

The modeling focus of PUB can only be successful if it is complemented by the establishment of focus drainage basins that cover a wide range of scales and climatic conditions, and that contain state-of-the-art instrumentation to measure a wide variety of variables required to characterize the hydrologic system. Data have to be available at multiple scales and be consistent with the requirements of the various sub-disciplines. These basins will form the focal points within which new hypotheses and models can be tested in an uncertainty framework. PUB therefore has a need for drainage basins over a range of scales, to test and evaluate models and methods, and to develop new and improved hypotheses.

Another promising development in the United States in this regard is the planned national center for hydrologic synthesis [CUAHSI, 2004], which will be a pioneer in the community's efforts to integrate multiple disciplines in hydrology toward common objectives. In addition, there has been an immense effort within PUB to develop science questions that enable and stimulate scientific integration, an effort from which discussions within CUAHSI can benefit. The PUB initiative has created momentum that can be used in this regard. New thinking and discussions, particularly on

a conceptual level, are required that allow the reevaluation of current assumptions and paradigms in light of new requirements for our field [e.g., Sivapalan, 2003; Wagener, 2003; Littlewood *et al.*, 2003; Lakshmi, 2004; McDonnell, 2004; Wagener *et al.*, 2004].

Through initiatives such as PUB and CUAHSI, we are at the threshold of exciting new opportunities that will help to further change the face of hydrology, nationally and internationally, to a new level of integrative science, and to unify the hydrologic community in addressing common problems collectively and collaboratively. PUB is a grassroots-level movement, enabling open participation to everyone who is interested, and with a minimum of bureaucracy.

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MEETINGS

Joint Discussion of Sedimentary Geochemistry Data Management Systems That Cross the Waterline

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Earth's evolution, its climate history, and the history of life are archived in the chemical and isotopic compositions of marine and terrestrial sediments and fossils found within them. This information provides evidence for crust-mantle recycling, bolide impacts, mass extinction events, gas hydrate expulsion, climate cycles, and much more. Much of this geochemical evidence, such as the discoveries of oxygen isotope cycles in Quaternary sediments, enhanced iridium at the Cretaceous/Paleocene boundary, and relationships between near-trench sediments and associated arc volcanics, have overturned paradigms, opened new avenues of inquiry, and helped launch international research programs (e.g., the Deep Sea Drilling Project [DSDP]).

In addition to revealing much about important Earth events and processes, geochemical records preserved in marine and terrestrial sediments are increasingly important for the correlation of global records; indeed, for Precambrian and anoxic sediments, chemical and isotopic methods are indispensable and provide the main basis for correlation.

The time is ripe to develop sedimentary geochemistry databases and interactive information systems that "cross the waterline," linking marine and terrestrial data. Technological

advances and discovery of new environmental proxies are yielding an explosion of chemical and isotopic data. During the last decade, advances in automation and the development of the inductively coupled plasma mass spectrometer (ICP-MS) have led to new and rediscovered chemical and isotopic approaches (e.g., Mg/Ca, Sr/Ca; Ca, Fe, Sr, Nd, Pb, Hf, Os, Mo isotopes), scientific advances, and new enthusiasm for paleo-geochemical studies.

Two workshops were recently organized with the main goal of developing a strategy to collect and make publicly accessible sedimentary geochemistry data to empower the scientific community with the data and tools needed to facilitate scientific discovery. The workshops brought together international leaders in sedimentary geochemistry and chemostratigraphy, and leading experts in geoscience data management and information and visualization technologies. Participants included both data producers and the modelers who use these data to understand oceanic chemical fluxes and the coupling between Earth's spheres. A total of 62 scientists, information technology specialists, and representatives of federal agencies attended the workshops and contributed to identifying the data needs of the community.

The workshop, Linking Information Systems in Marine and Terrestrial Geosciences (LISMTG), funded jointly by the U.S. National Science

Foundation (NSF) Divisions of Ocean Sciences and Earth Sciences, and held at the offices of the Joint Oceanographic Institutions in Washington D.C., originated from the working group for "Geochemistry of Igneous and Sedimentary Rocks" of ISES-CI (Cyber-Infrastructure for the Integrated Solid Earth Sciences). ISES is a grassroots effort to create a common voice for areas of geology that focus on the solid Earth.

The LISMTG workshop was motivated by community demand to apply the concepts of successful data management of igneous rock geochemistry by the PetDB (ocean floor igneous rocks), GEOROC (oceanic islands, arcs, and continental basalts), and NAVDAT (North American volcanics) projects to the development of complementary information systems for sediments. The PetDB, GEOROC, and NAVDAT management systems for geochemical data are based on a common data model, with similar interactive, dynamic user interfaces, that allows compilation of data from disparate sources into integrated datasets.

The development of these igneous rock databases has led to the new EarthChem initiative (<http://www.earthchem.org>) to advance a cyberinfrastructure for solid Earth geochemistry. A goal of the LISMTG workshop was to define the needs for sediment geochemical data management, emphasizing interoperability between different databases and integration of marine and terrestrial datasets.

The second workshop, CHRONOS Geochemical Cycles, was the latest in a series of workshops organized by the NSF-funded CHRONOS project (www.chronos.org). CHRONOS is an information technology (IT) project dedicated to providing sedimentary geology and paleobiology data and information, together with toolkits for data visualization and analysis, to the

broad geoscience community, the public, K-16 students and educators, policy makers, and the media. The workshop was designed to discuss what stratigraphically-defined sedimentary geochemistry data exist, and what data storage and visualization and computational tools are needed to compare and correlate geochemical data with other data (e.g., paleobiological, lithostratigraphic, and geochronological).

