U.S. Department of Energy
Office of Civilian Radioactive Waste Management

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Near-Field Chemistry

Presented to:
Nuclear Waste Technical Review Board

Presented by:
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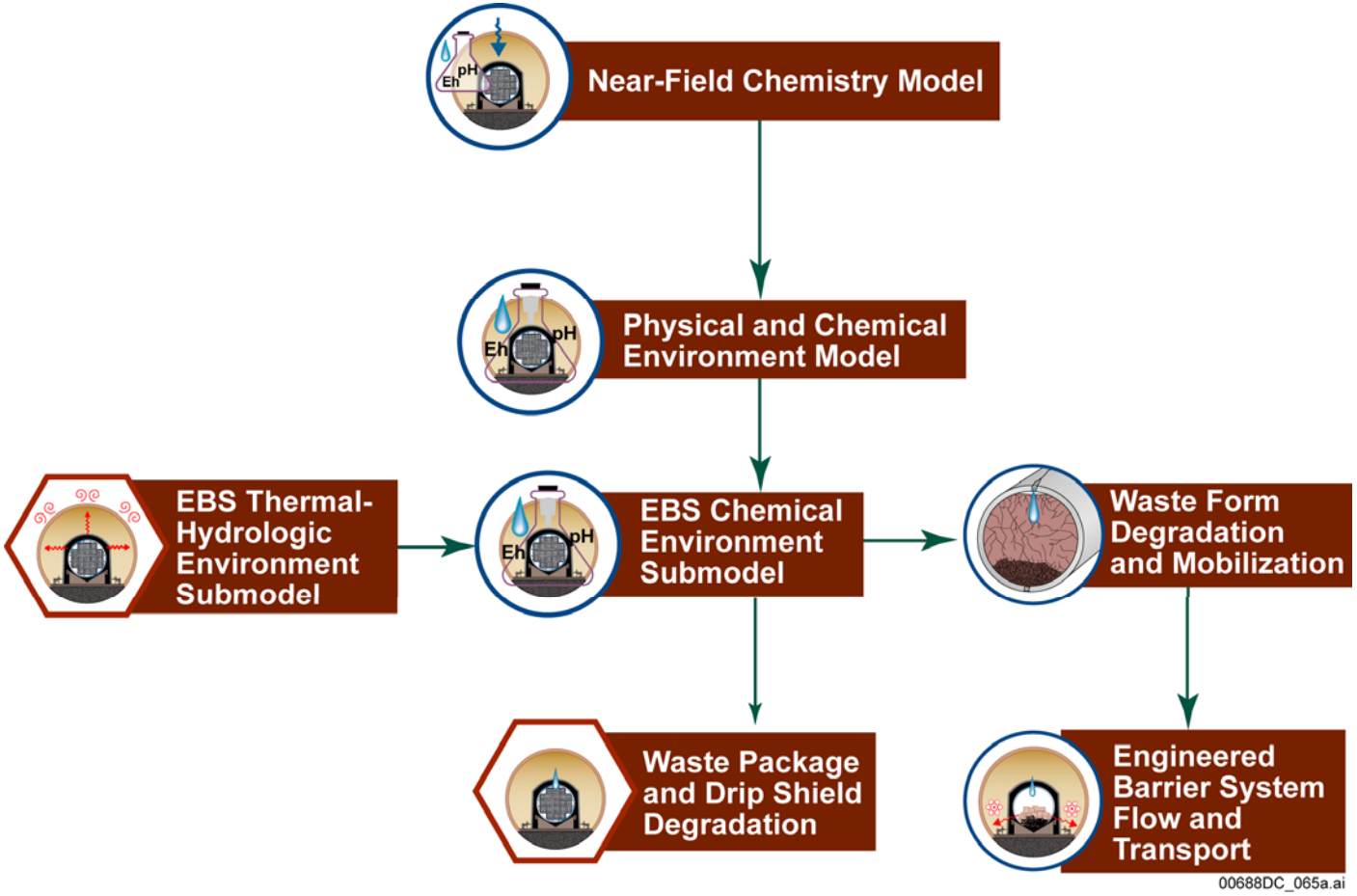
Outline

