SUMMARY DOCUMENT

Computational Fluid Dynamics Modeling of HLW Processes in Waste Tanks

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Introduction

Selection of baseline experimental and simulation data is a critical step in conducting a numerical simulation of waste mixing and transfer. An extensive literature review is performed in order to obtain precise information regarding different aspects of the problem, such as properties of supernatant and solid simulant, operating conditions and dimensions, as we as different reported metrics. These data will serve as inputs to multiple CFD simulations in regards to construction of computational domains, assignment of correct boundary conditions, and validation of simulation results.

FIU has reviewed different tests and simulations related to waste retrieval process from double-shell tanks (DST) at Hanford. The problem involves two mixer jet pumps (MJP) each having two opposing nozzles rotating in certain speeds in order to suspend solids that have settled in the bottom of the tank. Critical operational conditions are rotation rate and flow rate (may be expressed by nozzle velocity) of MJP's nozzles, suction velocity at the transfer line, and time duration for each batch transfer. FIU reviewed several tests and simulation runs carried out at different national laboratories and obtained information about performance metrics, such as Pre-transfer and batch transfer concentration of undissolved solids (UDS), effective cleaning rate (ECR) of MJPs, density of material at different height and radial locations, and the height up to which suspended particles can reach in the tank, known as cloud height (HC).

In addition, other relevant simulation studies of erosion in the literature were conducted. The aim was to obtain information about models and approaches that exist for simulation of erosion in the literature. FIU focused on numerical studies of mobilization of sediment layers exposed to a normal and shear stresses of fluid flows. In addition, a portion of study was dedicated to change of rheology due to change of slurry composition when solid particles were suspended in literature. A study was conducted on suitable multiphase models which can adapt to this change during simulation and exploitation of these models were investigated in our review. A summary of the data and information obtained from literature is provided in the following sections.

Baseline Experimental Data

In this research, attention will be given to properties of different simulants used in full-scale or scaled experiments related to Hanford retrieval processes, mixing and transfer, at or from DSTs. Focus is on reported data on tests conducted in 2010, 2011 and 2013 which are different in terms of liquid and solid simulants, as wells as operational conditions. We briefly explain the data and skip the details related to simulant development and refinement processes. Interested readers can find details in reports provided by [1-3].

Test 2010 (ZrO_2, 6 wt% in water)

This test was conducted using a single component solid simulant (ZrO_2) in water [1]. In this simple test (simplicity for working with single solid and single liquid), ZrO_2 had a 6 wt% of the tank material and specific gravity of 5.7. This test was also used as a baseline for a CFD simulation study conducted by Wells and his colleagues where simulation and test data about cloud height and UDS were compared (Table 1). According to recent communications between FIU and WRPS engineers, it was decided that FIU use data from this test as start-up for our simulation study, so more details about specifications of this test will be provided to FIU in the near future.

Table 1. Cloud height data for test 2010, 6 %wt ZrO2 [1]

Metric	43.2" tank Nozzle vel. (ft/s)			120" tank Nozzle vel. (ft/s)		
⬇	13	19	22	22	25	28
HC/HL	0.61	0.87	1.02	0.71	0.90	1.02
UDS	0.46	0.46	0.49	0.77	0.60	0.53

Test 2011-1 (four-part simulant in water)

This test was performed using a complex simulant composed of gibbsite, zirconium oxide, silicon carbide, and bismuth oxide in water and inside 43.2" and 120" tanks. [4,5] reported density variation along a riser near the tank center, referred to as riser 30, for different nozzle flow rates inside the 43" and 120" tank, respectively (Table 2). To date no simulation study based on data from this test was found in the literature.

Table 2. Density data (specific gravity) at different elevations inside 43.2" tank [4]

Elevation (inch)	Flow rate (gpm)							
	7	7.5	8	8.5	9	9.5	10	10.5
0.5	1.043	1.078	1.069	1.068	1.077	1.075	1.074	1.076
1.5	1.042	1.076	1.067	1.068	1.074	1.073	1.073	1.075
3.5	1.040	1.074	1.066	1.066	1.072	1.072	1.072	1.074
5.5	1.038	1.071	1.064	1.065	1.071	1.070	1.070	1.073
7.5	1.037	1.071	1.063	1.065	1.070	1.069	1.070	1.074
9.5	1.035	1.065	1.062	1.063	1.069	1.068	1.069	1.073
11.5	1.033	1.061	1.058	1.062	1.069	1.067	1.068	1.073
13.5	1.029	1.049	1.053	1.059	1.065	1.064	1.067	1.072
15.5	1.008	1.003	1.016	1.039	1.047	1.050	1.060	1.068

