

Liquid Waste Model Overview and Demonstration

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- **Purpose of the presentation**
- **What is modeling?**
- **How are models used?**
- **Introduction to current SRMC models**

The purpose of this presentation is to introduce the CAB to the concept of modeling and to introduce the CAB to the models being developed by SRMC and our teaming subcontractor DBD

A model is a program that runs on a computer that creates a digital representation, or simulation, of the real-world

“Outputs from computer models are used to create tables, charts, and schedules that are published in the System Plan and inform annual budget requests for cleanup activities.”*

Computer modeling allows SRMC to conduct thousands of simulated lifecycle scenarios by computer. The thousands of computer scenarios identify a handful of process or facility improvements that are most likely to accelerate the Liquid Waste mission.

❖ Nuclear Engineering

Front end engineering solutions to regulated industries.
De-risking engineering projects with our tools, technique and experience

❖ Mission Optimization

Providing digital tools and platforms to simplify key decisions and optimize our clients' complex missions.
Maximizing the value of clients existing data

❖ Safety and Assurance

Mitigating risk in the decommissioning of legacy nuclear sites.
Providing assurance to projects which keep the UK safe and secure.

Modeling Successes

❖ Dounreay – Site Closure Optimization and Risk Reduction

Re-structuring and streamlining a complex project plan to achieve site decommissioning in reduced time and at reduced cost, through automated task prioritization.

❖ Idaho AMWTP – Multi-stream Optimization

Speeding up a complex facility with many process lines, by utilizing all of the process lines more efficiently and reducing overall plant downtime, by coordinating repairs and shutdowns.

❖ AWE – Waste Repackaging and Relocation

Relocating schedule for waste material from an old storage facility to a new purpose-built one, safely, and in a timely fashion that removed the need to re-assure the safety of the old facility.

❖ Sellafield – Effluent, Sludge and HAW Treatment

Improving a wide range of chemical engineered processes including aqueous effluent treatment, chemically-reactive sludge management and waste vitrification processing.

❖ Strategic Petroleum Reserve – Cavern Management

Linking chemistry models of petroleum prediction, through engineering cavern management to financial modeling of gasoline sales to benefit US government and taxpayers.

Models Being Developed



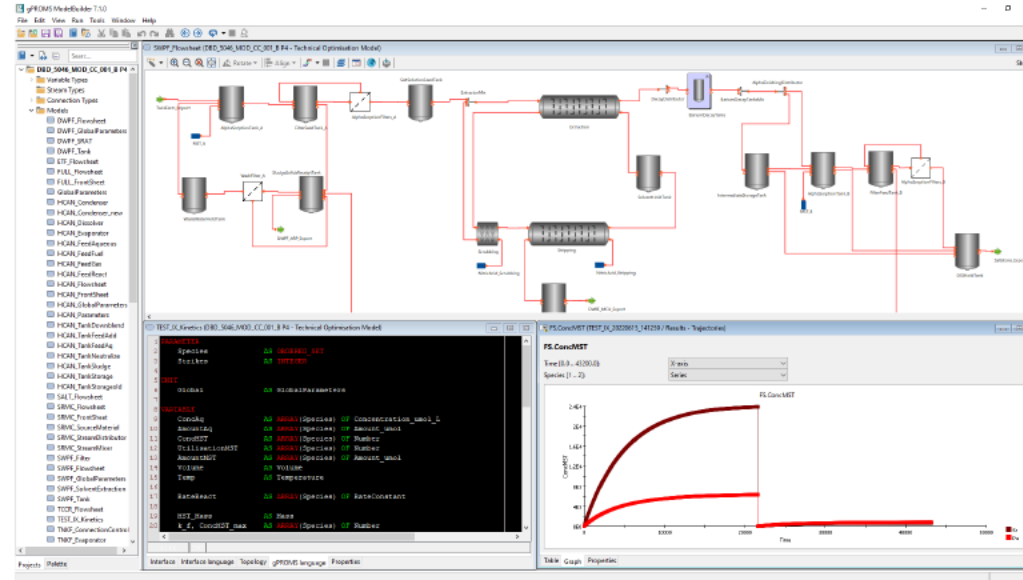
Two models are currently in development:

- 1. Technical Optimization Model (Process Chemistry)**
- 2. Process Optimization Model (Operations Research)**

Technical Optimization Model: TOM

Simulates Fluid Flow & Chemistry
Utilizes software called gPROMS

Fundamental chemical
engineering, first
principles theory



Specific Liquid
Waste processing
information

SRNL experimental
data

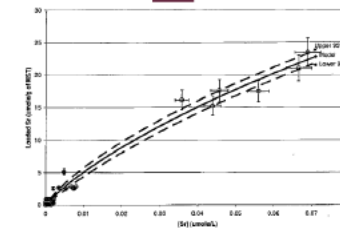


Figure 4. The Dubinin-Astakhov model predictions for the Sr loading data at 25 °C. The confidence limits are for the mean response. Please note the error bars on the data.

