NATIONAL RESEARCH PROGRAM OF THE WATER RESOURCES DIVISION, U.S. GEOLOGICAL SURVEY, FISCAL YEAR 1987

U.S. Geological Survey
Open-File Report 88-346

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Compiled by
Linda C. Friedman and Christine N. Donato

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DEPARTMENT OF THE INTERIOR

DONALD PAUL HODEL, Secretary

U.S. GEOLOGICAL SURVEY

Dallas L. Peck, Director

For additional information write to:

Chief, Office of Hydrologic Research
U.S. Geological Survey
436 National Center
12201 Sunrise Valley Drive
Reston, Virginia 22092

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THE NATIONAL RESEARCH PROGRAM OF THE WATER RESOURCES DIVISION, U.S. GEOLOGICAL SURVEY

FISCAL YEAR 1987

INTRODUCTION

The National Research Program (NRP) of the U.S. Geological Survey's Water Resources Division (WRD) had its beginnings in the late 1950's when "core research" was added as a line item to the Congressional budget. Since that time, the NRP has grown to encompass a broad spectrum of scientific investigations. The sciences of hydrology, mathematics, chemistry, physics, biology, geology, and engineering are used to gain a fundamental understanding of the processes that affect the availability, movement, and quality of the Nation's water resources. The knowledge gained and methods developed have great value to WRD's operational program. Results of the investigations conducted by the NRP are applicable not only to the solution of current water problems, but also to future issues, anticipated or unanticipated, that may affect the Nation's water resources.

The NRP is located principally in Reston, Va., Denver, Colo., and Menlo Park, Calif. A Chief, Branch of Regional Research (BRR), at each location is responsible for managing the program and serves as a liaison with the WRD's operational program. The Chief, BRR, reports directly to the Chief, Office of Hydrologic Research, who oversees the entire program. For technical administration, the NRP is subdivided into six disciplines with a Research Adviser assigned to each. The Research Adviser serves as a peer resource to the research projects and as a technical consultant to management. The six research disciplines are listed below along with the scope of their activity and current study emphasis:

(1) ECOLOGY--Studies biological and microbiological processes that affect solute composition and solute transport in surface and subsurface waters, and investigates the response of organisms, singly or in associations, to environmental factors to improve understanding of the biological effects of stress, hydrologic events, or climatic trends. Current investigations include studies of the influence of microbial processes on the fate of hazardous substances in ground water; the effect of geochemical processes on the transfer of hazardous substances to food chains that could include humans; the effect of hydrologic processes and associated environmental variables on the composition of benthic and pelagic communities; the use of organisms to help quantify and identify hydrologic events, such as floods or stress inputs; and the effect of microbial transformations of organic materials in the carbon, nitrogen, and sulfur cycles. Most studies are process-oriented and emphasize the interaction of physical and chemical aspects of hydrology with biological processes.

    The types of hydrologic regimes included in these ecological investigations vary from ground waters to lakes, rivers and estuaries, and from coastal wetlands to forests and deserts.

(2) GEOCHEMISTRY--Examines the processes by which mineralogic, geologic, and hydrologic conditions affect water quality. Current research includes the study of physical-chemical controls on dissolution and precipitation of carbonate and silicate mineral assemblages, and on the occurrence of major gases in water, and factors that control dissolution rates of carbonate and clay minerals and buffering of acidic waters by geologic materials. Comprehensive studies of geochemical reactions that affect the chemical composition of ground water, nutrient and metal fluxes between sediment and water, redox potentials in natural water systems, and migration of radionuclides from waste materials are being conducted. The use of stable isotopes to interpret past climates and characterize hydrogeologic processes is being investigated, as is the climatic effect of carbon fluxes in several hydrologic environments. The dispersion of several inorganic chemical constituents in surface-water and ground-water systems is being studied as well as the relation between water quality and health, and the emanation of volatile substances from active volcanic sites.

(3) GEOMORPHOLOGY AND SEDIMENT TRANSPORT--Focuses on understanding fluvial processes that govern the source, mobility, and deposition of sediment in surface waters. Currently, research is aimed primarily at providing the capability for deterministic and stochastic modeling, modeling sediment transport in alluvial channels, and assessing the causes of changes in stream-sediment loads with time, and the rates at which rivers adjust to changes in the quantity of water and sediment contributed to the channel.

(4) GROUND-WATER HYDROLOGY--Develops techniques for evaluating, understanding, and managing ground-water resources. Research into the role of the unsaturated zone is being conducted to provide information needed to evaluate the feasibility of ground-water conservation and management tasks, such as as artificial ground-water recharge, phreatophyte control, and the reduction of evapotranspiration loss. Currently, investigations of land subsidence are underway as are studies to determine how fracture zones, permeability distributions, and geothermal conditions affect, or are affected by, subsurface hydrologic processes. Comprehensive studies in borehole geophysics are being conducted to improve the resolution and effectiveness of these subsurface techniques. Efforts also are being made to develop new and to refine existing two- and three-dimensional models for use in understanding flow and solute transport in porous media in both the saturated and unsaturated zones. Parameter-estimation techniques to enhance and assess model accuracy also are being developed.

(5) SURFACE-WATER HYDROLOGY--Stresses studies to improve the ability to predict the occurrence, distribution, movement, and quality of the Nation's surface-water resources, and to explain quantitatively how these resources may be affected by natural or human-induced changes. Ongoing projects generally can be grouped into five areas: studies of (1) all hydrologic processes that govern the infiltration, evapotranspiration and runoff from basins, especially as they relate to an analysis of the effect of land-use practices, such as surface mining, agriculture, and urbanization; (2) the laws of random processes and how these laws are

related to the statistics of extreme events, such as floods, droughts, or other natural hazards, and the areal distribution of hydrologic information, or the accuracy and reliability of deterministic models of hydrologic systems; (3) the hydraulics or hydrodynamics of flow in single- or multi-dimensional surface-water systems and how this flow is related to the safety and welfare of man as he encroaches on the water body; (4) the sources, transport, and fate of constituents that are related to water quality in surface waters; and (5) the accumulation, movement and melting of snow or ice, particularly the ways in which its presence affects climate, water supply, and (or) safety.

(6) WATER CHEMISTRY--Involves an assessment of natural and contaminant chemicals in water and sediment, and study of fundamental chemical and biochemical processes that affect the movement of organic and inorganic solutes and gases through surface- and ground-water systems. Projects now underway include investigation of the mechanism by which trace metals and organics are sorbed on primary and secondary mineral surfaces; characterization of natural and man-made organic substances; identification of organic pollutants in natural waters; interaction of trace metals and radionuclides with natural organic substances; study of biodegradation processes of organic compounds; and study of the effects of volcanic gases on hydrogeologic systems.

This report provides current information about the NRP on an annual basis. Organized by the six research disciplines, the volume contains a summary of the problem, objective, approach, and progress for each project that was active during fiscal year (FY) 1987. Bibliographic information is included with each project summary in the form of reports published between April 1986 and May 1987.

The projects headquartered in each WRD Region are listed in Appendix I, which also lists the project number (five digits consisting of the appropriate two-letter WRD Region abbreviation followed by a three-digit sequencing number), the project short title, and the number of the summary. Appendix II is an alphabetic list of the Project Chiefs of all projects included in this volume along with the project short title, project number, and page number of the project summary.

This publication is intended for use primarily by the U.S. Geological Survey in program development, coordination, and review. Some of the project summaries may include tentative results that need further study and testing before they are verified. The publication is distributed to members of the Geological Survey staff and the general public that have a special interest in water-resources research.

ECOLOGY

CR286 ORGANIC-TRACE METAL INTERACTIONS

TITLE: Interactions Between Organic Solutes and Trace Metals in Natural Waters, and Their Ecological Role

PROJECT NUMBER: CR 84-286

LOCATION: Topical Research

PROJECT CHIEF: McKnight, Diane M.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: Aquatic humic substances and other classes of dissolved organic material present in natural waters can control the biogeochemistry of many important trace metals. These include trace metals that are (1) involved in weathering reactions, (2) important micronutrients, and (3) possible toxicants at natural or elevated concentrations. Recent advances in organic geochemistry can be used to determine the importance of interactions between organic solutes and trace metals in aquatic environments. Metal-binding sites of humic substances probably are composed of carboxylic-acid groups, but the exact chemical structure and mechanisms are not known. These data are critical to understanding the dependence of metal binding on pH, and concentration of major cations, such as calcium, magnesium, and sodium. Another unknown is the metal-binding properties of nonhumic organic solutes in natural waters, especially those associated with the growth and decomposition of aquatic microorganisms.

OBJECTIVE: (1) Isolate and characterize aquatic humic substances and other organic acids from several aquatic environments; (2) determine the dependence of trace-metal binding by humic substances on the nature and concentration of counter ions (H^+, Ca^{2+}, Mg^{2+}, Na^+), and use these results to develop a polyelectrolyte model for humic substances; (3) determine the processes that control the biogeochemistry of dissolved organic material and selected trace metals in several aquatic environments; and (4) characterize the uptake of iron and copper by freshwater algae as controlled by complexation by aquatic humic substances.

APPROACH: (1) Isolate and characterize aquatic humic substances and other organic acids from several current field sites using conventional methods; (2) conduct potentiometric titrations and other laboratory experiments to determine the dependence of copper and iron complexation by humic substances on pH and counter-ion concentration; (3) continue ongoing field studies of biogeochemical interactions between dissolved organic material and trace metals. Field sites include a mountain stream system, several alpine lakes, and a bog.

PROGRESS: A study of an ombrotrophic bog indicated that the main source of DOC (dissolved organic carbon) was the upper productive layer of the Sphagnum mat. A subsequent field study of the relation between humic substances and transport of trace metals in the bog is underway. A study of the temporal and spatial dynamics of trace metals and natural organics in a mountain stream system has shown that: (1) photoreduction of hydrous iron oxides is an important control on iron chemistry, and (2) a peak in instream microbe productivity is associated with the DOC peak during spring snowmelt. In a field study of phytoplankton dynamics in an alpine lake system, we have shown that the spring flood is a time of rapid growth of planktonic diatoms and that within-lake production of DOC is related to algal productivity. In the fall, a bloom of blue-green algae develops; these blue-green algae are more sensitive to acidic conditions than the diatoms in the spring.

REPORTS PUBLISHED:

Bencala, K. E., and McKnight, D. M., 1987, Identifying in-stream variability--sampling iron in an acidic stream, in Averett, R. C., and McKnight, D. M., eds., Chemical quality of water and the hydrologic cycle: Chelsea, Mich., Lewis Publishers, p. 255-269.

McKnight, D. M., Brenner, M., Smith, R. L., and Barron, J., 1986, Seasonal changes in phytoplankton populations and related chemical and physical characteristics in lakes in Loch Vale, Rocky Mountain National Park, Colo.: U.S. Geological Survey Water-Resources Investigations Report 86-4101, 64 p.

McKnight, D. M., and Feder, G. L., in press, Ecological Aspects of Humic Substances in the Environment: in McCarthy and others, eds., Humic Substances: Environmental Interactions: London, John Wiley and sons.

CR293 HYDROL-BIOL GEOCHEM INTERACTIONS

TITLE: The Role of Chemical Fluxes in the Biogeochemistry of Inland Surface Waters, Including Lakes, Reservoirs, and Wetlands

PROJECT NUMBER: CR 85-293

LOCATION: Topical Research

PROJECT CHIEF: LaBaugh, James W.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Most studies of the biogeochemistry of inland aquatic ecosystems have been confined to the water body. The effect of fluxes external to the water body on ecosystem biogeochemical processes has been ignored. Detailed studies of external chemical fluxes and their relation to the supply or loss of biologically important chemical elements are almost nonexistent, particularly for aquatic ecosystems that lack channelized surface-water inflow and outflow. Research on these external fluxes and their quantitative significance is critical for decisionmakers responsible for water quality and biological productivity of lakes, reservoirs, and wetlands.

OBJECTIVE: Determine the mechanisms controlling fluxes of biologically important chemical elements between surface waters and their watersheds. Examine the different transport pathways that affect the supply and loss of those elements from surface waters and use empirical and conceptual models of hydrological-biological interactions to identify mechanisms to be investigated further in the field.

APPROACH: Determine the mechanisms controlling supply and loss of biologically important chemical elements in surface waters (lakes, reservoirs, and wetlands) using data from new field work and using previously collected data from intensively studied field sites. Use field data to develop empirical and conceptual models that, in turn, will suggest areas of further field research into hydrological-biogeochemical interactions.

PROGRESS: One journal article was published. A paper summarizing studies of wetlands and lakes in the northern prairie of North America is in press. A paper on the role of ground-water flux on resource competition in Williams Lake, Minn., and a paper relating hydrogeologic setting to chemical characteristics of lakes and wetlands at three field sites were completed. Intensive studies of chemical fluxes including determination of ground-water flux and in-lake chemical and biological investigations continued at Cottonwood Lake wetlands, N. Dak., Crescent Lake refuge, Nebr., and Williams Lake, Minn.

WRD FEDERAL RESEARCH PROJECTS.....ECOLOGY

REPORTS PUBLISHED:

LaBaugh, J. W., in press, Chemical characteristics of wetlands and lakes in the northern prairie of North America, in van der Valk, A. G., ed., Wetlands of the northern prairies of North America: Society of Wetland Scientists Monograph.

LaBaugh, J. W., 1986, Limnological characteristics of selected lakes in the Nebraska sandhills and their relation to chemical characteristics of adjacent groundwater: Journal of Hydrology, v. 86, p. 279-298.

LaBaugh, J. W., Winter T. C., Adomaitis, V. A., and Swanson, G. A., in press, Hydrology and chemistry of selected prairie wetlands in the Cottonwood Lake area, Stutsman County, N. Dak., 1979-82: U.S. Geological Survey Professional Paper 1431.

CR295 MICROBIAL GEOCHEM OF ORGANIC MATTER

TITLE: Microbial Transformation of Dissolved Organic Carbon in Aquatic Environments

PROJECT NUMBER: CR 86-295

LOCATION: Topical Research

CHIEF: Smith, Richard L.

CITY: Arvada, CO

PROBLEM: Although it is recognized that microorganisms play an important role in the transformation of organic compounds in aquatic habitats, very little is known about the exact nature of these processes. This is true for pristine and contaminated environments. Within the context of in-situ environmental conditions, the mechanisms, pathways, rates, and factors controlling carbon cycling by microorganisms are poorly understood. However, these processes can significantly affect the entire range of biogeochemical and geochemical processes occurring within the aquatic environment.

OBJECTIVE: To study the mechanisms, pathways, and rates of transformation of organic compounds (both naturally occurring and contaminant) mediated by microorganisms in aquatic habitats and to identify some of the factors controlling these processes. The effect these transformations have upon other biogeochemical processes will also be examined.

APPROACH: Habitats of primary focus will be a pristine alpine stream and a sewage-contaminated ground-water aquifer. Microbial processes will be determined in both water and sediment samples using tracer techniques for both laboratory and field studies. These experiments will endeavor to maintain in situ conditions whenever possible and will therefore involve development of sample-handling techniques. When necessary, experiments with isolated cultures of microorganisms will be employed to help interpret the results obtained with natural samples.

PROGRESS: Research efforts continue to be focused upon carbon and nitrogen cycling at the Otis Air Force Base Groundwater Contamination Site in Cape Cod, Massachusetts. (1) Studies were continued on the relative rate of transport of ammonium, potassium, and nitrate within the contaminant plume. A divergent tracer test was conducted in the field in which these constituents were injected as a pulse and monitored as they moved past a multilevel sampling device. The results demonstrated that the rates of ammonium and potassium transport in the aquifer are retarded relative to a conservative constituent, whereas nitrate moves conservatively. During transport, ammonium and potassium sorb on aquifer solids displacing native cations such as calcium, magnesium, and sodium. The test results are consistent with the distributions of ammonium, nitrate, and major cations in the sewage plume. (2) In order to

assay in-situ rates of microbial processes that might be occurring within an aquifer, sampling and incubation techniques for selected microbial activities are being developed. Using a coring device (developed at the University of Waterloo) that takes complete cores from an aquifer with the interstitial porewater intact, techniques to pump substrates, inhibitors, or tracers directly into the cores to assay for microbial processes within intact cores are being developed. After an appropriate incubation period, the interstitial porewater is extracted from the cores and assayed for the product of interest. At present, this technique has been used successfully to study denitrification in cores. (3) As a consequence of our studies on nitrogen and carbon cycles at the Cape Cod site, dissolved gases within the contaminant plume, frequently end products of microbial metabolism, are assayed routinely. Depth profiles of dissolved N_2, CO_2, and N_2O demonstrate relatively high concentrations of these gases in certain zones of the plume. In the case of N_2, concentrations are well in excess of simple equilibrium with the atmosphere. To discover whether these gases were transported in a conservative manner within the contaminant plume, a tracer experiment was conducted to determine the relative rates of transport of two gases, Freon-116 and methane to a conservative tracer, NaCl. Results demonstrated that the gases were transported conservatively. When normalized to the injectate concentration, Freon-116 and chloride behaved in an identical fashion, but CH_4 was significantly attenuated. This attenuation was most likely the result of methane oxidation by the resident microbial population.

REPORTS PUBLISHED:

McKnight, D. M., Brenner, M., Smith, R. L., and Barron, J., 1986, Seasonal changes in phytoplankton populations and related chemical and physical characteristics in lakes in Loch Vale, Rocky Mountain National Park, Colo.: U.S. Geological Survey Water-Resources Investigations Report 86-4101, 64 p.

Oremland, R. S., Cloern, J. E., Sofer, Z., Smith, R. L., Culbertson, C. W., Zehr, J., Miller, L., Cole, B., Harvey, R., Iversen, N., Klug, M., DesMarais, D. J., and Rau, G., in press, Biogeochemistry and microbial processes of Big Soda Lake, Nev., in Kelts, K., ed., Lacustrine Petroleum Source Rocks: London, Geologic Society of London.

Smith, R. L., and Klug, M. J., 1987, Flow-through flasks to study microbial metabolism in whole sediments: Applied Environmental Microbiology, v. 53, p. 371-374.

Tarafa, M. E., Whelan, J. K., Oremland, R. S., and Smith, R. L., 1987, Evidence for microbiological activity in Leg 95 (New Jersey Transect) sediments, in Poag, C. W., Watts, A. B., and others, eds., Initial reports of the Deep Sea Drilling Project: Washington, D.C., U.S. Government Printing Office, v. 95, p. 635-640.

Whelan, J. K., Oremland, J. K., Tarafa, M. E., Smith, R. L., Howarth, R., and Lee, C., 1986, Evidence for sulfate-reducing and methane-producing microorganisms in sediments from sites 618, 619, and 622, in Bowman, A. H., and others, eds., Initial Reports of the Deep Sea Drilling Project: Washington, U.S. Government Printing Office, v. 96, p. 767-775.

NR027 PLANT GROWTH AND HYDROLOGY

TITLE: Basic Research Concerning Periodic Plant Growth Phenomena and Hydrology

PROJECT NUMBER: NR 66-027

LOCATION: Topical Research

PROJECT CHIEF: Phipps, Richard L.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Many plant growth phenomena are controlled in part by environmental conditions. Because water availability to plants seems to be the single most important factor limiting physiological processes in plants, relations must exist between hydrologic factors or conditions and various plant-growth phenomena. Studies to date indicate that such relations are complex and little understood. Such an understanding must be established before plants can be fully utilized to interpret hydrologic phenomena.

OBJECTIVE: Basic research objectives include the determination of relation between characteristics of the hydrologic environment and periodic plant-growth phenomena. The ultimate objective is to use data from interannual and intra-annual tree-growth parameters (tree rings) to estimate or reconstruct, on a temporal or spatial basis, parameters of the hydrologic environment. A specific long-range objective is to determine relationships between tree growth and environmental pollutants (including heavy metals as well as atmospheric pollutants). Short-range objectives are intended to contribute toward long-range objectives through methods development and establishment of a data base.

APPROACH: Collect data of growth responses of many species in innumerable habitats to ascertain types of information regarding hydrologic environment recorded in plant growth. Prepare a data base composed primarily of measured annual increments of radial growth of trees, and include other parameters of growth, such as wood anatomy and various ecological and mensuration statistics. The basic approach is to (1) identify a specific problem, examine the botanical growth processes involved, (2) describe the relationships between these processes and the aspect of the hydrologic environment under consideration, and (3) use botanical evidence to interpret, estimate, or extend records of the hydrologic environment.

PROGRESS: Trees growing over polluted ground water in Aberdeen, Md., were analyzed to determine the element content of individual rings, and to determine if concentrations over time could be used to estimate the past movement of the contaminated plume. A series of trees was sampled with Proton Induced X-ray Emission (PIXE) at successively greater distances from the burial site of contaminants. Large peaks of iron and cobalt within individual rings were found in the late 1930's in a tree nearest the burial site, in the mid 1960's in a tree still farther, and in the mid 1980's in a farthest tree. Assuming that each peak represents the respective passing of the contaminant front, a velocity of about 1.5 m/yr was calculated. As determined in 1986, the concentration of iron in ground water increased with distance from the burial site.

REPORTS PUBLISHED:

Weems, R. E., Obermeier, S. F., Pavich, M. J., Gohn, G. S., Rubin, Meyer, Phipps, R. L., and Jacobson, R. B., 1986, Evidence for three moderate to large prehistoric holocene earthquakes near Charleston, S.C.: U.S. National Conference on Earthquake Engineering, 3rd, Charleston, S.C., 1986, Proceedings, p. 3-14.

Yanosky, T. M., and Robinove, C. J., 1986, Digital image measurement of the area and anatomical structure of tree rings: Canadian Journal of Botany, v. 64, p. 2896-2902.

Whiton, J. C., in press, Trends in growth-rate of pines since 1930 in the Northeastern United States: International Symposium on the Ecological Aspects of Tree Ring Analysis, Proceedings.

Yanosky, T. M., Robinove, C. J., and Clark, R. G., in press, Progress in the image analysis of tree rings: International symposium on the Ecological Aspects of Tree Ring Analysis, Proceedings.

NR090 WETLAND STUDIES

TITLE: Remote Sensing and Ecological Research in Wetlands

PROJECT NUMBER: NR 73-090

LOCATION: Topical Research

PROJECT CHIEF: Carter, Virginia P.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Wetlands are hydrologically controlled ecosystems essential to estuarine, marine, lacustrine, and riverine productivity. To improve our understanding of these ecosystems we need information on: (1) Wetland hydrologic variables/budgets and their relation to wetland vegetation and nutrient cycling; (2) wetland dynamics and boundary fluctuations; (3) wetland functions and values; and (4) short and long-term temporal changes. Wetland plants may serve as sensitive hydrologic indicators of water (oxygen) stress; water-quality characteristics such as salinity, turbidity, pH, nutrients; presence of various pollutants; or frequency and duration of inundation. Submersed aquatic vegetation has many functional values including: (1) Habitat for invertebrate species; (2) food and (or) shelter for juvenile and adult fish, waterfowl, and other wildlife; (3) retarding flow velocities, stabilizing bottom sediments, and slowing erosion; and (4) oxygenating the water, recycling nutrients and heavy metals. Decline or disappearance of aquatic plant communities is of concern to scientists, ecologists, environmentalists, and managers. Overgrowth of submersed vegetation under nutrient-enriched conditions also is a problem. The processes affecting distribution and abundance and the factors contributing to the balance between phytoplankton and macrophytes are understood poorly.

OBJECTIVE: (1) Characterize wetland-transition zones and relate distribution of vegetation in Dismal Swamp in Virginia and North Carolina, to soils, hydrology, and elevation; (2) examine seasonal and long-term changes in wetland ecology as related to changes in environmental parameters including hydrology, water quality, and land use; (3) aid in the development of models that use remote sensing or biological hydrologic dates as part of their primary data base; (4) determine factors responsible for the changing distribution of aquatic beds and the resurgence of submersed macrophytes in the tidal Potomac River; (5) monitor the spread of Hydrilla and competition with other macrophytes; and (6) consider processes affecting flux of materials from vegetation to soil or water column or vice versa.

APPROACH: (1) Measure ground-water levels, surface-water inundation, ground and soil O_2, and recharge and discharge relation on the western transition zone of Dismal Swamp; (2) collect data on ground and surface water in major vegetation communities as well as data on elevation, depth of organic soil, water table, and surface flooding; (3) conduct field and laboratory

investigations of the survival of submersed aquatic plants under a variety of conditions and in different locations; (4) conduct yearly field surveys to document distribution, abundance, and species composition, and (5) develop models illustrating relation between plant success and other environmental factors.

PROGRESS: During 1986, submersed aquatic macrophytes spread about 8 miles downstream from their 1985 extent in the tidal Potomac River, Va. Plants were still scarce to nonexistent in the lower tidal river where our measurements show very low light penetration as a result of high chlorophyll-a concentrations. The correlation between soils, hydrology, and vegetation in the Dismal Swamp has been completed and written up in the form of a Ph.D. dissertation for George Washington University.

REPORTS PUBLISHED:

Carter V., 1986, An overview of the hydrologic concerns related to wetlands in the United States: Canadian Journal of Botany, v. 64, no. 2, p. 364-374.

NR136 MICROBIAL GEOCHEMICAL MODELS

TITLE: Modelling of Microbially-Catalyzed Geochemical Reactions in Aquatic Environments

PROJECT NUMBER: NR 87-136

LOCATION: Topical Research

PROJECT CHIEF: Lovley, Derek R.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Microorganisms catalyze most of the natural redox reactions involving carbon, sulfur, nitrogen, and metals. Thus, geochemical models of the distribution and fate of natural and contaminant compounds must include a microbiological component, which requires an understanding of the physiological characteristics of microorganisms that control the rate and extent of microbially-catalyzed reactions.

OBJECTIVE: (1) Quantify the rates of microbial process that influence the geochemistry of surface-water and ground-water aquifers; (2) determine the physiological characteristics that control the rate and extent of microbial processes; and (3) develop mathematical models of the distribution of microbial processes in surface-water and ground-water aquifers.

APPROACH: Rates and pathways of microbial processes will be quantified with radiotracer, stable isotope and inhibitor techniques. Microbial physiological characteristics will be determined with experimental manipulations of natural mixed populations and pure cultures. Data on physiological characteristics will be combined with appropriate geochemical models to generate models for the distribution of microbial processes.

PROGRESS: An organism that obtains its energy for growth by coupling the oxidation of organic matter to the reduction of ferric iron was isolated for the first time. This is a significant advancement for basic microbiology. The characterization of the physiology of this organism will provide information to develop models for microbial iron metabolism in surface- and ground-water sedimentary environments. It was demonstrated for the first time that dissimilatory microbial iron reduction can result in the production of fine-grained magnetite under anaerobic conditions. In addition to its geochemical significance, this finding is of central importance to such fields as paleolimnology and paleomagnetism as it provides a possible new source of magnetite and magnetism in sediments. The mechanisms by which sulfate reduction and methane production are excluded from the zone of ferric iron reduction in sedimentary environments were determined. These studies have demonstrated that when ferric iron is available in the appropriate form, iron-reducing organisms prevent sulfate reduction and methane production by maintaining the concentration of electron donors too low for sulfate-reducing

or methanogenic organisms to metabolize. These findings will contribute to the inclusion of an iron-reduction component in the developing conceptual and mathematical models for the distribution of microbially catalyzed redox reactions in aquatic environments. Progress was made in developing the use of hydrogen concentrations as an indicator for the predominant microbially catalyzed reactions in sedimentary environments. Laboratory studies with sediments from the Potomac River Estuary and measurements of hydrogen along the flow path of an aquifer further supported the validity of this novel hypothesis.

REPORTS PUBLISHED:

Lovley, D. R., in press, Organic matter mineralization with the reduction of ferric iron: A review: Geomicrobiology Journal, v. 5, p. 375-399.

Lovley, D. R., and Phillips, E. J. P., in press, Rapid assay for microbially reducible ferric iron in sediments: Applied and Environmental Microbiology, v. 53, p. 1536-1540.

Lovley, D. R., and Phillips, E. J. P., in press, Competitive mechanisms for inhibition of sulfate reduction and methane production in the zone of ferric iron reduction in sediments: Applied and Environmental Microbiology, v. 53, p. 2636-2641.

Lovley, D. R., and Phillips, E. J. P., 1986, Organic matter mineralization with reduction of ferric iron in anaerobic sediments: Applied and Environmental Microbiology, v. 51, no. 4, p. 683-689.

Lovley, D. R., and Phillips, E. J. P., 1986, Availability of ferric iron for microbial reduction in bottom sediments of the freshwater tidal Potomac River: Applied and Environmental Microbiology, v. 52, no. 4, p. 751-757.

WR012 LIMNOLOGY: BENTHIC COMMUNITIES

TITLE: Limnology: Controls on Distribution and Composition of Benthic Communities of Inland Aquatic Ecosystems

PROJECT NUMBER: WR 61-012

LOCATION: Topical Research

PROJECT CHIEF: Slack, Keith V.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Benthic invertebrates are the aquatic organisms most widely used as indicators of environmental quality in streams. Although many factors are known to affect the abundance and distribution of species, it is usually not possible to predict expected changes in benthic communities for a given impact. Improved understanding is needed of factors that control temporal and spatial distribution, abundance, and species composition of benthic invertebrate associations in different types of streams. The ability to predict such changes awaits greater knowledge of the functional relations between benthic invertebrates and other components of stream ecosystems.

OBJECTIVE: To study the organization and dynamics of benthic invertebrate species associations in streams. To study the relationships between environmental factors in streams, such as water and sediment chemistry, detritus, biotic interactions, and instream physical conditions, to the macroscale, mesoscale, and microscale distribution and the composition of stream biotic communities.

APPROACH: In a variety of small to large streams, sample benthic invertebrates and relate their spatial and temporal distribution and species composition to environmental differences using multivariate analysis. Test relationships derived from field studies in field and laboratory experiments.

PROGRESS: In a study of the impact of low pH and high concentrations of dissolved and precipitated metals on aquatic communities, invertebrate drift was collected in an acid- and metal-enriched Colorado Rocky Mountain stream (Snake River) and an adjacent undisturbed stream of similar size (Deer Creek). The nocturnal increase in drift abundance in both streams and below their confluence indicated that behavioral drift rather than catastrophic drift was occurring in the stressed and unstressed streams. About one-third of the total species regularly occurred in both streams and two-thirds occurred only in Deer Creek. Artificial substrate collections confirmed the low abundance of the benthic fauna in these streams compared to similar streams at lower altitudes. Preliminary results for the insect family Chironomidae suggest that in these high mountain streams, numbers of species in the subfamily Diamesinae decrease but numbers of individuals increase with environmental stress. This same response is shown by the subfamily Chironominae in lowland

streams as well as in Deer Creek-Snake River. Rearing Chironomidae in the laboratory produced 26 adults, 18 with all three life-cycle stages, from 128 larvae. Larvae collected from Snake River adapted to laboratory water quality (pH >7) indicating a wide ecological tolerance. These species may owe their abundance in Snake River to decreased competition with species less tolerant of low pH and high metal concentrations.

WR046 GEOCHEM RIVERS AND ESTUARIES

TITLE: Geochemistry of Riverine and Estuarine Waters

PROJECT NUMBER: WR 68-046

LOCATION: San Francisco Bay, California

PROJECT CHIEF: Peterson, David H.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Physical and chemical processes and rates (PAR) that control changes in water and sediment chemistry in river, estuary, and coastal-ocean systems are defined poorly. An understanding of PAR is essential to assess the response of these systems to variations in climate and human activities that can lead to changes in the amount, character, and timing of freshwater, toxic waste, sediment, and plant-nutrient inflows to these environments.

OBJECTIVE: Define dominant PAR that influence and control water and sediment chemistry (primarily oxygen, carbon, silicon, nitrogen, and phosphorous) in riverine, estuarine, and coastal ocean environments, including partially mixed and stratified environments.