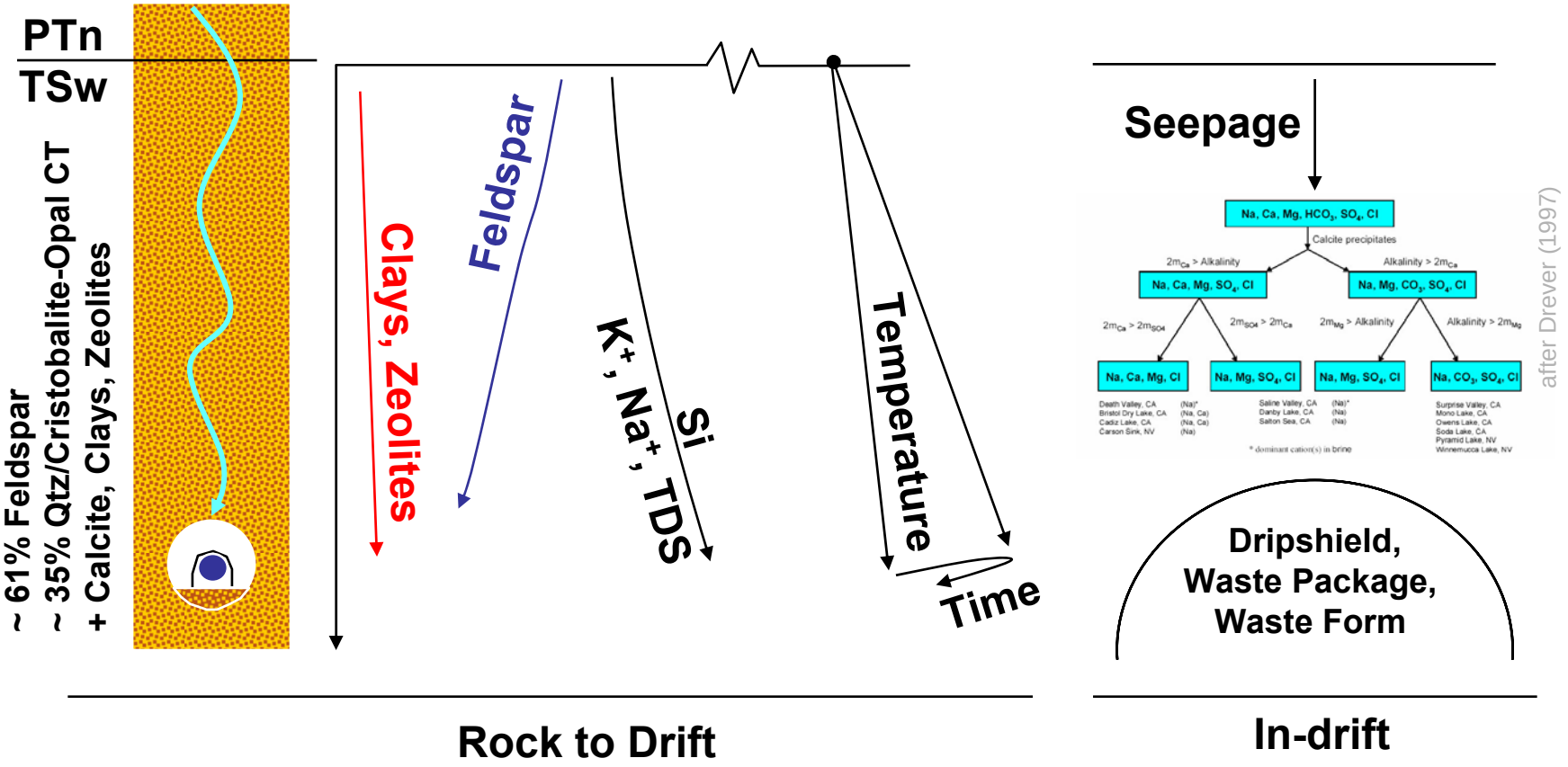
- Information flow from near-field chemistry model
- Near-field chemistry
- Hydrologic boundary conditions
- Field feldspar dissolution rate
- Median thermal path water–rock interaction parameter (WRIP) predictions
- Predicted rock alteration
- In-drift CO_2 levels
- Validation
- Summary

