

PNNL-36945

# Summary of Developing a Hanford Grout Modeling Framework Initial Workshop

October 2024

R. Matthew Asmussen

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R. Matthew Asmussen

Prepared for  
the U.S. Department of Energy  
under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory  
Richland, Washington 99354

## Summary

The “Development of the Hanford Grout Modeling Framework” project as part of the Network of National Laboratories for Environmental Management and Stewardship (NNLEMS) funding program is underway. An initial project team workshop was held in Richland, WA on June 4 and 5, 2024 with participants from PNNL, SRNL, SNL, WRPS and CRESO (VU and UCF). The workshop covered an overview of the current state of the art in grout modeling tools provided by the team. Based on a focus on liquid waste immobilization grout and encapsulation grout for solid wastes and tank closure grout at Hanford, the team identified preliminary conceptual models for these three applications which will be used to form the basis of the *Hanford Grout Modeling Framework*. The key processes that can drive mechanisms impacting the grout performance were identified for each test case. The programmatic plan was also identified with five core *Themes* being selected that will form the focus of the project. Within each theme, individual tasks for Year 1 were planned in support of the development of an updated *Hanford Grout Modeling Framework*. This report presents a summary of the information presented during the workshop.

## **Acknowledgments**

The workshop was sponsored by the project funding, and thanks are given to Ally Garza and Andy Ogrinc for planning support and to Shenyang Hu for technical review of this report and all team members for their participation.

## Abbreviations

Abbreviation	Definition
ACI	American Concrete Institute
BFS	blast furnace slag
CoPC	contaminant of potential concern
CRESP	Consortium for Risk Evaluation with Stakeholder Participation
DEF	delayed ettringite formation
DFLAW	Direct Feed Low-Activity Waste
DOE	US Department of Energy
EM	Environmental Management
FEM	finite element modeling
GCS	geochemical speciation in Orchestra
IDF	Hanford Integrated Disposal Facility
ILAW	immobilized low-activity waste
MS	mesoscale modeling
NNLEMS	Network of National Laboratories for Environmental Management and Stewardship
PA	performance assessment
PD	peridynamic modeling
PNNL	Pacific Northwest National Laboratory
RT	reactive transport modeling
SNL	Sandia National Laboratories
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
UCF	University of Central Florida
UHPG	ultra-high performance grout
VSF	variably saturated flow modeling
VU	Vanderbilt University
WRPS	Washington River Protection Solutions

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## 1.0 Introduction

This report has been prepared as a summary of the initial project workshop held in support of the “Developing a Hanford Grout Modeling Framework” project funded by the Network of National Laboratories for Environmental Management and Stewardship (NNLEMS) Roadmap program via the U.S. Department of Energy’s (DOE) Office of Environmental Management (EM). The workshop was held as a kick-off of programmatic efforts on the project, which included defining the initial conceptual models for grout at Hanford and developing five core themes as modeling targets in support of the *Hanford Grout Modeling Framework*. The *Hanford Grout Modeling Framework* will be integrated with flow and reactive transport software and made available to DOE, Hanford site contractors, and other interested parties. This report contains an overview of the project, a summary of the workshop, descriptions of the conceptual models proposed, and descriptions of the five core modeling themes.

### 1.1 Project Summary

Laboratory and field tests supporting the development of grouted waste forms and closure materials provide information for assessing the early aging and performance of such grouts and measuring important properties (e.g., leaching rates, physical stability) and to quantify intrinsic material parameters that control leaching of inorganic and some organic constituents. However, solely employing accelerated testing to model long-term performance can be limiting without the use of analogues. As such, numerical simulations and associated sensitivity cases have been relied on to predict grout performance over disposal time frames (beyond 100 years). Currently, the modeling of grouted waste forms (or other structural grouts) varies by site and application. The modeling used for grout at the Hanford Site (e.g., grouted secondary waste for the Integrated Disposal Facility [IDF] or tank closure) is simplistic due to prior data and computing limitations and as such calculations may be unnecessarily conservative related to the properties of the grout and predicted of the release of contaminants from grouts (e.g., radionuclides such as Tc-99 and I-129, regulated metals such as Cr, and chemical toxins such as nitrate). In the current modeling approach for the IDF, physical and chemical changes to the grout are handled via step function changes, resulting in overly conservative sensitivity cases. In turn, these unrealistically conservative results could limit evaluations of opportunities to implement grout in the mission or require extensive research and development (R&D) or risk mitigation that may not be needed. Continued conservative analyses of grout will limit the benefits to be gained in mission cost, duration, vitrification efficiency, worker safety, and long-term environmental management that have been projected to be realized from the expanded use of grout in the Hanford mission. The need to update and harmonize the modeling approach for grout materials at the Hanford Site to account for time-dependent processes (e.g., carbonation) that control bulk mechanisms (e.g., cracking) has been highlighted in several multi-lab reviews as a significant mission need (Asmussen et al. 2021, Bates 2022) and the need for improved grout modeling in PAs was identified in the NNLEMS Roadmap Concepts DL-3, TC-4, and TC-5 (NNLEMS 2022). This project is utilizing a multi-organization expert team to produce conceptual models for grout aging at Hanford that can be applied in PAs using a *Hanford Grout Modeling Framework*.

Updating the *Hanford Grout Modeling Framework* can facilitate more accurate performance projections of various grout formulations for both ongoing and future waste processing operations, enabling decision makers to pursue cost- and time-effective waste disposal strategies at the site, such as determining to dispose of a grout waste form off-site or on-site, or if specific wastes should be directed to vitrification or would be better candidates to be grouted. The project will also help to guide future formulation development by providing a better understanding of the long-term interactions of the multiple aging mechanisms and identifying what data needs to be collected on emerging grout materials while they are being developed to allow proper head-to-head assessments.

Implementing the *Hanford Grout Modeling Framework* will require developing a dynamic, reactive front conceptual model to better represent the aging processes of grout (including those used to model immobilized liquid wastes and encapsulated solid waste, and those used in other applications such as forming large enclosures such as tanks or structural fill grout). Grout aging processes include oxidation, carbonation, mineralogical evolution, reactive interfaces (e.g., tank walls and adjacent materials), which drive mechanisms that lead to material changes such as cracking. These processes can be coupled, and their effects can either accelerate contaminant release, for example through greater water exchange with the environment from cracking, or slow release by inducing chemical reactions or closing transport pathways (e.g., pore expansion or refinement due to carbonation).

This project is focused on three applications of grout in the Hanford mission: the immobilization of liquid wastes, the encapsulation of solid wastes, and the use of grout in tank closure. This project covers the four key developmental steps leading to a realistic conceptual model and modeling framework for grout aging and contaminant release at Hanford, which can be used to best inform decisions around expanded use of grout in the mission, decisions on areas to target for improvement, or to inform decision on disposal locations to use for grout waste forms (on-site vs. off-site):

1. *Conceptual model for the aging mechanisms of grout waste forms*: This conceptual model is a description of the aging mechanisms and their interactions as a dynamic, reactive front through the waste form. The conceptual model defines the processes of interest (e.g., controlling contaminant release or migration) that will be represented in the modeling framework and preliminary conceptual models are described within this report based on discussions during the workshop.
2. *Computational framework of grout aging (Hanford Grout Modeling Framework)*: The framework is composed of the equations and algorithms used to predict waste form behavior in PAs. These equations include numerical representations of the aging mechanisms identified in the conceptual model to compare against measured datasets in controlled lab conditions, field experiments, and analogues. The development of the *Hanford Grout Modeling Framework* will be supported by work in five themes that are described within this report based on workshop outcomes.
3. *Database of grout performance data*: To define the parameters and numerical representations to use in the *Hanford Grout Modeling Framework*, the data on grout currently available need to be accessible to developers and to future modeling efforts. This project will generate a database and design it in a manner that lends itself to future applications of machine learning (ML) techniques to grout behavior predictions.
4. *PA implementation of the Hanford Grout Modeling Framework*: The final goal of the project couples the refined and validated computational framework with the variably saturated flow and reactive transport models that support PA calculations at Hanford.