APPROACH: Identify and analyze vertical and horizontal PAR that control the supply, removal, and dilution of chemical substances in these environments by comprehensive field (shipboard and in-situ instrumentation) and numerical simulation methods. As data become available, systems variability is analyzed on various scales: for example, interannual variability (primarily climate-related), long-term trends (human factors) as well as seasonal and short term source-sink processes (photosynthesis/mineralization).

PROGRESS: The strong north-south gradient in precipitation along the West Coast makes this region an interesting laboratory for studying the influence of climate on runoff variability in general and riverine chemistry in particular. Interannual fluctuations in large-scale atmospheric circulation and associated precipitation and runoff can produce major disruptions in the "average" climatologic picture. The effect of the climate gradient along the western United States on the total dissolved-solids concentrations in rivers is summarized as a highly idealized force-response model of total dissolved-solids concentrations as a function of river flow. The response in dry climates to the south in wet years is more like the wetter climate response curves observed to the north and the response in dry years in the north is more like the drier response curves observed to the south. Over an annual cycle, production and mineralization processes have finite maximum rates per unit estuarine area. River basin process can be a fundamental cause of estuarine variability. In estuaries with a mean specific river flow close to the global average, the finite rates can exceed or be exceeded by riverine sources. In a generalized and very simple model, when the area of the estuary

is very small relative to the area of the river basin (that is, the river basin is hundreds of times larger), the within-estuary nutrient cycling processes can be overwhelmed by a strong riverine source. In this instance, the within-estuary plant nutrient recycling processes are probably relatively ineffective before the river water reaches the coastal ocean. When the area of the estuary increases relative to the area of the river basin (that is, the river basin is only about ten times larger), estuarine cycling processes can dominate the relatively weak riverine sources. In this instance, nutrients can be recycled many times before transit to the coastal ocean, atmosphere, or bottom sediment. If estuarine/coastal systems where recycling processes are especially important also remain stratified over long periods, then nutrient loss from the upper photic layer is inevitable and low nutrient concentrations could limit biomass production. In this latter case (for example, Chesapeake Bay) the magnitude of the anthropogenic nutrient factor is expected to be more important than in systems where nutrient recycling processes are relatively less effective (for example, San Francisco Bay).

REPORTS PUBLISHED:

Mooers, C. N. K., Peterson, D. H., and Cayan, D. R., 1986, The Pacific Climate Workshops: EOS, v. 67, no. 52, p. 1404-1405.

Peterson, D. H., Cayan, D. R., DiLeo-Stevens, J. and Ross, T. G., in press, Some effects of climate variability on hydrology in western North America: International Association of Hydrological Sciences Conference, Proceedings.

Peterson, D. H., Cayan, D. R., and Festa, J. F., 1986, Interannual variability in biogeochemistry of partially mixed estuaries--Dissolved silicate cycles in Northern San Francisco Bay in Douglas A. Wolfe, ed., Estuarine Variability, p. 123-138.

Schemel, L. E. and Hager, S. W., 1986, Chemical Variability in the Sacramento River and in Northern San Francisco Bay, Estuaries, v. 9, no. 4A, p. 270-283.

WR068 ORGANIC CHEMICALS IN SUBSURFACE

TITLE: Fate of Organic Chemicals in Subsurface Environments

PROJECT NUMBER: WR 71-068

LOCATION: Topical Research

PROJECT CHIEF: Ehrlich, Garry G.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Release of various synthetic organic compounds to the environment has caused soil and ground-water pollution in many places. The processes that control the persistence and movement of these materials are not well understood. A better understanding is necessary to aid in construction of models to predict movement and fate of pollutants in the subsurface and for design of control and abatement techniques.

OBJECTIVE: (1) Determine the transformation pathways of selected organic compounds using a combination of field observations and laboratory simulations of environmental conditions; (2) assess the relative importance of physical, chemical, and biochemical processes in the transformation of these compounds under natural ambient conditions; and (3) study relevant biotransformation processes occurring in the subsurface.

APPROACH: Select one or more field sites where ground water has become contaminated with organic compounds. Collect and analyze water samples to discover the chemical transformations that are occurring in the subsurface environment. Use laboratory simulation studies to elucidate the controls on these transformations.

PROGRESS: The movement and fate of the major water-soluble compounds in creosote are being studied, both in the laboratory and at the U.S. Geological Survey Hazardous Waste Study Site at Pensacola, Fla. The anaerobic microbial degradation pathways for several of the major components of the water-soluble fraction have been determined in laboratory digestors using high pressure liquid chromatography (HPLC) and gas chromatography-mass spectrometry (GC-MS) techniques. Computer programs to determine kinetic microbial growth parameters from laboratory growth studies and the adsorption of organic compounds in laboratory columns have been developed. The kinetic parameters and sorption characteristics have been determined for several of the major water-soluble compounds.

REPORTS PUBLISHED:

Goerlitz, D. F., Godsy, E. M., Troutman, D. E., and Franks, B. J., 1986, Chemistry of ground water at a creosote works, Pensacola, Fla., in Mattraw, H. C., Jr., and Franks, B. J., eds., Movement and fate of creosote waste in ground water, Pensacola, Fla.: U.S. Geological Survey Water-Supply Paper 2285, p. 49-53.

Godsy, E. M., Goerlitz, D. F., and Ehrlich, G. G., 1986, Effects of pentachlorophenol on methanogenic fermentation of phenol, in Ragone, S. E., and Sulam, D. J., eds., Program overview and selected papers from the toxic-waste program technical meeting, Tucson, Arizona, March 20-22, 1984: U.S. Geological Survey Open-File Report 86-324, p. 101-105.

WR125 TRACE ELEMENTS AVAILABILITY IN SEDIMENTS

TITLE: Availability of Trace Elements in Sediments to Aquatic Organisms

PROJECT NUMBER: WR 75-125

LOCATION: Topical Research
PROJECT CHIEF: Luoma, Samuel N.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Concentrations of potentially toxic elements in sediments are orders of magnitude higher than concentrations in water. The ability of the aquatic environment to assimilate many toxic wastes depends upon how available this concentrated sediment-bound pool of elements is to aquatic organisms. Development of realistic pollution regulations, in turn, depends on predicting assimilation capacities. Assessment of biological indicator data for mineral exploration and pollution assessment also depend upon understanding factors affecting the biological availability of trace elements bound to sediments. It is established that the same biota in different environments may differ widely in their susceptibility or their response to trace elements, and that these differences may, at least partly, be related to the differences in the availability of metals in sediments. However, little is known about the geochemical and physiological factors that influence the transport of metals from sediments to organisms.

OBJECTIVE: (1) Study the partitioning of trace metals among the components of sediments, and identify the processes that control partitioning; (2) study the influence of geochemical partitioning of trace metals in sediments upon metal uptake and metal effects in organisms that contact sediments directly; (3) study physiological characteristics of aquatic organisms that uptake metal; (4) improve methodology which uses biota and sediments as indicators of geochemical conditions; (5) develop indices or models for predicting the bioavailability of metals after their release to the aquatic environment; and (6) develop methods for assessing the presence of biological effects from toxic wastes in aquatic communities in nature.

APPROACH: (1) Collect organisms and sediments from rivers, lakes, or estuaries, across spatial or temporal gradients of physicochemical conditions; analyze geochemical partitioning through the use of chemical extractions, mathematical models, and statistics; statistically assess relation of metal concentrations in organisms to aspects of the specific geochemical gradient under study. (2) Use laboratory studies to assess the biological influences on metal burdens in animals, such as animal size, intraspecific differences in metal tolerance, and physiological controls on metal uptake and metabolism. (3) Geochemically modify sediments or use well-defined model sediments in laboratory studies of metal uptake by organisms to identify physicochemical factors that affect metal availablity, and to test models derived from field studies.

PROGRESS: (1) Developed method for separating natural variability of Cu concentrations in estuarine sediments from variability caused by human inputs of Cu. (2) Assessed causes of variability in metal concentrations in insects and sediments from Clark Fork River, Mont. Both seem to be tied to the geomorphology of sediment deposition in the floodplain of the river and to metal-specific geochemical processes that influence metal movement from floodplain sediments to the river. (3) Selenium distributions in benthic clams in North San Francisco Bay were shown to reflect Se inputs from local industrial sources rather than inputs from agricultural wastewater discharges to the Bay. (4) Reviewed current methods for assessing bioavailability of metals from sediments, emphasizing strong limitations of most approaches due to limited understanding of fundamental processes involved.

REPORTS PUBLISHED:

Luoma, S. N., 1987, Review of "Ecotoxicology" Ecological Bulletin: Earth Science Reviews, v. 24, p. 143.

Luoma, S. N., 1986, A comparison of methods for determining copper partitioning in oxidized sediments: Marine Chemistry, v. 20, p. 45-60.

WR137 TOXIC SUBSTANCES: AQUATIC ECOSYSTEMS

TITLE: Effects of Toxic Substances on Aquatic Communities

PROJECT NUMBER: WR 75-137

LOCATION: Nationwide

PROJECT CHIEF: Leland, Harry V.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Ecological effects of toxic materials in surface waters are of concern. Standard methods for evaluating effects of toxic substances at sublethal levels in aquatic ecosystems are not available. Several promising, but untested, methods are available to determine responses of individual species and are of potential value in monitoring programs. Data from the field and from laboratory streams on effects of continued low levels of toxicants on function and structure of aquatic communities are largely lacking.

OBJECTIVE: Determine through detailed studies of organisms, simplified ecosystems, and natural sites, the extent to which trace metals and stable organic compounds affect the production and structure of aquatic-plant assemblages and the growth and reproductive capacity of aquatic animals. Evaluate methods of assessing effects of chronic exposures of toxicants on individual species and natural aquatic communities.

APPROACH: Evaluate methods for assessing effects of chronic exposures of toxic substances released to the environment as a consequence of fossil-fuel extraction and combustion. These include tests of hatchability, embryogenesis, and respiratory response in fishes, specific birth rate and survival of critical life stages of aquatic invertebrates, and population growth rate of algae. Determine physico-chemical factors affecting responses and bioaccumulation of these toxic substances. Examine trophic dynamics of experimental streams exposed to chronic amounts of trace metals and stable organic compounds of fossil-fuel origin. Evaluate methods and results of laboratory and experimental stream studies by field experiments. Determine the utility of the biological test methods for detecting and monitoring small concentrations of toxicants. Examine the factors (physicochemical and biological) influencing responses of natural aquatic communities.

PROGRESS: Effects of saline, agricultural return flows on aquatic communities of the San Joaquin River, Calif., are being studied. Biological, chemical, and physical variables were monitored at six mainstem and five tributary sites during 1985 and 1986. Corbicula fluminea, the asiatic clam was shown to be enriched in Se, Hg, Cd, and possibly other trace elements at upstream sites, whereas stable organochlorine insecticide residues were higher in Corbicula at downstream sites. Relationships among trace elements in river water and tissues of Corbicula and the water hyacinth, Eichhornia crassipes, are being examined. Corbicula is a good monitor of Se bioavailability with concentrations of Se in soft tissue varying directly with the mean total Se concentration of river water. Distributions of phytoplankton, periphyton, and benthic invertebrate communities in permanent flow regions of the San Joaquin River have been determined for the low flow period of 1985. The structure of biological communities reflects concentrations of salts from upstream regions, the supply of nutrients, and the dissolved oxygen status of the water.

REPORTS PUBLISHED:

Leland, H. V., Fend, S. V., Carter, J. L., and Mahood, A. D., 1986, Composition and abundance of periphyton and aquatic insects in a Sierra Nevada, California, stream: Great Basin Naturalist, v. 46, p. 595-611.

WR145 VEGETATION ECOHYDROLOGY

TITLE: Ecohydrology of Arid Region Vegetation

PROJECT NUMBER: WR 76-145

LOCATION: Arizona, arid regions

PROJECT CHIEF: Turner, Raymond M.

HEADQUARTERS OFFICE: Tucson, AZ

PROBLEM: Water is becoming increasingly scarce in the arid region of the United States. In their attempt to manage or control this essential resource, humans constantly modify regional hydrology by changing watertable elevations, altering surface-drainage patterns, controlling streamflow, and altering erosion. These and other modifications may result in altered water quality and often result indirectly in vegetation changes that reflect the changed regional hydrology. Humans also change the vegetation directly through agricultural practices, urbanization, and vegetation management activities, all of which have an impact on the region's hydrology.

OBJECTIVE: Define the interrelation between the region's hydrology and its vegetation. Measure the effect that the changing patterns of vegetation have on the regional water supply, and, conversely, the effect that changes in water quality and quantity have on the vegetation.

APPROACH: Use historical documents and old photographs to determine the scope of vegetation changes over time. Use remote sensing products such as aerial photographs and satellite images to locate, map, and measure existing vegetation. Riparian and phreatic vegetation will be emphasized because, compared to the area they occupy, their hydrologic and ecological significance is disproportionately great. The communities are valuable wildlife habitats and recreation sites; at the same time they consume and transpire large amounts of water. Studies of desert plant populations will be made because vegetation changes at dry sites may be sensitive indicators of large-scale climatic change.

PROGRESS: The Santa Cruz River in southern Arizona represents one of the few western streams for which 19th century arroyo-cutting and subsequent channel changes can be reconstructed with confidence. Rich archives that accumulated as Tucson evolved from mud-walled village to modern metropolis have allowed us to establish watershed conditions prior to arroyo initiation; investigate when and how the arroyo developed; evaluate the effects of climate, geomorphic thresholds, and anthropogenic factors; and relate the continuum of historic channel changes to modern floodplain concerns. We have shown that discontinuous arroyos existed prior to the date of accelerated erosion. Headcut migration integrated these arroyos into a single channel during large flow events in summer and fall 1890, winter 1904-1905, and winter 1914-1915.

Channel aggradation during the dry period 1930-1960 was reversed by progressive urbanization of the floodplain. Sediment eroding from the Tucson Basin reach accumulated in the reach immediately downstream. The latter now supports several satellite communities under heavy development. Improved channel conveyance and more frequent tropical storms have produced an increase in flood peaks during the last 20 years. With increased stream power in the upper reach, the downstream zone of maximum aggradation is now prone to accelerated erosion should high-flow conditions arise in the near future. Should this occur, we anticipate catastrophic silting at the Gila River-Santa Cruz River confluence and points downstream. This could be the first time that the upper Santa Cruz has contributed significant amounts of sediment to the Gila River in centuries, if not millenia.

REPORTS PUBLISHED:

Betancourt, J. L., 1987, Paleocology of pinyon-juniper woodlands--summary: U.S. Department of Agriculture, Forest Service, General Technical Report INT-2115, p. 129-139.

Betancourt, J. L., Van Devender, T. R., and Rose, M., 1986, Comparison of plant macrofossils in woodrat (Neotoma spp.) and porcupine (Erethizon dorsatum) middens from the western United States: Journal of Mammalogy, v. 67, p. 266-273.

Davis, O. K., and Turner, R. M., 1986, Palynological evidence for the historic expansion of juniper and desert shrubs in Arizona, U.S.A.: Review of Paleobotany and Palynology, v. 49, p. 177-193.

Webb, R. H., Steiger, J. W., and Wilshire, H. G., 1986, Recovery of compacted soils in Mojave Desert ghost towns: Soil Science Society of America Journal, v. 50, p. 1341-1344.

WR164 ESTUARINE PLANKTON DYNAMICS

TITLE: Plankton Dynamics in Tidal Estuaries

PROJECT NUMBER: WR 79-164

LOCATION: San Francisco Bay area, Calif.

PROJECT CHIEF: Cloern, James E.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Because plankton are important sources of material and energy for other trophic levels, and because they interact rapidly with dissolved solutes, an understanding of plankton dynamics is a prerequisite for understanding other dynamic phenomena in estuaries. The composition and density of plankton populations vary temporally and spatially in response to natural and human-induced environmental changes. Therefore, assessments of human impact on estuarine ecosystems is dependent on a thorough understanding of the relation between natural environmental changes and plankton dynamics in unperturbed systems.

OBJECTIVE: (1) Study the distribution, abundance, species composition, and productivity of planktonic microalgae, animals, and bacteria in estuaries; (2) define and quantify processes that regulate population dynamics and productivity of planktonic organisms in estuaries; (3) define and quantify processes through which the plankton alter and reflect water quality in estuaries; (4) define and quantify benthic processes that affect plankton dynamics and productivity of estuaries; and (5) define anthropogenic impacts on estuarine ecosystems.

APPROACH: Integrate descriptive and experimental field studies and develop simulation models. Field studies suggest important mechanisms that must be acknowledged by models and provide a data base for model calibration and subsequent verification. Conversely, evolving ecological models suggest processes and environmental factors that deserve particular emphasis by field studies. Feedback between model development and field work will accelerate understanding of the natural system, and should produce ecological models having sufficient realism to predict gross effects of human-induced perturbations.

PROGRESS: During fiscal year 1987, articles were published on the following topics: (1) Production and sedimentation of organic matter in a stratified, saline lake (Big Soda Lake, Nev.); (2) phytoplankton as a component of seston in San Francisco Bay; (3) empirical models for estimating primary productivity in estuaries; and (4) models to elucidate the coupling between horizontal transport processes and phytoplankton blooms in San Francisco Bay. An intensive multi-agency, multi-disciplinary study of tidal redistribution of conservative and nonconservative constituents in San Francisco Bay was

designed and completed. A flume was constructed and a method developed for measuring particle grazing rates by benthic suspension feeders was begun. Use of a high-resolution CTD to quantify vertical density structures of San Francisco Bay was started.

REPORTS PUBLISHED:

Cole, B. E., Cloern, J. E., and Alpine, A. E., 1986, Biomass and productivity of three phytoplankton size classes in San Francisco Bay: Estuaries, v. 9, p. 117-126.

Cole, B. E., and Cloern, J. E., 1987, An empirical model of phytoplankton productivity in estuaries: Marine Ecology Progress Series, v. 36, p. 299-305.

Powell, T. M., Cloern, J. E., and Walters, R. A., 1986, Phytoplankton spatial distribution in South San Francisco Bay--mesoscale and small-scale variability, in Wolfe, D. A., ed., Estuarine variability: New York, Academic Press, p. 369-383.

Wienke, S. M., and Cloern, J. E., 1987, The phytoplankton component of seston in San Francisco Bay: Netherlands Journal of Sea Research, v. 21, p. 25-32.

WR174 MICROBIAL BIOGEOCHEMISTRY

TITLE: Microbial Biogeochemistry of Aquatic Environments

PROJECT NUMBER: WR 81-174

LOCATION: Topical Research

PROJECT CHIEF: Oremland, Ronald S.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Microorganisms alter the chemistry and fertility of aquatic systems by performing complex transformations of organic and inorganic molecules. The biogeochemical mechanisms by which these transformations proceed and their quantitative significance to the cycling of elements in the biosphere is poorly understood. In addition, microbes are geochemically active in environments representing biological extremes, such as volcanoes, hotsprings, spreading centers, and hypersaline waters, and at both low and high values of pH.

OBJECTIVE: Develop conceptual models of biogeochemical transformations and measure their quantitative importance in aquatic environments. Measure rates of biologically mediated geochemical reactions in volcanic regions and in other environments representing biological extremes. Compare these measurements and pathways to similar reactions occurring in aquatic environments that do not represent biological extremes.

APPROACH: Study pathways of biogeochemical transformations mediated by microorganisms in the laboratory using materials taken from the environment (for example, sediments). Conduct biochemical experiments with isolated cultures of microorganisms responsible for these transformations and determine their overall significance to the cycling of elements in aquatic environments. Use these in-situ measurements to discriminate between purely chemical reactions and biologically mediated reactions that occur in geothermal or volcanic regions and other extreme environments.

PROGRESS: Investigations on the biogeochemistry of Mono Lake, Calif., revealed that four sources of methane are present in the lake, including one which is derived from a deposit of natural gas. Other work on the lake included measures of methanogenesis, sulfate reduction, methane oxidation, phytoplankton, and bacterial productivity. The biogeochemistry of selenium was studed with respect to the ability of bacteria to: (1) demethylate dimethylselenide; (2) reduce selenate to selenide; and (3) reduce selenite to elemental selenium via assimilatory sulfate reductases. Methane flux was quantified from several types of lakes. Formation of methane and ethane from organosulfur compounds was studied.

REPORTS PUBLISHED:

Kiene, R. P., Oremland, R. S., Catena, A., Miller, L. G., and Capone, D. G., 1986, Metabolism of reduced methylated sulfur compounds in anaerobic sediments and by a pure culture of an estuarine methanogen: Applied Environmental Microbiology, v. 52, p. 1037-1045.

Oremland, R. S., in press, Biology of anaerobic microorganisms, in Zehnder, A. J. B., ed., The Environmental Microbiology of Anaerobes: John Wiley and Sons, p. 641-702.

Oremland, R. S., and Capone, D. G., in press, Use of "specific" inhibitors in microbial geochemistry and ecology, in Marshall, K. C., ed., Advances in Microbial Ecology, v. 10, Plenum Publishing Co.

Oremland, R. S., and Zehr, J. P., 1986, Formation of methane and carbon dioxide from dimethylselenide in anoxic sediments and by a methaogenic bacterium: Applied Environmental Microbiology, v. 52, p. 1031-1036.

Tarafa, M. E., Whelan, J. K., Oremland, R. S., and Smith, R. L., 1986, Evidence of microbiological activity of Leg 95 (New Jersey Transect) sediments, in Turner, K. L., ed., Initial reports of the Deep Sea Drilling Project, v. XCV: U.S. Government Printing Office, p. 635-640.

Whelan, J. K., Oremland, R. S., Tarafa, M., Smith, R., Howarth, R., and Lee, C., 1986, Evidence for sulfate-reducing and methane-producing microorganisms in sediments from sites 618, 619, and 622, in Bouma, A. H., and others, eds., Initial reports of the Deep Sea Drilling Project, v. XCVI: U.S. Government Printing Office, p. 767-775.

Zehr, J. P. and Oremland, R. S., in press, Reduction of selenate to selenide by sulfate-respiring bacteria: Experiments with cell suspensions and estuarine sediments: Applied Environmental Microbiology, v. 53.

WR186 BIOTA-SOLUTE TRANSPORT INTERFACE

TITLE: Biotic Interface with Fluvial Transport: Processes Associated with Dissolved Solutes in Transport

PROJECT NUMBER: WR 84-186

LOCATION: California Statewide

PROJECT CHIEF: Triska, Frank J.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Biogeochemical processes associated with the microbial community (algae, bacteria, fungi) constitute the interface between solute transport and biotic production in riverine environments. Identifying and estimating biotic transformations and adsorption of transported solutes are prerequisites for understanding both the biological structure and nutrient chemistry of streams and rivers. Specific chemical transformations and their rates, biotic community structure, and background water chemistry vary spatially and temporally along the drainage network. Comparison of biotic response to solutes in transport between pristine and anthropogenically modified riverine environments is poorly understood, but the comparison is necessary for long-term management of these surface waters.

OBJECTIVE: Identify and determine rates of biotic transformations of transported solutes at chemical-biotic interfaces in fluvial environments, including seepage areas, riparian zones, sediment/surface-water interfaces, intragravel-subsurface flow interfaces, and floodplains.

APPROACH: Use laboratory experiments on communities collected from small to large streams and use in-situ field experiments to estimate biotic transformation of dissolved solutes. Conduct field experiments both at background concentrations, and with mixtures of conservative and nonconservative solutes injected into pristine and human-impacted fluvial environments. Examine environmental factors regulating process rates (solute concentration, temperature, light, current velocity, and biotic interactions) in relation to biotic transformation of transported solutes. Emphasize cycling of elements which have high assimilative demand and can subsequently be passed to higher trophic levels (that is, carbon, nitrogen, phosphorous). Project orientation emphasizes process rates rather than community structure. Cooperate with other projects interested in biogeochemical cycling and biotic-abiotic transport interactions.

PROGRESS: Preliminary simulation models based on data collected during flume experiments of nitrogen uptake have been produced in conjunction with A. Jackman (University of California, Davis). Early results indicate hydrologic factors such as dispersion and dead-zone storage may be more important than biological factors (enzyme kinetics) in predicting uptake by epilithic algae in stream channels. An 18-month study (monthly sampling) of subsurface flows adjacent to Little Lost Man Creek, Humboldt Co., Calif., has been completed and the samples currently are being analyzed.

REPORTS PUBLISHED:

Jackman, A. P., and Ng, K. T., 1986, The kinetics of ion exchange on natural sediments. Water Resources Research, v. 22, p. 1664-1674.

Triska, F. J., Kennedy, V. C., Avanzino, R. J., and Stanley, K. C., in press, Inorganic nitrogen uptake and regeneration in a small stream at summer base flow--Long-term clearcutting and short-term storm related impacts: U.S. Geological Survey Professional Paper 1454.

WR190 SOLUTE TRANSPORT INVOLVING BIOTA

TITLE: Solute Transport Involving Biological Processes in Surface Waters

PROJECT NUMBER: WR 86-190

LOCATION: Topical Research

CHIEF: Kuwabara, James S.

CITY: Menlo Park, CA

PROBLEM: Availability of toxic substances and nutrients to biota is dependent on their chemical form or speciation. Toxicological models, for example, have emphasized the effect of solute speciation on biological processes. Conversely, it has been demonstrated that partitioning of contaminants and nutrients can be affected by biological processes. Chemical processes that control chemical speciation in natural waters are: solute complexation, precipitation/dissolution, sorption and redox. Each of these processes affect and are affected by biological activity. Therefore, understanding and quantifying solute interactions with biota can be important in developing accurate water-quality models. Although inorganic and organic complexation have been emphasized in previous toxicological studies in chemically defined media, it is clear that chemical processes suppressed in these experiments can be important in natural water systems. The effects of biological processes on solute uptake and transport need to be quantified and incorporated in transport models.

OBJECTIVE: Study transport of inorganic solutes between particulates and primary producers. Examine and quantify processes controlling that transport (for example, adsorption onto and desorption from particulates and uptake and release from plankton and periphyton.) Conduct laboratory studies using chemically defined particles and formulate a conceptual representation of the processes. Conduct culture experiments, using chemically analyzed natural sediment samples, to verify and calibrate these models. Establish how biological processes may contribute to the overall behavior of trace inorganic contaminants in surface-water systems.

APPROACH: Conduct field sampling and laboratory analyses to assess the chemical character of particulates and dissolved phases and to identify potentially important biological transport processes. Determine trace metal, macronutrient and organic carbon concentrations using various preparative techniques. Use chemically defined particles and unialgal cultures to describe processes controlling solute uptake and release by cells. Conduct laboratory culture experiments using field samples of suspended particulates and isolates from natural planktonic and periphyton populations and generate biological transport submodels for testing and eventual incorporation into comprehensive water-quality models.

PROGRESS: Results were published on algal uptake of orthophosphate (PO_4) and zinc (ZN) as an extension of particle interaction studies on algal growth. The initial uptake of both Zn and PO_4 were found to be passive for algae. In solute transport, this means that the algal cell is an adsorptive surface for these solutes with little cytoplasmic absorption over the first 24 hours of exposure. This observation had been reported before for metals, but not for an anionic nutrient. Laboratory adsorption studies at low suspended inorganic particle concentrations were published showing that the extrapolation of results determined in grams per liter for solids concentrations down to environmentally significant suspended solids concentrations (typically two orders of magnitude lower) may be inappropriate. Trace metal studies in San Francisco Bay are nearing completion. A paper being prepared describes the distribution of trace metals in the South Bay during and after a spring algal bloom, and discusses potentially important mechanisms controlling those distributions. A second paper examines the variability of dissolved and particulate trace metal concentrations during a tidal cycle. Arsenic transport parameters for a periphyton submodel for Whitewood Creek, S. Dak., are being determined. Although this study was started less than 1 year ago as part of the Surface Water Toxics Program, some interesting results already have been observed. First, algal cells exhibit an exclusion mechanism for preferential uptake of PO_4 over AsO_4. Diatoms also have been found to exclude As, and yet other microbes do not discriminate between As and P uptake. Secondly, like phosphate, initial AsO_4 uptake by algae has been found to be passive in our experiments. This is consistent with the hypothesis that the mechanism for As toxicity is an interference with P metabolism. Finally, based on data from our initial field trip to Whitewood Creek, it is very likely that the periphyton represent a significant reactive As pool during the summer months (the season when dissolved As concentrations peak in the water column).

REPORTS PUBLISHED:

Kuwabara, J. S., 1986, Physico-chemical processes affecting copper, tin, and zinc toxicity to algae--A review, in Evans, L. V., ed., Algal biofouling: Elsevier Publ., p. 129-144.

Chang, C. C. Y., Davis, J. A., and Kuwabara, J. S., 1987, A study of metal ion adsorption at low suspended-solid concentrations: Estuarine and Coastal Shelf Science, v. 24, p. 419-424.

WR191 BACTERIA-CONTAMINANT INTERACTIONS

TITLE: Interaction of Bacteria with Environmental Contaminants and Solid Surfaces in the Aquatic Environment

PROJECT NUMBER: WR 86-191

LOCATION: Topical Research

CHIEF: Harvey, Ronald W.

CITY: Menlo Park, CA

PROBLEM: Although efforts have been made to explain the behavior of heavy metals and refractory organic contaminants in aquatic habitats in the framework of known geophysical and geochemical processes, much remains to be learned about the role of bacteria in such behavior. Of particular interest are bacteria-contaminant interactions in ground water. Due to the persistence of some contaminants in the subsurface environment and to increasing demand for both high quality ground water and on-land disposal of toxic chemicals and radioisotopes, these interactions should remain important environmental problems for the next few decades. Since significant biotransformation/biodegradation of many environmental contaminants in aquifers and particle-laden surface waters can occur at particle surfaces, explanations for bacteria-contaminant interactions in such environments should take the presence of particles into account.

OBJECTIVE: Provide some of the microbiological information necessary for more realistic predictions of contaminant behavior in aquatic environments. Obtain information on specific mechanisms of interactions between environmental contaminants and aquatic bacteria, taking into account adsorption, active uptake, competition, biotransformation reactions, interaction with extracellular polymers, effects of nutrient and physiochemical gradients, and effects of particle surfaces. Investigate the effect of nutrient and physicochemical conditions upon subsurface bacterial transport since the role of bacterial transport upon the fate of environmental contaminants in ground water is unknown.

APPROACH: The complex nature of interactions between bacteria and organic and inorganic contaminants in particle-laden aquatic habitats necessitates an approach involving both field and laboratory studies: (1) Study the influence of surfaces and interfaces upon microbial heterotrophic activity in particle-laden aquatic environments, including freshwater aquifers. (2) Study of the effect of organic contaminants upon the distribution, transport, and activity of the bacterial population in ground-water habitats. These studies will be performed jointly with Richard Smith, Water Resources Division, Denver. (3) Use flow-through column experiments, both to assess the role of adherent bacteria upon the mobility of selected heavy metals and toxic organic compounds in simulated aquifer environments and to investigate factors affecting movement of bacteria through porous media. (4) Make microcosm studies of bacteria-heavy metal interactions.

PROGRESS: Small-scale natural and forced-gradient groundwater tracer-injection experiments have continued at the Cape Cod Groundwater Contamination Site in Massachusetts. Tests with both bacteria and bacteria-sized microspheres have suggested independent mechanisms for attenuation (immobilization within aquifer sediment) and retardation (slowing down of the transport process). Surface characteristics of bacteria and microspheres appeared to have had a much greater effect upon retardation than attenuation. Experiments with flow-through columns packed with aquifer sediments have idicated that importance of secondary permeability features in bacterial transport. Progress has continued on a series of interpretive reports on bacterial growth, transport, activity, and predation in an organically contaminated aquifer.