Information Flow from Near-Field Chemistry Model



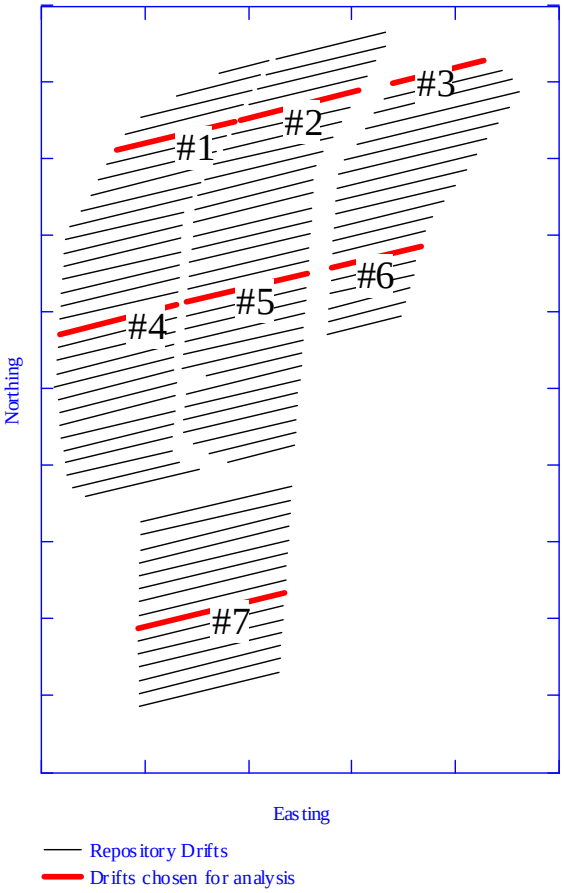
Near-Field Chemistry

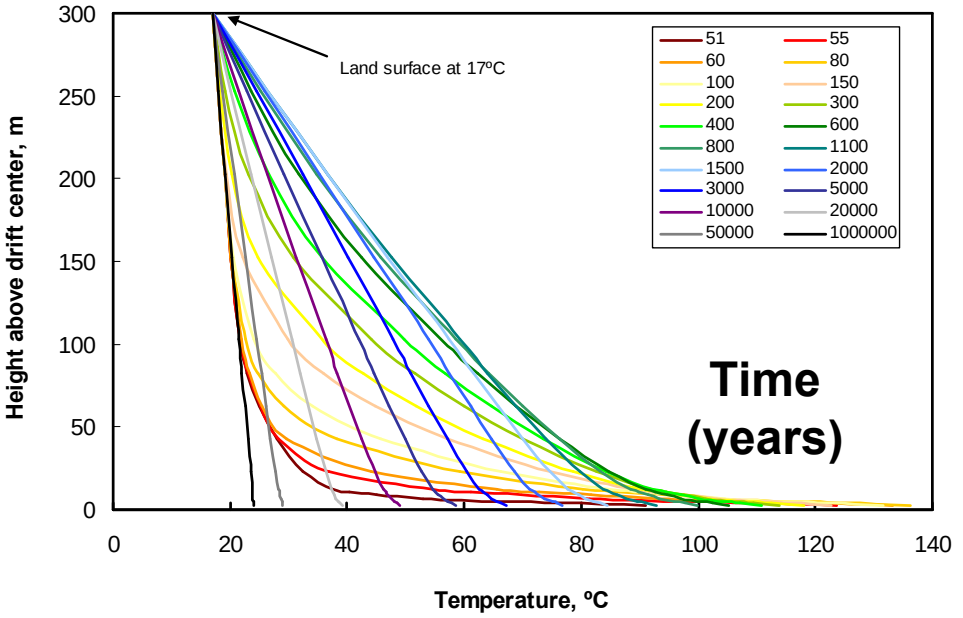
Charles R. Bryan and Katheryn B. Helean;
Sandia National Laboratories

