at various scales, it may be possible to provide independent constraints on the components of coupled models used to address field-scale reactive transport. Both laboratory "sand box" and in situ field experiments are recommended. This approach will provide insight into the limitations of conceptual models and parameterizations developed at the laboratory bench scale in accurately depicting a field-scale situation.

The need for calibration of field-scale reaction parameters in RTM should not be underestimated. Current limitations in characterizing multiscale variability in subsurface properties and observing in situ behavior result in knowledge gaps that will only be effectively addressed through process model calibration against field observations. While this may somewhat limit the robustness of model predictions, decisions based on RTM predictions can be justified if the conditions modeled are within the range of calibration conditions and the predicted outcomes can be bracketed to the extent that they clearly differentiate alternatives.

The WG concludes that addressing the research issues noted above would greatly improve the application of RTM to many public health issues where better predictions are needed, and ultimately result in cost savings to federal agencies.

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Predictions in Ungauged Basins As a Catalyst for Multidisciplinary Hydrology

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The face of hydrologic science is changing rapidly, on national as well as on international scales. The increasing complexity of the problems hydrology is asked to investigate in research and practice today often requires solutions that can no longer be obtained by a single hydrologist, but require a multidisciplinary team. One consequence of this trend is the establishment of initiatives that help formulate and implement science programs to engage and energize the scientific community toward achieving major advances.

The IAHS Decade on Predictions in Ungauged Basins (PUB) is an initiative of the International Association of Hydrological Sciences (IAHS) [*Sivapalan et al.*, 2003] to advance our ability to make reliable predictions in ungauged basins. Within PUB, the drainage basin (at various scales) is seen as the element that integrates all aspects of the hydrological cycle within a defined area that can be studied, quantified, and acted upon.

On the Need for PUB

Natural and human-induced climate changes and variability are beginning to exert increasing stresses on water resources around the globe [*Sivapalan et al.*, 2003]. The hydrologic community is increasingly called upon to respond adequately to these threats by supporting the development of sustainable management policies. Tools are required in this context that can generate reliable predictions of hydrologic responses over a range of space and time scales and climate.

Hydrologists have developed a wide variety of models to achieve this. These models vary widely in underlying philosophy, but have in common that they must be calibrated, to varying degrees, to the response of the river basin. In basins with a sufficiently long record of output observations, with streamflow as the main integrator of the system behavior, we can fall back on calibration to sufficiently constrain the model response, which enables us to obtain reasonably reliable predictions of the response behavior of the system under study.

However, the state of our knowledge can only be fully tested when we consider the "ungauged case" [*Sivapalan*, 2003], i.e., the case in which observations of the variable we are trying to predict are too short, of too poor a quality, or even nonexistent. In view of the tremendous spatiotemporal heterogeneity of climatic, landscape (surface and subsurface), and land cover properties, extrapolation of information or knowledge, from gauged to ungauged basins, remains challenging, with considerable difficulties and uncertainties, especially in light of our limited understanding of what flow path water takes to the stream.

A main bottleneck to modeling ungauged basins is the complexity of the problem at