WR192 ESTUARINE BENTHIC COMM. DYNAMICS

TITLE: Environmental Influences on Estuarine Benthic Community Dynamics

PROJECT NUMBER: WR 86-192

LOCATION: Topical Research

PROJECT CHIEF: Nichols, Frederic H.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Benthic communities are composed of sessile, relatively long-lived species. As such, they provide a continuing record of the effects of both short- and long-term changes in the environment through changes in species composition or abundance. This feature has lead to their use as indicators in water-quality studies. The necessary assumptions in such studies are that (1) the benthic community remains at some steady state condition during the period of observations, and (2) that changes seen in the community can be attributed to human activity. Recent findings from long-term investigations show, however, that benthic communities vary widely because of natural causes over both short (weeks) and long (years) time scales. Such natural variability often masks any changes that could be attributed to human activities.

OBJECTIVE: (1) Characterize long-term patterns in the structure of benthic invertebrate communities in estuaries and coastal regions; (2) determine the contribution of natural factors (climatic patterns and events, seasonal and interannual patterns of runoff, water chemistry, and circulation, sediment texture, and food availability) to benthic community variability; (3) assess the contribution of human influences (physical modifications of estuaries, waste disposal, accidental contamination, and control of river runoff to the remaining unexplained variability in benthic community dynamics; and (4) contribute to the development of conceptual and numerical models of river-estuary-ocean mixing systems through integration of studies of the processes and rates by which water, solutes, sediments, and organisms interact.

APPROACH: Quantitatively sample the benthos at regular intervals through time (and obtain access to data that have been collected by others) at fixed locations in various estuaries and nearshore habitats. Statistically analyze data from these samples for short- and long-term patterns of change in community structure and correlate these patterns through time series analysis with both natural environmental factors and anthropogenic factors associated with the water column and sediment. Determine the link between benthic community processes (feeding, respiration, substrate disturbance and stabilization) and changes in the water column (changes in planktonic biomass, nutrients, and organic matter) through field manipulation experiments using transplanted animals, and through laboratory experiments, using individual species and intact infaunal communities in flumes that simulate changing field conditions.

PROGRESS: During fiscal year 1987, reports were published on temporal variations in four intertidal benthic communities (Hopkins), a case study of human influence on an estuary (Nichols and Cloern), and the natural history and management of San Francisco Bay benthos (Nichols and Pamatmat). Studies on reproduction (Thompson) and effects of growth on trace metal uptake (Cain, Thompson, Luoma) in the common estuarine clam, Macoma balthica, were completed. A manuscript on possible links between continental shelf hydrodynamics and the behavior of a dominant infaunal invertebrate (Nichols, Cacchione, Drake, and Thompson) was completed. A seawater flume was constructed and its hydrodynamic properties characterized (Cole and Thompson). Investigation of long-term changes in estuarine and coastal benthic communities in San Francisco Bay and Puget Sound continued; laboratory and computer analysis of 1964-84 Puget Sound benthic community data were completed and manuscript preparation began (Nichols).

REPORTS PUBLISHED:

Nichols, F. H., in press, Benthic ecology and heavy metal accumulation, in Goodrich, D. M., ed., San Francisco Bay: issues, resources, status, and management: National Oceanic Atmospheric Administration Estuary-of-the-month Seminar Series No. 6, Washington, D.C., 1985, Proceedings, p. 65-68.

Nichols, F. H., and Pamatmat, M. M., 1987, The ecology of the soft-bottom benthos of San Francisco Bay: a community profile: U.S. Fish and Wildlife Service Biological Report 85.

GEOCHEMISTRY

CR189 GEOCHEMICAL KINETICS STUDIES

TITLE: Geochemical Kinetics Studies of Silicate Rock Hydrologic Systems

PROJECT NUMBER: CR 75-189

PROJECT CHIEF: Claassen, Hans C.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Adequate description of mass transport in hydrologic systems requires knowledge of the rates of the reactions among the gaseous, solid, and liquid phases present. This knowledge of reaction rates is necessary because many chemical reactions occur simultaneously in natural systems, and only a few of these appear to reach equilibrium, even after long contact times. Therefore, a complete description of the chemical processes and their rates will allow realistic modeling of mass transport in natural and perturbed hydrologic systems.

OBJECTIVE: Determine the relative importance of the factors controlling water quality and devise experiments to quantify the process by studying two model systems representing single lithologies--extrusive volcanic and shale. Determine the kinetics and mechanism(s) of these processes and the effects of natural variation on the controlling factors. Combining solution chemistry and the results of surface-alteration studies, suggest reaction models.

APPROACH: Monitor water quality from selected sources in the model study areas on a monthly basis. Monitor measurements of precipitation amounts and quality, soil temperature and moisture profiles, gravitational pore water quality and amount, and soil-pore carbon dioxide on either a continuous or periodic basis. These measurements will allow the relations between variations in input (recharge) and output (discharge) water quality to be described and will aid in design of controlled laboratory experiments, and the results of these laboratory experiments will provide data for kinetic mechanism elucidation. In addition to studies of the aqueous phase, describe changes that occur in the solid phase, using instrumental (nondestructive) and chemical-analytical techniques.

PROGRESS: An apparatus to quantitatively sample air moisture for hydrogen and oxygen isotopes under field (onsite) conditions was designed, modified, and tested. Sampling to verify the following hypotheses was begun: (1) air moisture is in approximate isotopic equilibrium with precipitation in the near-earth surface environment at a Rocky Mountain watershed; (2) the isotopic composition of air moisture determines the observed summer enrichment in soil moisture. Areal and temporal variability in chloride-ion deposition was investigated. Such knowledge is necessary for generalizing the effective-moisture model developed by Claassen and others to other sites and for paleo-groundwaters.

REPORTS PUBLISHED:

Reddy, M. M., Benefiel, M. A., and Claassen, H. C., 1986, Cadmium, copper, lead and zinc determination in precipitation--A comparison of inductively coupled plasma atomic emission spectrometry and graphite furnace atomization atomic absorption spectrometry: Mikrochimica Acta, 1, p. 159-170.

CR207 HYDROCHEMISTRY AND PALEOCLIMATOLOGY

TITLE: Arid-Basin Hydrochemistry and Paleoclimatology, Nevada

PROJECT NUMBER: CR 77-207

LOCATION: Southern Nevada (Nevada Test Site)

PROJECT CHIEF: Benson, Larry V.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: The partitioning of matter between aqueous and solid phases in arid regions is poorly understood. Hydrochemical processes occurring in arid-environment unsaturated zones remain almost unstudied. The residence time of the aqueous phase in both unsaturated and saturated zones of arid environments also is not known with any degree of certainty; however, certain arid regions such as the Yucca Mountain site bordering the Nevada Test Site (NTS), have been proposed as sites for the disposal of nuclear and chemical wastes. In addition, the cycling (transport and accumulation) of carbon in arid environments remains unquantified and impacts the calculation of the carbon dioxide changes.

OBJECTIVE: (1) Gain understanding of those arid hydrochemical processes that govern the transport of chemical species from the point of infiltration of precipitation to the point of discharge; (2) provide information on those hydrochemical processes that govern the migration rates of hazardous wastes emplaced in arid-environment settings (for example, NTS); and (3) reconstruct the Wisconsin paleohydrology and paleoclimatology of the Great Basin of the western United States from studies of the age and chemical composition of the aqueous phase in the unsaturated and saturated zones, as well as from the age, biological chemical, and mineralogical composition of sediments that have accumulated at major discharge points.

APPROACH: (1) Sample and chemically analyze the aqueous phase throughout selected points in the flow system; (2) collect data on the chemical and mineralogical composition of solid phases in contact with the aqueous phase; (3) develop conceptual models of the hydrochemical processes that govern transport and accumulation of chemical species in the unsaturated and saturated zones; (4) modify an existing chemical transport computer program to quantitatively simulate saturated- and unsaturated-zone hydrochemical processes; and (5) validate and apply the chemical transport computer program.

WRD FEDERAL RESEARCH PROJECTS.....GEOCHEMISTRY

PROGRESS: 65 m of Pyramid Lake sediment have been cored. Oxygen-18 isotope and carbon-13 isotope was determined on ostracodes from Walker Lake Cores 4 and 5. Storm trajectory analyses and isotope analyses for Southern Nevada are complete. Two major papers are in press. Sampling of the Lahontan surface-water system for oxygen-18 isotope continues. Weather and radiation equipment for Pyramid Lake are on hand.

REPORTS PUBLISHED:

Benson, L. V., and Thompson, R. S., in press , North America and adjacent oceans during the last glaciation, in The geology of North America: Geological Society of America.

Benson, L. V., and Thompson, R. S., in press, Lake-level variation in the Lahontan basin for the past 50,000 years: Quaternary Research, 17 p.

CR276 CLAY-WATER REACTIONS

TITLE: Geochemistry of Clay-Water Reactions

PROJECT NUMBER: CR 82-276

LOCATION: Topical Research

PROJECT CHIEF: Eberl, Dennis D.

HEADQUARTERS OFFICE: Denver, CO

PROBLEM: Clay minerals may influence the chemistry of ground water and other aqueous solutions through precipitation, dissolution and ion-exchange reactions. An understanding of these reactions also is crucial for predicting the behavior of toxic wastes in disposal areas. How do the various clays react with waters of varying composition at different temperatures and pressures? After the fundamentals of these processes are understood, how can they be applied to problems of predicting, enhancing, and ensuring water quality?

OBJECTIVE: (1) Develop a theory for ion exchange that would allow prediction of the exchange properties of a clay based on the clay's crystal chemistry; (2) gather basic information on clay mineral structure and chemistry; and (3) try to understand the precipitation and alteration of clay minerals in natural and synthetic systems.

APPROACH: Test and develop theoretical models through laboratory experiments (for example, measurement of exchange isotherms with well-characterized clay minerals). Study clay-water reactions in natural systems in the field.

PROGRESS: Work on the chemistry and structure of sericite has just been completed. Sericite is one of the most common hydrothermal alteration products. It was found that sericite is fine-grained muscovite. Its properties differ significantly from coarser grained micas because sericite particles are so thin that exposed basal surfaces comprise a significant proportion of the sample. The presence of these surfaces leads to swelling (expandability), to larger cation exchange capacities, and to smaller fixed cation contents in the structural formulae. Work on a nonpolluting, slow-release fertilizer (mixture of an exchanger and phosphate rock) has revealed that it is very effective in greenhouse experiments, that it actually can decrease yields for some soils by sequestering potassium, and that peat is a very effective exchanger for the system. Work on the effect of wetting and drying continues. Experiments have shown that some metals can be fixed in clay (smectite) structures during this process, thereby decreasing their availability to surface waters.

REPORTS PUBLISHED:

Eberl, D. D., 1986, Clays: Geotimes, v. 31, p. 10-11.

Eberl, D. D., 1986, The hydrothermal strategy, in Carins-Smith, A. G., and Hartman, H., eds., Clay minerals and the origin of life: Cambridge, Cambridge University Press, p. 65-70.

Eberl, D. D., Srodon, Jan, and Northrop, H. R., 1986, Potassium fixation in smectite by wetting and drying, in Davis, J. A., and Hayes, K. F., eds., Geochemical processes at mineral surfaces: Washington, D.C., American Chemical Society, p. 296-326.

Srodon, Jan, Morgan, D. J., Eslinger, E. V., Eberl, D. D., and Karlinger, M. R., 1986, Chemistry of illite/smectite and end-member illite: Clays and Clay Minerals, v. 34, p. 368-378.

CR284 CORROSION BY WET PRECIPITATION

TITLE: Corrosion of Building Materials as Determined From Solid Weathering Products Removed by Wet Precipitation

PROJECT NUMBER: CR 83-284

LOCATION: Topical Research

PROJECT CHIEF: Reddy, Michael M.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: Accelerated decay of stone cultural treasures and building materials is apparent in several areas of the United States. Its cause has been attributed to air pollution and acid deposition. Although this destructive process may have significant adverse effects on the economic well being of the country, little fundamental understanding of processes involved or quantitative relations between important variables are available. Processes involved in rock-precipitation reactions are poorly understood, leading to large uncertainties in estimates of acid-precipitation impacts. Information about the influence of acid precipitation on urban-runoff water quality also is lacking.

OBJECTIVE: Determine stone-dissolution processes and rates in the natural and polluted environment. To the extent feasible, separate the effects of wet deposition from the effects of dry deposition, as well as from normal weathering processes. Evaluate the influence of acid-precipitation interaction with materials on urban runoff water quality.

APPROACH: Collect and analyze rainfall leachate from selected materials at appropriate locations to obtain field measurements of acid rain damage. Washington, D.C., will be the first field site. A prototype field instrument that continuously monitors pH and conductance will be evaluated near Denver, Colo., before shipment and installation at the Washington, D.C., site. In support of the field study, use facilities and staff available at the U.S. Geological Survey Central Laboratory in Denver and establish appropriate, quality controlled, analytical methods compatible with the analysis of rainfall-leachate solutions.

PROGRESS: Two years of intermittent onsite measurement of acid rain weathering of limestone and marble at Research Triangle Park, N.C., were completed. Research sites at Newcomb, N.Y., Chester, N.J., and Washington, D.C., are fully operational. Weathering of limestone and marble was shown to be proportional to acid loading to the stone surface. This result was incorporated into several recent publications.

REPORTS PUBLISHED:

Claassen, H. C., Reddy, M. M., and Halm, D. R., 1986, Use of the chloride ion in determining hydrologic-basin water budgets--A 3-year case study in the San Juan Mountains, Colo., U.S.A.: Journal of Hydrology, v. 85, p. 49-71.

Reddy, M. M., Sherwood, S., and Doe, B., 1986, Limestone and marble dissolution by acid rain, in Materials Degradation Caused by Acid Rain, Robert Babioan, ed., American Chemical Society Symposium Series 318: Washington, D.C., American Chemical Society, p. 226-238.

Reddy, M. M., 1986, Effect of magnesium ions on calcium carbonate nucleation and crystal growth in dilute aqueous solutions at 25° celsius, in Mumpton, F. A., ed., Studies in diagenesis, U.S. Geological Survey Bulletin 1578, p. 170-182.

Reddy, M. M., and Werner, Marilyn, 1985, Composition of rainfall runoff from limestone and marble at Research Triangle Park, N.C.: U.S. Geological Survey Open-File Report 85-630, 6 p.

Reddy, M. M., See, R. B., and Liebermann, T. D., 1986, Protocol for collecting, processing, and shipping precipitation samples: U.S. Geological Survey Open-File Report 86-405A, 13 p.

Reddy, M. M., See, R. B., and Liebermann, T. D., 1986, Operational protocol for a continuous precipitation monitor: U.S. Geological Survey Open-File Report 86-405B, 24 p.

Reddy, M. M., and Youngdahl, C. A., 1987, Acid rain and weathering damage to carbonate building stone: Results of material loss measurements, in Corrosion 87: Conference of the National Association of Corrosion Engineers, San Francisco, 1987, Proceedings, p. 415/1-415/7.

NR020 MINERAL-WATER INTERACTION IN SALINE ENVIRONMENTS

TITLE: Mineral-Water Interaction in Saline Environments

PROJECT NUMBER: NR 69-020

LOCATION: Topical Research

PROJECT CHIEF: Jones, Blair F.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Saline hydrologic systems provide a wide range of conditions within which to examine hydrochemically important mineral reactions, alteration or genesis, and to better define reactants and products controlling the chemical composition of many natural waters. The effects of complex reactions, in addition to simple solution and hydrolysis, are reflected in relatively gross chemical change and interaction with fine-grained sediment.

OBJECTIVE: Use saline environments to determine mechanisms and relative importance of mineralogic processes that influence the solute composition of natural waters.

APPROACH: Study in the field and make laboratory analyses of saline waters and associated deposits, mostly from surficial sites or shallow cores in selected pilot or problem areas. Separate and examine solid and solution phases using high speed and gradient centrifugation, microscopy, x-ray diffractometry, and special potentiometric apparatus, as well as detailed constituent analysis of both solids and solutions. Relate composition of these materials to the hydrochemical environment, thermodynamic conditions, and structural elements of associated mineral species.

PROGRESS: Further testing of the SNORM program for diagnostic salt criteria of solute origin was continued, primarily as applied to the origin of brines in bedded salt and crystalline rock waste repository areas. With the late Marc Bodine, Geologic Division, a comprehensive evaluation of solute origin and contrasting brine chemistry in the Salado and Rustler formations of New Mexico was carried out. Analytical variance has been screened and at least four brine types were identified. Detailed SNORM characterization is helping to work out the history of possible movement and reaction of fluids. Additional analysis of ultrafine clays in sediment core from the Great Salt Lake has been done to better define the details of authigenic reaction. The less than 0.1 micron fraction magnesium/aluminum ratio, which increases with, and clearly defines, the extent of smectite trioctahedral interstratification, fluctuates directly with lake salinity. The very small variance in ultrafine clay chemistry in present river inflow sediment has allowed chemical definition of the authigenic component of lake strata by compositional subtraction. This calculation indicates that the ratio of magnesium to silica taken up from solution is 1:1, and permits estimate of an apparent stability constant for

neoformed magnesium-smectite. A new understanding of alluvial, lacustrine and saline lithology, mineralogy, and chemistry of Madrid basin aquifer materials is being used to construct basin ground-water flow models and related solute mass balance calculations. Using geomorphic evidence and a mass of dolomite dissolution predicted by computer modeling of the mixed pore fluids, dissolution rates for porosity development in the Edwards aquifer of Texas can be calculated that are consistent with dolomite dissolution rates determined for both the Madison and Floridan aquifer systems.

REPORTS PUBLISHED:

Rettig, S. L., and Jones, B. F., 1986, Evaluation of a suggested sequence for chemical extraction of soluble amorphous phases from clays: in Selected Papers on the Hydrologic Sciences, 1986, U.S. Geological Survey Water-Supply Paper 2290, p. 127-137.

Bodine, M. W., Jr., and Jones, B. F., 1986, The salt norm--A quantitative chemical-mineralogical characterization of natural waters: U.S. Geological Survey Water-Resources Investigations Report 86-4086, 130 p.

Jones, B. F., 1986, Clay mineral diagenesis in lacustrine sediments: U.S. Geological Survey Bulletin 1578, p. 291-300.

NR034 CHEMICAL CONSTITUENTS OF WATER

TITLE: Spatial Distribution of Chemical Constituents in Ground Water

PROJECT NUMBER: NR 57-034

LOCATION: Topical Research

PROJECT CHIEF: Back, William

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Reactions and processes that control the chemical character of ground water need to be identified to predict physical and chemical changes that occur in both natural and stressed environments. This project focuses on effects of these reactions in (1) regional limestone aquifers; and (2) contaminated environments.

OBJECTIVE: Study geochemical reactions that relate to: (1) Geologic processes, including karstification, diagenesis, and ore deposition; (2) generation, migration, and attenuation of leachate components; and (3) processes of isotopic fractionation.

APPROACH: Design field studies for the collection and interpretation of chemical and isotopic data within the hydrogeologic framework. Select areas that are feasible to demonstrate the occurrence, extent, rate, and consequences of chemical reactions. For example, (1) changes in porosity and permeability by karstification are being studied on the east coast of the Yucatan; (2) the degradation and migration of organic compounds and isotopic fractionation are being investigated at contamination sites, and in sulfide-rich ground water; and (3) comparative studies of regional systems in Ireland, Yucatan, Florida, and China are being undertaken to evaluate the environmental and geochemical consequences of hydrogeologic processes in limestone terranes.

PROGRESS: A manuscript has been completed on the Hydrogeology of North America. More than half the manuscript is largely a synthesis of the U.S. Geological Survey's Regional Aquifer Systems Analysis Projects. Two other studies were completed: (1) demonstrating the geologic and climatic controls on the incurrence and movement of ground water in islands, and (2) the hydrogeologic controls on development of karst in tropical environments and the effect of these karst features on the hydrogeologic regime. Studies are underway evaluating the hydrogeologic controls on the development and distribution of porosity and permeability and the diagenesis of both carbonate and silicate minerals by the chemical reactions and physical processes occurring in the ground-water mixing zones.

REPORTS PUBLISHED:

Back, William, 1986, Role of aquitards in hydrogeochemical systems: Applied Geochemistry, v. 1, no. 3, p. 427-437.

Back, William, 1986, Geologic significance of the ground-water mixing zone associated with sea-water intrusion: Fifth International Symposium on Water-Rock Interaction, Reykjavik, Iceland, 1986, Proceedings, p. 25-28.

Back, William, 1986, Foreward in Landa, E., and Ince, S., eds., History of geophysics (American Geophysical Union), v. 3, p. 75-80.

Herman, J. S., Back, William, and Pomar, L., 1986, Geochemistry of ground water in the mixing zone along the East Coast of Mallorca, Spain: International Association of Hydrologic Sciences Publication no. 161, p. 467-479.

Marinos, Paul, Herman, J. S., Back, William, and Xidakis, G., 1986, Structural control and geomorphic significance of groundwater discharge along the coast of the Mani Peninsula, Peleponnese, Greece: International Association of Hydrologic Sciences Publication no. 161, p. 481-495.

NR041 PALEOCLIMATOLOGY AND AQUIFER GEOCHEM.

TITLE: Interface of Paleoclimatology and Aquifer Geochemistry

PROJECT NUMBER: NR 74-041

LOCATION: Topical Research

PROJECT CHIEF: Winograd, Isaac J.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Reconstructions of continental paleoclimates of the Pleistocene Epoch have relied almost exclusively on the tree ring, packrat midden, and speleotherm records. The isotopic (denterium, oxygen-18 and carbon-13) record of old (10^3 to 10^4 year old)ground waters, and of calcitic veins marking the sites of fossil (10^5 to 10^6 year old) ground-water discharge, have not been used. Preliminary work indicates that such data will yield valuable new evidence regarding continental paleoclimate and paleohydrology of the Pleistocene and Pliocene Epochs. The data and interpretations also should be pertinent to selection of sites for the disposal and long term isolation of toxic wastes.

OBJECTIVE: (1) Infer paleoclimate and paleohydrology of selected regions based on variations in isotopic content of ground water and calcitic veins; (2) attempt correlation of inferred local variations in continental paleoclimate with global variations deduced from oceanographic studies; (3) differentiate between, and determine relative magnitude of, summer and winter recharge to major uplands receiving equal quantities of summer and winter precipitation; and (4) determine the fractionation of oxygen-18 and carbon-13 between ground waters and calcite deposits at modern springs.

APPROACH: Sample: (1) Water from regional aquifers for which quantitative hydrogeologic and geochemical studies have been completed; (2) rain, snow, snowmelt, and springs in major upland recharge areas; and (3) calcitic veins and dense travertine at modern and fossil springs. Analyze water and calcite deposits for denterium, oxygen-18 and carbon-13, uranium and thorium content, and date using carbon-14, thorium-230, uranium-234/238, as appropriate. Initial work using calcite deposits will be in the southern Great Basin, where a major fossil spring-discharge area (with a modern analog, the Ash Meadows region) has been exhumed by uplift and erosion.

PROGRESS: A report is in preparation which describes and interprets a 300,000-year record of oxygen-18 and carbon-13 obtained from uranium-series dated calcitic veins in Devils Hole, Nev. This record (developed in collaboration with T. Coplen, B. Szabo, and A. Riggs) is the longest, best dated, and most detailed continental paleoclimatologic record available to date. A comparison of this oxygen-18 record with the analogous marine records, indicates that key climate changes during the middle to late Pleistocene occurred much earlier than indicated by the standard marine oxygen-18 curves. This finding, in turn, calls into question orbital forcing (that is, the Milankovitch Theory) as the dominant cause of the Pleistocene ice ages.

REPORTS PUBLISHED:

Winograd, I. J., 1986, Archaeology and public perception of a transscientific problem--Disposal of toxic wastes in the unsaturated zone: U.S. Geological Survey Circular 990, 9 p.

NR056 MODELING MINERAL-WATER REACTIONS

TITLE: Kinetic and Thermodynamic Modeling of Mineral-Water Reactions in Natural Water Systems

PROJECT NUMBER: NR 76-056

LOCATION: Topical Research

PROJECT CHIEF: Plummer, Leonard N.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: In order to model the chemical quality of ground-water systems, it is necessary to determine what reactions are occurring and their rates. Very little is known of the rates of mineral-water interaction in ground-water systems. Furthermore, little is known of the effects of variable composition on the stability of minerals, as well as the stability of metastable and amorphous phases that apparently regulate, to a large extent, the composition of certain low-temperature natural waters. Much experimental and theoretical work is needed to define the thermodynamic properties of aqueous solutions of mixed electrolytes in order to model reactions between minerals and aqueous solutions.

OBJECTIVE: Obtain experimental data on the kinetics of mineral dissolution-precipitation reactions; investigate the effects of variable composition of minerals and the stability of metastable and amorphous phases in regulating the composition of natural waters; and relate these data to modeling the chemical evolution of natural waters. Develop theory and methods for determining reaction stoichiometry and rates from observed field hydrochemical data. Apply these methods to interpret the chemical evolution of ground-water systems. Develop improved thermodynamic models of aqueous solutions.

APPROACH: Study rates of dissolution and crystal growth of minerals using various methods including (1) change in weight of single crystals, (2) potentiometric and potentio-stat methods, (3) changes in solution composition, and (4) rotating disks. Investigate effects of single salts (and their mixtures) in solution on the rates. Obtain data on mineral stability from reversed solubility measurements. Use potentiometric measurements of aqueous solutions to refine thermodynamic models of aqueous solutions. Making extensive computer calculations, evaluate kinetic data, test thermodynamic models of aqueous solutions, and model the chemical evolution of ground water.

PROGRESS: Thermodynamic data on the strontianite-aragonite solid solutions were used to evaluate reaction paths for the dissolution of these solid solutions in non-stoichiometric solutions via theoretical Lippman diagrams which define conditions of equilibrium and stoichiometric saturation. The results show that stoichiometric saturation (not equilibrium) controls the reaction path. Solubility data on synthetic and biogenic magnesium-calcites are being evaluated to define stability as a function of defect density.

A thermodynamic evaluation of literature solubility data for potassium chloride-potassium bromide solid solutions shows that equilibrium is approached but not attained after several weeks of reaction. A report describing pH measurements in low-conductivity waters received Director's approval. An additional 24 wells in the Floridan aquifer, the overlying Miocene and underlying Gordon, Dublin, and Midville aquifers of Georgia were sampled in the summer of 1986. The sampling was conducted to extend well control to the outcrop along three flow paths currently under study and to provide chemical data for assessment of cross-formational leakage. Sulfur-34 isotope data for anhydrite from Madison cores in Wyoming and Montana became available and are similar to values predicted in earlier modeling supporting the modeling conclusions.

REPORTS PUBLISHED:

Plummer, L. N., 1986, Approach to equilibrium in solid solution--aqueous solution systems: the KCl-KBr-H_2O System at 25 °C, in Davis, J. A., and Hayes, K. F., eds., Geochemical processes at mineral surfaces: American Chemical Society Symposium Series no. 323, p. 561-573.

Busenberg, E., and Plummer, L. N., 1986, The solubility of $BaCO_3$ (cr) (witherite) in CO_2-H_2O solutions between 0 and 90 °C, evaluation of the association constants of $BaHCO_3$ (aq) and $BaCO_3$ (aq) between 5 and 80 °C, and preliminary evluation of the thermodynamic properties of Ba^{2+} (aq): Geochimica et Cosmochimica Acta, v. 50, p. 2225-2233.

Busby, J. F., Plummer, L. N., Lee, R. W., and Hanshaw, B. B., in press, Geochemical evaluation of water in the Madison aquifer in parts of Montana, South Dakota, and Wyoming: U.S. Geological Survey Professional Paper 1273-F.

NR064 ISOTOPE FRACTIONATION

TITLE: Physical Chemistry of Stable Isotope Fractionation in Hydrologic Processes

PROJECT NUMBER: NR 75-064

LOCATION: Topical Research

PROJECT CHIEF: Coplen, Tyler B.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: The stable isotopes of hydrogen, carbon, nitrogen, oxygen, silica, and sulfur show variations in their isotope abundances and may be useful in studying evaporation, ground-water mixing, lake or reservoir circulation and stratification, and associated hydrochemical phenomena. These isotope fractionations are related to: (1) Purely physical processes; (2) heterogeneous chemical equilibria; and (3) reaction kinetics. Many of these processes are neither sufficiently understood nor quantified to make the most effective use of stable isotope techniques in hydrologic research.

OBJECTIVE: Develop and refine theoretical and instrumental mass-spectrometric techniques through experimental investigation. Test theories in suitable field locations such as intermontane ground-water reservoirs, closed-lake basins, and suitable surface-reservoir, lake, or estuarine systems to aid in more complete use of light stable-isotope phenomena in hydrologic studies.

APPROACH: Analyze water and mineral samples from experimental studies, from evaporating surface-water bodies, and from ground-water basins, to determine light stable isotope abundances. Relate these experimental results and field data to other measurement factors, such as relative humidity, temperature, density, and salinity, in an attempt to develop an understanding and a theoretical predictive model of the processes involved.

PROGRESS: (1) Stable isotope study of Central West-side ground water of the San Joaquin Valley, Calif., was completed. The isotopic results are consistent with a tectonic model that calls for uplift of the Central Coast Ranges about 1,100 meters in about 300,000 to 400,000 years. (2) The major part of the software development of the laboratory information management system (LIMS) for sample handling in the stable isotope laboratory was completed. (3) Several hundred samples have been analyzed from NASQAN and BENCHMARK stations in a 3-year program to investigate processes affecting the spacial and seasonal distribution of deuterium and oxygen-18 in U.S. surface waters. (4) Manuscript preparation of Devils Hole isotopic results in a cooperative study with I. Winograd and B. Szabo (of Geologic Division) has nearly been completed. This continental record shows the same general peaks as the marine isotope record. Ages for each of the peaks can be calculated

and compared to the current ages associated with peaks in the marine isotope record. (5) The tritium laboratory under the leadership of R. Michel is being brought back into operation for Research and District programs.

REPORTS PUBLISHED:

Davis, G. H., and Coplen, T. B., in press, Stable isotopic composition of ground water of central California as an indicator of Mid-Pleistocene tectonic evolution: Vienna, Austria, International Atomic Energy Agency.

Wildman, J., 1986, Improvement of filament-protection circuitry in a Finnigan model 251 mass spectrometer: U.S. Geological Survey Open-File Report 86-484, 5 p.

NR065 SED.-WATER EXCHANGE OF NUT./METALS

TITLE: Sedimentary Geochemical Processes Affecting the Exchange of Nutrients and Transition Metals Between Sediment and Water in Riverine, Estuarine, and Lacustrine Environments

PROJECT NUMBER: NR 76-065

LOCATION: Topical Research

PROJECT CHIEF: Callender, Edward

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Benthic-sediment exchange processes are potentially a very significant source-sink of nutrients and metals within an aquatic system. Too often the quantitative effects of these processes only are estimated when considering biogeochemical cycling and ecological responses. Understanding geochemical processes that control nutrient and transition metal chemistry of natural waters is requisite for predicting the effects man-induced events will have upon natural geochemical cycles and for determining their utilization as a natural resource (for example, estuarine waters as food resources).

OBJECTIVE: (1) Study the important geochemical processes affecting the nutrient and metal composition of and exchange between sediment and water in several different aquatic environments; (2) aid in developing methods for determining nutrient and metal fluxes between sediment and water; (3) assess the influence man's activities exert on natural geochemical cycles.

APPROACH: Sample and analyze surface water, ground water, and sediment-pore water for nutrient and transition-metal content of aqueous phase and associated solid phases(s). Measure nutrient and metal exchange in natural and laboratory-controlled environments to determine the effects of changing environmental conditions (temperature, salinity, nature of inorganic and organic substrates, bioturbation). Analyze samples using colorimetry, ion chromatography, and flame and flameless atomic absorption spectrophotometry. Model results in terms of solution-mineral equilibria, ion exchange, and advective-diffusive transport through porous sedimentary media.