## 1.2 Workshop Details

The *Hanford Grout Modeling Framework* Workshop convened the project team with representatives from Pacific Northwest National Laboratory (PNNL), Savannah River National Laboratory (SRNL), Sandia National Laboratories (SNL), the Consortium for Risk Evaluation with Stakeholder Participation (CRESP: Vanderbilt University (VU) and University of Central Florida (UCF)), and Washington River Protection Solutions (WRPS). The two-day workshop was held June 4<sup>th</sup> and 5<sup>th</sup> in Richland, WA (PNNL). The list of attendees is given in Table 1. Day one of the workshop focused on overview discussions of the application of grout in the Hanford Mission and presentations from the subject matter experts on their unique modeling tools. The modeling tools were presented with their state of the art, prior applications in grout, cement, or waste forms and how the tool could contribute to

the *Hanford Grout Modeling Framework*. The second day focused first on the definition of the conceptual model for each of the three target grout applications and construction of the individual themes of the project for which modeling efforts will proceed. A summary of the discussion and planning from the workshop are presented in the proceeding sections.

Table 1 – List of Attendees for the Hanford Grout Modeling Framework Workshop

<b>Name</b>	<b>Organization</b>	<b>Name</b>	<b>Organization</b>
Alessandra Fujii Yamagata	Pacific Northwest National Laboratory	Nathaniel Adams	Washington River Protection Solutions
Chen Gruber	Vanderbilt University	Naveen Karri	Pacific Northwest National Laboratory
Christine Langton	Savannah River National Laboratory	Rodney Skeen	Washington River Protection Solutions
David Kosson	Vanderbilt University	Sarah Saslow	Pacific Northwest National Laboratory
Jeremey Trageser	Sandia National Laboratories	Sebastien Kerisit	Pacific Northwest National Laboratory
Jessica Rimsza (Virtual)	Sandia National Laboratories	Shenyang Hu	Pacific Northwest National Laboratory
Jiannan Chen	University of Central Florida	Suraj Rahmon	Pacific Northwest National Laboratory
Joelle Reiser	Pacific Northwest National Laboratory	Xiaonan Lu	Pacific Northwest National Laboratory
Jonathan Lapeyre	Pacific Northwest National Laboratory	Xuehang Song	Pacific Northwest National Laboratory
Kevin G. Brown (Virtual)	Vanderbilt University	Yilin Fang	Pacific Northwest National Laboratory
Matt Asmussen	Pacific Northwest National Laboratory		

## 2.0 Summary of Team Presentations

This section will provide overviews of the presentations given by the team members and the associated modeling tools to be incorporated in the project.

### 2.1 Hanford Overview and Modeling Framework – M. Asmussen

This introductory talk presented an overview of the Hanford mission focusing on the applications of grout. The three primary applications of grout presented can be grouped as the immobilization of liquid wastes, the encapsulation of solid wastes, and in filling of post-retrieved tanks; these three areas will be the focus of this project. A summary of the uses of grout in the Direct Feed Low-Activity Waste (DFLAW) mission at Hanford is shown in Figure 1.

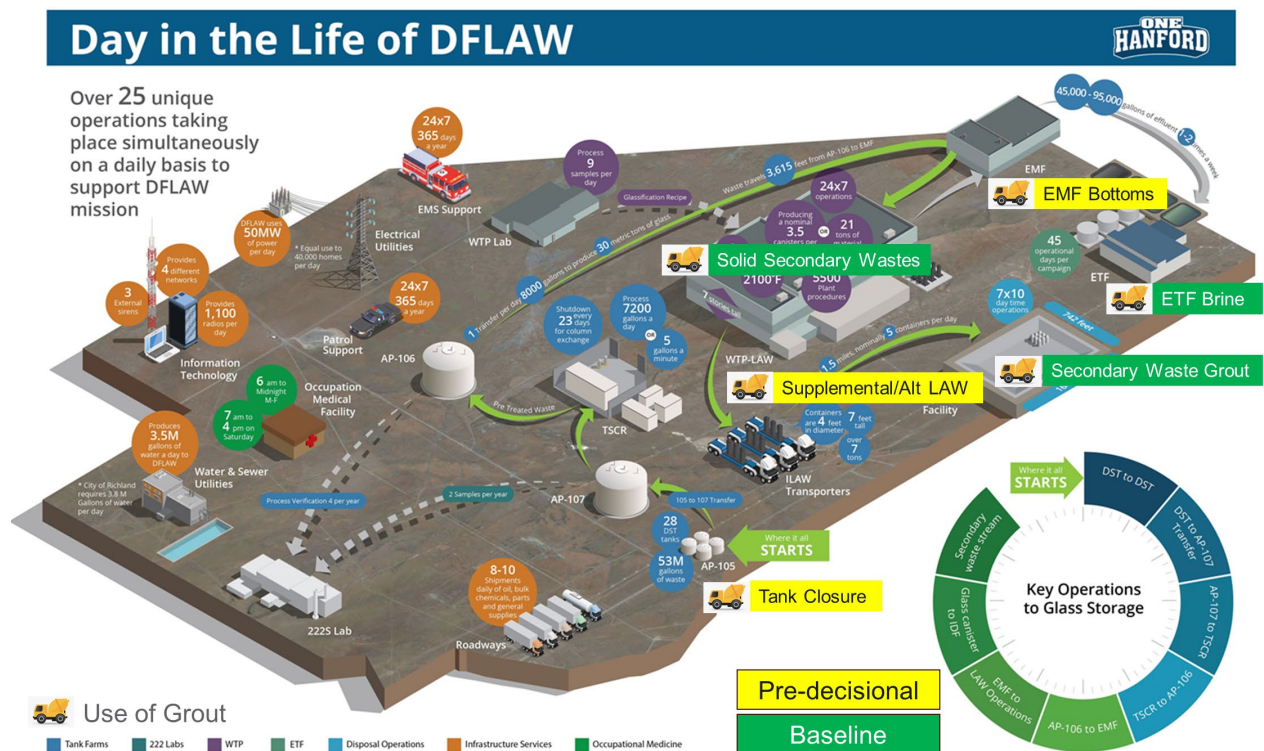


Figure 1 – Schematic showing the uses of grout, both baseline and pre-decisional, in the LAW treatment flowsheet.

### 2.2 Flow and Transport Modeling at Hanford – X. Song

The modeling of grout in PAs at Hanford (IDF, tank closure, subsurface remediation) is performed using reactive transport software. eSTOMP is the most well-established software platform for subsurface flow and multiple component reactive transport at Hanford. eSTOMP, developed by PNNL, has been widely used in programs involving waste form modeling (Fredman et al. 2016). The original version of the software used for the Hanford Site was STORM, which evolved to STOMP, allowing improved processing capabilities, and then eSTOMP, which allows coupling of different components. STOMP was used in the most recent IDF PA (coupled with GoldSim). eSTOMP was recently used to establish a

performance metric for grout in the IDF (Asmussen et al. 2019). This presentation covered the current uses of eSTOMP related to grout waste forms at Hanford.

### 2.3 Variable Saturated Flow Model for IDF – J. Chen

A full assessment of the disposal system containing grout waste forms is required, and having a comparative tool that directly links hydraulic conditions to waste form properties and disposal configurations in the facility would be highly beneficial for a more realistic PA. A variably saturated flow model using a finite element approach developed at University of Central Florida (using Seep/W and COMSOL Multiphysics software) was used to evaluate how hydrologic conditions and contaminant release in the IDF are influenced by the waste placement strategy and was covered in this presentation. This model has been used to study the hydraulic properties of backfill materials, arrangement of cementitious waste blocks, and degradation of the waste form (e.g., carbonation and oxidation of the cement in the waste form) (Chen et al. 2023). These assessments have been used to show that vertical alignment of the cementitious waste blocks and a more porous backfill within a disposal facility promote more rapid flow, shorter water-waste contact times and lower resulting contaminant release. A similar approach is currently being used to evaluate the hydrological conditions for the rate of contaminant release and carbonation of the single-shell tanks post-closure. This variable saturated flow model will be a crucial component for updating the *Hanford Grout Modeling Framework* in both capturing the impacts of mechanisms in the grout conceptual model and in the eventual full system performance modeling.

### 2.4 Saltstone Modeling – C. Langton

This presentation provided an overview of the modeling employed in the PA for the Saltstone Disposal Facility at the Savannah River Site (SRS). In the modeling of the saltstone waste form, a dynamic, reactive front model with input values specific to the saturated environment at SRS is used. First, the SRS model allows for time and spatial changes within the grout to be captured (in contrast to the step change approach used in Hanford modeling this model uses  $K_d$  step changes based on pore volume exchanges). For all species except Tc-99 and I-129, the hydraulic degradation (i.e., changes to the saturated hydraulic conductivity and the effective diffusion coefficients) is modeled using analytical solutions as a moving reactive front, with defensible assumptions to determine penetration rate coefficients (where corresponding data are currently being gathered in Hanford conditions in a lysimeter test). Using the penetration rate coefficients and the thickness of the saltstone monolith, the time required for conversion in various regions can be estimated. The properties of the grout are then changed only in the altered region, and the waste form interior retains the original properties.