The main topics discussed at both workshops related to the requirements for a data management system (DMS) for sediment geochemistry:

- (a) What data and metadata need to be included in a sediment geochemistry DMS that includes both terrestrial and marine sediments?
- (b) What functionality should user interfaces (UI) offer?
- (c) What visualization and computational tools should be provided to maximize user productivity and creativity?
- (d) How do we maximize outreach and CHRONOS applications in education at all levels?

Participants in both workshops agreed that the highest priority is the development of a database system for all geochemical data (i.e., stable and radiogenic isotope ratios, and major and trace elements). The system would include sufficient metadata (geographic, mineralogy and stratigraphic information, analytical and sample quality details, sample types such as leachates and residues, and size fractions) to be both comprehensive and practical to use, allowing data evaluation and re-evaluation. A key objective would be the seamless integration of multiple datasets to make them accessible through a common user interface as part of a networked distributed information system. In terms of visualization and computational tools for data analysis and presentation, participants in both workshops identified graphic correlation, age models, and the ability to place data points in a paleogeographic setting as most desirable.

At the LISMTG workshop, domain scientists—from paleoclimatologists to “subduction factory” researchers—urged the initiation as soon as possible of a pilot project to build a marine sediment geochemistry database (SedDB) using PetDB’s data model as a foundation, starting with post-cruise data for Ocean Drilling Program (ODP) cores. Breakout working groups focused on the challenge of interoperability with other information systems in the emerging geoscience cyberinfrastructure. Participants recommended the development of open and well-documented Web interfaces, standardized vocabularies, implementation of a unique sample identification protocol that is essential for linking sample-based data from different sources (e.g. different publications, labs, or

data systems), and collaboration with journals to enforce completeness of background information (metadata) for published analytical data.

The workshop concluded that only minor differences exist in the requirements for marine and terrestrial sediment data management, and that it is essential to be able to integrate them. Interoperability between data systems such as SedDB, PaleoStrat, and CHRONOS was, therefore, emphasized as a critical objective.

At the CHRONOS workshop, a lively discussion followed the break-out group discussion on how to maximize outreach and educational potential of these initiatives. Outreach tools should be designed to serve teachers, researchers, politicians, reporters, and industry. Features such as fact sheets, press releases, “ask a geologist,” and investigator biographies could be modeled after, and developed in cooperation with, museums, NASA, the U.S. Geological Survey, and the Integrated Ocean Drilling Program (IODP). Critical in these activities is the direct involvement of K-16 students and educators to ensure appropriate content and presentation. The universal view was that educational efforts should focus not on data, but on the scientific questions they answer, such as the end-Cretaceous extinction event, global warming in Earth’s past, and the evolution of life.

A key outcome of the CHRONOS workshop was the development of an organizational and implementation structure for geochemical cycles/sedimentary geochemistry within CHRONOS. Scientific working groups will collaborate with IT developers to test prototypes and ensure that the system meets community needs. Specifically, science working group members will: (1) help design and review specific aspects of the database schemas, metadata categories, and visualization and analytical tools; (2) serve as experts to answer questions from IT developers; and (3) enlist community support for populating and using this resource. The current list of participants in sedimentary geochemistry working groups is available at <http://www.chronos.org/workinggroups.html>.

Following the successful outcome of these workshops, SedDB and CHRONOS are working together to develop a data network system that fits the needs of the broader community and will allow for both sample-based and time-series geochemical data from marine and terrestrial sediments. Compatibility and interoperability are critical aspects of this collaboration. The joint IT and science teams will work closely to develop a schema that is tightly networked with CHRONOS main stratigraphic data engines, PaleoStrat (<http://www.paleostrat.org>) and Neptune (<http://services.chronos.org/databases/neptune/index.html>), and with the EarthChem infrastructure (<http://www.earthchem.org>).

As for scope, SedDB will focus on the assembly and digitization of all geochemical data from marine sediments, while CHRONOS will focus on the deep-time paleoproxy records from terrestrial sections and marine sediments. In collaboration with SedDB, CHRONOS is developing a module for geochemical samples and a metadata standard as part of PaleoStrat. This module will ensure the efficient connection between geochemical data and the associated stratigraphic information provided by PaleoStrat for terrestrial sections and Neptune for DSDP and ODP cores. It will also allow users to construct age versus depth plots online using CHRONOS Java-based, cross-platform Web application ADP (<http://services.chronos.org/webservices/adp/index.html>). The geochemical module will be named HERMES, after the messenger of the gods and father of alchemy of Greek mythology. Both CHRONOS and SedDB will also work on the further development of computational tools for data analysis and visualization.

CHRONOS and SedDB welcome participation from the geochemical, chemostratigraphic, and paleoceanographic community. Anyone wishing to contribute to this initiative and become involved in the sedimentary geochemistry aspects of CHRONOS is encouraged to contact Ethan Grossman (e-grossman@tamu.edu), John McArthur (j.mcarthur@ucl.ac.uk), or CHRONOS executive director, Cinzia Cervato (cinzia@iastate.edu). Those wishing to contribute to the development of SedDB or send data should contact Kerstin Lehnert (lehnert@ldeo.columbia.edu) or Steven L. Goldstein (steveg@ldeo.columbia.edu).

The Linking Information Systems in Marine and Terrestrial Geosciences: Sediment Geochemistry workshop was held 3–4 June 2004, in Washington D.C. The CHRONOS Geochemical Cycles workshop was held 25–26 June 2004, in San Antonio, Texas.

See <http://www.earthchem.org/workshop/> and <http://www.chronos.org/meetings/chemostratws.html>

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