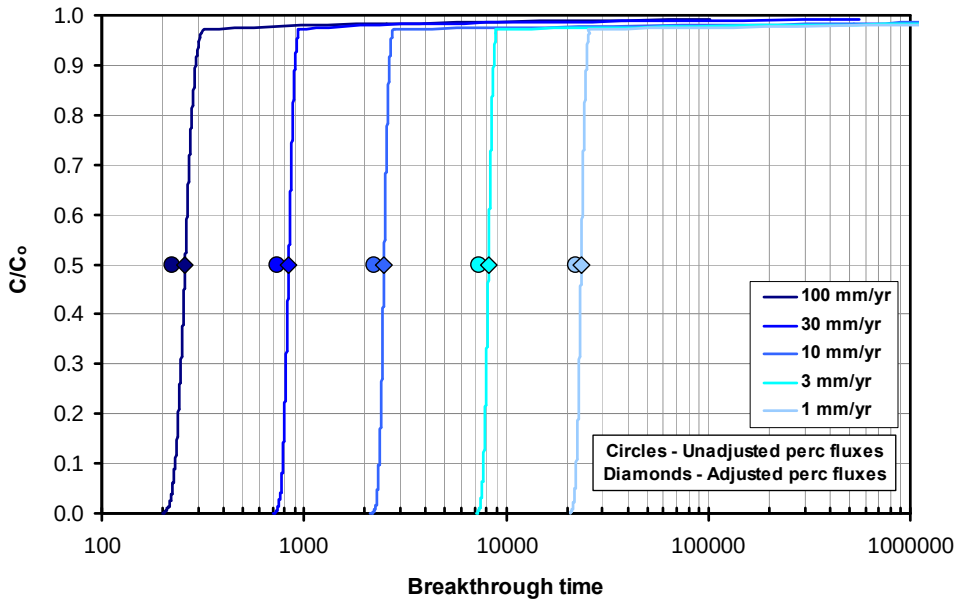


TDS = Total dissolved solids

Hydrologic Boundary Conditions







Field Feldspar Dissolution Rate

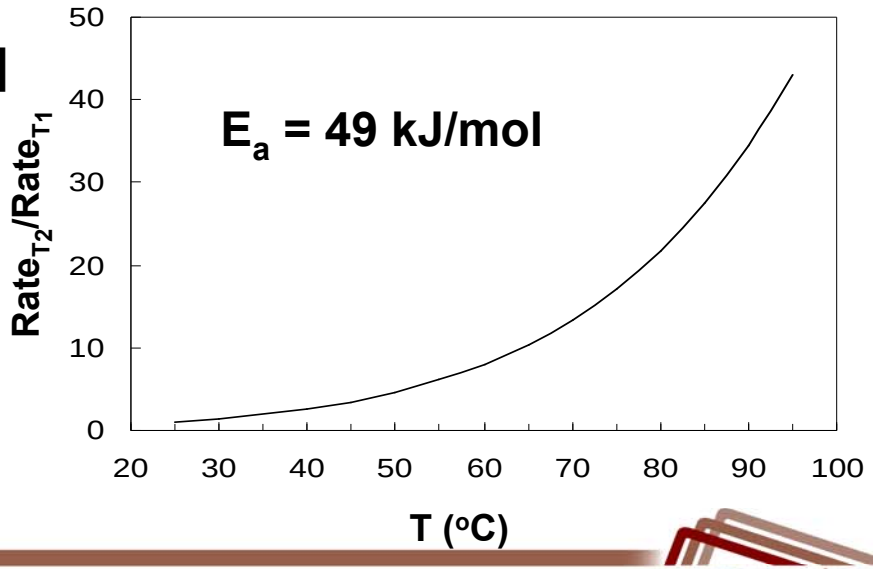
UNIT	smectite-illite		sorptive zeolite		feldspar	
	ave	std dev.	ave	std dev.	ave	std dev.
Tptpul	**2.5**	**1.37**	**0.06**	**0.14**	**61.38**	**7.87**
Tptpmn	**2.03**	**0.62**	**0.01**	**0.02**	**62.35**	**3.61**
Tptpll	**2.48**	**2.13**	**0.23**	**0.28**	**59.36**	**6.76**
Tptpln	**1.13**	**1.07**	**0.59**	**0.6**	**61.87**	**4.09**