PROGRESS: Approximately 24 gravity cores were taken from the Cheyenne River arm of Lake Oahe, S.D., during August 1986. These cores were sampled in 1- and 2-cm (centimeter) intervals for pore-water and solid-phase geochemistry; a few cores were sampled for radiometric age dating. Sediments from the upper part of the Cheyenne River arm are accumulating at a rate of between 12 and 23 cm/yr. Middle arm sediments are accumulating at rates of 6 to 10 cm/yr; lower-arm rates approximate 5 cm/yr. These extremely rapid sedimentation rates serve to preserve, at diminished concentrations, the original interstitial-water chemistry profiles. This is in contrast to the usual situation where there is sufficient time for molecular diffusion to

"smooth out" the original interstitial-water chemistry profiles. For the 2 years studied (1985 and 1986), the profiles are offset vertically by 12 cm in upper-arm sediments. Solid-phase constituents do not show a discernible repetitive pattern due to the extreme heterogenity of the sedimentary system. In addition, a decrease in sedimentary As (arsenic) of 1 micrometer per gram would result in an interstitial As increase of 300 micrometers per liter. Calculated upward diffusion/sediment-accumulation ratios for As suggest that very little sedimentary As is being recycled to the water column from rapidly accumulating sediments in the upper Cheyenne River arm. On the contrary, as much as 30 percent of the sedimentary As may be recycled to bottom water in the lower Cheyenne River arm.

NR092 URANIUM MILL TAILINGS

TITLE: Hydrogeochemical Controls on the Migration of Radionuclides from Uranium Mill Tailings

PROJECT NUMBER: NR 78-092

LOCATION: Topical Research

PROJECT CHIEF: Landa, Edward R.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Uranium mill tailings and related forms of low-level radioactive waste contain elevated contents of naturally occurring radionuclides that have been brought to the surface, processed for the recovery of uranium and other components, and then disposed of in near-surface impoundments. The long-term fate of the tailings and their constituents will be determined by surficial earth processes.

OBJECTIVE: Study the chemical form in which radionuclides and selected stable elements are retained in surficial earth materials, particularly uranium mill tailings, and identify processes operating in natural aqueous and terrestrial systems that may influence the transport of these constituents from these earth materials.

APPROACH: Determine the partitioning of nuclides and elements of interest in tailings, ores, soils, rocks, and waters through the use of leaching and sorption studies, particle-sizing, radon emanation measurements, and nuclear emulsion microscopy.

PROGRESS: Three ore samples of differing uranium mineralogies and rock types were leached with either sulfuric acid or sodium carbonate solutions under laboratory conditions to simulate acid or alkaline uranium milling practices. The radon emanation coefficients (REC's) of the initial ore and of the tailings derived from them were compared. No consistent pattern enabling the prediction of the REC's of tailings on the basis of ore types was evident. The similarities in the REC's of the acid-leach tailings suggests that the lixiviant solution plays an important role in determining the form, and hence, the emanating power of the radium retained therein.

REPORTS PUBLISHED:

Landa, E. R., Miller, C. L., and Updegraff, D. M., 1986, Leaching of 226 Ra from uranium mill tailings by sulfate reducing bacteria, Health Physics, v. 51, p. 509-518.

Updegraff, D. M., Miller, C. L., and Landa, E. R., 1986, Characterization of Arthrobacter isolated from uranium mill tailings: U.S. Geological Survey Open-File Report 86-527, 8 p.

Landa, E. R., 1987, Radium-226 and contents and Rn emanation coefficients of particle-size fractions of alkaline, acid and mixed U mill tailings: Health Physics, v. 52, p. 303-310.

Landa, E. R., in press, Colorado Radium--mining, processing and usage in medicine, science and industry: Colorado School of Mines Quarterly, v. 82, no. 2.

Landa, E. R., 1987, Radium at Jamestown, 1918-1919; a case study of metallurgy and mineral economics: Essays in Colorado History, no. 7, p. 27-47.

Miller, C. L., Landa, E. R., and Updegraff, D. M., 1987, Ecological aspects of microorganisms inhabiting uranium mill tailings: Microbial Ecology, v. 14, no. 2, p. 141-155.

Landa, E. R., 1987, Early 20th Century investigations of the radioactivity of waters in North America, in Landa, E. R., and Ince, S., eds., History of Hydrology; History of Geophysics (American Geophysical Union), v. 3, p. 75-80.

NR093 REDOX REACTIONS

TITLE: Redox Reactions in Ground Waters

PROJECT NUMBER: NR 79-093

LOCATION: Topical Research

PROJECT CHIEF: Thorstenson, Donald C.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Redox potential is the least understood major control on natural-water chemistry. The goal of this research is to better characterize the factors that determine redox potential in ground-water systems. An understanding of the major processes governing redox reactions must be available to model the ground-water geochemistry of compounds of multivalent elements such as iron, manganese, or uranium and other actinides.

OBJECTIVE: (1) Identify controls on redox potential in specific natural systems; (2) evaluate processes responsible for the distribution of oxygen and carbon dioxide in the unsaturated zone; (3) apply computer models to redox reactions in natural hydrologic systems; and (4) make a preliminary evaluation of redox conditions at radioactive waste disposal sites.

APPROACH: (1) Integrate fundamental thermodynamics of redox processes and natural water geochemistry; (2) measure gas composition and isotopic characteristics of carbon dioxide in the deep unsaturated zone; (3) apply computer models to specific redox problems in ground-water systems; and (4) measure gas compositions and tritium distribution in the unsaturated zone at waste disposal sites.

PROGRESS: Studies of gas composition in various unsaturated-zone boreholes at Yucca Mountain (Nevada Test Site) are continuing. The sampling program has been expanded to include boreholes UZ-6 (an open borehole; depth about 1,850 feet; cased for the upper 325 feet), UZ-6S (an open borehole adjacent to UZ-6; depth about 450 feet, uncased), and continued sampling at UZ-1 (a stemmed borehole, instrumented--including gas sampling piezometers--at 15 levels throughout its about 1,200 foot depth). The gas-analysis program also has been expanded to include hydrogen (by mercury-reduction detector), methane, ethane, and ethylene by methanizer-flame ionization detector gas chromatography, and the standard atmospheric gases nitrogen, oxygen, argon, and carbon dioxide. Isotopic analyses on some samples are carried out for carbon-13 and carbon-14 on the carbon dioxide, and for tritium, deuterium, and oxygen-18 on water vapor in the gas samples. Over the past year, on the order of 1,000 samples have been variously analyzed for these constituents. After nearly 4 years of sampling, the carbon dioxide concentrations in UZ-1 appear to be stabilizing at levels of 0.1 and 0.15 percent in most sampling intervals; the shallowest probe (42 ft) has about 1.5 percent carbon dioxide,

and the deepest probe (1,207 ft) shows about 0.3 percent carbon dioxide. Hydrogen, methane, and occasional trace amounts of ethane and ethylene are present at UZ-1. Hydrogen and methane range from about 0.5 ppm to about 3 parts per million (ppm), with a vaguely difined increase with depth. In the open boreholes, which are subject to atmospheric ventilation, the concentrations of minor gases are highly variable, ranging from atmospheric concentrations during inhalation to the following concentrations during prolonged exhalation: carbon dioxide about 0.1 percent; methane and hydrogen 0 to 0.1 ppm; ethane and ethylene undetectable.

REPORTS PUBLISHED:

Yang, I. C., Haas, H., Weeks, E. P., and Thorstenson, D. C., 1986, Analysis of gaseous-phase stable and radioactive isotopes in the unsaturated-zone, Yucca Mountain, Nev.: National Water Well Association Conference, Denver, Colo., 1985, Proceedings, p. 488-506.

NR099 GEOCHEMICAL CARBON FLUXES

TITLE: Carbon Fluxes in Hydrologic and Geologic Processes

PROJECT NUMBER: NR 79-099

LOCATION: Topical Research

PROJECT CHIEF: Sundquist, Eric T.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Carbon fluxes are an important aspect of many hydrologic and geologic processes. For example, on a global scale, rising atmospheric carbon dioxide concentrations and man's increasing use of fossil fuels have led to concern for the future effects of atmospheric carbon dioxide on global climate. Anticipating the effects of atmospheric carbon dioxide requires understanding of the affect of natural hydrologic and geologic processes on the global carbon budget. On a more local scale, ground-water and surface-water contamination problems often are associated with locally significant changes in the transport and sedimentation of carbon. This project evaluates carbon fluxes by studying the hydrologic and geologic processes responsible for them. These studies emphasize the need to understand the evidence for natural changes in local to global carbon fluxes before man's influence.

OBJECTIVE: (1) Evaluate local to global carbon fluxes associated with hydrologic and geologic processes; (2) investigate the possibility of past variations in the world's (natural) CO_2 balance, and apply this information to the prediction of future global CO_2 fluxes; (3) understand the role of fluxes of natural carbon compounds in selected local ground-water and/or surface-water contamination problems; and (4) determine the geochemical mass balance for carbon in selected hydrologic-geologic systems.

APPROACH: Derive estimates of carbon fluxes and quantities from direct measurements or from computer models of hydrologic and geologic processes. Characterize carbonate minerals by pyrolysis-gas chromatography and high-performance liquid chromatography. Determine dissolved inorganic carbon by gas chromatographic and titration techniques. Characterize carbonate minerals by both chemical and petrographic analyses. Apply stable isotope and ^{14}C measurements to all phases where appropriate. Incorporated these measurements into computer models using a mass balance approach, in which the estimated carbon fluxes and quantities are constrained by the principle of conservation of mass.

PROGRESS: Project activities have focused on aspects of the carbon cycle that are particularly relevant to the geochemical effects of carbon dioxide and long-term geochemical predictions. Matrix transformations and eigenanalysis show how carbon cycle models appropriate to short time scales can be systematically related to models appropriate for long time scales.

For long-term carbon dioxide predictions (hundreds to thousands of years), modeling techniques have been developed to accommodate carbonate dissolution and other sediment interactions. Ocean modeling suggests that, if man burns all of the world's fossil fuel reserves, the average lysocline and atmospheric carbon dioxide concentrations may remain perturbed for thousands to tens of thousands of years. The long-term predictions are subject to significant uncertainties because the present ocean/atmosphere/sediment system may not be at steady state. Based on the geologic record of oceanic carbonate dissolution, the model also suggests that geologic variations in atmospheric carbon dioxide must have been accompanied by significant oceanic alkalinity changes. In the laboratory, Sundquist and Doug Burns have implemented a gas chromatographic technique for analyzing carbon dioxide, carbon monoxide, and methane in 1-milliliter gas samples. They are also designing an automated remote soil gas sampler.

REPORTS PUBLISHED:

Sundquist, E. T., in press, Relation of future changes in atmospheric CO_2 to long-term changes in sea level: National Academy of Sciences, 33 p.

NR109 TRACE METALS AND NUTRIENTS

TITLE: Geochemical Cycling of Trace Elements and Nutrients in Natural Water Systems

PROJECT NUMBER: NR 81-109

LOCATION: Topical Research

PROJECT CHIEF: Bricker, Owen P.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Natural water systems provide a wide range of conditions in which to examine the geochemical behavior and cycling of trace elements and nutrients relative to hydrochemically important mineral reactions. Processes of mineral dissolution, alteration, and genesis exert strong controls on the concentrations of chemical species in natural water systems and thus on water quality. Chemical composition of atmospheric-precipitation input to terrestrial watersheds affects mineral-reaction rates and may regulate reaction pathways and products. Knowledge of the geochemical behavior and cycles of trace elements and nutrients is essential in order to understand and predict the consequences of deliberate or accidental anthropogenic additions of these substances to the environment.

OBJECTIVE: Define the affect of mineral-water interactions in determining the chemical composition of natural waters, with emphasis on trace elements and nutrients, to describe quantitatively the geochemical behavior of trace elements and nutrients in freshwater, estuarine, and marine environments. Assess the impacts of anthropogenic contributions on natural cycles in these systems and evaluate the hydro-geochemistry of trace elements and nutrients as a function of water resource utilization.

APPROACH: Develop geochemical mass balance studies of the flux of trace elements and nutrients in natural water systems by detailed sampling and chemical analysis of input waters and outflow waters. Identify and quantify the critical reactions that control changes in water chemistry through examination of the solids that the waters contact and react with and through laboratory studies of rock soil-water interactions. Separate solids from the solution phase requires special collection, filtration, and (or) ultra-centrifugation techniques. Examine the solid phases by chemical analysis, x-ray diffractometry, optical and electron microscopy (SEM, TEM), and special techniques for definition of the surface boundary layer. Perform chemical analysis of the aqueous phase using ion-chromatography and special potentiometric techniques. Interpret the chemical compositions of the solid and aqueous phases relative to thermodynamic and (or) kinetic behavior in the hydrochemical environment.

PROGRESS: Continuing investigations of the geochemical response of weathering processes and the resulting surface water chemistry in small forested watersheds receiving acid deposition show that the effects of acid deposition on surface waters in eastern United States watersheds having similar size, physiography, climate, and land use, are strongly related to the composition of the underlying bedrock. Watersheds developed on greenstone, calcareous shale, sandstone, granite, and schist differ in their ability to neutralize acid deposition. Surface waters in watersheds developed on greenstone and calcareous shale are not discernably affected by acidification. Watersheds developed on sandstone have little capacity to neutralize acid rain; consequently, stream acidity is similar to that of precipitation. Watersheds developed on granite and schist are intermediate in their capacity to neutralize acid deposition. Bedrock composition appears to be the major property controlling surface-water chemistry in these systems. Those watersheds containing bedrock with the highest percentage of weatherable minerals are the least affected by acidification. Hydrologic flow paths and the nature of surficial materials and vegetation also influence chemical responses to acid deposition in watersheds. Vegetation influences stream chemistry by modifying precipitation inputs, increasing sulfate inputs and retaining nutrients (ammonium and nitrate in particular), and evapotranspiration. The response of vegetation to water availability suggests a strong correlation between rainfall-runoff and near-surface water conditions. This response also reflects the distribution of subsurface barriers to hydrologic flow and sediment-soil facies changes. Biological activity elevates soil carbon dioxide and leads to carbonic acid weathering and production of alkalinity in ground water. However, shallow hydrologic flowpaths that bypass more alkaline ground waters contribute to stream acidification.

REPORTS PUBLISHED:

Baron, J., and Bricker, O. P., 1987, Hydrologic and chemical flux in Loch Vale watershed, Rocky Mountain Park, in Averett, R. C., and McKnight, D. M., eds., Chemical quality of water and the hydrologic cycle: Chelsea, Mich., Lewis Publishers, p. 141-156.

Bricker, O. P., 1987, Catchment flow paths: International symposium on acidification and water pathways, Bolkesjo, Norway, May 4-8, 1987, Symposium Volume Supplement, p. 1-22.

Puckett, L. J., 1987, The influence of forest canopies on the chemical quality of water and the hydrologic cycle, in Averett, R. C., and McKnight, D. M., eds., Chemical quality of water and the hydrologic cycle: Chelsea, Mich., Lewis Publishers, p. 3-22.

NR122 GROUND-WATER DISPERSION

TITLE: Dispersion of Toxic and Radioactive Wastes in Ground-Water Systems

LOCATION: Topical Research

PROJECT NUMBER: NR 81-122

PROJECT CHIEF: Wood, Warren W.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: The movement of toxic and radioactive substances in ground waters is principally the result of hydrodynamic forces and resistances acting in the system. This movement, however, can be greatly affected not only by physical dispersion, but also by other dispersive factors such as exchange capacities, chemical kinetics, ionic distributions, and selectivities. Without knowledge of how these physical and geochemical factors affect the movement of these hazardous substances, the prediction of dispersion of toxic and radioactive wastes is uncertain.

OBJECTIVE: Develop field methods and techniques that will yield values of critical parameters that are regionally significant in a ground-water system. Many of the factors which affect dispersion potentially can be determined by laboratory tests. But, the samples on which these tests are performed represent only a very small portion of an aquifer, and the results of the tests can be extremely misleading.

APPROACH: Undertake studies in which field methods and techniques are developed and applied to naturally stressed systems. Use these studies to define the importance of the various factors and find means for measuring the magnitude of each one.

PROGRESS: Research on the origin of playa lake basins in west Texas suggests that they are created by a combination of carbonate dissolution and piping in the unsaturated zone. This hypothesis is supported by hydrologic, solute, and gas chemistry data and contrasts with the prevailing view that the basins are eolian in origin. In addition to obtaining a better understanding of the geochemistry of unsaturated zones, the consequences of this hypothesis are important in the determination of surface stability at the proposed high level radioactive waste repository in Deaf Smith County, Tex. In a second study, initial evaluation of the reactive tracer data collected at the Cape Cod, Mass., natural gradient tracer test suggests that hydrodynamic dispersion may be different for conservative and reactive constituents in this glacial outwash aquifer. If this analysis holds up to more rigorous examination, it will require reevaluation of some of the assumptions commonly used in solute transport modeling of ground water. In a third area of interest, it has been determined that subtle changes in density of water in saline lakes of

west Texas, which are set within the High Plains fresh water aquifer, has a profound effect on the flow of ground water and solutes into, around, and out of lakes. Hydrologic control of density of saline lake water has been shown to affect the solute concentration and ratios in the surrounding ground water, and appears to have controlled the development of commerical deposits of mirabilite and bloedite in the lake sediments.

REPORTS PUBLISHED:

Wood, W. W., and Low, W. H., 1986, Aqueous geochemistry and diagenesis in the eastern Snake River Plain Aquifer System, Idaho: Geological Society of America Bulletin, v. 97, p. 1456-1466.

NR129 ORGANIC DEGRADATION

TITLE: Comparative Study of Organic Degradation in Selected Hydrogeologic Environments

PROJECT NUMBER: NR 83-129

LOCATION: Topical Research

PROJECT CHIEF: Baedecker, Mary Jo

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Degradation of organic material produces organic compounds that both alter the quality of water and affect the inorganic reactions. The hydrogeologic controls on organic-inorganic reactions, their rate, and progress are not well understood. This project focuses on the occurrence and fate of organic compounds in (1) contaminant aquifers, (2) soils, and (3) lake sediments.

OBJECTIVE: Increase our understanding of reactions involving organic matter and to evaluate the significance of these reactions in geochemical studies. Particularly: (1) identify organic and inorganic compounds that are present as a result of the degradation of organic material; (2) study the interaction of organic compounds with soil and aquifer materials; and (3) develop geochemical models in organic-rich environments.

APPROACH: Select several organic-rich environments that have chemical and hydrologic background data and obtain samples that can be analyzed for organic and inorganic constituents. Investigate the extent and effects of chemical reactions and processes in these areas where degradative processes are primarily anearobic. Determine the type of organic material present, the interaction of organic compounds with sediment, the migration of organic compounds, the fractionation of isotopes and generation of gases, and the fate of inorganic constituents in association with organic material.

PROGRESS: Progress was made in three areas of investigation on the degradation of organic material in shallow aquifers. (1) Detailed chemical analyses along vertical and horizontal sections delineate the formation of anoxic zones and show that the concentrations of constituents vary markedly over short distances. Important processes are the alteration of organic compounds, generation of large amounts of gases, solubilization of iron and sulfide phases, and the fractionation of carbon isotopes. (2) Petroleum hydrocarbons are significantly altered short distances from the source in a glacial outwash aquifer. Downgradient of the source, volatile hydrocarbons decrease exponentially in concentrations and the higher-molecular-weight hydrocarbons are sorbed on the sediments. The degradation of these compounds has altered the mineralogy of the aquifer and carbonates and silica are dissolved and reprecipitated. (3) An intermediate in the degradative processes

of organic material is the formation of organic acids. Their distribution and concentrations vary markedly in anaerobic plumes. In some areas, these acids contribute 50 percent of the total alkalinity and are of major importance in geochemical processes.

REPORTS PUBLISHED:

Franks, B. J., Goerlitz, D. F., and Baedecker, M. J., 1986, Defining extent of contamination using on-site analytical methods: NWWA/API Conference, Petroleum Hydrocarbons and Organic Chemicals in Ground Water--Prevention, Detection, and Restoration, Houston, Tex., 1985, Proceedings, p. 265-275.

Siegel, D. I., Baedecker, M. J., and Bennett, P., 1986, The effects of petroleum degradation on inorganic water-rock reactions: International Water-Rock Symposium on Water-Rock Interaction, 5th, Reykjavik, Iceland, 1986, Proceedings, p. 524-527.

NR132 WATER QUALITY AND HEALTH

TITLE: Relationship Between Chemical Quality of Natural Waters and Human Health and Disease

PROJECT NUMBER: NR 79-132

LOCATION: Topical Research

PROJECT CHIEF: Feder, Gerald L.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: In recent years, there has been increasing interest and study concerned with the possible relationships between the chemical quality of natural waters and human health and disease. Medical researchers recognize areal patterns of health and disease in the United States and suspect that these patterns may be controlled by both environmental and non-environmental factors. After excluding non-environmental factors, local and regional differences in water quality appear to have an effect on health and disease. Such differences influence the total dietary intake of necessary major and trace elements and the concentration of certain potentially toxic chemical constituents.

OBJECTIVE: Discover and quantify relations between the chemical quality of natural waters and human health and disease.

APPROACH: Identify chemical constituents occurring in natural waters that are most likely to affect health and disease and those medical conditions most likely to be affected by water quality. Use this information to determine the temporal and spacial associations between specific chemical characteristics of water and specific states of health and disease. Exclude known high-risk factors related to geographic areas (for example, urban environment, mining activity) in order to increase the likelihood of detecting risk factors associated with natural water quality. Initially, use existing data from sources such as the U.S. Geological Survey (USGS) and the Bureau of Vital Statistics (BVS) for both the medical and hydrologic aspects of the study. If data are lacking, collect new data in the field planned. Supplement data collection with cooperative programs with district and aquifer study water-quality specialists. Obtain information on chemical composition of soils, rocks, and plants through cooperation with the Branch of Regional Chemistry, Geologic Division. Cooperation with Dr. Howard C. Hopps, Curators Professor of Pathology, University of Missouri Medican School throughout this study.

PROGRESS: Studies were conducted through the U.S.-Yugoslavian Joint Scientific Board on the Mineral Nitrogen in Groundwaters Project. Initial analyses of ground water samples from an area in Yugoslavia where the fatal disease Balkan Endemic Nephropathy (BEN) occurs, indicates that aniline type compounds may be present in these wells. Aniline type compounds are

carcinogenic and biologically active, and may play a role in BEN. Work was begun with Kenneth Cantor, National Cancer Institute, exploring possible relationships between drinking water quality (especially ground water in rural areas) and certain types of cancers. Work continued with Dr. H. C. Hopps showing relationships between cardiovascular disease and human health. Data on sodium concentrations in ground water indicate that at the concentrations found in most ground waters it does not have an important effect on cardiovascular disease mortality. Work with L. Konikow and C. Brown helped to design the ground-water sampling plan for the Delmarva Peninsula NAWQA study.

REPORTS PUBLISHED:

Feder, G. L., 1986, Hydrogeologic controls on nitrogen species in ground and surface waters: International Association of Hydrologic Sciences Publication no. 156, p. 211-215.

Hopps, H. C., Feder, G. L., 1986, Chemical Qualities of water that contribute to human health in a positive way: The Science of the Total Environment, v. 54, p. 207-216.

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NR135 SPECIATION OF METALS

TITLE: Distribution and Speciation of Metals in Sedimentary Environments

PROJECT NUMBER: NR 86-135

LOCATION: Topical Research

CHIEF: Simon, Nancy S.

CITY: Reston, VA

PROBLEM: It is not sufficient to know only the total concentrations of metals in environmental samples. The partitioning of metals between solid and solution phases and the speciation of metals in these two phases among free ionic, metal compounds, and metal inorganic and organic complexes needs to be determined to develop correct models of environmental stystems. Prediction of the response of aquatic and sedimentary systems to environmental changes, and the determination of the toxicity of metals in these systems, are dependent on metal speciation. An example of an environmental problem involving organo-metal associations is the spread of toxic metals with the transport of sedimentary material. Metals readily bond to organic material. Organic coatings are found on particulate matter and smaller sedimentary materials have a large surface area per unit weight on which coatings can form. Therefore, higher metal concentrations can be found in the smaller size fractions of sedimentary material. These smaller particles are more easily transported by the water column than coarser sedimentary metal. This mobility means that toxic metals can extend beyond a point source. How environmental changes affect the partitioning and speciation of metals, and the rate at which these changes occur, needs to be evaluated.

OBJECTIVE: To determine inorganic-organic reactions by which toxic metals are retained in, or mobilized from, the sediment, and rates at which these processes occur.

APPROACH: Three sets of information are needed to meet the project goals. First, the distribution or partitioning of metals between the solution and solid phases needs to be determined. Second, the speciation of dissolved free, inorganic complexed metals and organic complexed metals must be evaluated. Third, the rate of change in species composition in response to changes in environmental conditions should be measured. Among the techniques to be used in this study are atomic absorption spectroscopy (total trace metal concentrations in aqueous and sedimentary samples), liquid chromatography (speciation of metal complexes), and electrochemical analysis (determination of free and liable metals ions in solution). This project differs from other projects because: (1) the techniques used will not only determine the distribution of metals between phases, but also the classes of organic compounds with which the metals are associated, and (2) the rates of

adsorption/desorption processes will be studied. More specifically, the speciation of metals in the systems to be studied will not be done by extraction methods or specific ion electrodes, but with biochemical methods coupled with liquid chromatography and electroanalytical techniques. In this way, more specific information about the rexdox chemistry, chemical associations, and bioavailability of toxic metals can be determined.

PROGRESS: Initial investigations of natural water samples with elevated metal concentrations using voltammetry and liquid chromatographic separations coupled with electrochemical characterization suggest that there is a direct relation between concentrations of metals in natural water samples and the presence of degradation products of organic matter. Anodic stripping voltammetry techniques have been applied to samples from hazardous waste study sites (Tar Creek, Okla., and Calcasieu River, La.) where toxic-metals transport is being investigated. Variations have been monitored in dissolved-free metal concentrations with pH changes caused by bacterial activity in water samples from the Tar Creek site. Changes in organic complexation, rather than dissolution of particulate matter, appeared to be the cause of fluctuation in concentrations of dissolved metal ions. Analyses of Calcasieu River sediment cores show that where adsorbed ammonium concentrations on sediment solids are elevated, interstitial-water concentrations of chromium are also elevated. Several electroactive organic compounds have been detected in the interstitial water using liquid chromatographic separation and electrochemical detection and characterization. The evidence suggests there is a relation between diagenesis of sediment organic material and elevated heavy-metal concentrations in sediment interstitial water. A detailed study by this project of sediment extraction techniques suggests that use of a complexing agent with oxidation of organic matter at neutral pH is an efficient technique for extracting metals from sediment samples taken from an anoxic environment.

SR075 RADIOISOTOPES IN GROUND WATER

TITLE: Uranium-Thorium Series Radioisotopes in Gulf Coast Ground-Water Systems

PROJECT NUMBER: SR 83-075

LOCATION: Topical Research

PROJECT CHIEF: Kraemer, Thomas F.

HEADQUARTERS OFFICE: NSTL, MS

PROBLEM: Little is known of the distribution and behavior of uranium-thorium series radioisotopes in ground-water systems despite their potential use as investigatory tools. Although an examination of these radioisotopes in deeply buried, moderately hot (150 °C) formations of the Tertiary Gulf Coast has led to some valuable observations concerning brine-rock interactions, more research must be done to understand fully the processes controlling these interactions. In addition, little research has been done on the behavior of uranium-thorium series radioisotopes in shallow brine and freshwater aquifer systems.

OBJECTIVE: Examine the behavior of uranium-thorium series radioisotopes in a variety of well studied subsurface environments, and relate the behavior to specific physical and chemical conditions and processes operating within the aquifer. Apply these results to other aquifers to determine conditions and processes occurring within them. For example, from examining the radiochemistry of produced fluids from a well, it should be possible to deduce (1) aquifer quality (clay content), (2) areal heterogeneity of an aquifer, (3) existence of a free gas phase, and (4) the presence of high concentrations of uranium or other naturally-occurring radioelements in aquifers and their potential health hazards, if any.

APPROACH: Collect and analyze water, rock, and hydrocarbon samples from a variety of aquifers and analyze for appropriate radioisotopes. Collect samples from wells for which there is available good-quality aquifer data from such sources as geophysical well logs, conventional core analyses, and reservoir production histories. Use these data to interpret results of radiometric analyses in light of known aquifer conditions. Conduct laboratory investigations including the determination of the exhalation rate of radioactive gas (radon) from sandstone and shale samples. Use results of field and laboratory studies to establish procedures for applying radiometric data to determine conditions and processes existing in aquifers.

PROGRESS: (1) Uranium in Gulf Coast sandstones seems to be at saturation in the formation water and in chemical equilibrium with a solid phase of either uraninite or coffinite; the uranium activity ratios of dissolved uranium are apparently influenced by this equilibrium. (2) Radium is quite abundant in Gulf Coast formation waters and very strongly correlated with chloride content of the water. Apparently high chloride content hastens the chemical reaction leading to the release of more radium. (3) Radon in geopressured-geothermal solution gas is higher than in coventional gas produced in the Gulf Coast, but within the range found for conventional gas produced in other areas of the United States. No greater risk to health is foreseen in using geopressured solution gas in industrial or commercial areas. (4) Progress is being made in determining the behavior of uranium, radium and thorium in shallow, cool, freshwater aquifers of the Gulf Coast. Areas where use of these isotopes is helping to understand hydrology have been examined in Mississippi, Missouri, and Florida.

REPORTS PUBLISHED:

Kraemer, T. F., Radon in unconventional natural gas from Gulf Coast geopressured reservoirs: Environ. Science Tech.

Kraemer, T. F., and Kharaka, Y. K., Uranium geochemistry in geopressured-geothermal systems of the U.S. Gulf Coast: Geochimica et Cosmochimica Acta, v. 50, no. 6.

WR044 SOLUTE TRANSPORT AT LOW FLOW

TITLE: Solute Transport Processes in Low-Flow Streams

PROJECT NUMBER: WR 65-044

LOCATION: Topical Research

PROJECT CHIEF: Kennedy, Vance C.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: The interaction of water and stream solids, such as abiotic material, organic detritus and biota, can affect the chemical composition of both water and solids, especially in the case of minor elements. Thus, when new solutes are added to a stream, they may behave as conservative constituents, may be adsorbed by stream solids (with or without displacement of previously adsorbed materials), may precipitate, or may combine with stream solutes to form complexes having properties quite different from the original solutes. In some respects, stream biota will behave much like abiotic solids on reacting with stream solutes, but in other aspects their behavior may be very different as, for example, in the case of nutrient uptake. A better understanding of the rate and nature of water-stream solids interaction is needed to allow quantitative predictions of the manner of transport of various dissolved constituents.

OBJECTIVE: Determine the nature and rates of the hydraulic and chemical processes involved in the interaction between introduced solutes and abiotic material plus organic detritus.

APPROACH: Inject a mixture of conservative and nonconservative solutes into streams for various time periods and intensively monitor their transport downstream. The conservative constituents serve as tracers for hydraulic transport processes independent of any reactions with stream solids, whereas the reacting nonconservative solutes (nutrients, trace and major elements) are removed from solution, permanently or temporarily, at various rates depending upon their chemistry and the nature of the stream solids (sediments and biota) with which they are interacting.

PROGRESS: A stream rise occurred during constant injection of strongly sorbed solutes. Additional dilution of strongly sorbed solutes occurred just below the injection site, but concentrations rose at downstream points demonstrating that increased water veolocity and depth in the channel reduced contact with reactive bed sediments and thereby allowed concentrations to exceed those present before the runoff event. These results were presented at an international conference.