Next, the chemical conditions ( $E_h$  and pH) of the saltstone matrix and the corresponding pore solution chemistry are estimated assuming chemical equilibrium, and these chemical conditions influence contaminant transport and release out of the waste form. Using an assumed mineralogical evolution and the assumed chemistry of SRS groundwater, a geochemical program, The Geochemists Workbench, is then used to estimate the number of pore volume exchanges required to influence changes in the  $E_h$  and pH of saltstone. Finally, flow of solution through the saltstone disposal units containing the saltstone waste form is simulated using near-field flow and transport models as implemented in PORFLOW (SRS, 2020).

For Tc-99 and I-129 releases, these transitions are applied to individual model nodes in PORFLOW, using an approach referred to as a “shrinking core model”. In the re-oxidation shrinking core model, dissolved oxygen migrates into saltstone and consumes the slag’s reducing capacity. The oxidized fraction of each cell is tracked through time accordingly, controlling the Tc-99 release.

## **2.5 IDF Solid Waste Form Simulations – D. Kosson**

This presentation provided an overview of recent work performed to develop models based on experimental data that allow for more accurate estimation of the release of constituents from grout waste forms under field conditions and efforts to model aging processes of grout. The specific objectives covered included the development of a geochemical speciation model accounting for solubility of constituents in grout waste forms and developing aging models for oxidation and carbonation of grout and assessing long-term leaching of radionuclides in field scenarios.

## **2.6 Geochemical Modeling for Waste Forms – S. Kerisit**

This presentation covered the modeling approach used to represent glass waste form corrosion using geochemical modeling. Geochemical modeling can develop, parameterize, and validate model forms to be used in simulations of waste form disposal and provides an excellent tool for verifying model frameworks against experimental data (e.g., laboratory tests, lysimeter tests). For example, automated approaches in PHREEQC have been developed in recent years (Kerisit et al. 2023) to accelerate the improvement of the immobilized low-activity waste (ILAW) glass corrosion model and its ability to accurately predict the long-term corrosion of low-activity waste glass in the IDF and replicate experimental data across various test conditions. These tools will be applied to grout modeling in this project, specifically in the dissolution of mineral phases in the grout.

## **2.7 Geochemical Speciation Modeling and Closure Behavior – C. Gruber**

The release of many species from grout waste forms is dictated by their speciation and needs to be captured in any modeling framework; the speciation can evolve during disposal timeframes. This presentation covered technical approaches developed by CRESO to carry out extensive geochemical speciation-based equilibrium and reactive transport modeling for cements, grout waste forms, and components thereof (Chen et al. 2021, Gruber et al. 2022). Equilibrium models typically include precipitation-dissolution, adsorption to mineral surfaces and solid organic matter, aqueous complexation, and activity coefficient models up to ionic strengths typical of pore water (up to 2 molar (Arnold et al. 2017)). Reactive transport models include diffusive and convective transport of water; ingress of reactive dissolved constituents and gases (sulfate, chloride, oxygen, carbon dioxide); and leaching of major and trace matrix constituents (radionuclides, metals, organic constituents) (Chen et al. 2021, Gruber et al. 2022). Specific applications have included grout waste forms (saltstone, Cast Stone (Chen et al. 2022)), single-shell tank integrity (Brown et al. 2013), mortars and concrete (Arnold et al. 2013), and a range of waste types (Van der Sloot et al. 2017). Examples were presented on modeling analogue cement samples and applicability to waste form behavior.

## **2.8 Mesoscale Modeling – S. Hu**

This presentation covered work performed in the Center for Hierarchical Waste Form Materials Energy Frontier Research Center, where the aim was to develop advanced nuclear waste form materials through advanced synthesis, characterization, and multiscale modeling. Specifically, PNNL efforts focused on developing a generic mesoscale model of ion exchange and leaching in multiphase porous structures. The model takes into account multi-physics coupling such as ion diffusion, interface reaction, porous media flow, elastic and electric interactions, phase transition, and microstructure evolution in a representative volume using a grout base case (geopolymer / zeolite particle composites) (Li et al. 2022b). During grout waste form aging, similar physics are expected, including diffusion in porous structures, microstructure change associated with oxidation and carbonation, deformation and cracking due to phase transition-induced volume change, leaching, and interface reaction (Li et al. 2022a). This multi-physics coupling

may be key to linking chemo-mechanical processes within the grout to bulk properties in the *Hanford Grout Modeling Framework*. The mesoscale modeling outputs are (1) the time and spatial evolution of species concentrations, stresses, and microstructures; (2) the effect of evolving microstructures on leaching kinetics; and (3) the effect of evolving microstructures on material properties such as effective diffusivity. These results can be directly compared with microstructures and material properties obtained from experiments. The mesoscale simulations can also generate huge virtual data of material performance and property degradation.

## **2.9 Peridynamic Modeling – J. Trageser**

This presentation covered the use of peridynamic modeling in cement and concrete research. Peridynamics is a particle-based fracture mechanisms method, which is ideally suited for systems that undergo brittle fracture and has been successfully applied for evaluation of cement fracture during decalcification and shrinkage (Jones et al. 2021). Based on prior work at SNL, a chemo-mechanical model that includes multiple aspects of materials aging, including degrading mechanical and fracture properties, reaction rates with the surrounding environment, and changes in porosity and/or shrinkage will be used by incorporating existing experimental data on laboratory leaching and aging. Through simulating relatively simple system geometries, uncertainty quantification on the impact of material aging on the stability of the grout will be bounded and will be used to guide further study and use of these materials.

## **2.10 Tank Integrity Modeling – N. Karri**

This presentation covered the use of a finite element analysis applied to model the structural integrity of the Hanford tanks. These analyses are utilized to evaluate the current integrity of the Hanford tanks and in eventual retrieval. The efforts evaluate the durability of the concrete and rebar comprising the tank superstructure, including integrity of the tank floor that experienced gravimetric and thermal loads over time.

## **2.11 Grout Database Development – S. Saslow and X. Lu**

To assess grout waste forms of various types in a model framework, a database presenting available data consistently is required. To date, information on the performance, aging, and degradation of waste forms relevant to Hanford is only present in individual reports/journal articles and a set of data packages supporting the 2017 IDF PA (which themselves only consider a small subset of samples). This presentation described an effort to be performed in this project to develop a comprehensive grout database. To facilitate future modeling updates (e.g., conceptual models, *Hanford Grout Modeling Framework*, PA simulations, predictive tools), a centralized database of grout data curated for general use must be developed. The database will also capture quality assurance status of the data to define use limits. Also, the database will be curated for use in future ML predictive model development for grout properties based on formulation and waste composition. The database will be based on an in-development database for glass properties.

## 3.0 Conceptual Models for Grout

### 3.1 Overview

The American Concrete Institute (ACI) defines durability as “*the ability of a material to resist weathering action, chemical attack, abrasion and other conditions of service*”.<sup>1</sup> Differing from concrete structures, waste form durability also includes the material’s ability to retain contaminants of potential concern (CoPC’s) (or in the case of tank closure with grout, impede exposure of residuals to infiltrating water). A durable waste form retains CoPCs to limit releases at a rate that is protective of the surrounding environment. Aging of grout waste forms may degrade the properties leading to accelerated release of CoPCs, but it could also improve other properties influencing CoPC retention. Prediction of grout behavior requires a comprehensive understanding of the different aging mechanisms that improve or degrade release of CoPCs. Such understanding would then lead to more carefully designed waste forms and disposal strategies that reduce the potential for identified significant degradation processes.

This section presents an overview of degradation mechanisms and processes expected to occur in the IDF or closed tank scenario that comprise the proposed conceptual models to be used in this project. Descriptions of the individual mechanisms and processes can be found in other relevant reviews (Pabalan et al. 2009, Asmussen et al. 2021). For this conceptual model development, the definitions of processes and mechanisms are:

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*Process: a material evolution or environmental interaction with the waste form matrix that causes a mechanism. These can be physical (e.g., freeze thaw) or chemical (e.g., oxidation) in nature.*

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*Mechanism: leads to a behavior or a bulk change in the waste form that is different from the unaltered state and projected aging. Examples include cracking or chemical changes to the radionuclides/CoPC.*

---

The different processes were considered for their relevant time frames and if the process was integral to grout integrity; if so the process would be included in the conceptual models as part of the *Hanford Grout Modeling Framework*. In the following sections, the grout applications and their associated conceptual model components are presented.