The corresponding DA equation for strontium at 25 °C follows. The "a" terms in the equations represent the standard error for the parameters.

$$4) \text{ Loaded Sr} = 22 \pm 19 \times \exp \left[-2.3 \pm 0.9 \times 10^{-3} \times 298^{10.19} \times \left(L_0 \left(\frac{0.07 \pm 0.12}{[\text{Sr}]} \right) \right)^{10.19} \right]$$

The pre-exponential and logarithm parameters may not be statistically significantly since they have strong correlations with the other parameters. We also fitted the data for all three temperatures simultaneously yielding the following equation. The Dubinin-Astakhov model equation for Sr loading follows with the same units as used for plutonium.

$$5) \text{ Loaded Sr} = 410 \pm 138 \times \exp \left[-0.09 \pm 0.02 \times \text{Temperature}^{4.01 \pm 0.09} \times \left(L_0 \left(\frac{0.42 \pm 0.12}{[\text{Sr}]} \right) \right)^{4.01 \pm 0.09} \right]$$

Mass balance:

$$\frac{dn}{dt} = n_{in} - n_{out} - r_{adsorption}$$

Rate kinetics:

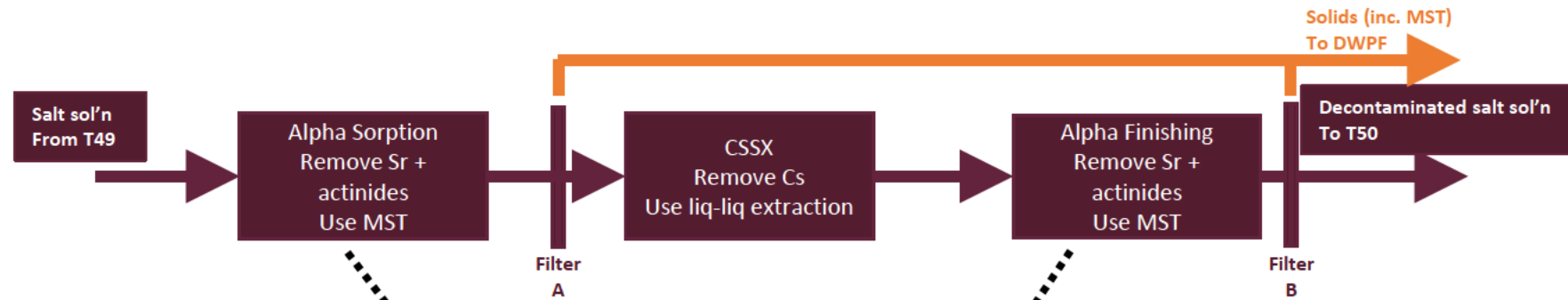
$$r_{adsorption} = k[\text{Sr}]^n \cdot [1 - \xi]^m$$

Technical Optimization Model Example



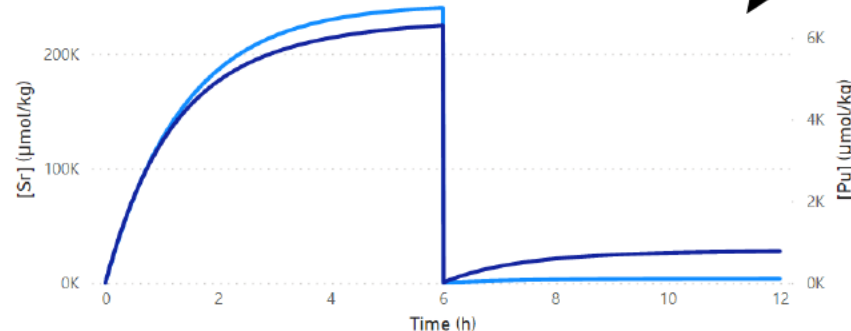
Background: Monosodium Titanate (MST) is used at SWPF to remove Strontium and Actinides such as Plutonium from salt waste

Objective: Compare Baseline Single MST Strike (12h at 0.4 g/L) vs Two ½ size MST Strikes (2x 6h at 0.2g/L)



Chemical Loading on MST: Two Equal MST Strikes

● [Sr] (μmol/kg) ● [Pu] (μmol/kg)



	Decontamination Factor	Waste Acceptance Criteria
Strontium	485 [170]	0.02% [0.05%]
Plutonium	258 [39]	0.3% [2%]