REPORTS PUBLISHED:

Avanzino, R. J., Bencala, K. E., Jackman, A. P., Kennedy, V. C., Triska, F. J., and Zellweger, G. W., 1986, Data on the solute concentration within the subsurface flows of Little Lost Man Creek in response to a transport experiment, Redwood National Park, northwest California: U.S. Geological Survey Open-File Report 86-403W, 72 p.

WR165 WESTERN U.S. GEOCHEMISTRY

TITLE: Chemical and Isotope Studies of Thermal Waters of the Western United States

PROJECT NUMBER: WR 79-165

LOCATION: Western United States

PROJECT CHIEF: Mariner, Robert H.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Reconnaissance and chemical and isotope sampling of thermal springs in the western United States generally has not provided information of sufficient detail to permit the geothermal potential of most individual areas to be determined with any certainty. This is especially true in the Cascade Mountian Range where the chemical geothermometers indicate much lower temperatures of water-rock equilibrium than the sulfate-isotope geothermometer and the geologic setting seem to require. This discrepancy could be due to simple mixing of thermal and fresh water or rapid equilibration of water with surrounding country rock as the fluids rise to the surface; alternatively, the sulfate-isotopic composition could be an artifact reflecting the original source.

OBJECTIVE: Investigate the origin of the dissolved constituents, water, and gases discharging in hot springs and determine their relation to fumaroles and cold mineral springs. Determine the recharge areas for the thermal springs and the amount of mixing of thermal and nonthermal waters. With this information, individual systems can be better understood and the geothermal potential of the individual thermal reservoirs estimated with greater accuracy.

APPROACH: Make chemical isotopic analyses on samples of water and gas discharging from thermal, cold, and mineral springs. Use the chemical and isotopic data to determine the extent of mixing and ascertain the probable recharge areas for the individual thermal systems. Investigate the factors that control the chemical and isotopic composition of the fluids. Although the initial area of investigation will be the Cascades of California, Oregon, and Washington, other geothermal areas in the western United States will be investigated as the project develops.

PROGRESS: Total gas compositions for hot springs of the Oregon Cascades based on dissolved gas determinations and assumed Rayleigh distillation show that the unusually high nitrogen to argon and nitrogen to neon ratios are due to excess nitrogen relative to the normal atmospheric source. Excess nitrogen is common in some oil field waters but is rare in geothermal waters, further, it indicates that the systems have never been much hotter than they are now. Higher temperatures would have degraded the organic material removing the

nitrogen source material. Anomalous chloride concentrations detected in the previous years regional sampling streams in the Oregon and Washington Cascades were quantified by detailed sampling and gaging near the anomalies. Only two large anomalies have been detected which are not associated with known thermal or mineral springs; one on the SE side of Mt. Baker, Wash., and one on the SE side of Mt. Mazama (Crater Lake), Oreg. Reevaluation of the production data from Newberry 2 (NB2) permits us to estimate the isotopic composition of the aquifer fluids. Hydrothermal minerals were used to confirm the oxygen isotope composition of the formation water at the bottom of the well, and to show that the hydrothermal minerals at shallower depth formed at the measured temperatures. Water/rock ratios for the system indicate a young system. Dissolved gas concentrations, stable isotope data, and carbon-14 data demonstrate the presence of two distinct aquifers in the low-temperature geothermal system at Twin Falls, Idaho.

REPORTS PUBLISHED:

Ingebritsen, S. E., Carothers, W. W., Mariner, R. H., Gudmundsson, J. S., and Sammel, E. A., 1986, Flow testing of research drillhole at Newberry Volcano, Oreg.: U.S. Geological Survey Water-Resources Investigations Report 86-4133, 23 p.

GEOMORPHOLOGY AND SEDIMENT TRANSPORT

CR098 SEDIMENT TRANSPORT PHENOMENA

TITLE: Measurement and Prediction of Sediment Transport Phenomena

PROJECT NUMBER: CR 74-098

LOCATION: Topical Research

PROJECT CHIEF: Stevens, Herbert H., Jr.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: In alluvial streams, for every different hydrologic condition, the bed configuration, sediment transport, and hydraulic characteristics mutually change to achieve quasi-equilibrium. These changes affect the ability of the stream to convey given quantities of water, accommodate navigation, transport and dilute solid and solute wastes, support aquatic biota, and perform a variety of other similar functions. As yet, the relation between pertinent hydraulic and sedimentologic variables are not completely understood; hence, the extent to which important variables, particularly bedform roughness and sediment transport, will change in response to natural or man-induced alterations to the flow regime cannot be predicted with desired reliability. As a result, optimum utilization and management of a waterway usually is not assured; often, modifications intended to enhance the utility of a waterway are ineffective or have adverse effects. Lack of understanding is due in part to inadequate instrumentation for measuring the bedload transport. This problem is particularly acute in areas where resources are being mined for energy development.

OBJECTIVE: Provide a more complete understanding of sedimentation phenomena in alluvial streams and the response of such streams to imposed changes through the use of improved instrumentation. In particular, consider the interrelationships between bed-form characteristics and the transport of bed-load and bed-material load.

APPROACH: Initially, analyze existing data to relate bed-form characteristics and hydraulic and sedimentologic variables, and develop one or more bedload samplers to permit accurate measurements of bedload transport. The development of bedload samplers will be accomplished through a comprehensive testing and calibration program with prototype samplers in a specifically designed laboratory facility capable of continuously measuring the discharge of bedload particles from 2 to 64 millimeters in diameter under different flow conditions. Later, study the characteristics of bed-forms, sediment transport, and other pertinent variables as required to meet specific needs. Use acoustic instrumentation, including side-scan sonar, to measure bed-form configuration and movement. Use suitable bedload samplers, and suspended load samplers, to define transport rates. Finally, analyze information to define criteria for predicting bed-form conformation and to provide a better understanding of sediment-transport phenomena. Study both sand-bed and gravel-bed streams.

PROGRESS: Data collected during laboratory calibration of bedload samplers were used to study the effect of length of sampling time and to make a spectral analysis of bed forms. The distribution of samples collected using varying sampling time periods closely agreed with the results using Einstein's distribution equation.

REPORTS PUBLISHED:

Hubbell, D. W., and Stevens, H. H., Jr., 1987, Laboratory data on coarse-sediment transport for bedload sampler calibrations: U.S. Geological Survey Water-Supply Paper 2299, 31 p.

Hubbell, D. W., Stevens, H. H., Jr., Skinner, J. V., and Beverage, J. P., 1986, Characteristics and use of Helley-Smith type bedload samplers: U.S. Geological Survey Open-File Report 86-415W, videotape.

CR102 SEDIMENT IN RIVERS

TITLE: Movement and Storage of Sediment in River Systems

PROJECT NUMBER: CR 75-102

LOCATION: Nationwide

PROJECT CHIEF: Meade, Robert H.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Sediment moves through a river system in response to specific events and changing conditions in the drainage basin. The movement of sediment is usually discontinuous. Episodes of movement are separated by periods of storage that can range from less than one year to more than one thousand. Understanding the movement and storage of sediment in rivers is important to navigation, flood control, and other aspects of river engineering, as well as to the prediction of the fate of contaminants absorbed on sediment particles.

OBJECTIVE: Assess: (1) changes in river sediment loads over periods of decades or longer, and the factors (natural or artificial) that cause the changes; (2) rates at which sediment is stored in river systems and the residence times of sediment particles in storage; and (3) sources, pathways, and sinks of sediment particles in river systems.

APPROACH: (1) Assess long-term changes in sediment loads from data previously collected by U.S. Geological Survey and other agencies; (2) assess sediment storage by repeated (annual) surveys of selected river channels, and by comparing old and new maps and aerial photographs of rivers and their flood plains in the upper Missouri River basin; and (3) assess sources, pathways, and sinks by intensive field studies (including tracer studies) of selected small rivers.

PROGRESS: One field excursion on the Apure River (Orinoco tributary) in Venezuela to sample sediment movement during the early rising stage (May 1986) was completed. A resurvey of cross sections in Powder River, Mont., showed very little change in a year of low runoff. An investigation of the distribution and fate of heavy metals associated with fluvial sediment in the channel and floodplain downstream from the Homestake Mine in South Dakota was continued. Preliminary results indicate that approximately one-third of the mining tailings discharged to the river have been incorporated within the floodplain.

WRD FEDERAL RESEARCH PROJECTS.....GEOMORPHOLOGY & SEDIMENT TRANSPORT

REPORTS PUBLISHED:

Marron, D. C., 1987, Floodplain storage of metal-contaminated sediments downstream of a gold mine at Lead, S.D., in Averett, R. C., and McKnight, D. M., eds., The chemical quality of water and the hydrologic cycle: Chelsea, Mich., Lewis Publishers, p. 193-209.

Marron, D. C., and Popenoe, J. H., 1986, A soil catena of schist in northwestern California: Geoderma, v. 37, p. 307-324.

Richey, J. E., Meade, R. H., Salati, Eneas, Devol, A. H., Nordin, C. F., Jr., and Santos, U. de M., 1986, Water discharge and suspended sediment concentrations in the Amazon River, 1982-1984: Water Resources Research, v. 22, no. 5, p. 756-764.

CR105 CHANNEL MORPHOLOGY

TITLE: Effects of Water and Sediment Discharges on Channel Morphology

PROJECT NUMBER: CR 65-105

LOCATION: Topical Research

PROJECT CHIEF: Williams, Garnett P.

HEADQUARTERS OFFICE: Lakewood CO

PROBLEM: Channels in alluvial streams change with time. Bed elevations and channel widths may change, meander bends may shift both laterally and downstreamward, the sizes of the bed particles may change, instream bars may grow and migrate, and the amount and type of vegetation along the river may increase or decrease. Sometimes the change is insignificant, even over decades, but in other cases catastrophic modifications occur in minutes. The transformations can be natural or human-induced, and they can have significant effects on humans and the environment.

OBJECTIVE: Determine and analyze the influence of the major variables, particularly water and sediment discharges, governing channel morphology.

APPROACH: Study the effect of large contribution of sediment to stream channels. Make field surveys and aerial-photograph analysis, preferably time-sequential, of stream reaches that have received exceptionally large sediment inputs. Document channel response, with a view toward eventually developing a general model of channel response.

PROGRESS: (1) With B. M. Troutman, completed a lengthy statistical manuscript on estimation and prediction of straight-line geologic relationships. The ordinary least squares (OLS) and structural-analysis (SA) methods of fitting straight lines to data were examined with respect to how closely each of these methods (a) estimates the parameters of "true" straight-line relations and (b) predicts values of the dependent variable. As expected, SA is superior to OLS for estimation of the true line. Differences between the two line-fitting methods decrease as error in X becomes small relative to error in Y. Also as expected, OLS is better than SA for predicting the dependent variable; again the difference grows smaller as X takes on less error relative to Y. (2) Completed first draft of a study of suspended sediment-water discharge relations for single hydrologic events (e.g., a flood) in rivers. Many features of the sediment-concentration water-discharge relation for a hydrologic event can be brought out by treating "smoothed" temporal graphs (discharge and concentration over time) as frequency distributions. Such distributions were analyzed qualitatively in terms of mean, spread, and skewness. Comparing concentration/discharge ratios on the discharge hydrograph's rising and falling limbs at a given discharge provides a consistent, reliable theory for explaining and categorizing the more common

types of concentration/discharge relations. Five categories of these relations emerged: single-valued line (straight or curved), clockwise loop, counterclockwise loop, single line plus loop, and figure eight. Of these, only the clockwise loop and perhaps the counterclockwise loop have received notable attention in previous studies for a single hydrologic event.
(3) Assembled a valuable and unique set of sediment-transport data for nearly 100 U.S. stream sites, representing a wide variety of environments. The data set is unique in that it will be the first one to present the total sediment load of streams along with the two main components of load--bedload and concurrently-measured suspended load. The associated hydraulic variables (water discharges, mean velocities, etc.) also are being listed. The entire data set will be published as a basic data open-file report; compilation is about 90 percent finished as of July 1987. The report will form the basis of various journal articles and other research papers.

REPORTS PUBLISHED:

Williams, G. P., 1986, River meanders and channel size: Journal of Hydrology, v. 88, p. 147-164.

Williams, G. P., and Wolman, M. G., 1986, Effects of dams and reservoirs on surface-water hydrology--changes in rivers downstream from dams, in National Water Summary 1985, Hydrologic events and surface-water resources: U.S. Geological Survey Water-Supply Paper 2300, p. 83-88.

CR187 BEDLOAD TRANSPORT RESEARCH

TITLE: Hydraulics and Mechanics of Bedload-Transport Processes

PROJECT NUMBER: CR 74-187

LOCATION: Topical Research

PROJECT CHIEF: Emmett, William W.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Of all processes operating in river channels, especially those of practical concern to engineers and others interested in river-channel behavior, perhaps the least understood are the hydraulics and mechanics of bedload transport. Before continuing advances in river-channel behavior can be made, the movement of bedload sediment must be understood.

OBJECTIVE: (1) Define spatial and temporal variations in bedload-transport rate for a single stage of flow; (2) define change in average magnitude of transport rate over a range in flow; (3) define change in average magnitude of transport rate over a range in channel geometry; and (4) analyze the data to evaluate the applicability of available bedload equations, suggest new coefficients for the existing equations, or propose new relations for predicting rates of bedload transport.

APPROACH: Use a conveyor-belt bedload-transport facility on the East Fork River near Pinedale, Wyo., as a control to evaluate variability factors in bedload transport and to field calibrate the Helley-Smith bedload sampler; to use the calibrated Helley-Smith sampler in the systematic collection of bedload samples, along with the concurrent measurements of streamflow hydraulics, from a variety of sand- and gravel-bed streams, and, within the laws of general physics, develop empirical relations of bedload transport and interpret the physical significance of the developed relations. Initiate at the conveyor-belt bedload-trap research facility a tracer study utilizing fluorescent particles to evaluate (1) residence time of sediment, (2) average speed of particles, (3) depth of bed material involved in transport, (4) dispersion of bed material, (5) short-term channel changes accompanying sediment transport, (6) influence of availability of sediment on transport rate, and other related aspects of sediment transport.

PROGRESS: (1) Measurements of bedload transport and associated hydraulic characteristics have been completed for the East Fork River, Wyo. Equipment and procedures have been described and process data are being analyzed and interpreted. (2) Six new field sites have been selected and bedload data are being collected at these sites by the U.S. Geological Survey. In addition to these six sites and the East Fork River site, several other sites provide information to the core data base.

WRD FEDERAL RESEARCH PROJECTS.....GEOMORPHOLOGY & SEDIMENT TRANSPORT

REPORTS PUBLISHED:

Mantz, P. A., and Emmett, W. W., 1986, Analysis of United States Geological Survey sediment transport data for some California streams: Euromech 192 Conference on Transport of Suspended Solids in Open Channels, Munich, Germany, 1985, Proceedings, p. 177-182.

CR266 ESTUARY SEDIMENTATION/EUTROPHICATION

TITLE: Transport and Deposition of Sediments and Sediment-Borne Contaminants in Tidal Rivers and Estuaries

PROJECT NUMBER: CR 81-266

LOCATION: Topical Research

PROJECT CHIEF: Glenn, Jerry L.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Sediments that contain large concentrations of nutrients and trace metals are accumulating rapidly in part of the tidal Potomac River, the Potomac Estuary, and the adjacent marginal embayments. Accumulations of sediments and sediment-borne contaminants may limit significantly the use of tidal waters and estuaries for commercial, recreational, and aquacultural purposes. The sediments decrease channel depths and widths to the detriment of commercial and recreational interests, and cover and destroy productive shellfish grounds. The nutrients are a factor in the development and maintenance of undesirable eutrophic conditions, including nuisance algae blooms and low levels of dissolved oxygen. Sedimentation and eutrophication problems in the Potomac are a consequence of essentially uncontrollable natural and anthropogenic influences. The problems began to develop naturally several thousand years ago when the current rise in sea level drowned the Potomac River and began the evolution of the modern tidal river-estuary system.

OBJECTIVE: (1) Identify modern sources of sediments and nutrients; (2) establish changes with time in sources or supply rates due to natural and anthropogenic influences; (3) determine sediment and nutrient transport and deposition patterns; (4) compute rates of accumulation and amounts of sediments and nutrients in selected hydrologic and geomorphic divisions of the Potomac system; and (5) compare supply and accumulation rates for prehistorical and historical periods with contemporary rates from concurrent transport studies.

APPROACH: Determine areal and stratigraphic distributions of sediments, nutrients, and trace metals by a combination of direct sampling (surface and core) and remote sensing (side-scan sonar and subbottom profiling). Analyze sediment samples for indicators of sources (particle size, mineralogy, nutrient and trace-metal concentrations) and accumulation rates (lead-210, carbon-14 pollen concentrations and distributions). Estimate sediment contributions from the shoreline source using a combination of field mapping, monitoring, and sampling at selected sites, and using laboratory measurements from available air photographs and maps. Integrate data with results from measurements and models of modern sediment and nutrient transport to provide past and present sediment and nutrient budgets for selected Potomac reaches.

PROGRESS: Bottom sediments collected from the transition zone were resuspended at other sites in the estuary where water-column characteristics differed greatly from those at the sampling site. Samples from each site were analyzed for total carbon and total phosphorus after approximately 8 days of resuspension. Statistical tests failed to establish significant differences in mean total carbon in original and resuspended samples from the transition zone and from anoxic near-bottom waters in the estuary; however, samples from oxic near-surface waters in the estuary had significantly less total carbon. Total phosphorus analyses were inconsistent, probably because of laboratory analytical errors.

REPORTS PUBLISHED:

Glenn, J. L., and Rice, C. A., 1986, Sediment data for computations of deposition rates in the tidal Potomac system, Maryland and Virginia: U.S. Geological Survey Open-File Report 86-279, 80 p.

CR273 HYDROLOGICAL-BIOLOGICAL INTERACTIONS

TITLE: The Interface of Hydrological and Biological Processes in Rivers

PROJECT NUMBER: CR 82-273

LOCATION: Topical Research

PROJECT CHIEF: Andrews, Edmund D.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: The geometry and pattern of river channels adjust to significant changes in the water discharge, size, and quantity of sediment supplied to the channel. When the quantity of water and sediment remains relatively constant over a period of years, the channel geometry and pattern vary about a mean or quasiequilibrium condition. Major watershed alterations that change the supply of water, sediment, and size of sediment reaching the channel necessitate an adjustment of the channel geometry and pattern and transform the channel from one quasiequilibrium state to another. Between the two quasiequilibrium states, there is a period of instability. Existing techniques for examining and predicting river-channel adjustment have been developed primarily from investigation of quasiequilibrium rivers. However, the dynamics and rate of river-channel adjustment during the period of instability rarely have been studied and are understood poorly. The length of time required for the complete adjustment is commonly a few decades to a century or more. In watersheds where various land-use changes occur every several years, the river channel may be adjusting continually to a different supply of water and sediment. An understanding of the dynamics and rate of river channel adjustment from one quasiequilibrium state to another is very important to managing fluvial resources. One of the most frequent and important adverse impacts of river-channel changes is damage to the aquatic ecosystem. When a river channel adjusts to a change in its watershed, the physical habitat of the aquatic organisms in the river may be reduced or even eliminated. In order to evaluate the biological impacts of watershed alteration, hydrologists frequently are asked to predict future hydraulic geometries and channel patterns so that changes in habitat can be assessed. The primary focus of this project is to understand the dynamics and rate of river-channel change as they affect the physical habitat. The greatest deficiencies in our present knowledge of river-channel adjustment as it relates to the aquatic ecosystem appear to be (1) the longitudinal sorting of bed material, especially gravel, (2) the formation of gravel bars, (3) adjustment of channel width, and (4) the rates at which the several hydraulic variables adjust.

OBJECTIVE: Describe the physical processes and rate at which a river channel adjusts due to a change in the water discharge, sediment size, and sediment load supplied to the channel concentrating on those aspects of the river channel known to influence significantly the aquatic ecosystem--the bed-material size distribution, the occurrence of bars, and channel width.

Describe the hydraulic processes controlling these characteristics of river channels as well as the rate at which they function. Develop mathematical models of the processes as required for longitudinal routing water and sediment. The ultimate goal of the project is to develop new analytical tools for describing river-channel adjustment.

APPROACH: Because adjustment of a river channel may extend over a few decades to a century, it is impractacal to observe the transition of a river channel from one quasiequilibrium state to another quasiequilibrium. The approach will be to study the movement of bed material through a reach of channel in detail, considering the transport of bed materials, distance transported, and location (bed, banks, or bar) of deposition for each size fraction. Two or three small, self-formed, gravel-bed streams will be selected for this part of the investigation that are also sites of active aquatic ecology research programs. Bedload-transport rates, tracer particles, and maps of channels features will be used to describe the movement of coarse bed material through the study reaches, and formulate a physical model of gravel movement by size fraction. In addition, the sequence and rate of adjustment will be reconstructed for historical examples of river-channel change to provide the temporal context in which to view a hydraulic characteristic at a particular point in time. Ideally, the study of hydraulic processes and aquatic ecology can be undertaken on the same river reaches that are used to reconstruct the historical data.

PROGRESS: Winter floods in the Sierra Nevada mountains kill buried eggs of brook trout and Paiute sculpin because bed-material transport increases greatly when high flows are constrained by snowbanks. From studies in 1952-61 in Sagehen Creek, Calif., winter floods were known to cause low populations of brook trout. In February 1982, dead Paiute sculpin were collected while sampling bedload during a rain-on-snow flood. Population estimates by electrofishing at nine permanent stations the following summer showed that density (3,586/hectare (ha)) and biomass (12.9 kilograms per hectare (kg/ha)) of Paiute sculpin were lower than the respective means (12,017/ha, 40.3 kg/ha) obtained during previous studies from 1952-61. These estimates were also below those obtained in 1956 after the largest winter flood during 1952-61. Brook trout fry also were less abundant in 1982 than the 10-year mean or the 1956 mean. Maximum flow depths, rather than discharge, were the likely cause of fish mortality. Winter floods are severe because accumulated snowpack increases the effective height of the streambank and confines a larger part, perhaps all, of a rain-on-snow flood within the channel. As a consequence, shear forces on the bed increase and bed-material transport increase rapidly. This increase is due primarily to an increase in the number of particles entrained by the flow at any instant. These conditions kill many benthic-living fishes such as the Paiute sculpin or buried eggs of fall-spawning fishes such as the brook trout.

WRD FEDERAL RESEARCH PROJECTS.....GEOMORPHOLOGY & SEDIMENT TRANSPORT

REPORTS PUBLISHED:

Andrews, E. D., 1986, Downstream effects of Flaming Gorge Reservoir on the Green River, Colorado and Utah: Geological Society of America Bulletin, v. 97, p. 1012-1023.

Andrews, E. D., 1987, Longitudinal dispersion of trace metals in the Clark Fork River, Montana, in McKnight, D. M., and Averett, R. C., eds., Chemical quality of water and the hydrologic cycle: Chelsea, Mich., Lewis Publishers, p. 210-223.

Andrews, E. D., and Parker, Gary, 1987, Formation of a coarse layer as the response to gravel mobility, in Hey, R. D., Bathurst, J. C., and Thorne, C. R., eds., Gravel-Bed Rivers: New York, John Wiley, p. 269-300.

NR081 INTERAGENCY SEDIMENTATION PROJECT

TITLE: A Study of Measurement and Analysis of Sediment Loads in Streams

PROJECT NUMBER: NR 39-081

LOCATION: Topical Research

PROJECT CHIEF: Skinner, John V.

HEADQUARTERS OFFICE: Minneapolis, MN

PROBLEM: Knowledge of factors governing the movement and deposition of sediment in streams and reservoirs is of major importance to Federal and State agencies involved in development of water and land resources of the Nation. A knowledge of the sediment discharge of streams is essential to the efficient design and operation of projects for the storage and use of streamflow. Movement of sediment also affects aquatic life and the transport of certain types of chemical pollutants. Complexity of sediment phenomena are such that comprehensive investigations are essential to support accurate conclusions.

OBJECTIVE: Develop new techniques for measuring and analyzing the sediment discharge of rivers. Coordinate studies to meet the common needs of two or more agencies. Serve as (1) a focal point for establishing standard methods for sediment discharge measurements; (2) a center for developing both manual and automatic samplers; and (3) a center for procuring, calibrating, and stocking sediment equipment used by federal agencies.

APPROACH: Use knowledge of hydraulics, physics, and electronics to develop new techniques for collecting sediment data. Evaluate new equipment under laboratory and field conditions. Distribute technical reports that explain research activities and manuals that explain equipment operation to all interested agencies.

PROGRESS: (1) An experimental sediment-concentration gage was installed on the Toutle River near Tower, Wash. Measured sediment concentrations ranged from 200 to 30,000 mg/L (milligrams per liter) during the initial 5 months of sampling. The probable measurement errors within the range of observed values are estimated to $\pm$ 200 mg/L. (2) Tests on an experimental frame for bedload samplers indicate certain dimensions are critical: the nozzle must be about 6.5 centimeters upstream of the frame to eliminate flow interference. (3) A special valve for point-integrating suspended-sediment samplers was designed and field tested to depths of about 5 meters. The new valve not only maintains ideal flow rates but also eliminates metallic contact with the sample water. (4) A paper describing techniques and equipment for collecting core samples was completed. Topics include terminology of core sampling, characteristics of different samplers, types of core distortions, methods for detecting and eliminating distortions, and techniques for dissecting and

preserving samples. The paper, which was recently accepted by the American Society for Testing and Materials committee on sediments, is being considered by the main committee. (5) A device for measuring particle-size distributions with X-rays is being evaluated by investigators at the USGS office in Iowa City, Iowa, as well as by several investigators at laboratories in Canada and Europe. In general, mean diameters obtained with the X-ray analyzer are smaller than mean diameters obtained by the pipet analyzer.

REPORTS PUBLISHED:

Beverage, J. P., 1987, Determining true depth of samplers suspended in deep, swift rivers, in A study of methods used in measurement and analysis of sediment loads in streams: U.S. Army Engineer District, St. Paul, 56 p.

Hubbell, D. W., Stevens, H. H., Jr., Skinner, J. V., and Beverage, J. P., 1987, Laboratory data on coarse-sediment transport for bedload-sampler calibrations: U.S. Geological Survey Water-Supply Paper 2299, 31 p.

Skinner, J. V., 1986, Measurement of scour-depth near bridge piers: U.S. Geological Survey Water-Resources Investigations Report 85-4106, 33 p.

Skinner, J. V., 1987, Report II-Progress Report--Temperature effects in vibrational-type sediment concentration gages, in A study of methods used in measurement and analysis of sediment loads in streams: U.S. Army Engineer District, St. Paul, 48 p.

Szalona, J. J., 1986, Report HH-Progress Report--Description and test of a straight-tube fluid-density gage for measuring suspended-sediment concentrations in streams, in A study of methods used in measurement and analysis of sediment loads in streams: U.S. Army Engineer District, St. Paul, 29 p.

NR107 SEDIMENT IMPACTS FROM COAL MINING

TITLE: Geomorphic and botantical impacts of sediment due to natural and unnatural land disturbance

PROJECT NUMBER: NR 84-107

LOCATION: Topical Research

PROJECT CHIEF: Osterkamp, Waite R.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Increased sediment yields from naturally stressed areas, such as mass-movement sites and devegetated lands, and man-stressed areas, such as mine spoils, urban areas, and agricultural lands, is one of the largest problems being addressed by agencies such as the U.S. Office of Surface Mining and U.S. Soil Conservation Service. The acquisition and interpretation of sediment data are among the most deficient areas that must be considered by these agencies. The impacts on geomorphology and botany that are caused by natural and induced sediment movement are sometimes intense; knowledge of these impacts is beneficial for understanding the effects of naturally occurring sediment movement.

OBJECTIVE: (1) Predict movement of sediment from naturally and unnaturally disturbed areas; assess existing techniques and develop new ones based on geomorphic, botanical, and statistical principles as aids in improving interpretive capabilities; evaluate geomorphic, botanic, and hydrologic changes changes caused by sediment movement from disturbed areas.

APPROACH: (1) Develop technology for determining amounts and rates of movement of sediment from disturbed areas based on factors such as land use, runoff, basin and landform morphology, and botanical indicators; (2) conduct research on the effect on landforms and vegetation of sediment movement using vegetation age, damage, and patterns of occurrence as indicators of the magnitude, frequency, and time of occurrence of destructive hydrologic events; (3) investigate the influence that ground-water movement exerts on sediment transport and changes in landforms by analyzing near-surface and subsurface rates of water and sediment movement (including piping, sapping and seepage erosion) in dynamic hydrologic systems; and (4) conduct research on the interactions between hydrology, water chemistry, and geochemistry as determinants of sediment movement through a hydrologic system, in conjunction and close coordination with other research and district personnel.

PROGRESS: Continuing studies in the Plum Creek basin, Colorado, have led to understanding how sand-bed streams adjust following historic flooding; the role of islands in causing channel narrowing has been defined. Investigations on Mount Shasta, Calif., are indicating that debris-flow activity on the mountain correlates better with warm summer temperatures than with heavy precipitation, such as during El Nino years. These findings offer the possibility of increasing our ability to predict debris flows and their hazard.

WRD FEDERAL RESEARCH PROJECTS..GEOMORPHOLOGY & SEDIMENT TRANSPORT

REPORTS PUBLISHED:

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Hupp, C. R., Osterkamp, W. R., and Thornton, J. L., in press, Dendrogeomorphic evidence and dating of recent debris flows on Mount Shasta, northern California: U.S. Geological Survey Professional Paper 1396-B, 39 p.

Osterkamp, W. R., ed., in press, Chapter 6, Great Plains, Geomorphic systems of North America: Decade of North American Geology Centennial Volume, Geological Society of America.

Osterkamp, W. R., Carey, W. P., and Hupp, C. R., 1987, Sediment impacts from coal mining, northeast Tennessee, in Glysson, G. D., ed., Proceedings of the advanced seminar on sedimentation, August 15-19, 1983, Denver, Colo.: U.S. Geological Survey Circular 953, p. 30-32.

Osterkamp, W. R., and Costa, J. E., 1986, Denundation rates in selected debris-flow basins: Fourth Federal Interagency Sedimentation Conference, Las Vegas, Nev., v. 1, p. 91-99.

Osterkamp, W. R., and Costa, J. E., in press, Changes accompanying an extraordinary flood on a sand-bed stream: Proceedings, 18th Annual Geomorphology Symposium--Catastrophic Flooding.

Osterkamp, W. R., and Hupp, C. R., in press, Dating and interpretation of debris flows by geologic and botanical methods at Whitney Creek gorge, Mount Shasta, Calif.: Geological Society of America Reviews in Engineering Geology, v. VII.

Osterkamp, W. R., Hupp, C. R., and Blodgett, J. C., 1986, Magnitude and frequency of debris flows, and areas of hazard on Mount Shasta, northern California: U.S. Geological Survey Professional Paper 1396-C, 21 p.

Osterkamp, W. R., and Wood, W. W., in press, Playa-lake basins on the Southern High Plains of Texas and New Mexico: Part I. Hydrologic, geomorphic, and geologic evidence for their development: Geological Society of America Bulletin.

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GROUND-WATER HYDROLOGY

CR085 GROUND-WATER QUALITY MODELING

TITLE: The Mathematical Simulation of the Transport and Reaction of Chemical Species in Ground Water

PROJECT NUMBER: CR 73-085

LOCATION: Topical Research

PROJECT CHIEF: Grove, David B.

HEADQUARTERS OFFICE: Denver, CO

PROBLEM: Mathematical techniques that describe the transport and reactions of dissolved chemical species during their flow through saturated porous media are necessary to predict water-quality changes in ground water. Such predictions are needed to help make decisions prior to possible injection of wastes and determine remedial actions after accidental contaminations of aquifers.

