Spatial Distribution of Geochemical Changes about an Oil Shale Retort

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**Oil Shale Samples**
Green River Formation, Piceance Basin, CO
Rio Blanco County
Duck Creek Mine

- TOC = 8.8%
- Oil Potential = 22 gal/ton
- Hydrogen Index = 777 mg HC/g TOC
- Oxygen Index = 10 mg CO₂/g TOC

Sample courtesy of Shell
Hydrous Retorting

150 g Oil Shale
300 g Water

Air purged from system
Pressure released, water/oil sampled
Sample gas

Oil retorted for 72 hours
Retort cooled to ambient T (24 hrs)
Geochemistry Of the Retort Water

Concentration (mmol/L)

Temperature (°C)

Concentration (mmol/L)

Temperature (°C)
Mineralogical Changes in Retorted Oil Shale
Objective:
To combine the geochemical information we have obtained from laboratory experiments with heat transport modeling to gain insight into the spatial distribution of the geochemistry about an in-situ retort.

Approach:
Use a one-dimensional finite element code to calculate the spatial and temporal distribution of temperature about a heat source and then “map” the temperature-dependent laboratory results onto the temperature field to obtain the spatial distribution of the geochemistry.
Heat Capacity of Oil Shale

Applied Kopp’s law of additivity of heat capacities:

Heat capacity is a weighted sum of the heat capacities of the minerals and organic fractions in the formation.

\[ C_p(\text{oil shale}) = f(\text{minerals}) \ C_p(\text{minerals}) + f(\text{kerogen}) \ C_p(\text{kerogen}) + f(\text{char})C_p(\text{char}) \]

\( f(\text{kerogen}) \) and \( f(\text{char}) \) are changing during retorting. This change is simulated with first-order reaction of kerogen and a proportionate increase in char.
Heat Capacity of the Mineral Fraction

Mineral Fraction

Heat Capacity, $C_p$ (J kg$^{-1}$ K$^{-1}$)

Temperature (K)

$C_p = aT + bT^2$

$r^2 = 0.982$
Heat Capacity of Kerogen

Kerogen

\[ C_p = a + bT + c/T^2 + dT^2 \]

\[ r^2 = 0.982 \]

Data from:
Hanrot et al. (1994)
Heat Capacity of Coke

Coke

Heat Capacity, $C_p$ (J kg$^{-1}$ K$^{-1}$)

Temperature (K)

$C_p = a + bT + cT^2$

$r^2 = 0.996$

Data from:
Hanrot et al. (1994)
Thermal Conductivity of Oil Shale

\[
\lambda = \frac{1}{a + bT + cG}
\]

\[r^2 = 0.961\]

Data from:
Wang et al. (1979)
Nottenburg et al. (1978)
Vosteen and Schellschmidt (2003)
Distribution of Temperature

![Graph showing temperature distribution with distance and time. The graph includes curves labeled 0.5, 1, 2, and 3 years, with a red shaded area indicating the retort zone.](image-url)
Dominant Aqueous Species

$Na^+, HCO_3^-$

Concentration (mmol/L)

Distance (m)
Fluoride
Total Nitrogen

- **Retort Zone**
- **Concentration Exceeds Background**

Concentration (mmol/L) vs Distance (m)
Carbonate Minerals

- Retort Zone
- Calcite
- Aragonite
- Ankerite
Aluminosilicate Minerals

Weight %

Distance (m)

Retort Zone

Aluminosilicates

Analcime

Ankerite

Low Albite

Fe-Mg Saponite
Quartz

Aqueous Silica
Summary

We have

• obtained data on the concentrations of dissolved and mineral components in retorted oil shale as a function temperature,

• simulated the distribution of temperature near a retort using a one-dimensional FEM code,

• mapped the temperature-dependent geochemistry laboratory results onto the spatially-dependent simulated temperature distribution to simulate the potential spatial distribution of the geochemistry near an oil shale retort,

• begun contemplating the results of these simulations.