Test 2011-2 (five-part/complex simulant in water)

According to [5], a complex 5-part solid simulant and water, as the liquid simulant, was used in SSMD testing in 2011. This 5-part solid simulant composed of Gibbsite, Zirconium Oxide, Silicon Carbide, Stainless Steel, and Bismuth Oxide, with properties given by [1]. The simulant mixture was a solids weight percent of 19% in water, with 10% being contributed by Zirconium Oxide (d50=12 micron), 6% Gibbsite (d50 =10 micron), and three spike particles at a concentration of 1% each of Bismuth Oxide (d50 = 38 micron), Silicon Carbide (d50=150 micron), and Stainless Steel (d50=128 micron) [6].

Other properties, such as critical shear stress (τ_c) and settling velocities (U_t), have been reported individually (for each solid constituent) by [5] and in bulk (mixture) by [1], respectively. The reported values are based on water (1.0 g/mL, 1.0 cP) as the eroding fluid, but can be recalculated or measured for other eroding supernatant as well. Two approaches can be considered; in the fist approach, based on the total solid content in the slurry, bulk values of τ_c will be used. This approach is more appropriate if a single solid component is involved. In the second approach summation of all weighted values ($\varepsilon_i \times \tau_{c,i}$) will be used. The second approach is more appropriate for multi-component simulant.

Information about operational conditions, such as nozzle velocity, capture velocity, and jet rotation rate, were obtained from [5-7]. We also extracted test results such as normalized ECR, normalized cloud height, fraction UDS mass transferred, and UDS concentration (in pre and batch transfers) from [5,7].

Table 3. Test conditions in 2011-2, [5]

Test case	Scale	Nozzle velocity (ft/s)	Jet rotation rate (rpm)	Solid simulant	Supernatant
1	1:21	16.9	1.53	5-part	water
2	1:21	22.1	1.53	5-part	water
3	1:21	24.8	1.53	5-part	water
4	1:21	27.6	1.53	5-part	water
5	1:8	22.3	0.77	5-part	water
6	1:8	28.7	0.77	5-part	water
7	1:8	31.9	0.77	5-part	water
8	1:8	35.4	0.77	5-part	water

Test 2013 (four-part/base simulant in suspension)

The 2013 test used supernatants composed of water, glycerin, sodium thiosulfate, and sodium bromide with different concentrations. Information about composition and physical properties of the liquid simulant were found in [3,8]. Solid simulant in this test was composed of four undissolved solids (UDS), which were Gibbsite or $Al(OH)_3$, sand, stainless steel (SS), and zirconium oxide (ZrO_2). This test was done using three configurations for solid, named low, high, and typical. The naming shows difficulty level of solid mixing and transfer. Information about composition and physical properties of solid simulants were found in [3].

This test had a very populated matrix and was done for three capture velocities, CV =3.8, 7.3, and 11.3 ft/s and five jet rotation rates. However, available information was limited to two tests; Test 2013-1 with capture velocity CV=7. 3 ft/s, typical solid (density = 2721 kg/m^3), modified high supernatant (density = 1.32 g/mL, viscosity = 8 cP), and CV=7.3 ft/s, and Test 2013-2 with capture velocity CV=11. 3 ft/s, typical solid (density = 3584.2 kg/m^3), high supernatant (density = 1.37 g/mL, viscosity = 15 cP), and CV=11.3 ft/s. One thing in common between these tests is that only 13% of the initial weight of slurry was solid, according to [8].

Test results in different nozzle velocities are UDS concentrations for both Test 2013-1 and Test 2013-2, information about effective cleaning rates for Test 2, and length and depth of cleaning for Test 1. Test results from Test 2013-1 and Test 2013-2 are of special interest since there were partially used in previous simulation studies by [5,9]. For this reason, it was highly recommended that FIU use data from Test 2013 for multi-component simulations for improvement evaluation purposes.

Data for full-scale tests

Available measurement and simulation data are limited to a number of studies in the literature. Simulated UDS and HCL data for single component solid test in 2010 [5]. Full-scale data related to ECR measurements in tank AZ-101 were found in [10]**.** Simulated UDS and ECR data for test 2013-1 with all dimensions and operating conditions of a full-size tank (AY-102) is given in Ref [9].

Geometrical dimensions and operational conditions

FIU reviewed key setup parameters related to previously-mentioned tests in order to obtain consistent and accurate information about operational conditions and geometrical dimensions of system elements such as tank, nozzle, and transfer line intake for both scaled tanks. Our review concludes that the same scaled tanks were used for various tests. Relevant data were extracted from [6,8], as shown in Table 4.