Ambient

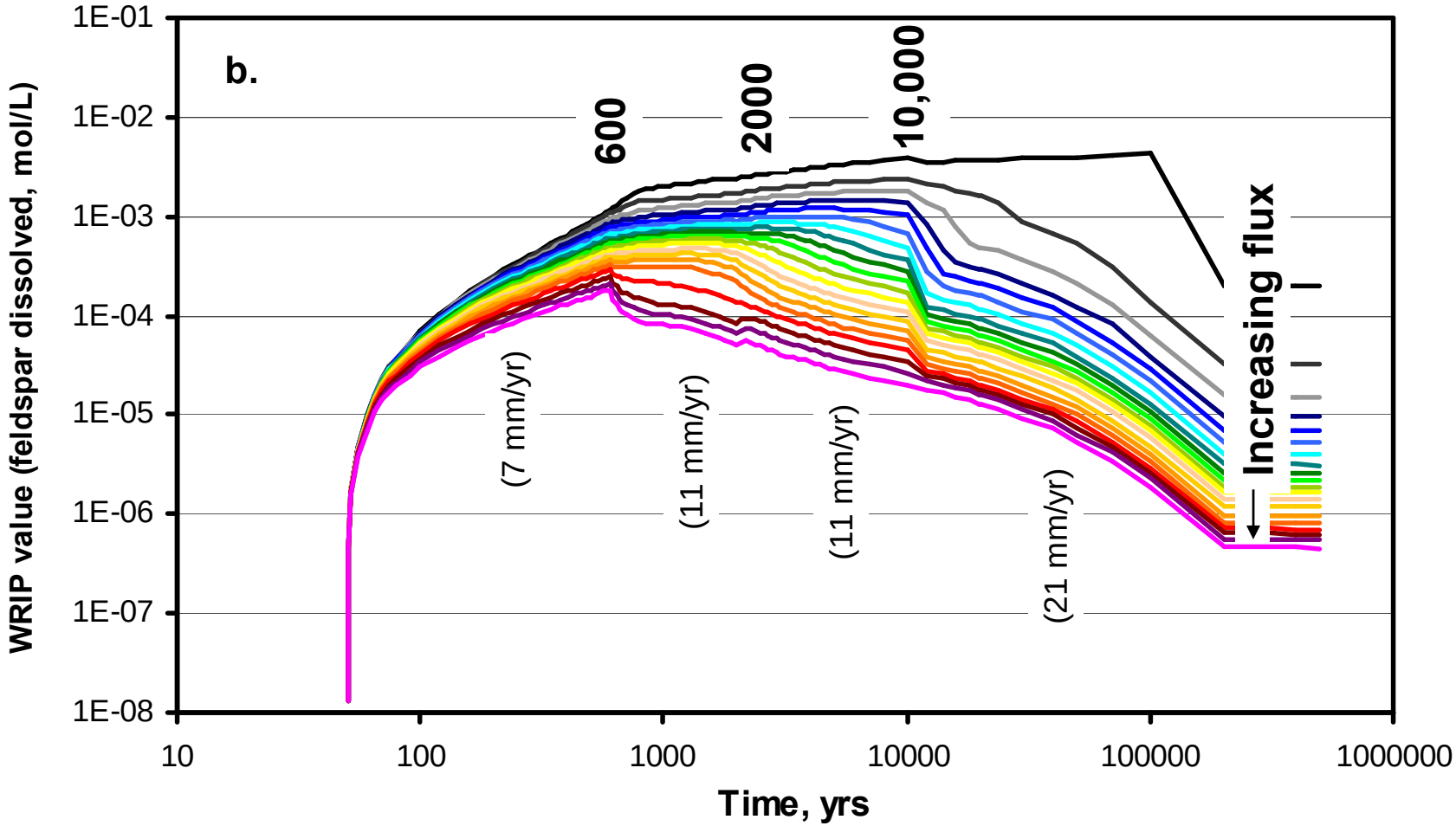
= 0.076 mol feldspar/kg
(assumes Al conserved) / **12.8 Ma** **= 5.94 x 10^{-9} mol kg^{-1} yr^{-1}**
Maximum, at 23°C

