiding plugging in slurry piping and other process piping components.

10. **Computational Fluid Dynamics (CFD) Simulations.** It is encouraging that efforts are underway to develop realistic CFD simulations of solids suspension/distribution by PJMs in WTP process tanks. By the time that the WTP comes on line, process simulators likely will be a common and relied upon source of real time information to plant operators. CFD simulations can be used to provide details relevant to higher level process calculations. For WTP, CFD can provide important insights into fluid-particle mixing under different operating conditions that will impact overall pretreatment performance for the range of waste types to be treated. It is important that DOE and its contractors are in position to take full advantage of these advances in simulation science by starting to develop the plant specific CFD simulations that will provide insights at the process level. Appendix B provides detailed comments and suggestions with regard to the current HLP-22 simulations.

Specific Comments

The following are additional specific comments that are narrower in scope but warrant consideration:

- 1. The CRESP team was impressed by the technologies that will be used with M-1 and M-3. Electrical Resistance Tomography (ERT) (also called Electrical Impedance Tomography) can lead to a highly instrumented pipeline (M-1) as this technology is inexpensive to implement and can be used in many of locations. The ultrasonic method used in M-3 is also an excellent choice. These technologies should be considered for implementation in the PEP.
- 2. Draft Test Plan document, page 8 indicates "The PEP will provide data with experiments conducted at "scale-time" (4.5 times shorter than plant time) and plant time to provide bounding conditions." The implication of this statement is that there is an expectation that the WTP will only run on plant time or faster, but not slower. So the statement of obtaining a bounding estimate seems to allow only for an upper bound on the rate of processing, not a possible lower bound.
- 3. The following statement appears on page A-4 of Shimsky et al, "Instead, the (total mass of solids)/(filter area) ratio will be 4.5 higher than in the full-scale facility, leading to less pore-plugging of the filters and presumably a higher filter flux." This is counter intuitive. It would seem that the filter cake would grow more quickly, leading to a lower flux. Are there data to confirm the statement on Page A-4?
- 4. Page 40 of the Draft Test Plan (bottom) refers to "the sample flows through a cooler to keep the sample from flashing when a hot sample is taken during the leaching operations at 100°C." Since solid solubility is a function of temperature, there is a concern that there might be precipitation during cooling. If this were to occur, the chemical analysis of a mixed solid-liquid sample (or for that matter any two-phase sample) is much more difficult. Perhaps the system is operated sufficiently far away from any solubility limit

that this is not an issue, but this is not clear. This issue is raised here just to insure that it has been considered.

The CRESP Review Team looks forward to further discussion regarding these topics and future review meetings.

Sincerely,

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Appendix A

Scaling of Micro-mixing and Meso-mixing Phenomena in Process Tanks

In the presentations and PEP documents, a common theme was to contrast PEP scale time versus WTP scale time to bound PJM mixing phenomena. Furthermore, constant velocity scaling was imposed to match 'the turbulence' on the PEP and WTP scales. These considerations may allow proper characterization of large scale mixing and overall (bulk) solids suspension, since the PJM pulsing rate sets the frequency of the time periodic convection currents or pseudo-turbulent² velocity fluctuations in the tanks. However, they may not capture the essential physics of processes that occur on small (micro-mixing) and intermediate (meso-mixing) length scales; that is, on the scale of individual solid particles or clusters of particles. During the meeting, the latter mixing phenomena were sometimes referred to as 'agitation of particles'.

Consider the discharge of a PJM jet in the absence of gas sparging. The turbulent macro length scale ℓ , of the jet is of the order of the jet diameter, so it is 4.5 times smaller on the PEP scale than on the WTP scale. The micro length scale or Kolmogorov microscale of turbulence is given by $\eta = (v^3 / \epsilon)^{1/4}$, where v is the kinematic viscosity, and ϵ is the local energy dissipation rate (power per unit mass of fluid). On average, this is just the power supplied per mass of fluid by the PJM. From a turbulence perspective, the energy dissipation rate is of order³ $\epsilon \sim u^3 / \ell$, where u is a characteristic macro scale turbulent jet velocity. For self-similar jets, u is proportional to the jet discharge velocity, so when the velocity is the same on both scales, the energy dissipation rate is 4.5 times larger and the Kolmogorov microscale is about 1.5 times smaller on the PEP scale. Constant velocity scaling results in a mismatch of the spectrum of turbulent eddies, and promotes better turbulent macro-mixing on the WTP scale and better micro-mixing on the PEP scale. This results in enhanced agitation of practical consequence on the particle scale in the PEP tanks. For $\ell \gg d \gg \eta$, the stress τ_d acting on a particle of diameter d is given by⁴:

³The approximation $\varepsilon \sim u^3 / \ell$ implies that locally turbulent energy production (that occurs on large scales) equals the dissipation (which occurs on small scales). This is a common assumption.