Table 4. Geometrical dimensions for scaled and full-size tanks and accessories, [8]

Property	**43.2" tank**	**120" tank**	**Full scale€**
Tank internal diameter (m)	1.1	3.05	22.9
MJP's Nozzle Diameter (m)	0.0071	0.0203	0.152
MJP's Nozzle Elevation (m)	0.0218	0.0610	0.457
MJP's Suction Diameter (m)	0.0135	0.0373	0.279
MJP's Suction Elevation (m)	0.0061	0.0170	0.127
MJP's Axial Offset in 0° & 180° angles (m)	0.323	0.8840	6.71
Transfer Pump Suction Inlet Diameter (m)	0.0064* 0.0071†	0.0081* 0.0081†	0.057-0.061* 0.057†
Transfer Line Diameter (m)	0.0095* 0.0079†	0.0095* 0.0095†	0.078* 0.078†
Transfer Pump Suction Velocity (m/s)	1.16 – 3.44*	1.16 – 3.44*	2.21 – 3.44†
Transfer Line Velocity (m/s)	0.53-1.56¤* 0.94-2.78¤†	0.84-2.50¤* 0.84-2.50¤†	1.19-1.86¤* 1.19-1.86¤†
Transfer Line flow rate (gpm)	1.15-2.17	1.5-2.8	90-140
Transfer Pump Suction Elevation (m)	0.0071	0.0203	0.152
Transfer Pump Axial Offset in 90° angles (m)	0.0884	0.244	1.83

€ Tank AY-102
* Lee and co-authors (2012, 2013), [2],[3],[8].
¤* Calculated based on data from Lee and co-authors (2012, 2013), [2],[3],[8].
† Jensen et al. (2012) for SSMD, [6].
¤† Calculated based on data from Jensen et al. (2012), [6].

Other considerations

To complete the problem set up in a simulation study, other important aspects were also considered. Slurry rheology, presence of air-lift circulators, solid layer thickness and simulation time are of special importance. Also, the presence of liquid inside the solid layer is important since sediment in several tanks is in form of sludge (BL sludge in AY-102 or P3 sludge in AZ-101 according to [11]). Presence of liquid in the sludge can be shown by packing density value which is ratio of the volume occupied by solid to the total volume sludge. The following sections address these important aspects.

Slurry rheology

Some solids in tanks at the Hanford site are composed of submicron particles of Boehmite and Gibbsite (form of AL_2O_3). The presence of these components can introduce particle gels with non-Newtonian behavior [12]. According to Lee, a Bingham plastic type of fluid may exist [2]. Similarly stated in [5], slurry rheology may change from Newtonian to non-Newtonian and can cause significant reduction of mobilization of clay layer. The effect can be a 40% increase of required flow rate to achieve the same waste mobilization metric, as usually identified by the effective cleaning radius (ECR). Suspending particles of a non-Newtonian slurry with higher yield stress is more difficult, but once erosion happens, particles stay suspended to a greater degree, as compared to situation with slurries with lower yields stress. The combined effect will be higher concentrations in the transfer lines [13].

It is critical to know how yield stress (τ_c) and consistency (k) of slurries in Hanford tanks vary with concentration of solids in slurries [11]. A simulant composed of 22 wt% and 28 wt% Kaolin clay in water will have yield stresses of 3 Pa and 10 Pa, respectively [2]. These stress values are recommended by RPP-PLAN-51625 for the simulant representing the slurry in Hanford tanks. In particular, this yield stress of sediment layer at the bottom of tank may be significantly different from liquid above the solid sediment, supernatant, which exists above this layer and contains suspended particles. This piece of information is very critical for simulation. If the mixture multiphase model is used, different rheograms are needed for the solid layer and the Supernatant during simulation. Therefore, part of the literature review will be dedicated to finding this variation.

Air lift circulators

AY-102 tank contains 22 air lift circulators (ALC) with 0.8-inch diameter which extend down to within 0.8 meters of the tank floor [7]. These air circulators are not functional according to [7] and their presence in scaled tanks is for simulating tank obstructions [2]. These obstructions can seriously affect waste mixing and will be remained in FIU's simulations. The presence of ALCs can be seen in reported simulations in [1,9,12].