$$Rate_{T2}/Rate_{T1} = EXP[(E_a/R)(T_1^{-1} - T_2^{-1})]$$

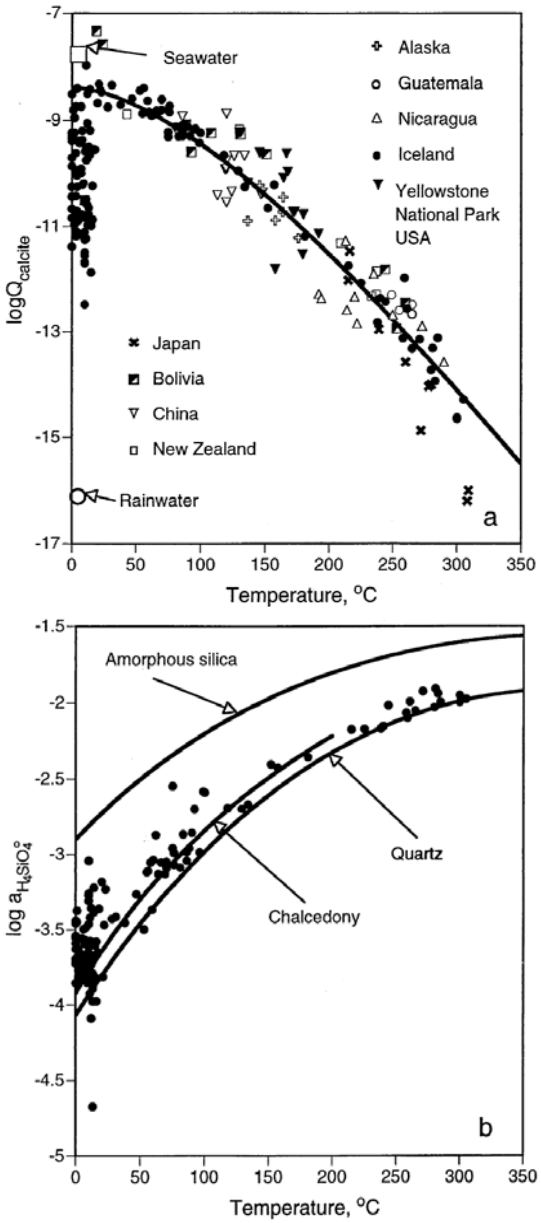
Thermally Perturbed



Median Thermal Path WRIP Predictions



Predicted Rock Alteration



Stefansson and Arnorsson, 2000; Geochimica et Cosmochimica Acta (64) 2567-2584.

$Na_{0.51}K_{0.46}Ca_{0.03}Al_{1.03}Si_{2.97}O_8 \rightarrow$
Smectite/Zeolite/Illite/Sep.