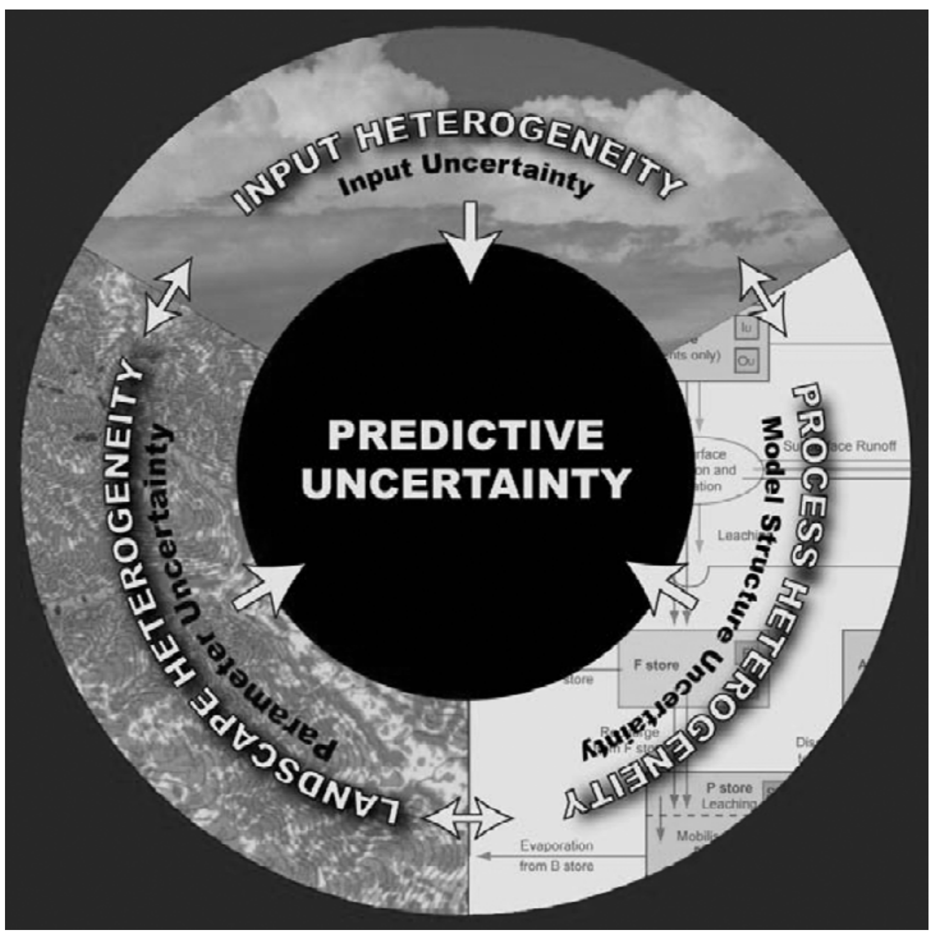

Fig. 1. Predictive uncertainty and links with climatic and landscape heterogeneity. Reproduced from Sivapalan et al. *[2003] with permission of IAHS Press.*

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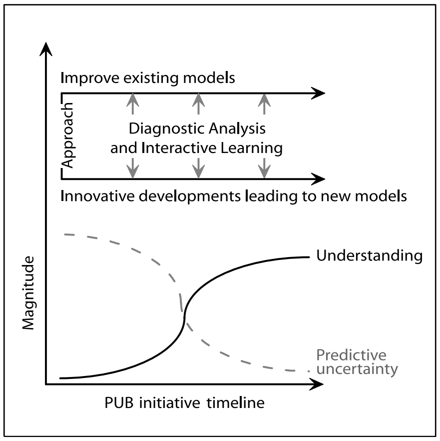

Fig. 2. Reducing predictive uncertainty and improving understanding through better modeling tools.

hand, and the scope and difficulties involved to be solved by individual scientists, often coming from a narrow disciplinary base. Significant new knowledge and understanding from a variety of cognate fields must be brought together to succeed in solving this dilemma (e.g., hydrometeorology, soil science, ecology, hydrogeology). Individual investigators can tackle only part of the problem, and only partial progress can be achieved. Therefore, a multidisciplinary approach is required if we want to solve this considerable problem comprehensively. The problem can serve as a perfect catalyst to bringing the hydrologic community together to work on a common problem using a multitude of approaches in an integrated manner.

The future face of hydrology is necessarily and decidedly multidisciplinary, and we need appropriate vehicles to move this integration forward. This multidisciplinary aspect is not just important from a research point of view, it is also requested from the operational part of the community, and most importantly for the future of hydrologic education in order to produce hydrologists that have the multidisciplinary background, training, and confidence required to solve complex environmental problems, today and in the future.

PUB Science Focus: Reduction of Predictive Uncertainty

A quantitative measure is required in PUB, as in any other scientific initiative, to assess whether science has been advanced. In this particular case, the progress is assessed in terms of our predictive capability. The chosen measure of performance for this purpose is a positive change, i.e., a reduction, in predictive uncertainty. Development of a framework for uncertainty analysis in which a multitude of approaches (models, data sources, etc.) can be compared with respect to their predictive uncertainty is underway as part of the initiative (www.hwr.arizona.edu/uncertainty). Major sources of uncertainty that have to be considered are heterogeneity in the input (climate forcing), in the landscape (model parameters), and in the processes (model structure) (Figure 1). It is assumed that an increase in understanding will lead to a reduction in predictive uncertainty (Figure 2).

