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(8) Research Objectives: Many highly radioactive wastes will be retrieved by installing mixer pumps that inject high-speed jets to stir up the sludge, saltcake, and supernatant liquid in the tank, blending them into a slurry. This slurry will then be pumped out of the tank into a waste treatment facility. Our objectives are to investigate interactions—chemical reactions, waste rheology, and slurry mixing—occurring during the retrieval operation and to provide a scientific basis for the waste retrieval decision-making process. Specific objectives are to

- Evaluate numerical modeling of chemically active, non-Newtonian tank waste mixing**,** coupled with chemical reactions and realistic rheology
- Conduct numerical modeling analysis of local and global mixing of non-Newtonian and Newtonian slurries
- Provide the bases to develop a scientifically justifiable, decision-making support tool for the tank waste retrieval operation.

(9) Research Progress and Implications: This report summarizes work done in 1.5 years of 3-year project.

(9.1) Yield strength of the waste: The chemically reactive, computational hydrodynamic code, TEMPEST, was modified to account for the yield strength of non-Newtonian tank waste sludge and saltcake that resist mobilization by mixer pump jets. The modified code was tested to model mobilization of sludge with and without yield strength. Test results showed that the 18-m/s slurry pump jets burrow into the sludge bank and erode only portions of the sludge where the shear and normal stresses acting on the sludge are greater than or equal to the sludge's yield strength. This modeling capability was used to assess pump jet mixing for Hanford Tank 401-AZ-102 and is now assisting in tank waste mixing test plans at Hanford. Once validated with the results of the Tank 401-AZ-101 mixer pump test, this added modeling capability could be used to determine how many pumps are needed to mobilize the tank waste, and, with a given number of pumps, how much and how fast tank waste will be mixed.

(9.2) Examine 2-D reactive transport simulation of tank waste: During mixing, the waste can undergo aqueous and solid dissolution/precipitation reactions. This phenomenon is being examined under four two-dimensional pump jet mixing setups: Newtonian and non-Newtonian wastes with and without chemical reactions having $NaNO_3$(s) and $NaNO_2$(s) dissolution during mixing. As shown in Figure 1, the study indicated that in addition to Newtonian and non-Newtonian rheology differences, dissolution of these solids changed the amount of the solids in the tank and the waste's physical properties and rheology, further affecting waste mixing.

(9.3) Examine realistic 3-D reactive transport simulation of tank waste: The TEMPEST code is being applied to more complex and realistic 3-D pump jet mixing with reactions of $NaNO_3$(s), $Na_2CO_3{\bullet}H_2O$(s), and Na_2SO_4(s) with aqueous species of Na^+ NO_3^-, $NaNO_3$(aq), OH^-, CO_3^{2-}, SO_4^{2-}, NO_2^-, $NaNO_2$(aq), H_2O, and $Al(OH)_4^-$. The results will be evaluated to examine interactions of chemical and hydrodynamic processes.

