Cyberinfrastructure Vision for Geochemistry, Petrology, and Volcanology

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Grand challenges in geochemistry and petrology, such as understanding the composition of and extent of fluxes between Earth's major reservoirs (core, mantle, crust, biosphere and hydrosphere), or the relationship between geologic processes and societal issues such as natural hazards and resources, require access and integration of large amounts of data and their seamless integration into dynamic models. Progress in scientific research will be greatly accelerated with a cyberinfrastructure that is guided by a community-endorsed vision. Recently, the geochemistry and petrology community has been charged with identifying key scientific and technical challenges, and next steps toward realizing the vision.

Scientific challenges are substantial in high impact, global scale research that currently is impeded by the dearth of accessible, integrated data, especially between terrestrial and marine data resources, thermodynamic models, experiments, and analytical data; lack of consistent coverage of geochemical sample specimens from geologic terrains of interest; lack of widespread sample curation and online sample catalogs; and lack of basic knowledge and communication within and outside the community.

The scientific challenges are augmented by technical challenges related to the discoverability, interoperability, and standardization of the geochemical, petrological, kinematic, and thermodynamic data currently in existence.

Steps have been proposed to reach the goal of science-supporting cyberinfrastructure in geochemistry: Data and metadata should be captured at the point of acquisition in a way that they can seamlessly be managed throughout their life cycle, including upload to repositories. Systems should be in place to promote spatial contextualization of analysis through sample registration, imagery, and links between samples (hand samples, thin sections, splits, etc.) and analytical data. Historical data should be properly brought into the integrated system. The community, especially early career scientists, must work together to produce the cultural shift to social networking, virtual collaboration, and sharing of data and knowledge.

With broad community participation and feedback, an integrated infrastructure can be lead more comprehensive, well-informed, and high impact scientific advances.

Anthropogenic impact on forest soil - Pollution with PAH, PCB and OCP in Germany

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While organic pollutants have been extensively studied in urban and agricultural areas, data from forested regions are relatively rare.

Within the framework of a forest soil inventory in Germany polycyclic aromatic hydrocarbons (PAH), polychlorinated biphenyls (PCB) and organochlorine pesticides (OCP) were analyzed in 1500 soil samples taken from 3 soil horizons at 447 sites. An analytical protocol was developed and validated for the simultaneous extraction and measurement of all analytes in humic rich soil at trace level range [1]. In line with the monitoring campaign a comprehensive quality assurance concept was implemented to guarantee constant analytical measurement conditions for two years.

At most sampling sites pollutant concentrations gradually decrease with depth. Only few spots showed highest concentrations in the upper mineral soil. In the O-horizon the sum concentrations of 16 PAHs range from 104 to 14.000 μg/kg, of 6 PCBs from <1 to 106 μg/kg and the sum of DDT and metabolites range from <1 to ca. 4.000 μg/kg.

The observed concentration of PAH, PCB and OCP reflect an ubiquitous background contamination at most sites. Relatively high concentrations of PAH and PCB are related to industrial areas and peak concentrations only of PAH are associated with open cast mining of brown coal areas. The spatial distribution of the contents of DDT and metabolites in German forest soils can clearly be attributed to historic application.

[1] Lehnik-Habrink *et al.* (2010), J Soils Sediments 10, 1487-1498

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