For each of the grout applications, a table summarizing the conceptual model component processes is presented. For each process, a shaded blue cell under a time frame indicates the process is relevant in said timeframe. Processes identified to be a component of the conceptual model, or key processes, are denoted in green with secondary processes denoted in yellow. Finally, the tools which can be used to evaluate the specific processes are listed. The summaries presented were assessed by the team during the workshop.

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<sup>1</sup> American Concrete Institute. 2021. Concrete Terminology. CTI-21. Available at: <https://www.concrete.org/store/productdetail.aspx?ItemID=CT21>

### 3.2 Liquid Waste Immobilization Conceptual Model

This application of grout is in the direct stabilization (or immobilization) of liquid waste streams. Here, the water in the liquid waste is used to activate the dry reagents and generate a final solidified waste form. The scenario considered in the Hanford grout modeling framework is one where the resulting waste form is emplaced in the IDF for disposal, Figure 2. The processes identified by the team to be most relevant to the performance of a liquid waste grout waste form are presented in Table 2.

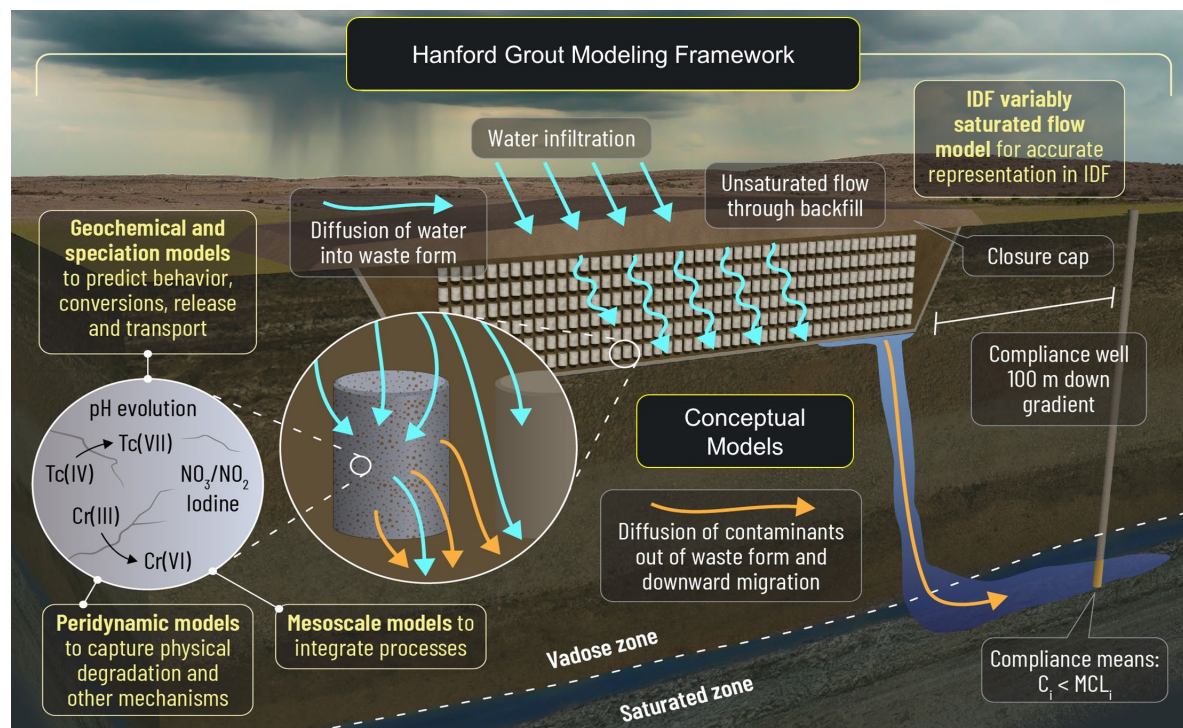


Figure 2 – Figure showing Hanford grout modeling framework and the IDF disposal concept for liquid waste grouts.

The key processes to comprise a conceptual model for liquid waste grout are as follows (in no order of priority). The project theme where the process will be evaluated is listed as well (see Section 4.0 for details):

**Moisture driven cracking:** a process by which moisture transport effects upon disposal in the arid Hanford environment could lead to cracking in a liquid waste grout. (Theme 2)

**Dimension:** a process by which shrinkage of the waste form leads to cracking. (Theme 4)

**Early exposure conditions:** prior to burial in the IDF, a liquid waste grout will experience various environmental factors including exposure to O<sub>2</sub> and CO<sub>2</sub>, which can alter the initial condition of the material prior to burial. (Theme 2)

**Carbonation:** a mechanism by which the pH of the liquid waste grout waste form can lower with time, driving mineralogical changes and physical property changes of the waste form. (Theme 3)

**Ca Leaching:** a mechanism by which the network making up the waste form matrix begins to alter due to leaching of the constituent phases. This mechanism is linked to carbonation. (Theme 2)

**Mineral Growth:** natural aging and contact with infiltrating water can drive mineralogical changes within the waste form that can be deleterious or beneficial to contaminant retention within a liquid waste grout. This includes delayed ettringite formation (DEF). (Theme 1)

**Moisture Transport:** The distribution of infiltrating water into the disposal facility and its behavior upon contacting a liquid will factor heavily in the aging processes and leaching of liquid waste grouts. (Theme 2)

**Oxidation:** Liquid waste grouts rely on maintaining reducing conditions in the waste form to limit the release of many contaminants and radionuclides. Therefore, the rate of oxidation of the material is a key process to predict long-term behavior. (Theme 3)

**Radionuclide/Contaminant Leaching:** The release of contaminants and radionuclides from liquid waste grouts can be dictated by the physical properties and localized chemistry within the waste form, and these factors need to be captured in a conceptual model. (Theme 3)

Secondary processes that will be considered in the project are:

**Early exposure conditions (temperature):** prior to burial in the IDF, a liquid waste grout will may experience environmental changes and freeze-thaw cycles in the open atmosphere, which could lead to the generation of cracks in the material. (Theme 4)

**Phase Segregation:** some liquid waste grouts (e.g., those prepared as geopolymers) may experience phase segregation or crystallization over time. (Theme 4)

**Sulfate attack:** a mechanism by which infiltrating sulfate can lead to expansion, cracking, and deterioration of a liquid waste grout due to mineral conversions. This mechanism is relevant to the high sulfate waste streams to be immobilized as grout. (Theme 3)

**Microbial:** The Hanford backfill and subsurface are home to microbes which can play a role in contaminant transport. While the likelihood of material degradation of liquid waste grouts via microbial activity is low, microbial activity can play a crucial role in determining contaminant transport in the near and far fields. It is unknown if the presence of organics or admixtures can drive enhanced activity. (Theme 3)

**Climate Change:** While direct effects of climate change cannot be predicted, sensitivity cases in modeling efforts should always be considered to identify impacts of possible climate changes (e.g., higher infiltration rates). (Theme 2)

Table 2 – Summary of the conceptual model component processes identified for liquid waste grouts. Blue represents a timeframe when the process is relevant, green is a key process to be included in the conceptual model while yellow is a secondary process which may be captured in specific cases for the conceptual model.

Mechanism	Process	Timeframe				Key Process	Tool(s)
		0 -1 year	> 1 year	1-50 years	>50 years		
Unaltered Evolution	Natural Processes						GC
Environmental Driven Cracking	Moisture Driven Cracking						PD/GCS
	Thermal Driven Cracking						
	Dimension Change (drying shrinkage)						PD/GCS/MS
	Early exposure conditions (atmosphere)						GCS/GC
	ASR					Only in vault/barrier	PD
	Steel Corrosion (outer package)						
	Phase Segregation (crystallization in GP matrix)						MS/RT/GC
	Rheological Properties						
	Creep						
	Wash-off/Bleed Effects						
Mineral Evolution/Cracking	Carbonation						GCS/RT
	Ca Leaching						GCS/RT/MS
	Sulfate Attack						GCS/RT
	DEF						GCS/RT/GC
	Mineral Growth						GCS/RT/GC
	Moisture Transport/Wet/Dry						VSF
Chemical/Waste Specific	Oxidation						GCS/RT/GC
	Radionuclide leaching						GC
	COPC Retention/leaching (org/LDR/solids)						GC
Environmental Changes	Microbial						RT
	Radiation						
	Extreme Heat						
	Acid Attack						
	Climate Change						RT (Sensitivity Case)

PD = peridynamics, MS = mesoscale, RT = reactive transport  
 GC = geochemical modeling GCS = geochemical speciation modeling , VSF = variable saturated flow

### 3.3 Solid Waste Encapsulation Grout

This application of grout is in the encapsulation (either microencapsulation/stabilization or macroencapsulation) of waste particulate or bulk solids, Figure 3. Here, a slurry is prepared then introduced to the solid waste. The grout functions to isolate the contaminated solid waste from infiltrating water and in some cases enhance binding of any released contaminants from the solids. The scenario considered in the *Hanford Grout Modeling Framework* is one where the resulting waste form is emplaced in the IDF for disposal. The focus of the formulations will be on ultra-high performance grout (UHPG) (Nichols and Kaplan 2021), paste, and mortar (Asmussen et al. 2020). The processes identified by the team to be most relevant to the performance of solid waste encapsulation grout waste form are presented in Table 3 and were influenced by a prior review on this waste form type (Asmussen et al. 2021).