Transfer line, return line, and tank floor in DST

According to Lee and Thien [8] transfer line is located with an offset from tank center, as shown in Table 4. This transfer line is equidistant from each MJP, as is schematically shown in [2]. Reported values of the capture velocity (CV) in transfer lines for different tests can be used to calibrate pressure values of a pressure boundary condition type in a CFD simulation. In addition, each MJP received slurry from an external slurry pump. Slurry is sucked by an external slurry pump and returned to the MPJ nozzle via a return line. Therefore, composition of slurry jet is the composition at the suction port which is just below the MJP's nozzle. Any CFD model must represent this cyclic behavior. All dimensions related to height and diameter of suction port are listed in Table 4. In the case of the tank floor, bottoms of both 43.2 and 120" tanks are flat with radius at corners are 0.6" and 1.6" inch, respectively [2,9].

Thickness of sediment layer and liquid layer

According to Jensen et al. [6], AY-102 DST contains up to 1.78 m of settled solids. This number is 1.4 meters in [4,7]. However, no records of solid layer thickness inside the scales tanks were found to date. One possible estimate can be scaled-down solid layer via scale factors (1:8 and 1:21). For calculations, we used values reported by Greer and Thien [7] and obtained H_{solid} =1.4/8= 0.175m and H_{solid} =1.4/21= 0.067m, for large and small tanks, respectively. Using the same estimate for the liquid layer, we obtained H_{iquid}=9.2/8= 1.15m and H_{liquid} =9.2/21= 0.43m, for large and small tanks, respectively. Here, 9.2m is the liquid height in AY-102 tank, as reported in [7]. If scaling estimate is accurate, a 13 wt% solid containment, as reported in [8], must be attained. Using the total solid density of 3584.2 kg/m^3 and liquid density of 1370 kg/m^3, we obtained the solid to liquid mass fraction of $\rho_{solid}*H_{solid}*A_{tank}/(\rho_{liq.} * H_{liq.}*A_{tank})$ = 3584.2 *0.175/ (1370*1.15) = 0.398, which is approximately 29 wt% of solid in slurry for scaled 43.2" and 120" tanks. This calculation is based on the assumption that solid covers the bottom of the tank and volume fraction of solid inside the solid layer is one. This scaling can be accurate if a maximum solids packing ratio of 15 wt% exists. This discrepancy suggests that a reconfirmation on solid and liquid heights in scaled tanks is needed.

Data collection time

According to Jensen et al. [6] for the 120" vessel, batch transfer times corresponding to suction velocities of 6 and 11.3 ft/s are approximately 127 to 237 minutes, respectively. For the 43.2" tank, these times are approximately 8 to 14 minutes for the same velocities. These times are 1071 and 1667 minutes for the full-scale AY-102 tank corresponding to 7.26 to 11.3 ft/s velocities at the suction inlet, respectively. Measurement data [6] show periods of 12500 to 60000-second data collection. Data collection times for tank level, MJP discharge, sample density, tank temperature, and transfer flow rate are 80000 seconds in [5]. In the case of simulation work, a 50000-second data collection time for ZrO_2's batch transfer concentration was reported in [5]. Data collection time for UDS concentration was 8000 seconds in [9].

Baseline Simulation data

Existing simulations of waste retrieval in the literature used single and multiple-particle solid simulant. In single-particle studies, ZrO_2 with 6wt% in water was used in both scaled (43.2" and 120"-diameter) and full-size tanks. Data regarding HCL and UDS concentration were found in [1,4,12]. A simulation study using a four-particle simulant (Test 2013-1) was conducted by Rector et al. (2013, [9]) and information about UDS concentration, ECR, and cleaning radius were provided to FIU through private communications with WRPS. This simulation data was carefully reviewed to complete the information regarding problem setup which was not found in the literature and also to distinguish potentials for accuracy and performance improvements.

Results and Discussion

Preliminary Simulation Study of Erosion Conducted at FIU

In review of simulation studies of erosion, a number of numerical studies of sediment or wall erosion were found that used Eulerian-Eulerian and Eulerian-lagrangian approaches [14-23]. In some of these works, mesh on the sediment surface was updated within each time step to adapt to displacement of the sediment surface, which itself was modeled based on the erosion model. Examples of jet-induced erosion are in [12,16,17]. Some works calculated erosion rate on walls or sediment layers based on an erosion model and did not change the mesh or geometry of sediment [14,15,20,22,23]. In other works, no modeling was used for erosion and solid sediment surface was tracked by volume fraction scalar [18-19].