OBJECTIVE: Demonstrate the applicability of numerical-modeling techniques to the prediction of water-quality changes during transport of solutes through the saturated ground-water systems; and analyze the effects of these changes on the ground-water environment. This will provide the capability to predict the effects of chemical and physical stresses on the quality of ground water.

APPROACH: Solve the mass-transport equation through numerical means using finite-difference and finite-element methods and produce a water-quality model that will predict the effects of chemical disturbances on the ground-water system. Evaluate the effects of the disturbances on the aquifer. Concentrate on the use of field data and laboratory experiments to verify the model. Work closely with District, Federal, and State research projects involved in similar studies.

PROGRESS: Research activities have concentrated on field and laboratory data collection and preliminary analysis of results from the Cape Cod, Mass., and the Globe, Ariz., field sites. More than 25,000 water samples have been analyzed for molybdenum at the Cape Cod site. Preliminary analyses have shown four factors to be important in predicting the transport of molybdate: (1) adsorption of molybdate increases with decreasing pH; (2) molybdate adsorption decreases as dissolved solids increase (primarily due to competition for surface sites with phosphate and possibly other anions such as sulfate); (3) the amount of molybdate adsorbed increases with solution concentration; and (4) variations in hydraulic conductivity affect the rate of molybdate transport in solution. Data from laboratory experiments were used to predict the actual location of the molybdenum plume in the field. The Globe, Ariz., site involves a study of acidic ground-water contamination from copper mining. Laboratory column experiments have been used to estimate the

capacity of the alluvium to remove constituents from the acidic ground water. The principle mechanism for this removal is related to the neutralization of H+. A rise in pH causes the solubility of most metals to be exceeded and the metals precipitate. The unconsolidated alluvium, through which most of the plume is moving, has the capacity to neutralize approximately 1 to 2 pore volumes of acidic water. Estimates of plume breakthrough range from 1 to 15 years.

REPORTS PUBLISHED:

Eychaner, J. H., and Stollenwerk, K. G., 1987, Acidic ground-water contamination from copper mining near Globe, Ariz.--I. Overview, in U.S. Geological Survey Program on toxic waste--ground-water contamination: U.S. Geological Survey Open-File Report 87-109, p. D13-D18.

Stollenwerk, K. G., and Grove, D. B., 1987, Natural-gradient tracer test in sand and gravel--Nonconservative transport of molybdenum, in U.S. Geological Survey Program on toxic waste--ground-water contamination: U.S. Geological Survey Open-File Report 87-109, p. B17-B24.

Stollenwerk, K. G., and Eychaner, J. H., 1987, Acidic ground-water contamination from copper mining near Globe, Ariz.--II. Neutralization capacity of alluvium, in U.S. Geological Survey Program on toxic waste--ground-water contamination, U.S. Geological Survey Open-File Report 87-109, p. D19-D24.

CR090 HYDROLOGY OF LAKES

TITLE: The Role of Lakes in the Hydrologic System with Emphasis on Their Relation to Ground Water

PROJECT NUMBER: CR 74-090

LOCATION: Topical Research

PROJECT CHIEF: Winter, Thomas C.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Many hydrological and geochemical processes associated with lakes are poorly understood. Characteristics of wind and vapor profiles, which are basic controls on evaporation, over lakes of various sizes in different climatic and topographic settings have been studied in detail in only a few large Western U.S. reservoirs. Many commonly used methods of estimating surface runoff to lakes are highly inaccurate. Hydrogeologic controls in seepage have never been studied adequately, either from theoretical or field perspectives. Research into these components of lake hydrology is especially critical to those responsible for lake management, protection, and restoration.

OBJECTIVE: Gain understanding of the basic principles controlling the interaction of lakes and ground water, including associated chemical fluxes. Emphasize integration of theoretical and experiment fieldwork. Emphasize the study of ground water, but include state-of-the-art studies of the atmospheric and surface-water components of lake hydrology, as needed for the evaluation of the ground-water component. Evaluate error in hydrologic methodology for the various aspects of lake-water balances.

APPROACH: Construct theoretical and field-related mathematical models of steady-state and transient, variably-saturated ground-water conditions as related to lakes. Choose field experimental sites in selected parts of the United States for calibration and modification of models, instruments, and methods. Measure all components of the hydrologic system, as related to the experimental lakes, by various methods in support of the ground-water studies. Use multiple-level sensors on the lake for evaporation research purposes. Integrate chemical flux and biological studies with the hydrologic work at selected sites.

PROGRESS: (1) Current knowledge of the hydrology of lakes and wetlands for the North American continent was synthesized. This was presented as a broad classification based on hydrogeology and climate, and a comparative analysis of the types based on dominant components of their water balance was made. (2) A conceptual framework that unifies the fundamental hydrologic processes related to nearly all types of wetlands was developed. This was done as a foundation upon which cumulative effects of human disturbances on

wetlands were assessed. (3) Data on direct measurement of seepage in surface-water beds indicated the wide variety of near-shore hydrologic processes that affect the complex and dynamic patterns of seepage commonly observed.

REPORTS PUBLISHED:

LaBaugh, J. W., Winter, T. C., Adomaitis, V. A., and Swanson, G. A., in press, Geohydrology and chemistry of prairie wetlands in the Cottonwood Lake area, Stutsman County, N. Dak.: U.S. Geological Survey Professional Paper 1431.

Swanson, G. A., Winter, T. C., Adomaitis, V. A., and LaBaugh, J. W., in press, Chemical characteristics of prairie lakes in south-central North Dakota: U.S. Fish and Wildlife Service, Technical Report.

Winter, T. C., 1986, Effect of ground-water configuration of the water table beneath sand dunes and on seepage in lakes in the sandhills of Nebraska: Journal of Hydrology, v. 86, p. 221-237.

Winter, T. C., in press, Hydrologic studies of wetlands in the northern prairie of North America: in van der Valk, A. G., ed., Wetlands of the northern prairie of North America, Society of Wetland Scientists Monograph.

Winter, T. C., in press, Stream gaging: McGraw-Hill Encyclopedia of Science and Technology, New York, McGraw-Hill.

Winter, T. C., LaBaugh, J. W., and Rosenberry, D. O., in press, Direct measurement of differences in hydraulic head between ground water and surface water using a hydraulic potentiomanometer: Limnology and Oceanography, v. 33.

Winter, T. C. and Woo, Ming-Ko, in press, Hydrology of lakes and wetlands, in Moss, M. L., Wolman, M. G., and Riggs, H. C., eds., Surface water hydrology of North America: Geological Society of America, The Geology of North America, v. O-1.

CR103 DRILLING TECHNIQUES

TITLE: Research of Drilling Techniques as Applied to Hydrologic Investigations

PROJECT NUMBER: CR 75-103

LOCATION: Nationwide

PROJECT CHIEF: Teasdale, Warren E.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Many hydrologic studies need means to identify hydraulic and transport properties of porous media. Improved techniques for obtaining undisturbed and disturbed geologic samples for laboratory analyses and for conducting isolated-zone tests by use of inflatable packers are needed.

OBJECTIVE: (1) Develop methods to obtain the best quality and quantity of undisturbed cores and lithologies by experimenting with rotary-drive, stationary-piston, and hydraulic-push coring; (2) determine the most efficient use of various types of drilling muds under any drilling conditions encountered and the relation of hole size and lithologic conditions to borehole geophysical logging, using air or mud, rotary or auger drilling; and (3) determine the most efficient use of pneumatic and hydraulic packers for aquifer testing in shallow depths (1,000 feet) and for hydrofracting or deep testing (in excess of 1,000 feet).

APPROACH: Collect cores and samples that are adequate for laboratory analyses, and evaluate and adapt existing tools and design new ones for isolated aquifer testing. This will involve developing drilling techniques and techniques for holding drill holes open for geophysical logging, making evaluations of existing core barrels and the physical and chemical properties of drilling muds and additives according to their abilities to prevent invasion of sample material, and looking in detail at mud-rotary drilled holes. Provide consulting and advisory assistance to U.S. Geological Survey field offices. Coordinate all efforts with Borehole Geophysical Research Project. All final testing will be done in the field and all methods will have have transfer value to other field projects.

PROGRESS: (1) Mud-rotary coring of lake sediments using a prototype conventional core barrel was successfully accomplished at Pyramid Lake, near Reno, Nev. About 97 percent recovery of the core was obtained for the Paleoclimate Research Project. The hole ended in basalt at about 213 ft. (2) About 22 ft of unconsolidated sediments were cored at Walker Lake, near Hawthorne, Nev., with the same core barrel. (3) Three well installations were drilled, cased, and grouted near Hayes, S. Dak., for the Pierre Shale experimental site.

REPORTS PUBLISHED:

LeBlanc, D. R., Garabedian, S. P., Quadri, R. D., Morin, R. H., Teasdale, W. E., and Paillet, F. L, 1987, Hydrologic controls on solute transport in a plume of sewage-contaminated ground water, Cape Cod, Mass. U.S. Geological Survey Toxic Waste Technical Meeting, Hyannis, Mass., 1985, U.S. Geological Survey Open-File Report 86-481.

Shuter, Eugene, and Teasdale, W. E., in press, Application of drilling, coring, and sampling techniques to test holes and wells: U.S Geological Survey Techniques of Water-Resources Investigations, Book 2, ch. F1.

CR140 BOREHOLE GEOPHYSICS

TITLE: Borehole Geophysics as Applied to Geohydrology

PROJECT NUMBER: CR 64-140

LOCATION: Topical Research

PROJECT CHIEF: Paillet, Frederick L.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: A large amount of geophysical data is recorded in water wells and test holes but interpretation is subject to significant uncertainties. The data are used in ground-water models to evaluate potential waste-disposal sites, the effects of ground-water contamination, and to guide aquifer development, including geothermal reservoirs. The development of quantitative log-interpretation techniques to derive more accurate data and to evaluate the statistical uncertainty in the data will reduce costs in ground-water investigations.

OBJECTIVE: (1) Evaluate presently available logging equipment and log-interpretation techniques and develop improved instrumentation and analytical techniques for specific ground-water problems, such as site selection and monitoring for disposal of radioactive, municipal, and industrial wastes; (2) improve log-derived data such as porosity values; (3) attempt to relate the log character of fractures to their hydraulic conductivity and to refine computer techniques for plotting hydraulic conductivity profiles from logs; (4) develop the capability of making quantitative interpretation of borehole gamma spectra, and (5) make a statistical analysis of the magnitude and sources of errors in log-derived data.

APPROACH: Log selected drill holes with core analysis, hydraulic test data, and calibration pits and research the logs in both analog and digital form. Develop computer models to predict the behavior of gamma photons and acoustic energy in borehole environments. Compare field-log data, theoretical predictions and hydraulic tests, core analyses and test-pit values. On the basis of these comparisons, modify equipment, develop log corrections, and calculate the statistical accuracy of log data.

PROGRESS: A. E. Hess published a report describing the application of the heat-pulse flowmeter to the determination of fracture permeability in fractured granite. R. M. Morin published journal articles on fracture permeability characterization and aquifer heterogeneity. F. L. Paillet produced a review paper on the application of acoustic logging techniques to radioactive waste storage. The first journal article on the application of the heat-pulse flowmeter to fracture permeability characterization during a pump test was published and additional flowmeter data under ambient conditions were obtained at a Canadian crystalline rock research site. Extensive nuclear log-data were

obtained at the Cape Cod research site in Massachusetts; preliminary analysis suggested several specific improvements for future field work. Journal articles describing these results are being published. Development and additional tests of low-frequency acoustic sparker source were also conducted during the preceding year. Acoustic-waveform estimates of fracture permeability were compared to vertical seismic-profile data at a site near Mirror Lake, N.H.

REPORTS PUBLISHED:

Barrash, Warren, and Morin, R. H., 1986, Defining patterns of ground water and heat flow in fractured Brule Formation, Western Nebraska, using borehole geophysical methods: National Water Well Association Conference and Exposition, Denver, Colo., Proceedings, p. 545-569.

Morin, R. H., and Olsen, H. W., 1987, Theoretical analysis of the transient pressure response from a constant flow rate hydraulic conductivity test: Water Resources Research, v. 23, no. 8, p. 1461-1470.

Olsen, H. W., Morin, R. H., and Nichols, R., in press, Flow pump applications in triaxial testing: American Society of Testing and Materials Symposium on Advanced Triaxial Testing of Soil and Rock, Louisville, Ky., Proceedings.

Paillet, F. L., Morin, R. H., and Keys, W. S., 1986, Borehole geophysical applications in the characterization of geothermal energy resources: McKelvey Forum on Research in Energy Resources, Denver, Colo., 1986, Proceedings.

Paillet, F. L. and Hess, A. E., 1986, Geophysical well-log analysis of fractured crystalline rocks at East Bull Lake, Ontario, Canada: U.S. Geological Survey Water-Resources Investigations Report 86-4052, 37 p.

Paillet, F. L., Cheng, C. H., and Meredith, J. A., 1986, New applications in the inversion of acoustic full wave logs: Society of Professional Well Log Analysts Annual Logging Symposium, 27th, Houston, Tex., Transactions, p. VV1-VV25; Log Analyst, 1987.

Paillet, F. L., Hess, A. E., Cheng, C. H., and Hardin, E. L., 1986, Characterization of fracture permeability with high-resolution vertical flow measurements during borehole pumping: Ground Water, v. 25, no. 1, p. 28-40.

Paillet, F. L., Cheng, C. H., Hess, A. E., and Hardin, E. L., 1986, Comparison of fracture permeability estimates based on tube-wave generation in vertical seismic profiles, acoustic waveform log attenuation, and pumping test analysis: National Water Well Association Conference and Exposition, Denver, Colo., Proceedings, p. 398-416.

Paillet, F. L., Morin, R. H., Hodges, R. E., Robison, L. C., and others, 1986, Preliminary report on geophysical well-logging activity on the Salton Sea Scientific Drilling Project, Imperial Valley, Calif: U.S. Geological Survey Open-File Report 86-544, 99 p.

Paillet, F. L., and Kim, Kunsoo, 1986, Distribution and acoustic character of borehole wall breakouts in deeply buried basalt: Journal of Geophysical Research, v. 92, no. B-7, p. 6223-6234.

Taylor, T. A., 1986, Application of gamma spectral logging to ground-water investigations: National Water Well Association Conference and Exposition, Denver, Colo., 1987, Proceedings, p. 527-544.

CR191 SIMULATION OF SUBSURFACE-WATER FLOW

TITLE: Mathematical Simulation of Subsurface-Water Flow Using Uncertain and Incomplete Data

PROJECT NUMBER: CR 76-191

LOCATION: Topical Research

PROJECT CHIEF: Cooley, Richard L.

HEADQUARTERS OFFICE: Denver, CO

PROBLEM: Satisfactory formulations and solutions of equations approximately describing (1) movement of fluids and components contained in fluids through consolidated and unconsolidated rocks, and (2) interactions of the fluids and rocks accompanying fluid movement are needed for proper understanding and management of ground-water resources. Such formulations and solutions of equations that apply to general field situations, where the flow system is complex and hydrologic data are inexact, are not available in general.

OBJECTIVE: (1) Reformulate, where necessary, the equations describing the flow of fluids through porous or fractured rock to include stochastic processes, emphasizing equations that are suitable for field use; (2) derive techniques to solve for dependent variables and estimate parameters in the equations; (3) assess the degree of reliability and significance of both the model formed by the basic equations and the parameters estimated for it in terms of the input data; and (4) assess the degree of reliability and predictive capability of the model.

APPROACH: Develop fundamental equations using methods of mathematical physics, stochastic processes, and statistics, and basic physical concepts from geology, geochemistry, geophysics, and so forth. Develop solutions to the equations analytically or numerically, depending on the problem. Analyze error propagation, stability, and convergence using techniques of linear and nonlinear algebra where feasible and appropriate. Use techniques of nonlinear regression to estimate parameters so that the reliability and significance of estimated parameters and the predictive capability of the model can be assessed.

PROGRESS: (1) The finite-element model for two-dimensional and radial flow of ground water was completed and tested by R. L. Cooley. New features of the model include an accurate and efficient transient leakage method, ability to desaturate and resaturate nodes, an accurate and efficient method for storage conversions, nonlinear leakage functions, and a preconditioned conjugate-gradient matrix solver. Documentation is presently being completed. (2) Methods for efficiently computing exact simultaneous confidence and prediction intervals for dependent variables of nonlinear regression models, and

conservative simultaneous confidence and prediction intervals for hand-calibrated models that are nonlinear in the parameters were completed. Work is continuing on removing the approximation from the intervals for hand-calibrated models and deriving individual intervals for both nonlinear regression and hand-calibrated models. (3) Work on depth-averaging effects on hydraulic head for a medium with stochastic hydraulic conductivity was completed. The correlation structure of heads for a depth-averaged model and for a two-dimensional model are quite different. Work on the variance of hydraulic head in the presence of a constant-head boundary is nearing completion. (4) Estimation procedures for spatial random processes were refined and computer programs were revised by A. V. Vecchia to allow efficient estimation for large spatial data sets with irregularly spaced observations.

REPORTS PUBLISHED:

Cooley, R. L., Konikow, L. F., and Naff, R. L., 1986, Nonlinear-regression ground-water flow modeling of a deep regional aquifer system: Water Resources Research, v. 22, no. 13, p. 1759-1778.

Cooley, R. L. and Vecchia, A. V., 1987, Reliability analysis for ground water models--an approach through use of confidence and prediction intervals: National Water Well Association Conference, Denver, Colo., 1987, Proceedings, v. 1, p. 613-625.

Naff, R. L. and Vecchia, A. V., 1986, Stochastic analysis of three-dimensional flow in a bounded domain: Water Resources Research, v. 22, no. 5, p. 695-704.

Naff, R. L. and Vecchia, A. V., 1987, Depth-averaging effects on hydraulic head for media with stochastic hydraulic conductivity: Water Resources Research, v. 23, no. 4, p. 561-570.

CR200 UNSATURATED ZONE FIELD STUDIES

TITLE: Field Applications of Unsaturated Zone Flow Theory

PROJECT NUMBER: CR 69-200

LOCATION: Various States - in Colo., Kans., Nebr., Tex.

PROJECT CHIEF: Weeks, Edwin P.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Knowledge of flow through the unsaturated zone is needed to evaluate natural recharge and return flow from irrigation, and the impact of land-use changes on recharge and overland runoff. In addition, such knowledge is needed to evaluate water-management schemes involving artifical recharge and vegetation and water-table manipulation to increase water supply. Finally, unsaturated-flow theory is needed to evaluate pollution hazards from surface sources. Although much research has been done on unsaturated-flow phenomena, operational methods are lacking for many of the above problems.

OBJECTIVE: Develop and test methods for field measurement of hydraulic head, saturated and unsaturated hydraulic conductivity, and moisture content in the unsaturated zone. Develop and test an operational computer program for simulation of saturated-unsaturated flow phenomena on a structure-imitating basis for small-scale problems, and a more empirical watershed-type model for large-scale problems.

APPROACH: Test various methods for field determination of hydraulic parameters in the unsaturated zone at field experimental sites. Conduct experiments at these sites to test the simulation models being developed by the project staff.

PROGRESS: (1) Measurements of ET (evapotranspiration) from wildland vegetation in the San Luis valley were continued, and results to date suggest that previous estimates of potential ET salvage are too large by a substantial factor. Previous problems involving the measurement of net radiation, used in the ET measurements, were diagnosed and corrected. A new ET measurement technique, based only on net radiation and air-temperature variance, appears promising for routine measurements. (2) Measurement of convective airflow from two wells located at the crest of Yucca Mountain, Nev., and tapping unsaturated fractured rock continued, with flow-meter logs, temperature logs, and gas-composition profiles being obtained quarterly. Measurements indicate that this convective circulation results in a large net heat flux, on the order of 3 to 5 kilowatts from each well during winter conditions. However, currently hypothesized mechanisms for producing such flow appear to be inadequate to explain its magnitude and constancy of direction of the flow. (3) Documentation of the VS2D unsaturated flow computer code has been published. In addition, the code has been adapted to simulate trickle

irrigation, and that adaptation documented. (4) Background soil-moisture tension measurements at the Jackass Flat (Nevada Test Site) caisson site have been automated, and the background data collection continues.

REPORTS PUBLISHED:

Stannard, D. I., 1986, Theory, construction, and operation of simple tensiometers: Ground Water Monitoring Review, v. 6, no. 3, p. 70-78.

Weaver, H. L., Weeks, E. P., Campbell, G. S., Stannard, D. I., and Tanner, B. D., in press, Phreatophyte water use estimated by eddy-correlation methods: American Society Civil Engineers Water Forum, Long Beach, Calif., 1986, Proceedings.

CR292 SOLUTE-TRANSPORT SIMULATION

TITLE: Ground-Water Solute-Transport Simulation

PROJECT NUMBER: CR 85-292

LOCATION: Topical Research

PROJECT CHIEF: Kipp, Kenneth L.

HEADQUARTERS OFFICE: Denver, CO

PROBLEM: Ground-water solute-transport modeling is an important tool that aids in the analysis of ground-water contamination problems, both actual and potential. Accidental spills, leakage, and waste disposal operations can lead to ground-water contamination. The ability to analyze and predict the movement of solutes in ground-water systems is necessary to assess the effects of a contamination situation or properly design a waste-disposal operation. Modeling also is used to compare alternative strategies for aquifer reclamation. In some cases, the solute of interest is thermal energy. Heat-transport modeling is useful in analyzing geothermal systems, waste-heat storage systems, and some deep-aquifer systems.

OBJECTIVE: (1) Develop and apply new analytical, quasianalytical, and numerical techniques to the field of saturated ground-water solute-transport simulation modeling; (2) develop mathematical representations of solute porous-medium interactions and chemical reactions and develop and apply efficient algorithms for numerical calculation; and (3) apply analytical and numerical simulation modeling to field-scale situations, both actual and experimental.

APPROACH: Formulate transport equations for systems being studied, develop or adapt various methods for solving the equations, develop and test various algorithms for numerical computation or simulation calculations, and apply the methods to laboratory- or field-scale experiments and actual field situations. Work closely with District, Federal, and State research projects involved with similar studies.

PROGRESS: Testing the computer program of the new heat- and solute-transport simulation (HST3D) continued with application to a thermal injection field experiment and with cross-code comparison problems. The program documentation was published as a U.S. Geological Survey Water-Resources Investigations report. A preprocessing program was designed and partly written. The HST3D program was modified to simulate gas flow in porous media and applied to the investigation of topographically enhanced thermal circulation of the atmosphere within Yucca Mountain, Nev. Preliminary simulation of the ammonium and nitrate plumes at the Otis research site in Cape Cod, Mass., showed that additional data were necessary to understand the reactions taking place. A utility program that renumbers and reformats FORTRAN-77 routines

was completed. This program executes much faster than previous renumbering programs because the characterstring handling functions of FORTRAN-77 are employed. A post-processing program was written to create contour and vector plots of HST3D program output.

REPORTS PUBLISHED:

Kipp, K. L., Jr., 1987, A computer code for simulation of heat and solute transport in three-dimensional ground-water flow systems: Water-Resources Investigations Report 86-4095, 517 p.

Kipp, K. L., Jr., 1987, Preliminary one-dimensional simulation of ammonium and nitrate in the Cape Cod sewage plume, in U.S. Geological Survey Program on toxic waste ground-water contamination: U.S. Geological Survey Open-File Report 87-109, p. 45-46.

Kipp, K. L., Jr., in press, Effect of topography on gas flow in unsaturated fractured rock--numerical simulation, American Geophysical Union Fall meeting, San Francisco, Calif., 1987, Proceedings.

NR035 CRETACEOUS SHALE HYDROLOGY

TITLE: Hydrologic Behavior of Cretaceous Shales

PROJECT NUMBER: NR 81-035

LOCATION: Topical Research

PROJECT CHIEF: Neuzil, Christopher E.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Studies of the Dakota regional aquifer system suggest that the overlying Cretaceous shales that confine the aquifer are low in permeability. An understanding of the hydrologic behavior of these low permeability shales is important; the shale may be able to confine wastes for long periods of time. In addition, the behavior of aquifers and confining layers are interrelated closely. The hydraulic behavior of low permeability argillaceous-rock units is poorly understood. Basic data on properties such as hydraulic conductivity and specific storage generally are unavailable. Because hydrologic interest in these types of rocks is relatively recent, the techniques for determining these properties must be developed. The importance of secondary permeability, such as transmissive fractures, is unknown.

OBJECTIVE: Develop and use techniques to determine hydraulic properties of the shale at field sites and in the laboratory. Determine whether connected, transmissive fractures are present, and if present, determine their size, density, and distribution. Use the information obtained to (1) evaluate under what specific condition the thick Cretaceous shales of the midwestern United States can be used for waste disposal and (2) determine the significance of leakage to and from the aquifer through confining layers.

APPROACH: Complete the hydrologic model analysis of South Dakota as a prototype area for studying Cretaceous shales. Concurrently, begin a core drilling and in-situ testing program to obtain laboratory and field data on the permeability of Pierre Shale. Drill a series of four shallow holes strategically located to sample the entire stratigraphic sequence of Cretaceous shales above the Dakota aquifer. Drill additional holes as required to investigate transmissive fractures. Conduct laboratory work, model development, and model analysis concurrently, interrelating laboratory experiments, fieldwork, and model analysis. Based on measured permeabilities, make an analysis of jointing and fracturing that will account for the permeabilities. Coordinate activities with Geologic Division research on rock-mechanics problems and factors affecting nuclide transport.

PROGRESS: Analysis of flow in sediments undergoing burial and heating has demonstrated that interaction between flow and sediment deformation in these systems can be much more complex than previously believed. Distinct nonlinearities and discontinuities appear when realistic descriptions of matrix strain are used. These properties (1) impart a "memory" of system history in its flow behavior, (2) can produce cyclical pressure and stress changes from a negative feedback phenomenon, and (3) limit ability of pressure-producing mechanisms to reduce effective stress and hydrofracture the medium. An in-situ experiment to study coupled (water-ions) fluxes in the Pierre Shale was begun in four boreholes in October 1986. Data are being collected showing a diffusive flux of ions and osmotic flux of water between boreholes and shale. A thermal "slug" test was completed in Pierre Shale, permitting computation of the shale's in-situ thermal conductivity. Precision measurements of the shale's thermal gradient also were completed and suggest a temperature transient at ground surface in the last 2 to 3 centuries.

REPORTS PUBLISHED:

Neuzil, C. E., 1986, Ground-water flow in low permeability environments: Water Resources Research, v. 22, no. 8, p. 1163-1195.

NR089 SUBSURFACE TRANSPORT PHENOMENA

TITLE: Investigations of Single and Multiphase Fluid Flow, Mass and Energy Transport, and Fluid Phase Change in the Subsurface Environment

PROJECT NUMBER: NR 78-089

LOCATION: Topical research

PROJECT CHIEF: Voss, Clifford I.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: The subsurface environment is subject to both natural and human imposed stresses, the interaction of which determines both its preservation and its employment as a multifaceted natural resource for water supply, energy production, and subsurface storage of energy and materials. Subsurface problems of current interest include: geothermal-energy development, thermal- and mechanical-energy storage in aquifers and tunnels, radioactive-waste isolation, ground-water development in permafrost regions, oil pollution of ground water, and saltwater encroachment in aquifers. Study of these various problems is unified by the theoretical framework of the physics of single and multiphase fluid flow, mass and energy transport, and fluid-phase change as applied to the subsurface environment.

OBJECTIVE: Develop quantitative methods for analysis of systems in the subsurface environment involving single and multiphase fluid flow, mass and energy transport, and fluid phase change. Apply these methods to field problems to illuminate hydrological relationships that are important in both the preservation and optimal employment of the subsurface.

APPROACH: Develop a mathematical description of the system based on the relevant single or multiphase flow, transport, and phase-change processes. Study system behavior using analytical and numerical solutions of the mathematical description based on either hypothetical or field conditions. Models and analytical methods for general classes of subsurface problems are by-products of the investigations.

PROGRESS: A family of finite-element simulation models for analysis of broad classes of subsurface fluid flow and transport processes has been developed (SUTRA, SATRA, SATRA-CHEM). These models simulate subsets of saturated-unsaturated variable-density ground-water flow with single or multi-species reactive-solute transport or thermal-energy transport in two spatial dimensions. New developments in nonlinear optimization methodology were implemented in a coupled simulation-optimization computer program that has been applied to management of solute-transport problems in aquifers and to identification of aquifer transport parameters. Further methods have been developed for estimating parameter values and identifying significant

processes, boundary conditions, and flow geometries in one-dimensional solute transport from field data. Results allow optimal network design for parameter estimation and transport model identification. Variable-density flow and solute-transport simulation models have been applied to a number of difficult problems involving saltwater intrusion with narrow transition zones, flow near salt domes, and natural fluid convection in aquifers.

REPORTS PUBLISHED:

Knopman, D. S., and Voss, C. I., 1987, Behavior of sensitivities in the one-dimensional advection-dispersion equation--Implications for parameter estimation and sampling design: Water Resources Research, v. 23, no. 2, p. 253-272.

Miller, R. T., and Voss, C. I, 1986, Finite-difference grid for doublet well in an anisotropic aquifer: Ground Water, v. 24, no. 4, p. 490-496.

Souza, W. R., and Voss, C. I., 1986, Modeling a regional aquifer containing a narrow transition between freshwater and saltwater using solute-transport simulation--Part II, analysis of a coastal aquifer system, in Boekelman, R. H., and others, eds., 9th Salt Water Intrusion Meeting: Delft University of Technology, Delft, The Netherlands, 1986, Proceedings, p. 457-473.

Voss, C. I., and Souza, W. R., 1986, Modeling a regional aquifer containing a narrow transition between freshwater and saltwater using solute transport simulation--Part I, theory and methods: in Boekelman, R. H., and others, eds., 9th Salt Water Intrusion Meeting: Delft, The Netherlands, Delft University of Technology, p. 493-514.

NR120 TRANSPORT MODELING -- SATURATED ZONE

TITLE: Digital Modeling of Transport in the Saturated Zone

PROJECT NUMBER: NR 81-120

LOCATION: Topical Research

PROJECT CHIEF: Konikow, Leonard F.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Management of ground-water resources requires that the extent and rate of movement of contaminants in the saturated and unsaturated zones be understood. The contaminants have been and will continue to be both accidentally and deliberately introduced into ground-water systems. Some of these contaminants constitute very hazardous conditions. Because of the immediacy of such contamination problems, understanding of the physical and chemical processes needs to be increased rapidly, and mathematical models derived from this understanding validated and documented.

OBJECTIVE: Investigate the parameters in basic mathematical transport models developed for ground-water systems to increase understanding of the factors influencing these parameters and of the interrelation between parameters. Derive appropriate two-dimensional and three-dimensional mathematical models to describe contaminant movement in complex field situations, including the unsaturated zone. Study the appropriate computer algorithms used to approximate the numerical solution to the transport equations.

APPROACH: Develop numerical models, emphasizing those ground-water systems and contaminants for which transport model needs seem most critical. This emphasis will dictate the order in which particular models are initiated. Evaluate the accuracy and efficiency of new and existing modeling techniques through comparisons with analytical solutions, other numerical methods, and observed data from practical field problems.

PROGRESS: The potential for porosity development and permeability enhancement in coastal carbonate rocks by the dissolution of calcite in the freshwater-saltwater mixing zone was analyzed by coupling results from the chemical-reaction computer model PHREEQE with a variable-density ground-water flow and solute-transport model. Results show that the process is controlled primarily by equilibrium chemistry and ground-water velocity. Porosity develops mostly at the tip and toe of the mixing zone on the freshwater side of the interface. This asymmetric dissolution causes a landward migration of the interface. Several new modifications to the MOC solute-transport computer model have been documented. These include the options to use SIP or D4 algorithms to solve the flow equation.