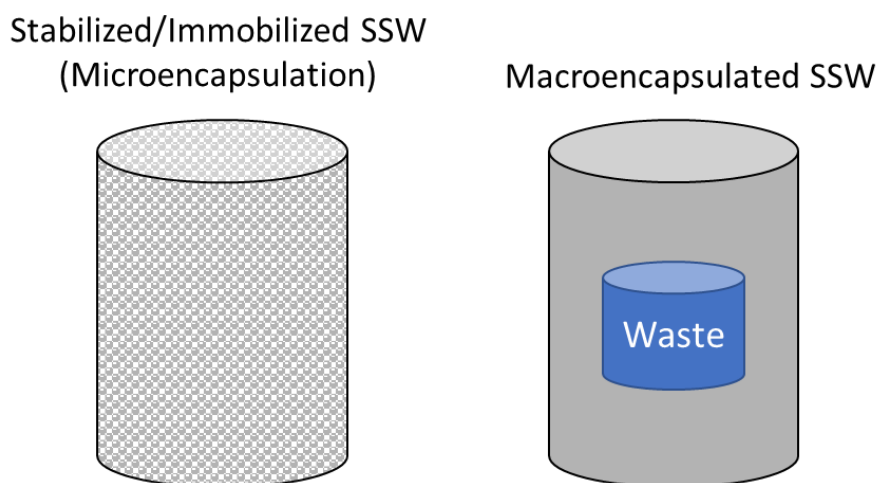


Figure 3 – Schematic showing the two types of encapsulation used for solid waste grouts.

The key processes to comprise a conceptual model for solid encapsulation grout were as follows (in no order of priority). The testing theme where the process will be evaluated is listed as well (See Section 4.0 for details):

**Moisture driven cracking:** a mechanism by which moisture transport effects upon disposal in the arid Hanford environment could lead to cracking in a solid waste encapsulation grout, including the reaction of unreacted cement. (Theme 2)

**Dimension Change:** a mechanism by which shrinkage of the waste form leads to cracking or the volume of the encapsulated solid changes over time. (Theme 4)

**Early exposure conditions:** prior to burial in the IDF, a solid waste encapsulation grout will experience various environmental factors including exposure to  $O_2$  and  $CO_2$  which can alter the initial condition of the material prior to burial. (Theme 2)

**Carbonation:** a mechanism by which the pH of the liquid waste grout waste form can lower with time, driving mineralogical changes and physical property changes of the waste form. (Theme 3)

**Ca Leaching:** a mechanism by which the network making up the waste form matrix begins to alter due to leaching of the constituent phases. This mechanism is linked to carbonation. (Theme 3)

**Mineral Growth:** natural aging and contact with infiltrating water can drive mineralogical changes within the waste form that can be deleterious or beneficial to contaminant retention within a solid waste encapsulation grout; including DEF. (Theme 1)

**Moisture Transport:** The distribution of infiltrating water into the disposal facility and its behavior upon contacting a liquid will factor heavily in the aging processes and leaching of solid encapsulation grouts. (Theme 2)

Secondary processes that will be considered in the project are:

**Early exposure conditions (temperature):** prior to burial in the IDF, a solid waste encapsulation grout may experience environmental changes and freeze-thaw cycles in the open atmosphere, which could lead to the generation of cracks in the material. (Theme 4)

**Oxidation:** Some solid waste encapsulation grouts are designed with reducing conditions in the waste form, however, is not a primary retention mechanism in these systems. (Theme 3)

**Radionuclide/Contaminant Leaching:** The release of contaminants and radionuclides from solid waste encapsulation grouts is more strongly influenced by the physical properties of the grout than by leaching from the solid waste material itself. Cracking would be a primary driver of radionuclide/contaminant transport. (Theme 3)

**Microbial:** The Hanford backfill and subsurface are home to microbes which can play a role in contaminant transport. While the likelihood of material degradation of solid waste encapsulation grouts via microbial activity is low, microbial activity can play a crucial role in determining contaminant transport in the near and far fields. It is unknown if the presence of organics or admixtures can drive enhanced activity. (Theme 3)

**Climate Change:** While direct effects of climate change cannot be predicted, sensitivity cases in modeling efforts should always be considered to identify impacts of possible climate changes (e.g., higher infiltration rates). (Theme 2)

Table 3 - Summary of the conceptual model component processes identified for solid waste encapsulation grouts. Blue represents a timeframe when the process is relevant, green is a key process to be included in the conceptual model while yellow is a secondary process which may be captured in specific cases for the conceptual model.

Mechanism	Process	Timeframe				Key Process	Tool(s)
		0 -1 year	> 1 year	1-50 years	>50 years		
Unaltered Evolution	Natural Processes	Blue	Blue	Blue	Blue		GC
Environmental Driven Cracking	Moisture Driven Cracking Sealing (UHPG)	Grey	Blue	Blue	Blue	Green	PD/GCS/MS
	Thermal Driven Cracking	Blue	Grey	Grey	Grey		
	Dimension Change	Blue	Blue	Blue	Blue	Green	PD/GCS/MS
	Environmental Exposure	Blue	Blue	Blue	Grey	Green	GCS/GC
	ASR	Grey	Grey	Grey	Blue		
	Steel Corrosion (Outer package/fibers)	Blue	Blue	Blue	Blue		
	Phase Segregation	Blue	Grey	Grey	Grey		
	Rheological Properties	Blue	Grey	Grey	Grey		
	Creep	Grey	Grey	Grey	Blue		
	Scaling	Grey	Grey	Grey	Blue		
Mineral Evolution/Cracking	Carbonation	Grey	Blue	Blue	Blue	Green	GCS/RT
	Ca Leaching	Grey	Blue	Blue	Blue	Green	GCS/RT/MS
	Sulfate Attack	Grey	Blue	Blue	Blue		
	DEF	Grey	Blue	Blue	Blue	Green	GCS/RT/GC
	Mineral Growth	Blue	Blue	Blue	Blue	Green	GCS/RT/GC
	Moisture Transport/Wet/Dry	Blue	Blue	Blue	Blue	Green	VSF
Chemical/Waste Specific	Oxidation	Blue	Blue	Blue	Blue	Yellow	GCS/RT/VSF
	Radionuclide leaching	Blue	Blue	Blue	Blue	Yellow	PD/GC
	COPC Retention/leaching (org/LDR/solids)	Blue	Blue	Blue	Blue	Yellow	PD/GC
Environmental Changes	Microbial	Grey	Grey	Grey	Blue	Yellow	RT
	Radiation	Blue	Blue	Blue	Blue		
	Extreme Heat	Blue	Blue	Blue	Blue		
	Acid Attack	Blue	Blue	Blue	Blue		
	Climate Change	Grey	Grey	Grey	Blue	Yellow	RT (Sensitivity cases)

### 3.4 Tank Closure Grout

This pre-decisional application of grout is the bulk filling of retrieved tanks for closure. Here the grout would be poured into the tank following the conclusion of retrieval activities and rests on top of any solids remaining in the tank. The grout functions to provide structural fill to the tank void space and limit ingress of water to the residuals, which in-turn can limit release of contaminants and radionuclides to the subsurface. A schematic of a closed tank farm is presented in Figure 4. The processes and mechanisms identified by the team to be most relevant to the performance of tank closure grout are presented in and were influenced by a prior review on closure grout (Pabalan et al. 2009).