Assume equilibrium with calcite (0.01-0.41% in TSw), silica.

A. $NaKAl_2Si_6O_{16} + SiO_{2,aq} + Ca^{++} + 7H_2O \rightarrow CaAl_2Si_7O_{18}{\bullet}7H_2O + Na^+ + K^+$

B. $NaKAl_2Si_6O_{16} + SiO_{2,aq} + CaCO_3 + CO_2 + 8H_2O \rightarrow CaAl_2Si_7O_{18}{\bullet}7H_2O + Na^+ + K^+ + 2HCO_3^-$

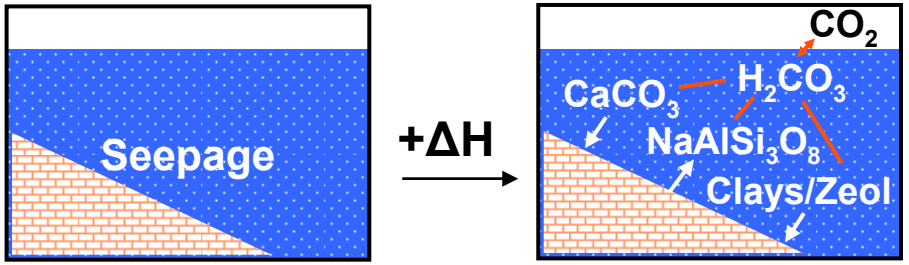
C. $3NaKAl_2Si_6O_{16} + 4SiO_2 + 2CaCO_3 + 2Mg^{++} + 16H_2O \rightarrow 2KMgAlSi_4O_{10}(OH)_2 + 2CaAl_2Si_7O_{18}{\bullet}7H_2O + K^+ + 3Na^+ + 2CO_2$

Increasing alteration ↓

(Use EQ3/6)

