

Regime of volatile components in magmatism of LIP (Siberian traps)

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To assess the formation conditions of Siberian traps we investigated melt and fluid inclusions in the phenocrysts of these rocks, which were analyzed for major and trace elements (EMPA and SIMS methods).

Ion microprobe data for reheated melt inclusions show relatively low concentrations of water by comparison with non-volatile components of comparable incompatibility ($H_2O/Ce=4.5$ vs 170 for MORB). Similar decoupling of H_2O and light REE was found for OIBs which belong to EM2 mantle reservoir. This has been interpreted as diffusive dehydration of the EM2 source during its storage in a drier ambient mantle (Workman *et al.* 2006). Similar mechanism of diffusive loss of water to the surrounding mantle may be proposed for magmas in Siberian Trap Province. Fluorine whose partition coefficients for major minerals of mantle rocks are similar to those of water is characterized in the investigated melts by close correlation with its non-volatile analogue ($F/Nd=17$ vs 21 for MORB+OIB). Concentrations of volatiles other than water in the mantle source of Siberian magmas are similar to the estimates for the sources of OIB magmas.

Low concentration of H_2O and moderate contents of other volatiles imply that the estimates of near-solidus temperature based on comparison with volatile free systems would not be changed significantly. Comparison of the estimated from melt inclusion data pressures with experimental data shows that the temperature of rising plume material was ca 400°C higher by comparison with the convecting upper mantle at the same depth. This proves that plume material arrived from deep levels in the mantle below certain thermal boundary layer.

Predicting the properties and behavior of multiphase materials in disposal environments

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Multiphase materials such as cement, ceramics, metals, glasses, and glass-ceramics, are being considered for stabilization of primary and secondary radioactive wastes. These materials are hydrophysically, chemically, and structurally complex with properties varying across multiple length scales. Hydrophysical properties exert control over percolation processes that help to define the relationship between microstructure and transport properties. Chemically, each form contains several components and phases, some of which can be amorphous or poorly crystalline with metastable solid-solution compositions varying over a fairly wide range. Transport properties are generally not well understood; their dependences on microstructure are non-unique such that empirical relations cannot be universally applied with confidence and modeling of interactions is under-constrained. In addition, the characteristics, and thus performance, of multiphase materials will change as the system evolves and degrades. Prediction of these changes is necessary for an improved understanding of service life in the disposal environment. A direct consequence of this complexity is that the evolution and degradation of waste form systems (comprised of the waste form and the near-field environment) are difficult to measure and, consequently, long-term performance is difficult to predict.

This research uses an integration of computational materials science, multiphase hydraulics, and geophysical techniques with careful experimentation to develop the tools necessary for analyzing and predicting the changes accompanying the evolution and degradation of multiphase waste form systems. Two waste form systems have been chosen for analysis: corroded HLW glass and cementitious cast stone. Both subject materials are multi-scale in their heterogeneity, with variations in microstructure from nanometers to millimeters. Inverse modeling techniques are coupled with physically-realistic composite physico-chemical models to determine critical parameters. These are then investigated with targeted experiments utilizing a suite of experimental techniques covering the range of scales of interest to these particular problems, including nuclear magnetic resonance, electron microscopy, x-ray tomography, and impedance spectroscopy.