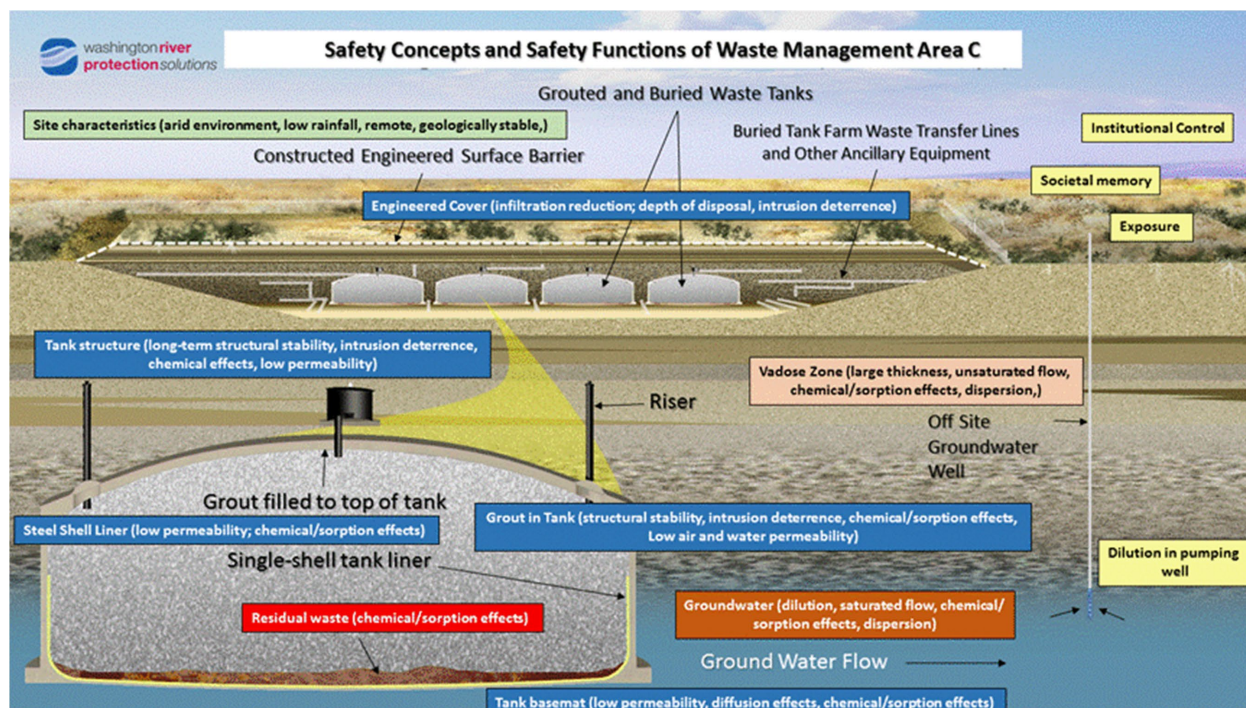


Figure 4 – Schematic showing a closed tank farm at Hanford (Mehta et al. 2016)

The key processes to comprise a conceptual model for tank closure were as following (in no order of priority). The testing theme where the process will be evaluated is listed as well:

**Thermally driven cracking:** a process by which the thermal history of the existing concrete structures or thermal history of the grout upon emplacement lead to changes in the initial condition of the structures; including extreme heat events. (Theme 4)

**Steel Corrosion:** a process that involves the imbedded steel rebar in the tank superstructure corroding and leading to changes in the immediate vicinity of the rebar. This process can also apply to the steel infrastructure (e.g., risers, pipes) within the closed tank. (Theme 4)

**Carbonation:** a mechanism by which the pH of the emplaced grout or concrete structure can lower with time, driving mineralogical changes and physical property changes of the matrix. (Theme 2)

**Ca Leaching:** a mechanism by which the network making up the grout matrix begins to alter due to leaching of the constituent phases. This mechanism is linked to carbonation. (Theme 3)

**Moisture Transport:** The distribution of infiltrating water into the closed tank and its behavior upon contacting the closure will factor heavily in the aging processes and migration toward residuals. This process includes any hydraulic head that may be present during emplacement. (Theme 2)

**Radionuclide/Contaminant Leaching:** The release of contaminants and radionuclides from the residuals (or, if any inventory is present in the concrete superstructure, from waste leaks) is a key driver in closure PAs. The release is dictated by both the initial condition of the radionuclides/contaminants and by the interfacial behavior between the grout and residuals. (Theme 3)

Secondary mechanisms that will be considered in the project are:

**Oxidation:** Oxidation is relevant in tank closure only if an amendment (e.g., Fe) is placed in the first layer of grout to interact with the residuals and impede release. (Theme 2)

**Microbial:** The Hanford backfill and subsurface are home to microbes which can play a role in contaminant transport. While the likelihood of material degradation of solid waste encapsulation grouts via microbial activity is low, microbial activity can play a crucial role in determining contaminant transport in the near and far fields. It is unknown if the presence of organics or admixtures can drive enhanced activity. (Theme 3)

**Climate Change:** While direct effects of climate change cannot be predicted, sensitivity cases in modeling efforts should always be considered to identify impacts of possible climate changes (e.g., higher infiltration rates). (Theme 2)

Table 4 - Summary of the conceptual model component processes identified for tank closure grouts.

Mechanism	Process	Timeframe					Key Processes	Model Tool(s)
		Pre-condition	Operations					
		<50 to 0 year	0 -1 year	> 1 year	1-50 years	>50 years		
Unaltered Evolution	Natural Processes							
Environmental Driven Cracking	Moisture Driven Processes (Drying/Seasonal)						VSF/GCS/MS	
	Thermal Driven Cracking/Shrinkage						GCS/MS/FEM	
	Dimension Change (Shrinkage, Long-term)							
	Freeze Thaw							
	ASR							
	Steel Corrosion (Rebar)						GCS	
	Phase Segregation							
	Processing Condition (Rheological/Shrinkage)							
	Creep							
	Scaling							
Mineral Evolution/Cracking	Carbonation						GCS/MS	
	Ca Leaching						GCS/MS	
	Sulfate Attack							
	DEF							
	Mineral Growth							
	Moisture Transport/Wet/Dry						VSF	
	Saturation and Hydraulic Head (spatially)							
Chemical/Waste Specific	Oxidation						GCS/RT	
	Radionuclide leaching						GCS/RT	
	COPC Leaching (Interface of grout/residual)							
Environmental Changes	Microbial							
	Radiation							
	Extreme Heat						PD	
	Acid Attack							
	Climate Change						RT (Sensitivity cases)	

## 4.0 Project Direction

Based on the conceptual models described in Section 3.0 for each of the grout applications, the team members developed a set of focus themes required to develop the *Hanford Grout Modeling Framework*. Each of the themes contains a number of specific tasks to mature modeling tools, incorporate processes into the modeling of grout at Hanford, and improve the predictive capability of grout degradation and release models. The preliminary list of tasks presented here will be pursued in Year 1 of the project but is subject to change based on team discussions as work progresses. The findings of Year 1 will be compiled in a Guidance Report targeted for issue in April 2025.

### 4.1 Theme 1 – Grout Mineralogy

Cementitious materials, and other ambient temperature-formed materials, are comprised of complex mineral assemblages that dictate material properties. During their lifetimes, these mineral assemblages evolve through hydration processes, conversion to other phases, or dissolution based on environmental exposures. These mineral growth and conversion processes are integral in determining the properties of grouts during their service and disposal lifetimes, as such they were identified as key conceptual model processes for the liquid waste grouts and solid waste encapsulation grouts. In current Hanford grout modeling, the mineral assemblages are based on cured compositions (i.e., early life from X-ray diffraction, XRD) and the phases can only dissolve through kinetic reactions. The databases used to assign these mineral properties in current Hanford modeling are also not designed for cementitious material use. As such, Theme 1 was composed to update the handling of mineral evolutions in Hanford grout modeling. Two tasks are currently planned:

#### 4.1.1 Theme 1 – Task 1 Hanford Mineral Network

This task will focus on updating the handling of mineral phases within grout modeling of Hanford systems. The first effort will be placed on updating the databases used to define the thermodynamic and chemical properties of assigned mineral phases and move towards an equilibrium phase-based approach, where appropriate. The CEMDATA-18 database (Lothenbach et al. 2019), that has been developed specifically for hydrated Portland, calcium aluminate, calcium sulfoaluminate and blended cements, as well as for alkali-activated materials, will be incorporated into eSTOMP modeling. The database includes thermodynamic properties determined from various experimental data published in recent years, compared with the existing mineral network from the Lawrence Berkeley National Laboratory database designed specifically for subsurface. This database will allow reactive and phase transitions to be captured through an equilibrium approach. The CEMDATA-18 database will be incorporated either through PHREEQC or Leachxs-ORCHESTRA where phase evolution is calculated at each time step.