REPORTS PUBLISHED:

Konikow, L. F., 1986, Predictive accuracy of a ground-water model--lessons from a postaudit: Ground Water, v. 24, no. 2, p. 173-184.

Person, M. A., and Konikow, L. F., 1986, Recalibration and predictive reliability of a solute-transport model of an irrigated stream-aquifer system: Journal of Hydrology, v. 87, p. 145-165.

Konikow, L. F., and Person, M. A., 1986, Influence of irrigation on salinity and nitrate in a stream-aquifer system: International Association of Hydrologic Sciences Publication no. 156, p. 217-229.

Cooley, R. L., Konikow, L. F., and Naff, R. L., 1986, Nonlinear-regression modeling of a deep regional aquifer system: Water Resources Research, v. 22, no. 13, p. 1759-1778.

NR130 SURFACE GEOPHYSICS AND HYDROLOGY

TITLE: Development of Surface Geophysical Methods and Applications to Ground-Water Hydrology

PROJECT NUMBER: NR 84-130

LOCATION: Topical Research

PROJECT CHIEF: Brown, Charles E.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Ground-water investigations require the definition of the geologic nature and hydraulic properties of media that store and transmit ground water. With recent regulations regarding ground-water contamination and disposal of toxic wastes, methods need to be calibrated for monitoring and detecting waste products and leachates around landfills and storage lagoons. Surface-geophysical methods offer a means of quickly detecting and measuring characteristics of geologic media and fluids.

OBJECTIVE: (1) Apply and extend theory and methods underlying the use of a variety of surface geophysical techniques and develop new theoretical and field models, and interpretive techniques; (2) test and demonstrate the effectiveness of geophysical techniques in practical field applications and as monitoring tools; (3) evaluate the limitations of the electromagnetic, electrical resistivity, gravity, and magnetic methods in hydrologic studies using statistical techniques and error analysis; and (4) improve existing techniques and (or) devise new techniques as required.

APPROACH: Evaluate and improve existing quantitative methods and develop new techniques for analysis of hydrogeologic systems using higher mathematics, statistics, geophysical models, and carefully designed field studies. Emphasize techniques having immediate applications for needs established during current field studies. About 50 percent of this effort will be spent in the development and calibration of methods, and about 50 percent in field testing existing techniques and instrumentation and quantitatively ascertaining limitations of methods. Complete comprehensive literature survey.

PROGRESS: Water-quality data for the Delmarva Peninsula (Delaware, Maryland, and Virginia) have been compiled and summary statistics for key chemical variables have been studied.

REPORTS PUBLISHED:

Brown, C. E., 1986, Determination of rock properties by borehole-geophysical and physical-testing techniques, and ground-water quality and movement in the Durham Triassic basin, North Carolina: U.S. Geological Survey Professional Paper 1432, 86 p.

Brown, C. E., 1987, Modeling and analysis of direct-current electrical resistivity in the Durham Triassic Basin, North Carolina: Geoexploration, v. 24, p. 429-440.

NR134 TRANSPORT IN FRACTURED ROCK

TITLE: Transport Phenomena in Fractured Rock

PROJECT NUMBER: NR 84-134

LOCATION: Topical Research

PROJECT CHIEF: Shapiro, Allen M.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: There has been an increasing awareness that, in many circumstances, the theories associated with the description of hydrogeologic phenomena in granular porous media are unacceptable in the description of these same phenomena in fractured rock and geologic formations having similar characteristics. Because of the wide extent that fractured formations naturally occur and have been used for various purposes by humans, including proposed repositories for radioactive waste, a need exists to describe and better understand the physics of fluid movement, deformation, contaminant migration, and energy transport under the broad range of physical situations where fractured formations exist.

OBJECTIVE: Develop mathematical models of transport phenomena in fractured rock. Because the description of fractured rock is highly dependent on scale of observation, use alternative conceptualizations of the medium in the development of these models. Investigate the parameters that arise, and evaluate physical situations where each conceptualization is applicable and the adaptability of field measurements to these conceptualizations.

APPROACH: Consider fractured rock and similar formations as a series of discrete fractures, and also in various continuum conceptualizations. Develop mathematical models of transport phenomena. Use hypothetical physical situations and later, if possible, field data and field investigations to examine the applicability of these model conceptualizations and the adaptability of field measurements to these conceptualizations.

PROGRESS: Field testing of a fractured dolomite beneath a low-level radioactive-waste disposal site southwest of Chicago, Ill., was continued. The drilling and coring of three new boreholes was completed, bringing the total to seven boreholes distributed spatially over the study area. Laboratory testing of the dolomite cores was conducted to determine permeability and porosity of the rock matrix. Geophysical logging was conducted on the new boreholes to further support hypotheses concerning the lithologic character and fracture geometry in the dolomite. Hydraulic testing of one of the subhorizontal fractures indicated that a hydraulic connection within that fracture exists between all boreholes. Tracer tests also were conducted in an individual subhorizontal fracture to determine transport properties. Thermal profiles of the boreholes were taken under natural and hydraulically stressed

conditions to assess the presence of vertical fracturing; the thermal profiles indicate a possibility of vertical fracturing between two boreholes. A method of assessing the statistical properties of the fracture aperture using field-scale hydraulic and tracer tests has been developed and will be tested using the hydraulic and tracer-test data that were collected at the field site. In a related topic, research on a stochastic description of three-dimensional contaminant movement in heterogeneous porous media also was continued. A method was developed for analyzing the uncertainty associated with the contaminant arrival time at a given location based on a stochastic description of porous medium properties, such as the hydraulic conductivity and the effective porosity.

REPORTS PUBLISHED:

Silliman, S., Nicholas, J., and Shapiro, A. M., 1987, Estimating fracture connectivity using measurements of borehole temperatures during pumping: National Water Well Association Conference, Indianapolis, Ind., 1987, Proceedings, p. 231-248.

WR024 INFILTRATION AND DRAINAGE

TITLE: Application of the Unsaturated Flow Theory to the Phenomena of Infiltration and Drainage

PROJECT NUMBER: WR 63-024

LOCATION: Topical Research

PROJECT CHIEF: Rubin, Jacob

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Surface runoff and various ground-water processes often are influenced significantly by water flow through the unsaturated zone. For many situations of hydrologic interest, inadequate knowledge prevents these influences from being taken properly into account in water-resources analyses.

OBJECTIVE: Critically test present theories of water flow through the unsaturated porous media, and in particular theories of infiltration and drainage. Use these theories to develop experimental techniques that will enhance studies of ground water, runoff, and other hydrologic problems in the unsaturated zone. Study unsaturated zones of various environments, especially deep unsaturated zones in the field, to measure their natural water rates, and explain these rates in terms of soil, plant, and atmospheric conditions. Use the results of such studies for the assessment of possible movement of wastes, including radioactive wastes, towards ground water.

APPROACH: Test the validity and accuracy of present predictive theories of water flow through unsaturated porous media experimentally in laboratory. Devise improved laboratory and field methods to measure such flows and to evaluate the flow-determining characteristics of soils and sediments. Use these methods and the unsaturated-flow theory for field studies of flow rates of unsaturated-zone water in settings relevant to hydrologic problems involving ground-water recharge, surface-runoff formation, or movement of radioactive and chemical pollutants.

PROGRESS: A study on the influence of soil compaction on the water permeability and pore-size-distribution curves of a sandy soil was completed. Under unsaturated conditions, this influence depends less on soil density than on the nature of the compaction process (vertical-drop impacts of air-dry soil columns versus moist-soil centrifugation). To increase versatility of the previously developed, steady-state centrifuge method (SSCM) for measuring unsaturated permeabilities, the centrifuge and the SSCM apparatus was modified, making it possible to carry out electrical measurements within soil columns during centrifugation. The modified instrumentation can determine essential soil-water parameters during SSCM measurements. A field study using SSCM to determine vertical, ground-water-recharging fluxes in deep unsaturated zones was started. The initial test involves the unsaturated zone

below an intermittent stream in California's Central Valley. SSCM was used to determine the unsaturated permeabilities of undisturbed soil cores. Four codetermined parametric functions that govern water and air flow in unsaturated soils were compared. The study: (1) firmly establishes trapped-air contents as monotonic functions of water content, functions that probably form a hysteretic family; (2) reveals a number of contrasting features of water and air permeabilities; and (3) suggests a basic reason for the contrasts. Results obtained strongly suggest that ephemeral, microscale water blockages play an important role in air permeability and air trapping. Hence, the connectivity of pores filled by a given fluid as well as capillary phenomena must be taken into account by the microscopic theories of the four macroscopic functions studied.

REPORTS PUBLISHED:

Nimmo, J. R., and Miller, E. E., 1986, The temperature dependence of isothermal moisture vs. potential characteristics of soil: Soil Science Society of America Journal, v. 50, no. 5, p. 1105-1113.

Nimmo, J. R., Rubin, Jacob, and Hammermeister, D. P., 1987, Unsaturated flow in a centrifugal field--measurement of hydraulic conductivity and testing Darcy's law: Water Resources Research, v. 23, no. 1, p. 124-134.

Rubin, Jacob, Nimmo, J. R., and Hammermeister, D. P., 1987, Method and apparatus for steady-state measurement of liquid conductivity in porous media: U.S. Patent, temporary no. 901,360.

WR082 NEVADA GEOTHERMAL

TITLE: Hydrologic Reconnaissance of Geothermal Areas in Nevada and California; Geohydrology of Geothermal Areas in Nevada

PROJECT NUMBER: WR 72-082

LOCATION: California and Nevada

PROJECT CHIEF: Olmsted, Franklin H.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Geothermal energy is receiving attention as a source for electricity and for various nonelectrical uses. Optimum development of the resource must be preceded by a rational program of exploration and evaluation. Improved understanding is needed of conditions that control the occurrence of hydrothermal convection systems in the Basin and Range physiographic province of the western United States. Such understanding will greatly aid evaluation of known systems and prediction of the occurrence of hitherto unknown systems.

OBJECTIVE: Develop and evaluate geohydrologic-reconnaissance techniques chiefly related to shallow-test drilling, to explore the following geothermal areas in northern and central Nevada: (1) Beowawe; (2) southern Grass Valley (Leach Hot Springs area); (3) Stillwater (eastern Carson Desert); (4) western Carson Desert; and (5) Bradys Hot Springs. For each area, describe the hydrologic environment; determine the most probable recharge areas and ground-water flow paths; interpret geologic, geochemical, geophysical, thermal, and hydrodynamic information in terms of the configuration of the hydrothermal reservoir and its hydrologic properties; provide the basis for analytical or numerical modeling studies of the reservoir and the associated hydrothermal-flow systems; and evaluate the utility of shallow-exploration techniques, such as measurement of temperature at 1 meter depth, in delineating a prospective geothermal area.

APPROACH: (1) Review literature and canvass public agencies and private companies for available hydrologic data; catalog available data and prepare a tabular summary of deficiencies; (2) in collaboration with geologists and geochemists who will be making companion studies, select geothermal areas to be studied; (3) inventory wells and springs, measure the discharge of flowing wells and springs and of streams into which these drain, and compile precipitation and runoff data pertinent to ascertaining areas and magnitude of recharge; compilation of geologic data may be required where the recharge area for a system is inferred to be far from the discharge area; (4) assist in sampling water sources for chemical analysis; sample selected wells and springs for carbon, oxygen, and hydrogen isotopes where required for hydrologic analysis; (5) design and carry out a program of shallow-test drilling for supplementary data; (6) prepare geohydrologic maps and cross sections of several kinds from information gathered in activities 3, 4, and 5 listed

above; and (7) develop conceptual models of the flow systems in collaboration with personnel of Geologic and Water Resources Divisions, using results of geologic, geochemical, geophysical, thermal, and hydrodynamic studies.

PROGRESS: Substantial progress was made on two final reports that will finish work on this project. The first report is a revision of a 1981 open-file report on the geothermal system of southern Grass Valley, south of Winnemucca, Nev. Geologic, hydrologic, geophysical, and geochemical data are used to derive an internally consistent model of the system. The second report will summarize knowledge about the geothermal resources of the Carson Desert area in west-central Nevada. The objectives of the study are to: (1) relate the geothermal hydrology to the hydrology of the Carson Desert area as a whole; (2) characterize the several known hydrothermal convection systems; (3) determine the predevelopment flux of heat and fluid through the systems, both before and after development.

REPORT PUBLISHED:

Olmsted, F. H., Welch, A. H., and Ingebritsen, S. E., 1986, Shallow subsurface temperature surveys in the Basin and Range province, U.S.A.--(I) Review and evaluation: Geothermics, v. 15, no. 3, p. 251-265.

Olmsted, F. H., and Ingebritsen, S. E., 1986, Shallow subsurface temperature surveys in the Basin and Range province, U.S.A.--(II) Ground temperatures in the Upsal Hogback geothermal area, west-central Nevada: Geothermics, v. 15, no. 3, p. 267-275.

WR102 MODELING GEOTHERMAL SYSTEMS

TITLE: Modeling Heat and Fluid Flow in Geothermal Systems

PROJECT NUMBER: WR 73-102

LOCATION: Topical Research

PROJECT CHIEF: Sorey, Michael L.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Analysis of heat and fluid flow in geothermal systems is needed to test the adequacy of alternative conceptual models of the natural state of such systems and the effects of fluid production for energy development on related hydrologic features, such as hot springs and geysers. In addition, because geothermal systems commonly occur in regions of active volcanism and seismicity, analysis of changes in such systems can provide precursory evidence of future eruptions and earthquakes.

OBJECTIVE: Elucidate the processes involved in the evolution of geothermal systems in areas of active volcanism with shallow magmatic heat sources and the implications for existence of viable geothermal reservoirs. Quantify the effects of geothermal energy development on naturally occurring thermal discharge features. Collect and analyze data on changes in the geothermal system in Long Valley caldera, Calif., caused by ongoing magmatic and tectonic processes to provide warnings of future eruptive activity.

APPROACH: Apply numerical simulators describing heat and fluid flow in three-dimensional porous media with multiphase (steam and water) fluid to quantify the conditions under which geothermal systems in areas of active volcanism could evolve. Specific areas to be studied include Lassen Volcanic National Park, Calif. Valles caldera, (NM), and Long Valley caldera, Calif. After the development of satisfactory models of the natural state of hydrothermal activity in these systems, carry out numerical simulation of the effects of fluid withdrawal for energy development to assess the impacts on related hot springs and fumaroles. At Long Valley, monitor and analyze changes in thermal discharge and pressures and temperatures in wells for evidence of renewed magmatic activity and possible volcanic eruptions.

PROGRESS: In collaboration with the California District, two interpretive reports on changes in the hydrothermal system related to earthquakes and magmatic intrusions in Long Valley caldera, Calif., were published. Two workshops on hydrologic and geochemical monitoring were organized and a 2400-foot core hole was drilled and tested. Results of the Lassen Park, Calif., work include preparation of an Environmental Impact Statement (EIS) for geothermal leasing and collection and analysis of 4 years of data on variations in hot spring and steam discharge from thermal areas in and around the park.

REPORTS PUBLISHED:

Sorey, M. L., Farrar, C. D., and Wollenberg, H. A., 1986, Proceedings of the Second Workshop on hydrologic and geochemical monitoring in the Long Valley caldera: Lawrence Berkeley Laboratory Report LBL-22852, 80 p.

Ingebritsen, S. E., and Sorey, M. L., 1987, Conceptual models for the Lassen hydrothermal system: Geothermal Resources Council Bulletin, February 1987, p. 3-9.

Farrar, C. D., Sorey, M. L., Rojstaczer, S. A., Janik, C. J., Winnett, T. L., and Clark, M. D., in press, Hydrologic and geochemical monitoring in Long Valley caldera, Mono County, Calif., 1985: U.S. Geological Survey Water-Resources Investigations Report 87-4090.

WR108 GEOTHERMAL COORDINATION

TITLE: Technical Coordination and Support of WRD Geothermal Studies

PROJECT NUMBER: WR 00-108

LOCATION: Menlo Park, California

PROJECT CHIEF: Olmsted, Franklin H.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Geothermal studies in the Water Resources Division (WRD) are part of a nationwide research and mapping program of the Geological Survey. These studies require planning, coordination, technical surveillance, and logistical support.

OBJECTIVE: Provide planning, technical surveillance, coordination, and logistical support services to WRD geothermal investigations.

APPROACH: Plan, arrange for staffing, approve budgets, maintain technical surveillance and advise the Chief Hydrologist on the geothermal program. Review needs for test drilling and other logistical support as work progresses, and make necessary support funds available.

PROGRESS: The WRD Geothermal Studies Coordinator continued his activities of coordinating geothermal research in WRD with that of other divisions in the U.S. Geological Survey and with that of other Federal agencies. The WRD research projects, treating principles, processes, and specific geothermal systems, were continued over a wide range of subject areas and in diverse geographic areas. Support was given to several projects, funded in part under geothermal program, for purchase of equipment, contracts, and other miscellaneous activities.

WR121 HEAT AND MASS TRANSPORT--CASCADES

TITLE: Hydrologic Studies of Heat and Mass Transport in the Cascades

PROJECT NUMBER: WR 74-121

LOCATION: Oregon and California Cascades

PROJECT CHIEF: Olmsted, Franklin H.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: The U.S. Geological Survey has assumed much of the responsibility for making reconnaissance surveys as a first step in the the exploration and evaluation of known geothermal resource areas. High-temperature igneous-related geothermal resources are known to exist in the Cascade Mountain Range, but the magnitude of these resources is unknown. To evaluate the most promising areas, it will be necessary to develop quantitative conceptual models of the Cascades hydrothermal systems, using the information provided by concurrent geologic, geochemical, and geophysical studies.

OBJECTIVE: (1) Describe the hydrologic environments of several identified but unevaluated hydrothermal systems in the Oregon and California Cascades Mountain Range; (2) ascertain probable recharge and discharge areas; (3) determine modes and quantities of recharge and discharge; (4) interpret geologic, geochemical, and geophysical data in terms of the size, shape, and hydraulic characteristics of hydrothermal systems; and (5) use analytical and numerical modeling techniques to develop quantitative conceptual models of various systems.

APPROACH: (1) In collaboration with geologists, geochemists, and geophysicists making concurrent studies, select specific areas to be studied; (2) collect and tabulate available hydrologic data from the literature and from the files of public and private agencies; (3) supplement deficient data by field inventory, measurement, and sampling; and (4) develop quantitative conceptual models. If available modeling methods are found to be inadequate in dealing with supercritical temperatures, vapor-dominated conditions, transport in fractured media, the presence of noncondensable gases, and other potentially important factors, improve existing methods.

PROGRESS: A program of geophysical, geochemical, and hydrologic data collection in the hot spring areas on the west side of the central Oregon Cascades was completed. A digital data base is being developed. An analysis of flow-test data from a drill hole at Newberry Volcano, Oreg., and a modeling study of Newberry Volcano were completed. Additional work on vapor-dominated zones was done. A series of talks on work in the Cascades and on vapor-dominated zones was given in Japan during November 1986. Also, a version of a single-phase geothermal simulator was developed in which carbon dioxide, rather than water, is the working fluid.

WRD FEDERAL RESEARCH PROJECTS.....GROUND-WATER HYDROLOGY

REPORTS PUBLISHED:

Ingebritsen, S. E., in press, Vapor-dominated zones within hydrothermal convection systems: Twelth Workshop on Geothermal Reservoir Engineering, Stanford University, Palo Alto, Calif., Proceedings.

Ingebritsen, S. E., Carothers, W. W., Mariner, R. H., Gudmundsson, J. S., and Sammel, E. A., 1986, Flow testing of the Newberry 2 research drill hole, Newberry Volcano, Oreg.: U.S. Geological Survey Water-Resources Investigations Report, 86-4133, 23 p.

WR127 ENERGY TRANSPORT IN GW

TITLE: Mathematical Modeling of Energy Transport in Multiphase Ground-Water Systems

PROJECT NUMBER: WR 75-127

LOCATION: Nationwide

PROJECT CHIEF: Moench, Allen F.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Subsurface formations serve as conduits, barriers, and reservoirs for water and heat energy. Meteoric water percolates through openings in the rock and exchanges heat with its environment as it moves. The physics involved in the simultaneous transfer of mass and heat in porous or fractured rock under multiphase conditions needs further study so that it can be effectively applied to the use of ground water and geothermal energy.

OBJECTIVE: Predict temperature and pressure distributions in single-phase and multiphase ground-water systems under normal and stressed conditions. Determine rates of water and heat movement in subsurface formations under natural and stressed conditions. Test equations developed for physical work.

APPROACH: Simulate field and laboratory data on transient pressure and temperature by numerical and analytical techniques. Develop and modify controlling equation to account for the physical processes that occur in earth materials. Develop models using laboratory results. Use field data for case studies.

PROGRESS: New analytical solutions that can be used to evaluate aquifer dispersive and adsorptive properties in homogeneous and in double-porosity formations have been developed. These solutions were derived in the Laplace domain for inversion by numerical techniques. The solutions involve tracers either introduced in an injection well and observed in another well, or introduced in one well and observed in a nearby pumping well. A paper was presented at the 1986 American Geophysical Union Annual Fall Meeting in San Francisco that involved radial dispersion from a large-diameter injection well and a paper was presented at the 1987 Annual Workshop on Geothermal Reservoir Engineering at Stanford that involved radial dispersion in a double-porosity formation with diffusion in sphere-shaped blocks with fracture skin.

WR171 HYDROLOGIC ANALYSIS OF PETROFABRICS

TITLE: Hydrologic Analysis of Petrofabrics--Sandstones

PROJECT NUMBER: WR 76-171

LOCATION: Topical Research

PROJECT CHIEF: Getzen, Rufus T.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Techniques for analyzing ground-water flow and for predicting the response of ground-water systems to natural and human-made stresses require quantitative descriptions of spatial variation in permeability. New techniques for three-dimensional simulation of ground-water flow and solute transport require detailed quantitative descriptions of dispersion characteristics and the permeability tensor that are difficult and expensive to obtain with current measurement techniques.

OBJECTIVE: (1) Determine the geologic factors affecting ground-water flow and the transport of heat and solutes in porous media; (2) develop methods for estimating the relative importance of these geologic factors in various geologic settings and under various stress conditions; and (3) develop simple and inexpensive methods for measuring the requisite geologic factors and for estimating the dispersion characteristics and permeability tensor from them.

APPROACH: Develop and test methods of field samples since sand-body geometry and the permeability tensor within a sand-body are related to the fabric of the deposits. Use trend analysis, multivariate correlation and regression, and other statistical techniques to relate sandbody geometry and permeability tensor to petrofabric. Use sensitivity analyses, including digital simulation, to determine the degree of accuracy for permeability and dispersion measurements required for adequate analyses under various conditions of stress and in various geologic settings.

PROGRESS: More than 90 percent of the manpower has been directed toward designing a data-acquisition system for the Nuclear Hydrology Program. That effort has produced a design for a 4000-channel instrumentation/data-acquisition system (I/DAS) that is well on its way to completion. When implemented, the I/DAS will economically produce laboratory-quality hydrologic measurements in the unsaturated ground-water zone that are fully verified and documented, while operating in a desert environment.

WR176 WELLS-STRAIN METERS

TITLE: Water Wells as Strain Meters

PROJECT NUMBER: WR 75-176

LOCATION: Topical Research

PROJECT CHIEF: Bredehoeft, John D.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Water wells commonly show earth-tide fluctuations. Often the magnitude of the tidal fluctuation in the well is 1 to 2 centimeters. This fluctuation is produced by a tidal dilatation, the sum of the normal strains, of approximately 1×10^{-8}. This indicates that the water well is as sensitive to strains of the crust as the strain seismometer. The problem with the water well is that other factors such as changes in barometric pressure, aquifer recharge, and pumping also can cause the water-level to fluctuate. Using the well for crustal-strain measurements requires that the strain response (the signal) be separated from other effects like noise. Careful experiments need to be conducted in areas where the crustal strain is known.

OBJECTIVE: Use water wells as crustal-strain indicators.

APPROACH: Instrument a set of wells along the San Andreas fault in California and in the Palmdale area for the express purpose of sensing crustal strains. Increase the network with improved instrumentation that uses satellite telemetering of the data.

PROGRESS: Real-time monitoring in seven wells in the Parkfield area along the San Andreas fault in California was continued. Tidal frequency analysis was completed on the data from each site in an effort: (1) to demonstrate that we are observing earth tide responses; and (2) in an effort to develop procedures to filter barometric and tidal effects. Removing both earth tides and barometric fluctuations makes it possible to observe crustal dilatation at a level of approximately 10^{-9} to perhaps 10^{-10}. Real-time programs to process and filter the data have been developed and installed on the Water Resources Division Prime computer in Menlo Park, Calif.

REPORTS PUBLISHED:

Belitz, K., and Bredehoeft, J. D., 1986, Comment on safe disposal of toxic radioactive liquid wastes by J. S. Bradley: Geology, March, p. 266-267.

Djevanshir, R. D., and Bredehoeft, J. D., 1985, Mathematical analysis of lateral fluid filtration and pore pressure development in compacting sandy-clayey sediments: Izvestiia: Academy of Sciences of Azerbaijan SSR, Earth Sciences Series, no. 2, p. 93-104.

Essaid, H. I., 1986, A comparison of the coupled freshwater-saltwater flow and the Ghyben-Herzberg sharp interface approaches to modeling of transient behavior in coastal aquifer systems: Journal of Hydrology, v. 86, p. 169-193.

Roeloffs, E., and Bredehoeft, J. D., 1986, Possible role of fluid injection--fluid pressure changes in epicentral area and conclusions, in Wesson, R. L., and Nicholson, C., eds., Studies of the January 31, 1986, northeastern Ohio earthquake: U.S. Geological Survey Open-File Report 86-331, p. 20-23.

Roeloffs, E., Nicholson, C., Wesson, R. L., and Bredehoeft, J. D., 1986, Possible role of fluid injection--estimation of the state of stress, in Wesson, R. L., and Nicholson, C., eds., Studies of the January 31, 1986, northeastern Ohio earthquake: U.S. Geological Survey Open-File Report 86-331, p. 15-19.

WR178 MODELS FOR GW MANAGEMENT

TITLE: Models for Ground-water Management

PROJECT NUMBER: WR 82-178

LOCATION: Topical Research

PROJECT CHIEF: Gorelick, Steven M.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Human activities influencing ground-water systems need to be properly managed. Ground-water hydraulic, solute, and thermal transport models often are used to explore aquifer-management options. Generally, models are executed repeatedly under different management scenarios and the results compared. Using such an approach often avoids rigorous formulation of ground-water management objectives and fails to consider important physical and operational restrictions. It is unlikely that optimal management alternatives will be discovered using simulation techniques alone.

OBJECTIVE: Develop techniques that unify ground-water models with management-optimization methods for studying aquifer-management options. Explore capabilities and limitations of various combined simulation and optimization methods.

APPROACH: Develop techniques for optimizing aquifer management by joining numerical-simulation techniques with optimization methods of mathematical programming and statistics. Develop linear management formulations amenable to the set of available optimization methods; problem linearization or decomposition may be required. Include models as constraints in the optimization models; these constraints will be in the context of other physical and operational restrictions.

PROGRESS: A methodology for parameter estimation in advective-dispersive systems was developed and published. The general problem of ground-water contamination control under uncertainty was investigated. Two approaches were developed: one that deals with the problem of spatially variable hydraulic conductivities, the other employs simulation-regression-stochastic programming. Three technical papers were prepared for publication on the above topics.

REPORTS PUBLISHED:

Gorelick, S. M., 1987, Sensitivity analysis of optimal ground-water contaminant capture curves--Spatial variability and robust solutions: National Water Well Association Conference, Denver, Colo., 1987, Proceedings, p. 133-146.

Gorelick, S. M., and Umari, A. M. J., 1986, Evaluation of the matrix exponential for use in ground-water flow and solute-transport simulations--theoretical framework: U.S. Geological Survey Water-Resources Investigations Report 86-4096, 33 p.

Lefkoff, L. J., and Gorelick, S. M., 1986, Design and cost analysis of rapid aquifer restoration systems using flow simulation and quadratic programming: Ground Water, v. 24, no. 6, p. 777-790.

Wagner, B. J., and Gorelick, S. M., 1986, A statistical methodology for estimating transport parameters--theory and application to one-dimensional advective-dispersive systems: Water Resources Research, v. 22, no. 8, p. 1303-1316.

WR179 NONISOTHERMAL MULTIPHASE FLOW

TITLE: Nonisothermal Multiphase Flow

PROJECT NUMBER: WR 82-179

LOCATION: Topical Research

PROJECT CHIEF: Herkelrath, William N.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Water plays an important role in the movement of energy and mass near the earth's surface. To describe the transport process in porous materials, the interactions between the fluid in its liquid and vapor state with the granular materials must be understood. The effects of phase change and two-phase flow upon transport processes also are important. The interactions are documented to some degree for low temperature, low pressure fluid. However, documentation at high temperatures and high pressures is needed for geothermal applications and at high temperatures for nuclear waste applications. Very little information is available.

OBJECTIVE: Determine the adequacy of the present limited description of the mechanism of transport in porous material and the various fluid-rock interactions due to temperature and pressure changes, and develop a more general and realistic model of fluid movement and mass and energy transport in porous media. Experimentally evaluate the theory of moisture movements due to temperature and pressure gradients and the effect of evaporation and condensation on the flow of moisture at elevated temperatures. Make a theoretical evaluation of various characteristics to obtain a realistic description of the transport process in the form of differential equations and to seek solutions by analytical and numerical methods.

APPROACH: Conduct experimental studies involving the use of laboratory scale models of moisture movement due to a heat source in a high temperature and high pressure environment. Use methods developed by soil physicists to measure moisture contents and pressure. Generate data to provide information on effects of absorption, evaporation, and condensation upon head and water transport. Apply fundamental laws of physics to develop equations, and solve the equations by standard numerical and analytical means. Perform limited field experiments in order to test the applicability of methodology developed in theoretical and laboratory studies.

PROGRESS: W. N. Herkelrath carried out laboratory and field investigations of multiphase flow in porous media. The flow of mixtures of steam and noncondensable gas in high-temperature porous media was studied in laboratory experiments. Methodology was developed for measuring hysteretic, water-vapor-adsorption isotherms for rocks and soils over a wide range of temperatures. A numerical model was written to describe the transport of steam and gas in

adsorbing porous media. A laboratory method was developed for measuring the volume saturation of nonpolar liquids in porous materials. An automated time-domain reflectometry system was developed for continuous monitoring of soil moisture content in remote field areas. Using this system, rapid movement of water through the unsaturated zone was studied in a watershed.

WR180 UNSATURATED ZONE THEORY

TITLE: Theories of Water Flow and of Solute Transport in the Unsaturated Zone

PROJECT NUMBER: WR 82-180

LOCATION: Topical Research

PROJECT CHIEF: Rubin, Jacob

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: The unsaturated zone has a significant influence on the quantity and quality aspects of water resources. The existing theoretical methods of evaluating and predicting this influence, for a particular set of field conditions, cannot account adequately for the complexity of the processes involved and for interactions among them. In order to achieve such an accounting, it is necessary to improve the current theoretical approaches to water-flow and solute-transport problems of unsaturated-zone hydrology.

OBJECTIVE: Determine which conditions are or are not essential to realistically refining the commonly used mathematical models for unsaturated flow. Combine water-flow and water-mixing models with models for chemical reactions and biological processes, using models that are rigorous and appropriate to analyses of solute transport in the unsaturated zone. For both water-flow and solute-transport processes, explore situations of hydrologic interest and those that may be valuable in connection with model validation or parameter determination. Experimentally test the theoretical conclusions reached in cooperation with other projects.