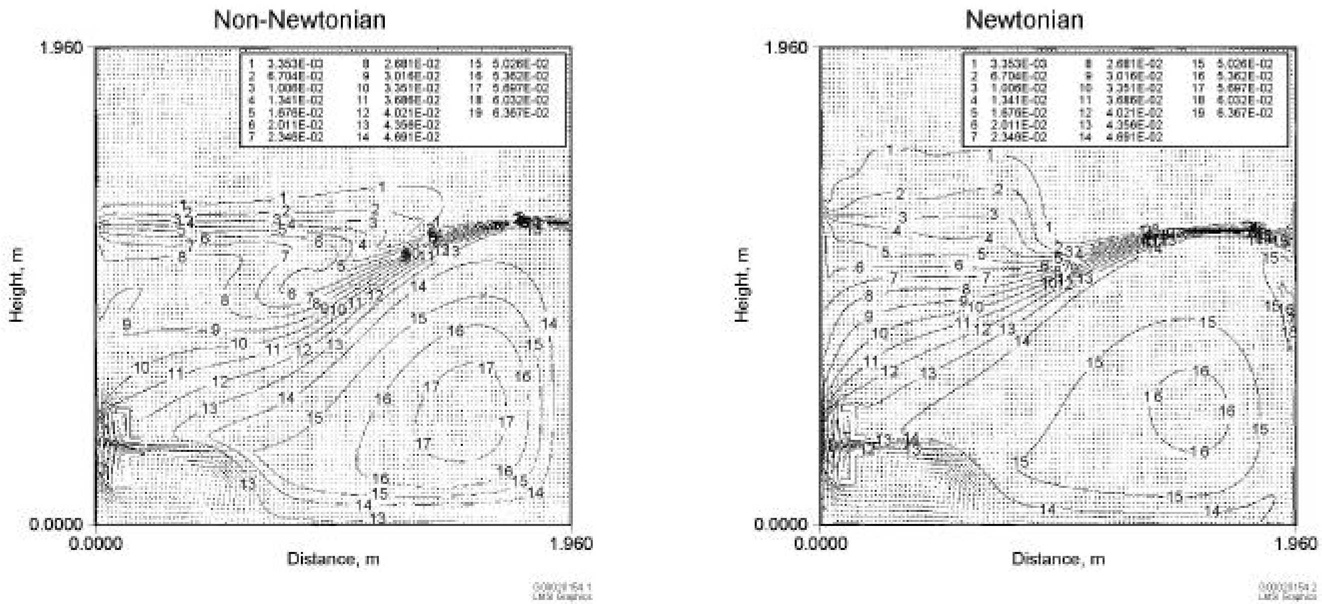

Figure 1. Predicted $NaNO_3$(s) distributions for 2-D Newtonian and non-Newtonian cases with chemical reactions at 20 simulation seconds

(9.4) Numerical modeling analysis of local and global mixing of non-Newtonian and Newtonian slurries. It is important to evaluate local areas of unwanted chemical reactions not anticipated from small-scale laboratory experiments or coupled reactive slurry modeling by TEMPEST with coarse resolution. Thus, we will use the 2-D velocity field predicted by TEMPEST (Sec. 9.2) to conduct numerical modeling analysis of local and global mixing of non-Newtonian and Newtonian slurries. We will use a line method that is an extension of the particle method with the particles redistributed on the line dynamically with each time step. From mixing analysis, the Newtonian medium revealed a greater amount of stretching than the non-Newtonian material, which offers a natural scale-dependent resistance to deformation, preventing efficient mixing at smaller length scales (see http://bobby.msi.umn.edu/mixing/).

(9.5) Gibbsite and boehmite interactions and their mixing: During waste retrieval operations, if boehmite were to form instead of gibbsite, the slurry would become a gel and would be impossible to retrieve from the tank waste. We are developing a hypothesis for gibbsite and boehmite interactions and their associated rheology changes. This concept will be incorporated into TEMPEST to test its validity under 1-D test cases.

(10) Planned Activities for Remainder of FY 2000 and FY 2001: We plan to continue to simulate coupled chemistry and mixing for tank waste for the 1-, 2- and 3-D test cases described above. Using the predicted velocity field obtained by TEMPEST, we will perform detailed local and global mixing for the 2-D cases. We will examine differences of mixing scales and degrees of Newtonian and non-Newtonian slurries and their implications on chemical reactions and slurry rheological changes. We will then compare these results with the coupled mixing and chemistry modeling results by TEMPEST, and we will use these findings to improve the scientific basis for developing retrieval operation decision-making support tools needed to determine the safety, design, and operational conditions of waste retrieval.

(11) Information Access

Onishi Y and DS Trent. 1999. "Mobilization Modeling of Erosion-Resisting Radioactive Tank Waste." *Proceedings of Rheology in the Mineral Industry II*. United Engineering Foundation, New York, pp. 45-56.

Onishi Y, DS Trent, TE Michener, JE Van Beek, and CA Rieck. 1999. "Simulation of Radioactive Tank Waste Mixing with Chemical Reactions." FEDSM99-7786, *Proceedings of 3rd ASME/JSME Joint Fluids Engineering Conference*, San Francisco.

Ten AA, YY Podladchikov, DA Yuen, TB Larsen, and AV Malevsky. 1998. "Comparison of mixing properties in convection with the particle-line method." *Geophys. Res. Lett.*, 25(16):3205-3208.

Ten AA, DA Yuen, and YY Podladchikov. 2000. *Electronic Geosciences*, in press.

http://bobby.msi.umn.edu/mixing/