The second effort in this task will involve defining a mineral reaction network for the near-field region of grout waste forms in the IDF. Similar to glass dissolution, where an incongruent dissolution reaction (IDR) network is utilized, the team plans to generate a similar network for grout (Neeway et al. 2023).

The activity is led by PNNL with support from CRESP (VU).

#### 4.1.2 Theme 1 Task 2 – Geochemical Modeling of Reactive Grout Phases

Within grout waste forms, unreacted reagents can commonly be found, and their continued hydration can drive mineral changes. One reagent's evolution is of particular interest: blast furnace slag (BFS). BFS is a supplementary cementitious material that is involved in the core hydration reactions forming the

solidified grout; but most importantly it provides reduction capacity to suppress the release of redox sensitive contaminants and radionuclides (e.g., Cr and Tc). BFS is an amorphous material (glassy) that is ground for use in the cement industry but retains its glassy features. Within grouts glass particles remain in the cured material, Figure 5. As time progresses these particles will continually react, releasing reduction capacity at a currently unknown rate. This task will focus on applying glass dissolution models developed for Hanford and applying them to predict slag glass dissolution rates within cured grout waste forms. Identifying and building tools to assess these conversion rates will help support predictive capability for oxidation rates of grout waste forms.

This task will be led by PNNL with support from SRNL.

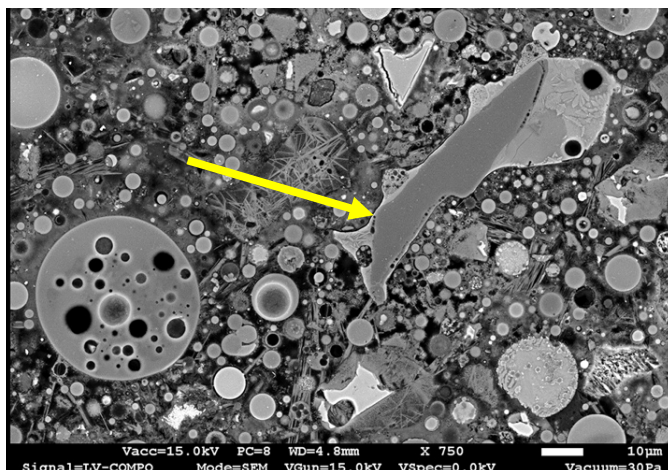


Figure 5 – Electron micrograph showing the presence of a slag glass particle within a cured Cast Stone matrix (Asmussen et al. 2020).

## 4.2 Theme 2 – Dynamic Modeling of Moisture Driven Processes

As discussed previously, a significant limitation of the modeling of grout currently applied at Hanford is the lack of dynamic processes occurring within the grout and disposal facility. This theme was designed to directly address this limitation but adapting contemporary tools for use in predictive modeling for Hanford grouts. A specific focus will be placed on moisture behavior both in the disposal facility and around waste forms coupled with the rate of key processes (e.g., oxidation, carbonation) in confirmed porous geometries of grout.

### 4.2.1 Theme 2 – Task 1 – Integration of variable saturated flow modeling to eSTOMP

This task will focus on integrating the recent developments of variably saturated flow and transport modeling into the existing eSTOMP construct used at Hanford. The current approach at Hanford assumes a constant infiltration rate that is not affected by seasons or position in the IDF. The variably saturated flow model that has been developed shows that, within the IDF or in a closed tank scenario, there will be large variations in the degree of saturation across the IDF. This means the water flux near individual waste forms will vary based on their position within the IDF, and the release of contaminants from the grout (or rate of processes such as oxidation) will vary spatially. In other words, the current projections using constant infiltrating and wetting are overly conservative. In Year 1, a 2-D representation of the IDF

will first be constructed in eSTOMP, then simulations will be performed to benchmark against those produced by the variably saturated flow models. Refinements will be performed as necessary. Benchmarking will also be performed using data from the PNNL field lysimeter test.

This task will be a collaborative effort between PNNL and CRESP (UCF).

#### 4.2.2 Theme 2 – Task 2 – Maturation of Geochemical Speciation Models for Hanford Grouts

Geochemical modeling has been successfully applied in recent years to replicate the aging processes seen in natural cement samples from arid environments similar to Hanford. These studies have been expanded to assess the aging processes of closure grout scenarios in Hanford single shell tanks and coupled with hydrologic modeling. This task will build on these advancements to apply similar modeling of aging processes to grout waste forms in IDF disposal. Initial efforts in Year 1 will focus on 2-3 specific grout examples where appropriate data is available (e.g., Cast Stone, hydrated lime grout), followed by efforts to integrate into eSTOMP and the Hanford grout modeling framework.

This task will be led by CRESP (VU).

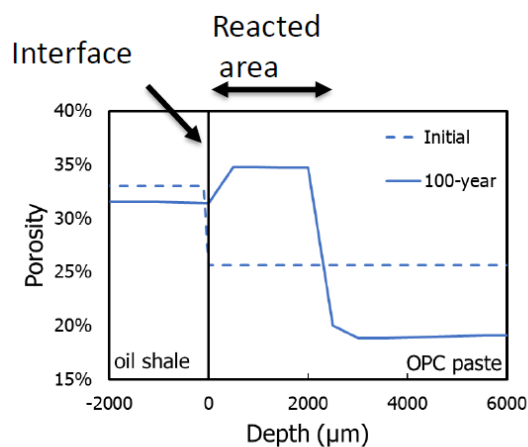


Figure 6 – Example of simulation for porosity changes in natural cement sample from an arid environment showing projected changes over 100 years (Presented by C. Gruber at workshop).

#### 4.2.3 Theme 2 – Task 3 – Evaluation of Moisture Transport Using Mesoscale Models

This task will mature mesoscale models to assess moisture transport within the pore space of cementitious waste form and materials. It will begin in Year 2 after the mesoscale models of grout systems have been constructed and can be used to assess chemo-mechanical links between physical properties of the grout matrix and long-term transport processes.

This task will be led by PNNL.

### 4.3 Theme 3 – Dynamic Modeling of Processes Impacting Contaminant and Radionuclide Behavior

#### 4.3.1 Theme 3 Task 1 – Application of Geochemical Speciation Modeling to Other Hanford Grout Examples

In the development of the geochemical speciation models for grout, a Hanford specific test case was evaluated using Cast Stone fabricated using a liquid secondary waste simulant, Figure 7. This work showed that the geochemical speciation model was able to replicate the release behavior of a multitude of elements from the grout, including Tc-99 (Chen et al. 2021). A geochemical speciation component to the *Hanford Grout Modeling Framework* will likely improve the fidelity of contaminant releases, but further assessment against grout datasets is required. This prior developmental work will be expanded to assess the predictive capability of the geochemical speciation model against other Hanford grout datasets. In Year 1, this will involve performing geochemical speciation modeling on 2-3 relevant Hanford systems where sufficient data exists (e.g., hydrated lime-based grout, getter-containing grouts).

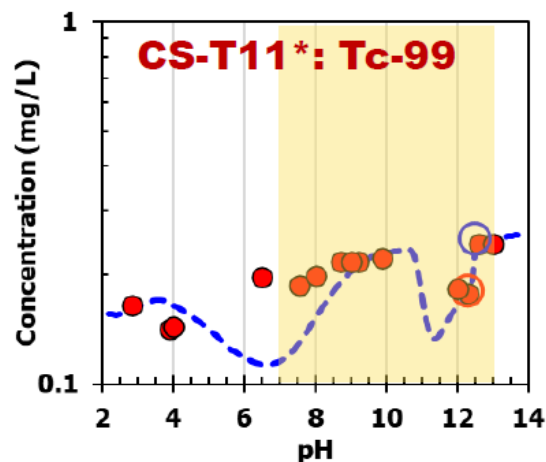


Figure 7 – Example of the predictive capability of the geochemical speciation model for the release of Tc-99 from grout.

This task will be led by CRESP (VU).