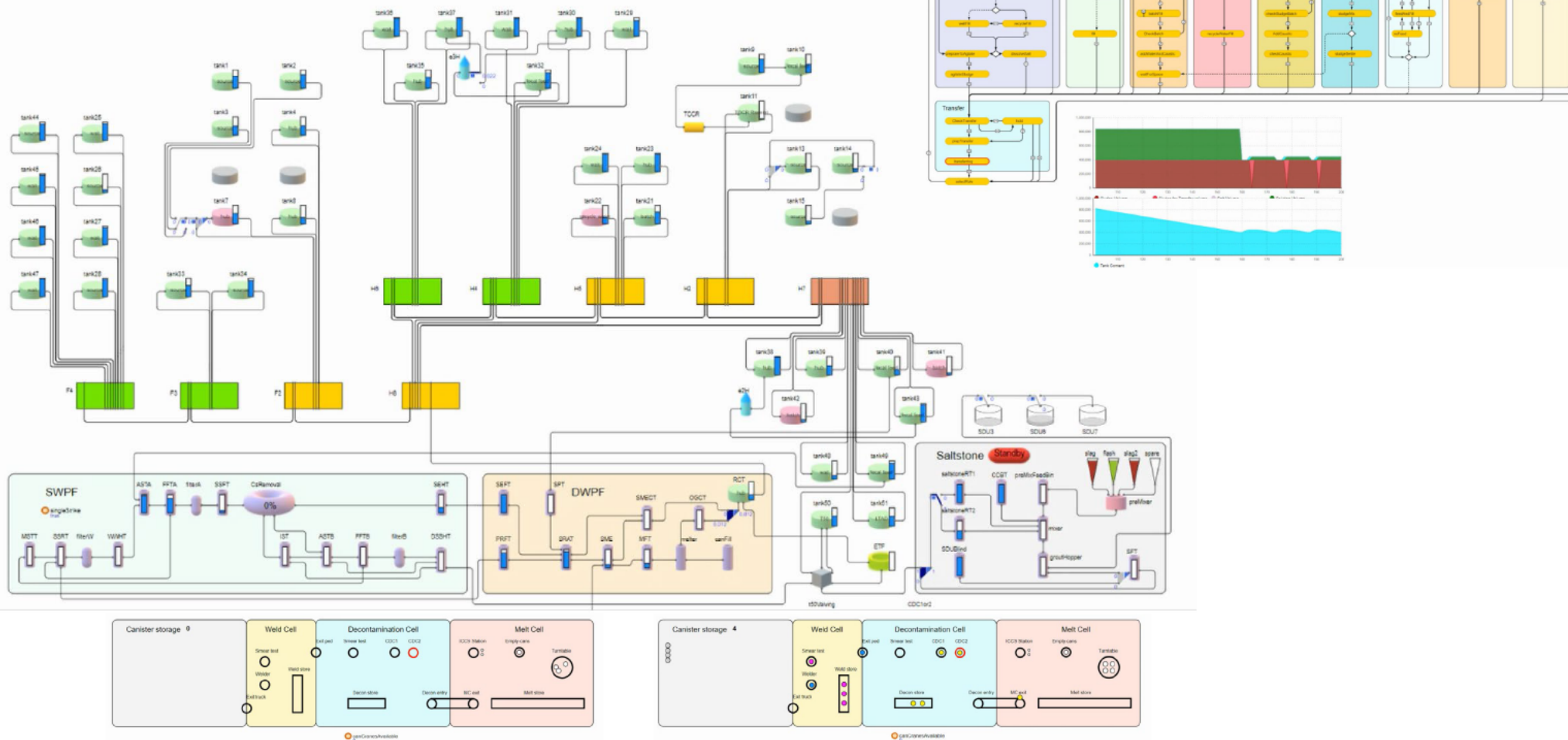
Values in [] are baseline values – 12h single strike @0.4g/L MST

Program Optimization Model: POM



Tracks Fluid Movements & Resources
Utilizes software called AnyLogic

Tank farm test : Simulation - AnyLogic Professional



Model Demonstration

Model Output Analytics (Power BI Demo)

Verification at 3 Levels

Subject Matter Experts provide input to develop the model design basis

Model Design
Basis
Document

DBD modelers use the SME
input to build the model

Model “checked” against the model
design basis by an independent DBD
modeler

Model

Current Liquid
Waste Facilities
Performance

Subject Matter Experts validate the
model against current physical plant
performance

Lifecycle scenarios are compared to lifecycle modeling performed
using the previous tools. Previous modeling was
audited/validated independently by the 3 different external
groups [the GAO/HQ(Regalbuto) team/HQ(MITRE)]

Previous
Lifecycle
Modeling

Questions?