 4 For the larger size particles the assumption that $\,\ell\,>>\eta$ is strictly valid. The relationship

 $\tau_d \sim \rho(u'_d)^2 \sim \rho \epsilon^{2/3} d^{2/3}$ follows from Kolmogorov's theory for the inertial subrange of turbulence. A

²The discharge and suction cycles of the PJMs create large scale, time periodic motions that appear as velocity fluctuations at sampling times that are long compared to the PJM pulsing rate. As a result, a peak appears in the turbulent energy spectrum at the PJM pulsing frequency. This peak must be subtracted out or removed to obtain the actual turbulent energy. These non-turbulent time periodic motions are not turbulent velocity fluctuations and are referred to as pseudo-turbulence. They do not contribute to the energy that cascades to and the stresses that occur on smaller scales. (Turbulence is produced by energy input at large scales and is dissipated by viscosity at small scales. The large scale eddies are said to decay or breakdown into smaller eddies and so fourth. In this way energy is transported from large to small scales where it is dissipated. This is referred to as the energy cascade, where energy is transferred from large to small scales.)

derivation and references can be provided. For the smallest particles $d < \eta$ and a different scaling relationship, that would lead to similar conclusions, is obtained.

 $\tau_d \sim \rho(u'_d)^2 \sim \rho \epsilon^{2/3} d^{2/3}$, where ρ is the fluid density and u'_d is the characteristic fluid velocity fluctuation on the particle scale. u'_d , in turn, determines the slip velocity. That is, mass transfer rates to/from small particles, as well as the ability to suspend small particles from the tank bottom are governed by turbulence phenomena that occur on the scale of the particle, and therefore depend on the local energy dissipation rate, which is 4.5 times larger on the PEP scale.

The above arguments only hold for Newtonian fluids. However, they can be extended to more complex fluids if it is assumed that the only relevant non-Newtonian phenomenon is that associated with yield stress/strength. Another consequence of the dependence of τ_d on length scale is that the stress imparted by turbulent eddies as they decay down to smaller sizes, decreases with length scale. That is, it becomes more difficult to impose a stress on a fluid element as the element size decreases. Furthermore, for relative motion to occur on smaller scales, the local stress must exceed the yield stress/strength. A particle, or a cluster of particles ("held together" by the yield stress), can be contained within fluid elements, with no internal fluid motion that are convected to other parts of the tank (macro-mixing) by larger scale motions (much like a puff in a smoke stack plume). That is, there may be stagnant fluid layers and no slip velocity on the particle surfaces. Such localized dead zones can significantly affect particle-fluid mass transfer rates. Since τ_d depends on ε , yield stress/strength would tend to be more easily overcome at the smaller scales in the PEP than in the WTP.

The above considerations suggest that jet power per mass (or volume) of fluid, rather than equal jet velocity, would provide the correct scaling for agitation of particles. Jet power depends on the discharge flow rate and pressure driving force. While the above discussion focused on the PJM discharge stroke, similar arguments would apply to the suction stroke.

Similar arguments can also be applied to scaling of particle agitation by gas spargers. The power imparted to the broth (liquid - particle slurry) is the product of the gas volumetric flow rate and the pressure drop across the discharge orifice.

The conclusion from the discussion here is that in the scaling analysis, jet power per mass (or volume) of fluid, rather than equal jet velocity, should be used to provide the correct scaling for agitation of particles. If not, then tests should be conducted to show that it is not important.

Appendix B

Comments on Computational Fluid Dynamics (CFD) Modeling of Solids Distribution in HLP-22

If steady progress is to be made toward the development of full plant simulations, it is important that the current efforts take advantage of what can presently be accomplished at the cutting edge. It is in this context that we have questions, comments and suggestions about the current HLP-22 simulations.