#### 4.3.2 Theme 3 Task 2 - Integration of Oxidation and Carbonation Processes with Existing Models

In both the SRS PA and in geochemical speciation modeling, two of the main processes as part of the grout conceptual models, oxidation and carbonation, are evaluated dynamically. However, as stated previously, in the modeling of grout at Hanford these processes are not captured as dynamic processes. This task is focused on remediating this significant gap by developing approaches to model these two processes in Hanford relevant materials and disposal environments. Year 1 will focus on two components. First, the integration of oxidation and carbonation processes into grout waste forms using eSTOMP will be evaluated by incorporating the approach used at SRS. The second component will focus on the integration between the existing reactive transport models and the assessments done to date on the carbonation and oxidation of grouts using geochemical modeling.

This task will be a joint effort between PNNL and CRESP (VU).

#### 4.3.3 Theme 3 Task 3 – Contaminant Interactions with Microbial Processes

Within the Hanford subsurface a range of microbial processes can lead to natural attenuation of contaminants. One such contaminant is nitrate, a major component of LAW (Asmussen et al. 2024). Microbial conversion rates for nitrate (and nitrite) are available from prior subsurface models. This task in Year 1 will perform an evaluation of the impact of nitrate conversion on the overall impact to groundwater from a grouted inventory of LAW in the IDF.

This task will be performed by PNNL.

#### **4.3.4 Theme 3 Task 4 – The Interactions Between Grouts and Waste Solids**

This task will perform a data gathering on the interactions between grouts and Hanford tank waste solids. In the grouting of tanks for closure, the grout will directly interact with the residual solids. The composition of the solids will vary by tank. To assess if any chemistry-specific interactions should be built into the Hanford grout modeling framework, this task will perform a literature review of possible interactions in Year 1, and if confirmed, will integrate these interactions into the Hanford grout modeling framework in Year 2.

This task will be led by PNNL with support from WRPS.

### **4.4 Theme 4 – Modeling of Cracking in Grout**

#### **4.4.1 Theme 4 – Task 1 – Peridynamic Modeling**

Cracking remains the prominent mechanism that can drive failure of grout and can be caused by several processes. Yet, predicting and representing cracking in grouts remains a challenge, and rarely pursued for grouts used in waste management applications. Peridynamics (PD) modeling has potentially beneficial features for the modeling of grouts used in waste disposal such as ease of implementation and an intrinsic ability to represent brittle fracture, which makes this effort distinct from previously employed classical continuum methodologies. With the success of PD application to the aging of hardened cement pastes (Jones et al. 2021), this task will be focused on a novel effort integrating peridynamic modeling into the prediction of physical properties of grouts used in waste management. Year 1 will be focused on constructing first-of-their-kind peridynamic models for Hanford applications. The first test case will involve developing peridynamic models of Hanford tank floors that have experienced varied thermal histories then will expand to the properties of tank closure grouts (due to their similarities to concretes previously assessed with PD). This work will then target waste grouts in Year 2. This work will also leverage the finite element modeling used in Hanford tank integrity models.

This task will be led by SNL with support from SRNL and PNNL.

#### **4.4.2 Theme 4 – Task 2 – Maturation of Mesoscale Models for Hanford Grout**

As grouts age, there will be spatial changes in the bulk material properties due to natural evolution of hydration products and interactions with the near-field environment. These bulk properties can directly impact the release behavior of contaminants from the grout. One key property is the porosity of the grout as this dictates the flow of water within the grout, and hence, the flow of contaminants from the grout. This concept is the basis of the use of UHPG for waste encapsulation. While the geochemical modeling targeted in Theme 2 Task 2 can calculate properties such as porosity and tortuosity changes, the micro-scale features of the porous grout network (e.g., connectivity) are not replicated. And as such there remains a gap in the link between the grout's chemo-mechanical processes occurring on the microscale and the bulk properties. This task aims to begin to bridge this fundamental gap in grout modeling by constructing mesoscale models of selected grout systems (e.g., Cast Stone, UHPG) and assessing conversions between cured and aged samples. Year 1 efforts will be focused on constructing the mesoscale models of waste grouts for the first time using grouted Ag-zeolites as a test case. Future work may focus on capillary effects or evolution of cracks.

This task will be led by PNNL with support from SRNL.

## 4.5 Theme 5 – Grout Database

As described in Section 2.11, this task will assemble a central resource for Hanford grout properties from the literature and prior reports. The database to be designed and developed in Year 1 will be based on an in-progress online database for glass properties. A similar online interface to the glass database will be used (see Figure 8). The goals of this effort are to provide a centralized reference for grout data to support modeling efforts, identify significant data gaps for key processes that require further R&D to fill, and potentially develop, machine learning assessments for predictions of grout properties.

This task will be led by PNNL for database construct development with support from all partners.

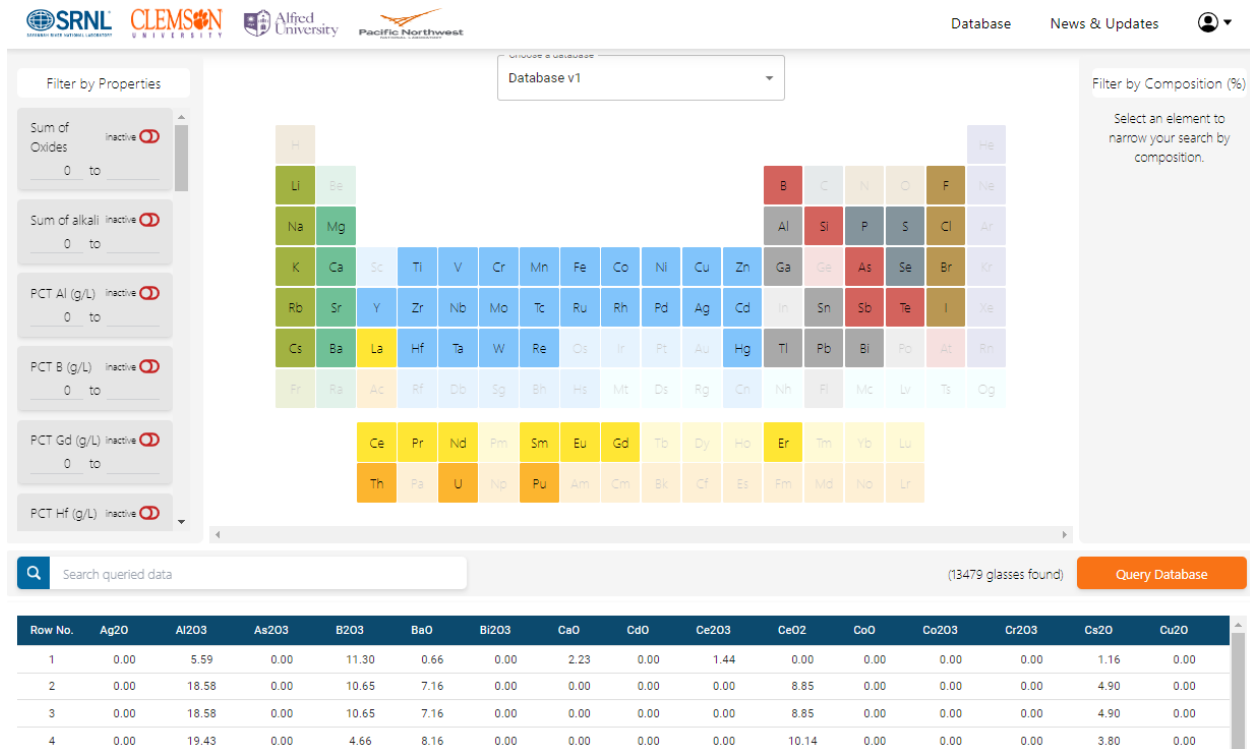


Figure 8 – Example online interface of the glass property database that will be utilized in this work.

## 5.0 Summary

In summary, the “Development of the Hanford Grout Modeling Framework” project as part of the NNLEMS program is underway. An initial project team workshop was held in Richland, WA on June 4<sup>th</sup> and 5<sup>th</sup>, 2024 with participants from PNNL, SRNL, SNL, WRPS and CRESO (VU and UCF). The workshop covered an overview of the current state of the art in grout modeling tools provided by the team. Based on a focus on liquid waste immobilization grout, encapsulation grout for solid wastes and tank closure grout at Hanford the team identified preliminary conceptual models for these three applications. The key processes that can drive mechanisms impacting the grout performance were identified for each test case. The programmatic plan was also identified with five core *Themes* being selected that will form the focus of the project. Within each theme individual tasks for Year 1 were planned in support of the development of an updated *Hanford Grout Modeling Framework*.

## 6.0 References

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