Small Angle X-ray Scattering from Yucca Mountain Groundwater Colloids

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Abstract

We demonstrate the use of small-angle x-ray scattering (SAXS) to characterize groundwater-borne colloids. The samples included groundwater from the USGS J-13 well, one of which was treated by heating it to 90 degrees C in contact with crushed Topopah Spring Tuff from the Yucca Mountain site. The SAXS measurements used the UNICAT undulator beamline at the Advanced Photon Source at the Argonne National Laboratory. Power-law plots (scattering intensity verses momentum transfer) were fitted to the SAXS data. Colloids in the untreated J-13 groundwater were shown to have a fractal dimension of nearly 3, whereas colloids in the treated groundwater ("EJ-13") have a dimensionality of approximately 2.4 over a length scale of approximately 3 to 300 nm. Similar power-law plots with dimension 3 characterized concurrent SAXS measurements from aqueous suspensions of Na-montmorillonite and NIST Brick Clay (NBS-67). We attribute these results to the sheet silicate layered structure of the clay colloids present in J-13 well water, montmorillonite, and "brick clay" systems. The differences between treated EJ-13 and as-received J-13 colloids are perhaps owing to exchange of calcium for sodium with the tuff. These data mirror earlier SAXS results obtained by others on bulk clay minerals, but the groundwater systems are far more dillute, perhaps, than any previously measured with reliability. Our results demonstrate the application of SAXS to study the physical nature of groundwater colloids essential for understanding phenomena related to colloid stability, size, morphology, aggregation, and adsorption properties. These characteristics may be important in determining the role of groundwater colloids in the transport of environmental contaminants.

The Fractal Dimension, *D*

•Find the minimum number N of balls of radius a needed to cover a surface completely.

•For a fractal surface, $N = N_0 a^{-D}$ where $2 \le D \le 3$.

Small Angle X-ray Scattering

•SAXS: $Q\lambda << 1$, where $Q = |\mathbf{k}_f - \mathbf{k}_i|$ and $k = 2\pi/\lambda$

•Colloids are known or suspected in groundwaters, but characterization elusive owing to low concentrations

Fractal Scattering

$I(q) = Aq^{-\alpha} + B$

•*Mass fractal:* $\alpha = D$,

D = fractal dimension

•*Surface Fractal:* $\alpha = 6 - D$

The UNICAT USAXS instrument adds a geometric factor of q to above equation.

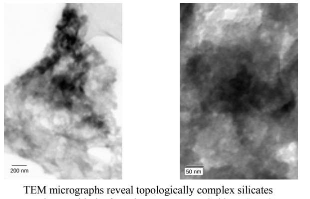
"EJ-13" water

•Ground water from USGS J-13 well, SE Nevada ("J-13" water).

•Heated to 90 °C for 30 days in contact with crushed Topopah Springs tuff (so-treated is now "EJ-13 water").

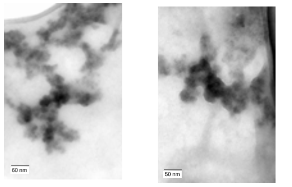
	Ca (ppm)	Na (ppm)	Si (ppm)
J-13	16000	44000	30000
EJ-13	5000	55000	40000

TEM: EJ-13 Colloids



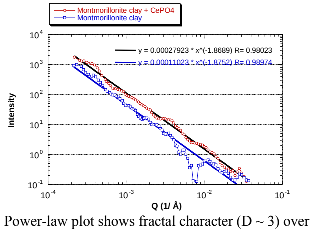
TEM micrographs reveal topologically complex silicates consistent with the fractal geometry revealed by USAXS.

TEM: J-13 Colloids



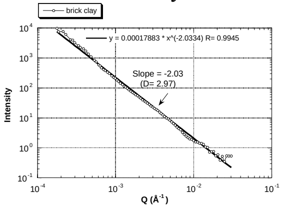
TEM micrographs of the untreated J-13 colloids also reveal a convoluted topology.

Montmorillonite Clay Colloids



Power-law plot shows fractal character (D ~ 3) over large scattering range from suspended Na-montmorillonite clays. A mixture of montmorillonite and cerium orthophosphate colloids is characterized by an increase in scattering intensity with no change in slope.

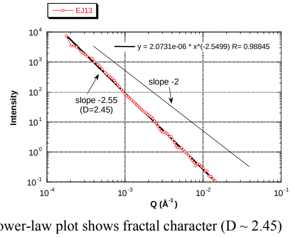
NIST Brick Clay Colloids



Power-law plot shows fractal character (D ~ 3) over large scattering range from colloidal brick clay.

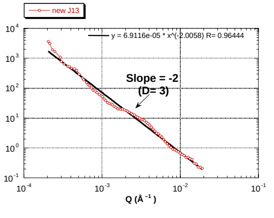
USAXS instrument

EJ-13 ground water



Power-law plot shows fractal character (D ~ 2.45) over large scattering range from treated EJ-13 water.

USGS J-13 water



Power-law plot shows fractal character (D ~ 3) over large scattering range from untreated J-13 water.

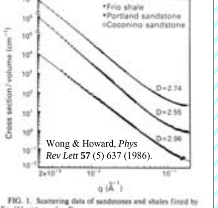


FIG. 1. Scattering data of sandstones and shales fitted by Eq. (1) with $\alpha = 6 - D$.

Note similar surface fractal dimensions to our dilute colloid findings.

Conclusions

•USAXS can determine topology of colloids even in dilute groundwater.

•Fractal geometry of colloidal silicates matches remarkably well with previous studies of bulk clay minerals

•Topology (fractal geometry) may be determined, in part, by interlayer cation.

UNICAT

Acknowledgement

The UNICAT facility at the Advanced Photon Source (APS) is supported by the Univ of Illinois at Urbana-Champaign, Materials Research Laboratory (U.S. DoE, the State of Illinois-IBHE-HECA and the NSF), the Oak Ridge National Laboratory (U.S. DOE under contract with UT-Battelle LLC), the National Institute of Standards and Technology (U.S. Department of Commerce) and UOP LLC. The APS is supported by the U.S. DoE, BES, OER under contract No. W-31-109-ENG-38.

Advanced Photon Source