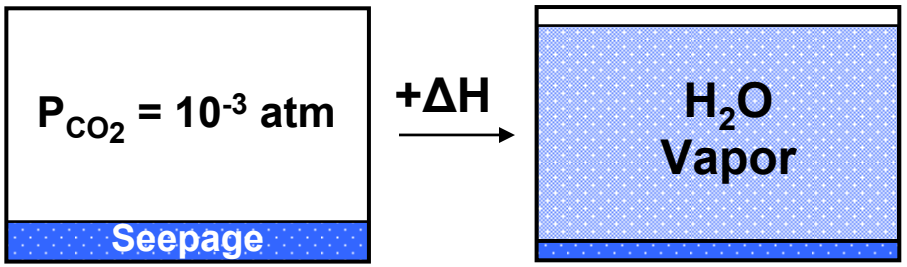
In-drift CO_2 Levels

Maximum



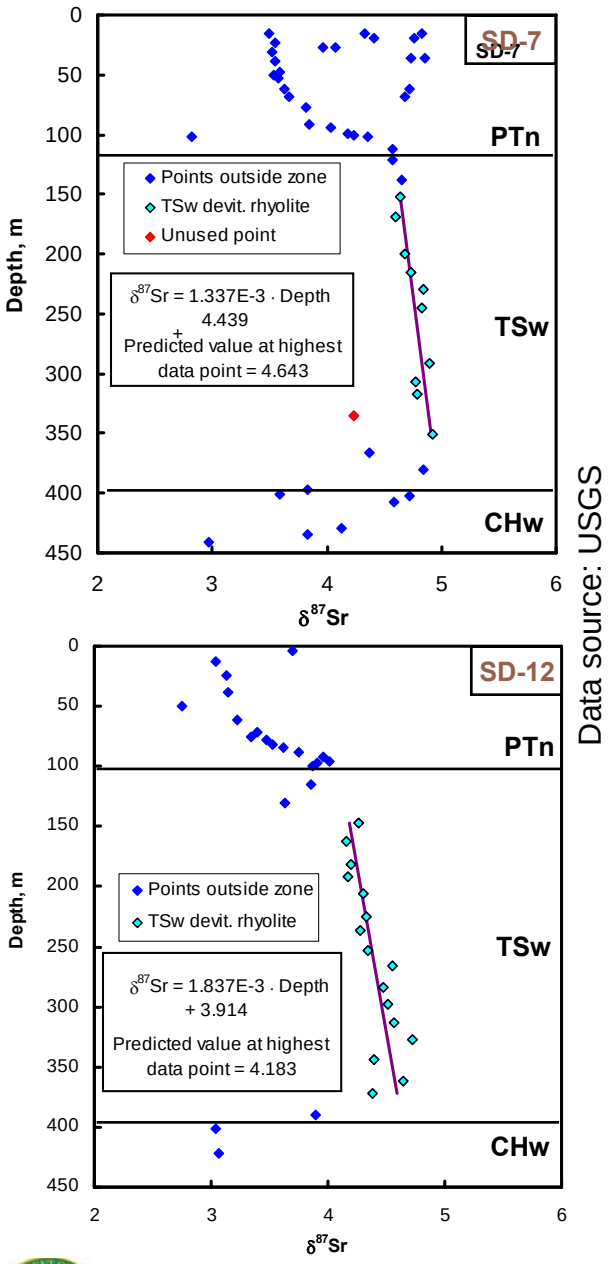
Equilibrium CO_2: CO_2 addition from calcite/smectite/zeolite growth, CO_2 loss from calcite/silicate dissolution

Minimum

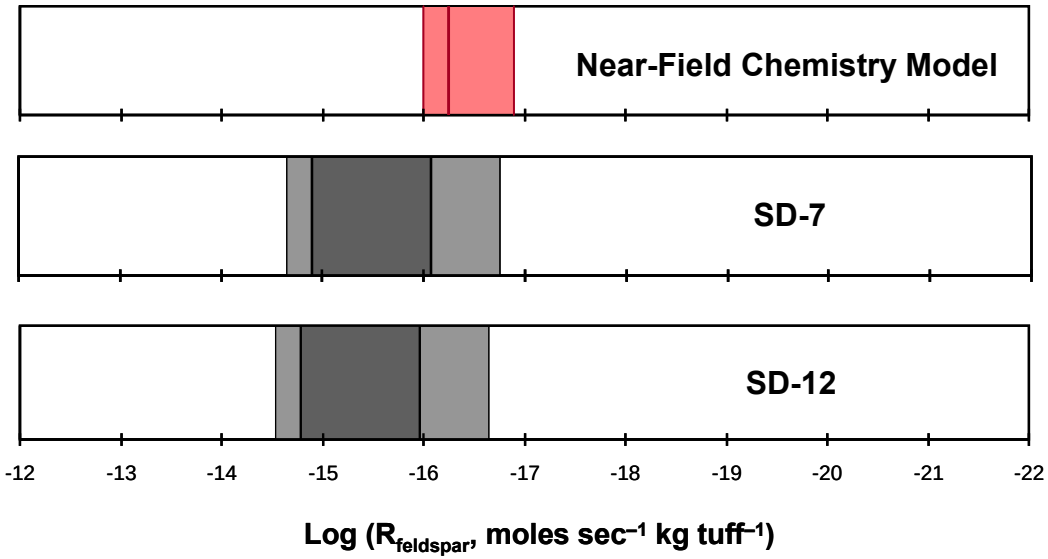


Ambient CO_2 levels displaced by water vapor, plus CO_2 from evaporated seepage

Validation



δ^{87}Sr Calculated TSw Feldspar Dissolution Rate



Summary

- **Near-field chemistry model inputs = thermal field, percolation fluxes**
- **Near-field chemistry model outputs = seepage chemistries**
- **Near-field chemistry model validation = δ^{87}Sr, PTn waters, Drift-Scale Test**