ILAW Glass Testing Status

Elvie Brown
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Mission Need

ILAW Glass testing is needed to support the Integrated Disposal Facility (IDF) Performance Assessment (PA) and ongoing PA Maintenance

- Selected ILAW glasses will be subjected to accelerated testing to estimate the parameters needed for the IDF PA and ongoing PA Maintenance.
- Representative ILAW glasses will be tested in an actual subsurface environment at the Hanford Field Lysimeter Test Facility (FLTF) to corroborate results of lab scale testing and PA modeling.

IDF PA Source Term Model

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Kinetic Rate Law based on Transition State Theory

$$r = \vec{k}\, a_{H^+}^{-\eta} \exp\left(\frac{-E_a}{RT}\right)\left[1 - \left(\frac{Q}{K_g}\right)^{\sigma}\right] + r_{IEx}$$

Rate law term [1] — Ion Exchange term [2]

$\vec{k}$= intrinsic rate constant (mol/m²•s)	T= temperature
η= power law coefficient w/ respect to hydrogen ion activity (a_{H^+})	Q= ion activity of orthosilici acid ($SiO_2(aq)$)
E_a= apparent activation energy (kJ/mol)	K_g= pseudo-equilibrium constant
R= gas constant (kJ/mol•K)	σ = Temkin coefficient (=1)
	r_{IEx}= ion exchange rate

References:
[1]Grambow B. (1985). "A General Rate Equation for Nuclear Waste Glass Corrosion." Materials Research Society Symposium Proceedings, 44, 15–27.
[2]Grambow B. and Muller R. (2001). "First-order dissolution rate law and the role of surface layers in glass performance assessment." Journal of Nuclear Materials 298: 112-124.

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Main Data Sets Required

1) Rate Law Parameters
   - k, η, E_a, K_g
2) Ion Exchange Rate
   - r_{IEx}
3) Secondary Phase Reaction Network
   - The set of reactions that occur when in the glass-water interface, forming minerals/zeolites

Rate Law parameters and IEx rate are traditionally obtained via ASTM C1662, Glass Dissolution Rate Using the Single Pass Flow Through (SPFT) Test Method.

Data on secondary phases may be obtained via the Long Term Product Consistency Test (LT PCT), ASTM C1285 Method B.

Reference and Baseline ILAW Glasses Performance Parameters for 2017 IDF PA

	Parameters						
	$\bar{k}_0$		K_g[a]	η	E_a	σ	r_{IEX}
Glass	Reported Forward Rate Constant (g/[m² d])	Converted[b] Forward Rate Constant (mol/[m² s])	Glass Apparent Equilibrium Constant Based on Activity Product $a[SiO_2(aq)]$	pH Power Law Coefficient	Glass Dissolution Activation Energy (kJ/mol)	Temkin Coefficient	Na Ion-Exchange Rate (mol/[m² s])
LD6-5412	9.7×10^6	1.8×10^0	1.14×10^{-4}	0.40 ±0.03	74.8 ±1.0	1	1.74×10^{-11}[c]
LAWABP1	3.4×10^6	5.7×10^{-1}	4.90×10^{-4}	0.35 ±0.03	68 ±3.0	1	3.4×10^{-11}
LAWA44	1.3×10^4 ($R^2 = 0.78$)	2.2×10^{-3}	1.87×10^{-3} ($R^2 = 0.95$)	0.49 ±0.08	60 ±7	1	5.3×10^{-11}
LAWB45	1.6×10^4 ($R^2 = 0.90$)	3.0×10^{-3}	1.79×10^{-3} ($R^2 = 0.78$)	0.34 ±0.03	53 ±3	1	0.0×10^0[d]
LAWC22	1.0×10^5 ($R^2 = 0.98$)	1.8×10^{-2}	1.80×10^{-3} ($R^2 = 0.94$)	0.42 ±0.02	64 ±2	1	1.2×10^{-10}

$$r = \underbrace{\vec{k}\, a_{H^+}^{-\eta} \exp\left(\frac{-E_a}{RT}\right)\left[1 - \left(\frac{Q}{K_g}\right)^{\sigma}\right]}_{\text{Rate law term}} + \underbrace{r_{IEx}}_{\text{Ion Exchange term}}$$

Reference and Baseline ILAW Glasses Principal Secondary Phase Reaction Network

Phase	Reaction	Log K (15 °C)
Analcime [$Na_{0.96}Al_{0.96}Si_{2.04}O_6 \cdot H_2O$]	Analcime + $3.84H^+ \leftrightarrow 0.96Al^{3+} + 0.96Na^+ + 2.04SiO_2(aq) + 2.92H_2O$	6.55
Anatase [TiO_2]	$TiO_2 + 2H_2O \leftrightarrow Ti(OH)_4(aq)$	-6.56
Baddeleyite [ZrO_2]	$ZrO_2 + 2H^+ \leftrightarrow Zr(OH)_2^{2+}$	-5.50
Calcite [$CaCO_3$]	$CaCO_3 + H^+ \leftrightarrow Ca^{2+} + HCO_3^-$	2.00
Chalcedony [SiO_2]	$SiO_2 \leftrightarrow SiO_2(aq)$	-3.64
$Fe(OH)_3(s)$	$Fe(OH)_3(am) + 3H^+ \leftrightarrow Fe^{3+} + 3H_2O$	6.16
Gibbsite [$Al(OH)_3$]	$Al(OH)_3 + 3H^+ \leftrightarrow Al^{3+} + 3H_2O$	8.37
Sepiolite [$Mg_4Si_6O_{15}(OH)_2 \cdot 6H_2O$]	Sepiolite + $8H^+ \leftrightarrow 4Mg^{2+} + 6SiO_2(aq) + 11H_2O$	46.27
$Zn(OH)_2$-γ	$Zn(OH)_2\text{-}\gamma + 2H^+ \leftrightarrow Zn^{2+} + 2H_2O$	11.88

$$r = \underbrace{\vec{k}\, a_{H^+}^{-\eta} \exp\left(\frac{-E_a}{RT}\right)\left[1 - \left(\frac{Q}{K_g}\right)^{\sigma}\right]}_{\text{Rate law term}} + \underbrace{r_{IEx}}_{\text{Ion Exchange term}}$$

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Path Forward: PA Maintenance

- Enhanced Waste Loading vs. Baseline Glasses
  - Opportunity for significant increase in waste loading
  - Translates to reduced container count and shorter mission duration

- Glasses are formulated to meet WTP product specification and processability constraints
  - Meet short term (PCT-A) and Vapor Phase Hydration Test (VHT) limits
  - Need confirmation that Enhanced glasses will have acceptable long term durability under IDF disposal site conditions