Keeping the focus on predictive uncertainty in mind, the PUB Science Plan [*Sivapalan et al.*, 2003] includes a suite of enabling research programs, integrating across various hydrologic sub-disciplines, which are articulated through the following six key science questions:

1. What are the key gaps in our knowledge that limit our capacity to generate reliable predictions in ungauged basins?
2. What are the information requirements to reduce predictive uncertainty in the future?
3. What experimentation is needed to underpin the new knowledge required?
4. How can we employ new observational technologies in improved predictive methods?
5. How can we improve the hydrological process descriptions that address key knowledge elements that can reduce uncertainty?
6. How can we maximize the scientific value of available data in generating improved predictions?

PUB aspires to the development of new predictive approaches that will be based on improved understanding of hydrological functioning at multiple space and time scales. Indeed, PUB could herald a major paradigm change in surface hydrology from one that is presently dominated by the need for calibration to a new one based on a new level of understanding. This desire is encapsulated in the following interconnected targets:

- Target 1: Examine and improve existing models in terms of their ability to predict in ungauged basins through appropriate measures of predictive uncertainty.
- Target 2: Develop new, innovative models to capture space and time variability of hydrological processes for making predictions in ungauged basins, with a concomitant reduction of predictive uncertainty.

Progress of PUB So Far

The PUB initiative was developed through a series of meetings starting in 2001 and culminating in its official launch in Brasilia, Brazil, in December 2002. The Science and Implementation Plan of PUB was launched at the International Union of Geodesy and Geophysics (IUGG) Meeting in Sapporo, Japan, in July 2003. A summary version was published in December 2003 [*Sivapalan et al.*, 2003].

The focus of the PUB initiative has now switched to its implementation stage in various parts of the world. The main focus in its next set of activities will be the formation of working groups, formed in self-organized fashion, from the grassroots level. With this in mind, a number of meetings have already been completed in Paris, France, Perth, Australia, and Yellowknife, Canada. Various working groups have already been formed, and others will be launched in the future. A number of workshops and symposia have been held this year or are being planned for the near future (see http://cee.uiuc.edu/research/pub/):

- Workshop on "From new descriptions of catchment form and function to new model blueprints" at Oregon State University, 14–16 June 2004. This was CUAHSI Vision Workshop and kickoff meeting for a new PUB working group on catchment theory.
- Workshop on "Uncertainty analysis in environmental modeling" in the Villa Vigoni in Menaggio, Italy, 6–8 July 2004 (www.es.lancs.ac.uk/hfdg/uncertainty_workshop/uncert_intro.htm). During this workshop of the PUB working group on uncertainty in hydrologic modeling, the way forward toward a common uncertainty framework was discussed.
- NATO Advanced Research Workshop on "Physical models of river runoff and their application to ungauged river basins," 7–10 September 2004, Moscow, Russia.
- IAHS Scientific Assembly in Foz do Iguaçu, Brazil, 25–29 April 2005 (www.cig.ensmp.fr/~iahs/). This assembly will include a range of sessions covering all aspects of the PUB initiative.

Outlook and Links to the U.S. Community

Hydrologists worldwide have come to recognize the multidisciplinary nature of their discipline and the need to establish efforts that will enable scientists from various sub-disciplines to integrate their work. This will surely lead to novel opportunities for scientific progress that would be unachievable by individual scientists working alone. In this context, the PUB activities described above will undoubtedly lead to new predictive approaches based on a combination of current and new theories, and of existing and potentially new data sets, that are unimaginable at the present time.

In particular, over the next 10 years PUB will lead to:

- Development of a framework for, and implementation of, routine estimation of predictive uncertainty in all future hydrological predictions;
- A new suite of models and methodologies that can be used with confidence for predictions in ungauged basins in different hydroclimatic zones;
- A network of scientists and groups around the world, especially in developing countries, with the necessary scientific expertise and experience to solve emerging hydrological problems;
- An array of measurement networks in selected basins around the world and associated databases of hydrological measurements to serve as a reference pool for new emerging questions.

This international initiative to foster and enable multidisciplinary approaches to hydrology must be matched by national initiatives with similar objectives in individual countries or regions. The U.S.-based Consortium of Universities for the Advancement of Hydrologic Science (CUAHSI, www.cuahsi.org) is gaining momentum in this context. Links between CUAHSI and PUB are manifold, e.g., planned CUAHSI observatories as part of the larger international network of experimental drainage basins over a wide range of scales and hydroclimatic regimes [*Hooper*, 2004].

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 paleogeochemical 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