The current 2-D simulation for 1/8 geometry at 750,000 nodes is based on an axi-symmetric assumption that ignores the dependency of the velocity field on the angular (θ) coordinate. Given PJM placement, momentum and swirl, the jet plume that impacts the tank bottom will spread in all directions. It is not clear that a 2-D flow will result relative to the tank axis in the absence of more detailed information on tank geometry and PJM operation. Therefore, justification for the 2-D assumption needs to be provided.

The current approach to predict solids distribution using a RANS (Reynolds Averaged Navier Stokes Equations) based two fluid/dispersed phase model may be too ambitious given what can be accomplished using current computer architectures. It may be more prudent to redefine the current goal to take full advantage of current/proven computationally efficient approaches.

After a simulation is started, the velocity field created by the PJMs operating at a specified cycling frequency will soon become time periodic; that is, the flow field throughout the tank can be correlated with the discharge/suction profile for PJM operation. In the absence of particles, the time periodic steady state imposed by steady PJM operation can be realistically computed on a well resolved 3-D grid of 3 to 5 million cells for the full tank geometry using a relatively modest-sized Linux cluster. For instance, for a RANS simulation of the turbulent flow of water using Fluent with the standard or realizable k- ε model and a variety of wall functions, the solution will probably converge to a time periodic steady state in 5 to 10 PJM pulse cycles. This can be accomplished on a 24 processor cluster with 2 GB memory per node on the order of a month or months. Once satisfied that the mesh and numerical settings have been adequately chosen, there is little manpower cost to running a number of simulations at varying conditions compared to hot testing. The primary interest is in capturing the final computed velocity field of the steady periodic motions of the PJM cycles that can be exploited to gain insight about particle phenomena as described later.

If particles at high solids loading are introduced, an approach must be used that is based on a two fluid/dispersed phase model and accounts for yield stress/strength. Starting from an initial condition in which the particle phase is either settled on the tank floor or is uniformly distributed throughout the fluid volume, it will take numerous PJM pulse cycles before the solids distribution within the tank reaches a time periodic steady state. As concluded by Bechtel personnel, such a computation is not possible with current computer resources, even for the 2-D, 1/8 tank, 750,000 cell geometry. Therefore, an alternate approach may be warranted.

For the suspension of large, high density particles, the limiting case is at low solids loading where the broth (liquid in the tank) is water like or of low viscosity. Under these conditions, it is possible to decouple the calculation of the fluid velocity field and particle trajectories (often referred to as one-way coupling in CFD). This is a currently tractable problem for the largest and most dense particles. These particles cannot respond to the small scale velocity fluctuations (known as the crossing trajectories effect), which cannot be predicted by a RANS formalism. If the interest is in solids suspension (not leaching - mass transfer and reaction), it is doubtful that the trajectory of a 50 μ m particle that is 5 to 10 times more dense than water can be influenced by small scale turbulent velocity fluctuations. As a result, a pragmatic approach would be to assume that the particle motion is governed by the RANS predicted mean (time averaged) flow field and that the presence of particles does not significantly influence the flow dynamics of the surrounding fluid.

With these assumptions, the mean flow field in the absence of particles, as described above, can be used to simulate particle trajectories throughout the tank by repeatedly superimposing the final predicted time-periodic fluid velocity field discussed earlier without further CFD simulations. Fast particle tracking schemes to accomplish this are available, so this is a realistic computation within current resources. The selected tracking scheme must account for drag, gravity/buoyancy, pressure, fluid acceleration and apparent mass effects on particle motion.

Prediction of the spatial distribution of solids within the tank at low solids loading can be realistically accomplished by the approach above suggested. Prediction of the suspension of solids is a completely different issue. The use of wall functions precludes a realistic description of particle deposition onto, or re-suspension from, solid surfaces. Within the RANS formalism, the only work around is to use empirical rules to treat particles in the vicinity of the tank bottom. These "rules" would have to be tuned based on accurate experimental data acquired for the off-bottom suspension of solids. Such data could be provided from carefully designed experiments conducted in the PEP or within the M-3 test facilities.