FIU conducted a preliminary study on capability of STAR-CCM+ in conducting jet-erosion simulation using a two-fluid model and without introducing any erosion modeling. In this study, sediment was considered a small region (fully packed with Aluminum particles of size 0.001 m) which was connected to a larger region (filled with water) through four interfaces. In the solid region, viscosity was set to ten times larger than the fluid viscosity to represent a region of higher flow resistance. The simulation was run for 60 seconds and results are shown in Figure 1. As this figure shows, it was possible to simulate erosion of the solid without any mesh deformation or modeling for erosion. However, more realistic timing could be obtained using calculated solid viscosity using granular temperature values.

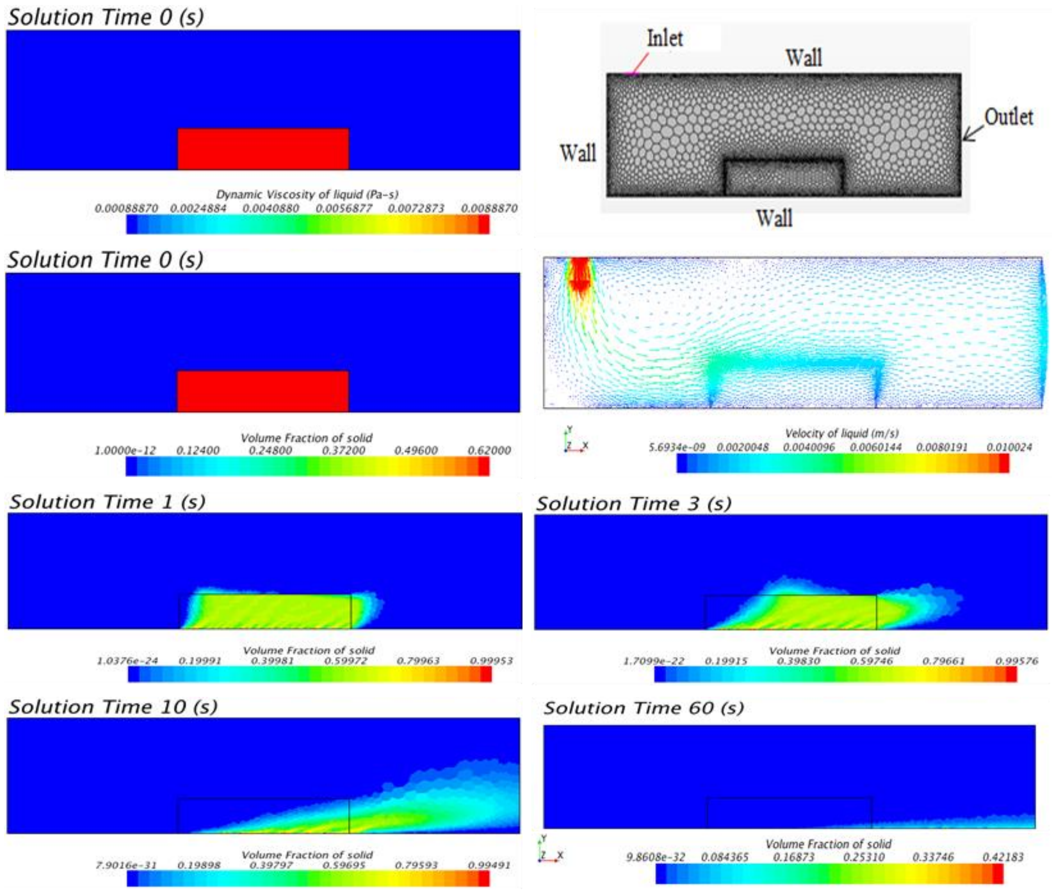

Figure 1. Evolution of Flow From 0 Sec To 60 Sec, Contour Of Solid Volume Fraction.

Summary

FIU obtained information regarding different metrics for various tests and simulations. These data can be used a basis for validation and verification of future simulations. Properties of different single and multi-component liquid and solid simulants along with dimensions of system elements and operating conditions were obtained. FIU engaged in discussions with WRPS to complete missing data and define cases that were relevant for startup of simulation studies.

As a conclusion remark, priority will focus on single particle simulation following test 2010. This simulation requires more information included in RPP-48358 report, which as of this date has not been obtained. The next step will be multi-component simulation according to the test 2013-1. For this purpose, critical shear stress will be calculated according [1]. For both these studies, a viscosity model with variable critical shear stress depending on solid content in slurry will be built using the mixture multiphase model. Also, use of pressure outlet at the transfer line intake and velocity inlet at the jet seem appropriate. In addition, the use of Star-CCM+ in direct simulation of erosion was demonstrated, this approach will be applied to future simulations of waste retrieval at FIU.

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