APPROACH: For unsaturated flow, consider model refinements dealing with effects of parameter hysteresis, air trapping, pore-geometry transformations and medium heterogeneity. Determine the conditions under which such refinements are essential. Develop computer-aided theoretical analyses of the interactions between unsaturated-zone waters and ground or surface waters. For solute transport, attempt to integrate the hydrodynamic dispersion approach to transport with the chemist's or ecologist's approaches to chemical equilibria, chemical kinetics, and population ecology. In addition, modify the above standard approaches to treat more realistically the special conditions encountered in natural unsaturated zones, such as the presence of two fluid phases, changes in water content, wide range of soil water fluxes, chemical heterogeneity of the porous medium. Use or adapt existing mathematical methods, especially numerical methods, and, if necessary, develop new mathematical methods.

PROGRESS: A study was completed of the significance of special, dimensionless parameters, which make it possible to assess whether a given reaction-affected, solute-transport problem can be analyzed adequately with the aid of the local-equilibrium assumption. The chemical significance of these special parameters was assessed. For the cases studied, they were identical with the exponential terms that appear in the integrated rate-law of the corresponding batch reaction. Work on the mathematical formulation and modelling of solute-transport processes affected by multi-segment chemical reactions was continued. Hybrid cases in which the segments belong to different classes of chemical reactions were stressed. Reactions are either homogeneous or heterogeneous; if heterogeneous, reactions are either surface or classical.

REPORTS PUBLISHED:

Willis, C. M., and Rubin, J., 1987, Transport of reacting solutes subject to a moving dissolution boundary--numerical methods and solutions: Water Resources Research, v. 23, no. 8, p. 1561-1574.

James, R. V., and Rubin, J., 1986, Transport of chloride ion in a water-unsaturated soil exhibiting anion exclusion: Soil Science Society of America Journal, v. 50, no. 5, p. 1142-1149.

Rubin, J., 1987, Development of National Water Quality Assessment Program: a perspective of the U.S. Geological Survey: Water Science and Technology Board, National Water Quality Monitoring and Assessment, Report of a Colloquium, May 21-22, 1986, National Academy Press, p. 57-70.

Bahr, J. M., and Rubin, J., 1987, Direct comparison of kinetic and local equilibrium formulations for solute transport affected by surface reactions: Water Resources Research, v. 23, no. 3, p. 438-452.

Lewis, F. M., and Voss, C. I., and Rubin, J., 1987, Solute transport with equilibrium aqueous complexation and either sorption or ion exchange--simulation methodology and applications: Journal of Hydrology, v. 90, p. 81-115.

WR184 HYDROLOGY OF FRACTURED ROCKS

TITLE: Hydrology of Fractured Rocks

PROJECT NUMBER: WR 83-184

LOCATION: Topical Research

PROJECT CHIEF: Hsieh, Paul A.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Understanding the process of fluid flow in fractured rocks is important to assess the suitability of underground hazardous-waste storage sites, as well as to predict waste movements if contamination occurs. Although porous-media theory provides a feasible modeling approach, the low permeability and highly heterogeneous nature of fractured rocks require extensions in current theory and field methods. It is particularly important that theoretical developments can be applied to the field on a scale that is compatible with test equipment and borehole dimensions.

OBJECTIVE: Develop a comprehensive methodology of hydraulic testing in fractured rocks, and investigate the relation between hydraulic properties measured on different scales by characterizing the heterogeneity and anisotropy of the rock mass.

APPROACH: Develop theory and application of hydraulic testing methods to determine hydraulic properties of fractured rocks. Design single-hole and cross-hole packer tests using geologic and geophysical information. Theoretically investigate the effects of scale by computer simulation using stochastic and geostatistical techniques. Using results of field tests conducted on a small scale, predict rock characteristics on a larger scale and compare the predicted results to those from large-scale tests.

PROGRESS: (1) Completed 4 weeks of field testing (single-hole and cross-hole packer tests) at the Oracle site (Arizona) to characterize the hydraulic properties of fractured metamorphic rocks at the site. (2) Completed 3 weeks of field testing (aquifer tests) at the Lee Valley site (California) to study the water resources of a bedrock valley. (3) Prepared equipment to use a newly developed hydraulic testing method to determine the vertical hydraulic conductivity of the basalt sequences underneath the island of Oahu, Hawaii.

REPORTS PUBLISHED:

Hsieh, P. A., 1986, Discussion of "Aquifer test analysis in fractured rocks with linear flow pattern" by Zekai Sen: Ground Water, v. 24, no. 4, p. 530-531.

WR193 TEMPERATURE EFFECTS, UNSAT. ZONE

TITLE: Temperature Effects in the Unsaturated Zone

PROJECT NUMBER: WR 87-193

LOCATION: Topical Research

PROJECT CHIEF: Constantz, James E.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Transport in the unsaturated zone is strongly dependent upon temperature. However, there is a lack of quantitative information concerning the influence of temperature upon water retention characteristics, unsaturated hydraulic conductivity values, and water fluxes in natural porous materials. When compared to experimental results, existing theories underestimate the magnitude of temperature-induced changes in many pore water and interfacial properties. Consequently, models incorporating the effects of temperature upon water retention and transport in the unsaturated zone are inadequate.

OBJECTIVE: (1) Measure the influence of temperature upon water retention characteristics, unsaturated hydraulic conductivity, and coeffecients derived from these primary parameters, such as water diffusivities and capacities; (2) ascertain whether the behavior of water in close proximity to mineral surfaces is altered sufficiently to result in modified temperature coefficients for gas solubilities, adsorption, viscosity, interfacial surface tensions and contact angles, as well as other properties important to transport in porous materials; and (3) examine the influence of temperature upon primary hydrologic processes occurring in the unsaturated zone, such as infiltration, moisture redistribution, evaporation, and drainage.

APPROACH: Perform laboratory experiments designed to measure the temperature dependence of water retention characteristics and unsaturated hydraulic conductivities in natural porous materials, using both field cores and repacked samples. Examine relationships between the matric potential, the volumetric water content, and temperature in these materials, using experimental equipment and procedures which have been modified for high temperature. Perform field experiments to determine the influence of temperature upon water retention and transport.

PROGRESS: The importance of air encapsulation during infiltration was demonstrated for several different soil materials and a new method for high temperature measurement of pore water properties was successfully tested in the laboratory.

SURFACE-WATER HYDROLOGY

CR228 RAINFALL-RUNOFF MODELING

TITLE: Precipitation-Runoff Modeling of Watershed System

PROJECT NUMBER: CR 77-228

LOCATION: Topical Research

PROJECT CHIEF: Leavesley, George H.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: (1) Energy-resource development, urbanization, forestry practices, and other land-use changes can have a significant effect on watershed hydrology. Computer modeling techniques that simulate the physical processes of the hydrologic cycle, using measurable watershed and climatic characteristics, must be developed to adequately predict and assess the effects of current or proposed land-use changes on watershed hydrology. (2) Eruptions of Mount St. Helens deposited large quantities of volcanic ash in major tributary basins to the Columbia River. An understanding of the infiltration and erosion processes taking place on the ash deposits must be obtained to estimate the effects of this ash on runoff and erosion rates.

OBJECTIVE: (1) Test, verify, and enhance the distributed parameter Precipitation-Runoff Modeling System (PRMS) which was developed by this project to predict runoff, sediment yields, and water-balance relations for normal and extreme rainfall and snowmelt on land used in a variety of ways; develop a statistical theory of errors for the PRMS; develop model parameter estimates to relate parameters to measurable watershed and climatic characteristics. (2) Determine the infiltration and erosion characteristics of volcanic ash on selected study plots; evaluate the processes influencing these characteristics; extrapolate the plot-study results to larger basin areas using the PRMS to estimate the impacts of the ash deposits on watershed hydrology.

APPROACH: (1) Examine data from past and current small-watershed studies of the U.S. Geological Survey (for example, small-streams, coal, and oil-shale programs), other Federal Agencies, and universities for the physiographic and climatic regions of the United States. Evaluate the PRMS components with regard to the significant hydrologic processes in each region, and enhance through modification and additional research where required. Assess the sources of model error and the transfer of these errors to the model output. Evaluate rainfall simulator for infiltration and erosion parameter estimation. (2) Install small plots to monitor runoff and erosion from rain and snowmelt; determine infiltration and erosion rates from these data, and relate to hydrologic and ash characteristics.

PROGRESS: The sources and magnitudes of precipitation input errors and their effect on snowmelt-runoff-simulation errors were and are being investigated using the Precipitation-Runoff Modeling System (PRMS) for selected basins in different climatic and physiographic regions of the western United States. Ratios of high-elevation precipitation to low-elevation precipitation computed by storm, month, and season show a large temporal and spatial variability. Techniques and procedures that account for some of this variability when distributing point-precipitation data by elevation and area are being developed and tested to minimize this major source of simulation error. A procedure to automate the segmentation of a watershed into hydrologic-response units using digital terrain data, satellite imagery, basin-characteristic data bases, and the ARC/INFO and TINS geographic information systems is being developed and tested. A microprocessor-based version of PRMS was developed and packaged with a microprocessor-based version of ANNIE. A weighted least-squares regression analysis (WLS) was applied to a data matrix consisting of observed and map-model estimates of T-year annual floods for 200 small basins east of the 105 Meridian. The WLS accounts for the variability in the accuracy of observed flood estimates on regression-line parameters (slope and intercept), and also yields an assessment of model error. A Monte Carlo experiment was designed and conducted to evaluate the utility of two competing time-sampling error-variance formulations and their impact on evaluation of model error. Bridge scour, including constriction scour and local scour at piers and abutments, was analyzed and equations for predicting these values were developed. A 1-dimensional open-channel flow model is being developed to simulate highly dynamic floods and resulting stream-channel erosion and deposition.

REPORTS APPROVED FOR PUBLICATION:

Leavesley, G. H., Lumb, A. M., and Saindon, L. G., in press, A microcomputer-based watershed-modeling and data-management system: Western Snow Conference, Vancouver, British Columbia, 1987, Proceedings.

CR279 ERRORS ANALYSIS

TITLE: Statistical Analysis of Errors in Hydrologic Models

PROJECT NUMBER: CR 83-279

LOCATION: Topical Research

PROJECT CHIEF: Troutman, Brent M.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Application of hydrologic models without an analysis of the errors can be misleading. Proper interpretation of model output through analysis of errors can eliminate economic consequences of over- and under-design resulting from model-related errors.

OBJECTIVE: (1) Develop unified approach to analyzing and partitioning errors in hydrologic modeling; (2) develop improvements to existing practices; and, (3) develop new approaches to managing error levels within the constraints of reduced budgets.

APPROACH: Use concepts of linear and nonlinear regression and optimal interpolation and prediction to estimate the individual contributions of space, time, and model error in hydrologic modeling.

PROGRESS: The value of the instantaneous unit hydrograph (IUH) theory in defining the runoff-response characteristics of a drainage basin was examined, and new expressions for the IUH of a basin were derived. These expressions are functions of only a few quantities, some of which are readily obtained from a map of the basin: number and mean length of first-order streams (external "links") in the network, mean length of the internal links, mainstream length, order of the basin, and mean hydraulic properties. Derivations of these expressions utilized results in geomorphology for so-called topologically random channel networks and probabilistic methods in branching theory. Under certain conditions, runoff predictions using the derived IUH compare favorably to predictions of complicated rainfall-runoff models which require considerably more input data. Sensitivity analyses were performed which tested the extent to which the derived IUH depends on the amount of detail in the network description. Methods for estimating the parameters, especially celerity, of the IUH were examined and applied to a number of drainage basins in the Western United States. Application to actual storm-event data yields very satisfactory agreement with observed runoff hydrographs.

REPORTS PUBLISHED:

Srodon, Jan, Morgan, D. J., Eslinger, E. V., Eberl, D. D., and Karlinger, M. R., 1986, Chemistry of illite/smectite and end-member illite: Clays and Clay Minerals, v. 34, no. 4, p. 368-378.

Troutman, B. M., 1986, Reducing bias in parameter estimation caused by model-input errors: 6th Annual Front-Range American Geophysical Union Hydrology Days, Colorado State University, Fort Collins, Colorado, 1986, Proceedings, p. 71-86.

Troutman, B. M., and Karlinger, M. R., 1986, Averaging properties of channel networks using methods in stochastic branching theory, in Proceedings of the Symposium on Scale Problems in Hydrology, Princeton University, 1984: Boston, Massachusetts, Reidel Publishing Company, p. 183-214.

Karlinger, M. R., Guertin, D. P., and Troutman, B. M., 1987, Use of topological information in hydrograph estimation: Water Resources Bulletin, v. 22, no. 2, p. 271-279.

NR019 NUMERICAL SIMULATION

TITLE: Numerical Simulation of Hydrodynamic Processes in Rivers, Estuaries, and Embayments

PROJECT NUMBER: NR 69-019

LOCATION: Topical Research

PROJECT CHIEF: Baltzer, Robert A.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Technical solutions to the problem of investigating and managing waste movement and disposal in regulated rivers, estuaries, and embayments require qualitative and quantitative assessment of the interactions among waste constituents undergoing dynamic transport. Mathematical, numerical, computer-simulation models offer one very powerful solution. Because water is both the vehicle by which the waste constituents are transported and the media in which the constituent interactions occur, the temporal and spatial variations of the flow appreciably govern the interactions both qualitatively and quantitatively. Design of the desired simulation models depends in large measure on accurate mathematical-numerical representation of the hydrodynamics of the transient-flow process.

OBJECTIVE: (1) Thoroughly explore the hydrodynamics of one-, two-, and three-space dimensional transient flows in waterways and waterbodies (including the transport and interaction of constituents); (2) develop mathematical-numerical techniques with which to simulate these processes; and (3) provide the hydrologist with a simulation system comprised of rational mathematical-numerical models for evaluating the effect of past, present, and projected changes in prototype-waterbody systems.

APPROACH: Derive mathematical models, comprised of sets of nonlinear, partial, differential equations, representing various transient flow conditions. Develop numerical techniques to simulate the various flow regimen represented by the models. Use field data gathered at specific field sites and (or) hypothetical data reflecting a projected change to provide the necessary boundary-condition information and driving function with which to particularize model solution. Use large-capacity, high-speed digital computers and videographic output equipment in making the simulations.

PROGRESS: Study and further development of a one-dimensional (1-D) test model based on an implicit method-of-characteristics (IMOC) numerical technique underscores the soundness and high operational potential of this approach. Solution techniques, one utilizing Q,Z as the dependent variable set and another using Q,A as the variable set, are being developed and compared. The Q, A-based solution, which is the more unorthodox of the two, appears at this point to offer specific benefits with minimal operational penalties. All numerical simulation schemes depend in one way or another upon numerical interpolation. Much effort has been and is being directed toward developing one (or more) computationally efficient procedures for high order numerical interpolation between two adjacent points within a model grid. One such two-point, fourth-order scheme is generally useful for a Courant number less than one. A spline-based scheme for this same two-point, interpolation problem appears almost as good, but is suitable for Courant numbers in excess of one as well. The problems of off-channel storage and internal boundary conditions have been analyzed in anticipation of adding these operational capabilities to the BRANCH one-dimensional model and to an operational IMOC model. The types of off-channel storage have been categorized for purposes of subsequent numerical treatment and model implementation. Efforts are underway to revise all 1-D and 2-D model support systems (GDAS, TDDS, CGAP) so as to operate interactively on super microcomputers and so-called engineering work stations.

NR074 WATER QUAL. MODEL DEVEL. AND IMPLE.

TITLE: Water Quality Model Development and Implementation

PROJECT NUMBER: NR 71-074

LOCATION: Topical Research

PROJECT CHIEF: Baltzer, Robert A.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Existing and (or) potential water quality conditions in regulated rivers, estuaries, and coastal embayments can be investigated best using mathematical-simulation models. These models also can be used to assess the interactions between waste constituents (including heat) dispersed throughout the hydrodynamic framework. Computational models are available currently for only a limited class of prototype situations wherein vertical stratification does not exist. Also, data handling and digital graphics techniques to be used with all models require improvement.

OBJECTIVE: (1) Provide efficient data-handling and computer graphics techniques with which to fully implement the existing, two-dimensional, non-stratified simulation models, and a highly transferable computational model for the simulation of three-dimensional transient flows and water-quality parameters under conditions of nonisotropic density; and (2) provide hydrologists or water-resources managers with an economically viable simulation model with which to evaluate the effects of past, present, and prospected changes in a given prototype water body.

APPROACH: Organize model-data input and output to permit fast, economical computer implementation of the models. Using a system with extensive digital graphics comparison capability, including interactive graphic capability. Develop three-dimensional models by carefully selecting the appropriate form of the mathematical expressions for motion of incompressible but variable-density fluid, continuity of total fluid mass, for continuity of solutes, for thermal energy in fluid, and for relations between fluid density and solute concentrations. Transform these expressions to finite difference expression and design the computational grid to account for conservational properties.

PROGRESS: In support of a cooperative effort with Federal Highway Administration (FHWA) and U.S. Geological Survey (USGS) District projects, the SIMSYS2D finite-difference, flow/transport modeling system has been adapted for upland riverine watercourse and flood plain, right-of-way crossing investigations. Changes made to the system improve estuarine and coastal-embayments study capabilities. Means were devised for selecting hydrography and hypsography data from USGS data files to produce bottom configuration data. The problem of "nesting" fine-scale models within coarser scale models is being studied, with particular attention to the transfer between models of boundary condition data.

NR096 COMPUTATIONAL HYDRAULICS

TITLE: Computational Hydraulics for Surface Water Problems

PROJECT NUMBER: NR 79-096

LOCATION: Topical Research

PROJECT CHIEF: Lai, Vincent C.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Because of rapid change in computer capability and computing milieu and involvement of Water Resources Division in computer modeling of various practical water problems, many research hydrologists find little time for carefully appraising up-to-date numerical tools and modeling techniques. Use of inadequate computational methods and numerical analysis, improper handling of parameters and data for numerical modeling, and application of questionable or outdated modeling techniques, all lead to serious simulation errors or total information losses. Relatively little work has been done for numerical analysis; moreover, the previous work largely has been limited to simple, linear, and idealized flow conditions far from real-world problems. Also, relatively few people are aware that present-day computer modeling requires much broader knowledge and techniques than numerical analysis.

OBJECTIVE: (1) Investigate, compare, or appraise various numerical approaches, methods, schemes, or modeling techniques for hydraulic or hydrodynamic simulation, explore or test newly introduced numerical methods for their adequacy and applicability in hydrologic projects, and devise or develop new numerical modeling approaches for simulating surface-water problems; and (2) conduct studies on numerical stability, convergence, accuracy, efficiency, parameter identification, and sensitivity analyses associated with nonlinear schemes or models in computational hydraulics and water resources problems that are more complex but physically more realistic than linear schemes and models.

APPROACH: (1) Review existing and newly introduced numerical approaches, methods, schemes, and modeling techniques. Investigate, for given flow problems, the effect that changes in numerical schemes and modeling methods have on simulation results. Compare relative merits of different methods and techniques from various viewpoints; and (2) review physical concepts of nonlinear effects in various flow problems, rapidly-varied unsteady flows in particular; study the roles of nonlinear and higher-order terms in partial differential equations, and investigate the effects of these terms in different numerical schemes.

PROGRESS: Continued efforts were made to the two themes of computational hydraulics--model assessment and numerical methods. A third theme, "innovation" has been added to the research program of this project and several new and significant advancements and breakthroughs have been made in the following three areas: (1) Complex Variable Boundary Element Method (CVBEM): The CVBEM modeling technique has been successfully applied to stratified flows. The model awaits some field data for practical applications. (2) Modeling unsteady fixed-bed open-channel flow by the method of characteristics using specified-time-intervals (MOC-STI for fixed-bed channel flow) (a) IMOCDS model. A new implicit scheme has been implemented in this model, which enables the user to compute unsteady flow with the Courant number considerably larger than 1. (b) SPRMOS/NEWMOS model, combines several implicit and explicit schemes into one, thus possessing all the advantages of individual schemes involved, in addition to its newly endowed robustness and versatility and its inherent MOC strength. (3) Modeling unsteady movable-bed open-channel flow by the method of characteristics using specified-time-intervals (MOC-STI for alluvial channel flow). By combining the implicit scheme and the reachback scheme, it is possible to couple the rapidly propagating hydrodynamic-waves and slowly moving bed-deformation waves in one model--XRACMB model.

REPORTS PUBLISHED:

Hromadka II, T. V., and Lai, C., 1987, The complex variable boundary element method in engineering analysis: New York, Springer Verlag, 389 p.

Lai, C., 1986, Analysis of stratified flows by the complex-variable boundary-element method: International Conference on Computational Mechanics, Tokyo, Japan, 1986, Proceedings, p. XI. 149-154.

Lai, C., and Chang, F. F. M., 1987, A new approach for modeling unsteady flow in alluvial channels by the method of characteristics--basic theory and formulation of computational algorithm: American Society of Civil Engineers Specialty Conference, Buffalo, N.Y., 1987, 16 p.

Lai, C., and Hromadka II, T. V., 1986, Some advances in CVBEM modeling of two-dimensional potential flow: American Society of Civil Engineers Conference, Minneapolis, Minn., 1986, Proceedings, p. 492-499.

NR104 MODELING OF HYDRODYNAMIC SYSTEMS

TITLE: Simulation Modeling of Hydrodynamic Systems

PROJECT NUMBER: NR 80-104

LOCATION: Topical Research

PROJECT CHIEF: Schaffranek, Raymond W.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: Managing water use in riverine and estuarine systems requires an understanding of the governing supply, circulation, mixing, and flushing processes. Qualitative and quantitative evaluation of the hydrodynamic and transport properties of such water bodies can be computed via mathematical/numerical simulation models. To accurately simulate both the temporal and spatial variations of the flow, which significantly define the transport processes, the simulation model must be capable of accounting for hydraulic and tide-induced fluctuations, water withdrawals, discharges, winds, non-uniform geometric configurations, and other human-made or natural factors.

OBJECTIVE: (1) Investigate and develop various mathematical-numerical techniques with which to simulate the hydrodynamics of one-, two-, and three-space dimensional transient flows in various waterbodies; (2) evaluate and (or) develop methods to describe the transport of solutes in such waterbodies utilizing the comprehensive flow information derived from flow simulation models; and (3) develop and implement an operational system in support of flow/transport simulation models.

APPROACH: Use large-capacity, high-speed digital computers and various supporting peripheral equipment. Derive and develop mathematical models, constituting approximate numerical solutions to the governing nonlinear, partial, differential equations, to simulate the transient flow and transport processes. Use data, collected at specific locations or hypothetically-imposed, use to provide the required boundary-condition information with which to effect the numerical solution.

PROGRESS: A modularized, personal computer compatible version of the branch-network model has been developed and tested. Improvements made in the model include removal of measured-data time-step constraints, addition of self-setting external boundary conditions, special handling of time-series boundary-value data, computation of Courant values, incorporation of global specification of momentum and friction coefficients, and printout of array dimension utilization information. A paper describing the initial calibration effort of the 2-D model of the Potomac Estuary transition zone has been prepared and presented at a national conference of the American Society of Civil Engineers. Advances were made in converting, enhancing, and documenting systems developed in support of hydrodynamic simulation models. Consultation,

direct assistance, and (or) training have been provided to district offices proposing or actively conducting model-based investigations using methods and techniques developed within the research project.

REPORTS PUBLISHED:

Schaffranek, Raymond, W., 1986, Hydrodynamic simulation of the Upper Potomac Estuary, in Water Forum '86 (vol. 1): American Society of Civil Engineers, p. 1572-1581.

NR125 REGRESSION AND DATA-NETWORK DESIGN

TITLE: Hydrologic Regression and Data-Network Design in Coal Mining Regions

PROJECT NUMBER: NR 82-125

LOCATION: Topical Research

PROJECT CHIEF: Tasker, Gary D.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: There is a need to develop methods by which the Water Resources Division's hydrologic-data-collection activities in coal-mining regions can be evaluated objectively and modified, when necessary, so that the efficiency of its operations will be maximized.

OBJECTIVE: Produce objective methods for hydrologic network design and methods for information transfer in coal-mining regions.

APPROACH: Use cross-validation and computer simulation of hydrologic processes to evaluate the statistical and economic measures of the hydrologic-data-collection programs.

PROGRESS: The operational generalized least squares (GLS) regression method was programmed, along with the network analysis technique, to include networks of up to 275 stations. The general applications technique also was developed and applied to urban water quality studies on a nationwide basis. Various methods of estimating low-flow characteristics were compared and tested using bootstrap computer-intensive methods. This was the first application of bootstrap methods for comparing methods of estimating low-flow characteristics.

REPORTS PUBLISHED:

Stedinger, J. R., and Tasker, G. D., 1986, Regional hydrologic analysis 2--Mean-error estimators, estimation of sigma, and log-Pearson Type 3 distributions: Water Resources Research, v. 22, no. 10, p. 1487-1499.

Tasker, G. D., 1986, Generating efficient gaging plans for regional information: Design of Hydrologic Networks, International Association of Hydrologic Sciences Publication No. 158, p. 269-281.

NR133 REGIONAL HYDROLOGIC PROCESSES

TITLE: Stochastic Structure of Regional Hydrologic Processes

PROJECT NUMBER: NR 84-133

LOCATION: Topical Research

PROJECT CHIEF: Landwehr, Jurate M.

HEADQUARTERS OFFICE: Reston, VA

PROBLEM: The regional nature of hydrologic processes long has been considered from the viewpoint of shared basin and climatic characteristics. Inferences have been attempted by regressing the measures of hydrologic interest against such basin characteristics. However, such treatment has been insufficient to characterize either the magnitude of flows or the water-quality variations observed within a geographic area. Consequently, the stochastic structure of the regional hydrologic process itself needs to be studied.

OBJECTIVE: Develop hydrologic statistics within a regional context and identify the apparent effect of persistence in developing regional statistics.

APPROACH: Examine the composition of a hydrologic region for the applicability of Bernoullian trials. Use the statistical theory of extremes to analyze the distribution of flows as expressed through different flow regimes. Measure persistence by treating it as both a random variable and as a constant property of the stochastic process. Derive empirical flow information using the recently developed Mini-Regions File, water-quality data from the National Stream Quality Accounting System (NASQAN) Database, and surrogate hydrological records, such as tree-ring chronologies, as necessary.

PROGRESS: An automated data base of monthly and annual discharge records from throughout the world has been completed (through 1979); this data base will allow comparison of large-scale, long-term hydrologic phenomenon. An analysis of patterns of persistence in eastern versus western dendrochronologies shows that they are similar in finite memory but the fine structure of the stochastic processes are different.

REPORTS PUBLISHED:

Landwehr, Jurate Maciunas, and Matalas, N. C., 1986, On the nature of persistence in dendrochronologic records with implications for hydrology: Journal of Hydrology, v. 86, p. 239-277.

SR029 SURFACE-WATER HYDRAULICS

TITLE: Development and Validation of Computational Techniques in Surface-Water Hydraulics--HIF

PROJECT NUMBER: SR 73-029

LOCATION: Southern Mississippi

PROJECT CHIEF: Lee, Jonathan K.

HEADQUARTERS OFFICE: NSTL, MS

PROBLEM: Flow and transport in surface-water systems are governed by conservation equations for mass, momentum, and energy. There is a need to develop solutions of these equations for increasingly complex field applications (such as the analysis of the effects on flow distribution and backwater of multiple bridge openings in complex flood plains, the attenuation and travel time of flood peaks as meandering rivers inundate large flood plains, and the routing of extremely abrupt floods induced by dam breaks and volcanic eruptions). The general non-existence of appropriate analytical solutions both complicates and necessitates the careful validation of computational techniques developed.

OBJECTIVE: Develop and validate computational techniques for the solution of flow and transport problems in surface water using hydraulic theory to the maximum extent possible, leading to improvement in nationwide surface-water analysis procedures and techniques.

APPROACH: Develop computational techniques and advance the basic understanding of hydraulic processes by conducting theoretical transport and numerical experiments. Conduct and use controlled experiments in the floodplain simulation facility and indoor hydraulics laboratory to define unknown coefficients and to refine, test, and validate computational techniques.

PROGRESS: Work continued on the development and enhancement of the two-dimensional finite-element surface-water flow model FESWMS. The interactive program for network entry was improved. A version for personal computers was developed, and GKS graphics were added to the system. Work continued on model documentation. The simulation of data collected in the Flood Plain Simulation Facility (FPSF) during experiments on steady flow through contracted openings continued. During this numerical work, it was found that additional data were needed on vertically averaged velocities, momentum-correction coefficients, recirculation zones, and jets downstream from the contracted openings. To collect these data, experiments on steady flow through concentric contracted openings were carried out for three contraction ratios at each of three discharges. A Layered Lagrangian Transport Model (LLTM) that simulates laterally averaged transport in steady flow has been developed and tested. The LLTM extends one-dimensional (longitudinal) Lagrangian techniques to two dimensions

(longitudinal and vertical), which significantly improves our ability to simulate suspended-sediment transport due to the settling property of sediment. The one-dimensional Lagrangian Transport Model (LTM) has been applied in a quasi two-dimensional manner to simulate suspended sediment. Development and testing of the Branched Lagrangian Transport Model (BLTM) for simulation of transport and water quality in networks of tidal channels has been completed and the BLTM is being documented. Documentation of the HYDRAUX flow model is nearing completion.

REPORTS PUBLISHED:

Lee, J. K., 1987, Discussion of "Fourier analysis of dissipative FEM channel flow model," by N. D. Katapodes: Journal of Hydraulic Engineering, American Society of Civil Engineers, v. 113, no. 2, p. 267-270.

Lee, J. K., 1987, Physical modeling of contracted flows: American Society of Civil Engineers National Conference, Williamsburg, Va., 1987, Proceedings, p. 25-30.

Schoellhamer, D. H., 1987, Lagrangian modeling of a suspended-sediment pulse: American Society of Civil Engineers National Conference, Williamsburg, Va., 1987, Proceedings, p. 1040-1045.

Schoellhamer, D. H., and Jobson, H. E., 1986, Programmer's manual for a one-dimensional Lagrangian transport model: U.S. Geological Survey Water Resources Investigations Report 86-4144, 101 p.

Schoellhamer, D. H., and Jobson, H. E., 1986, User's manual for a one-dimensional Lagrangian transport model: U.S. Geological Survey Water Resources Investigations Report 86-4145, 95 p.

SR055 ORGANIC SUBSTANCES IN STREAMS

TITLE: Transport and Degradation of Organic Substances in Streams

PROJECT NUMBER: SR 77-055

LOCATION: Topical Research

PROJECT CHIEF: Rathbun, Ronald E.

HEADQUARTERS OFFICE: Bay St. Louis, MS

PROBLEM: Organic substances discharged into streams affect water quality and possible uses of the water. To quantify the effect of organics on water quality, the chemical, physical, and biological processes involved in the transport, degradation and determination of the ultimate fate of these substances must be understood.

OBJECTIVE: (1) Determine the fundamentals of the microbial degradation and the fundamentals of the volatilization, dispersion, adsorption, and other physical processes that affect the concentrations of organic substances in streams; and (2) develop sub-models of these processes and integrate these sub-models into an overall model describing the transport and degradation of organic substances in streams.

APPROACH: Perform controlled laboratory studies (stirred tank or flume) to determine the degradation characteristics of specific organic compounds, both as single components and as mixtures, and controlled studies of the transport and degradation of these substances in the small model river at the Gulf Coast Hydroscience Center. Apply the results of these studies to the testing, adapting, or developing of transport models for organics in streams. Test these models under field conditions.

PROGRESS: The dependences of liquid-film coefficients on the molecular-diffusion coefficient and molecular weight for benzene and eight alkyl-substituted benzene compounds were only partially in agreement with two commonly used equations from the literature. Deviations for the low-molecular weight compounds were attributed to molecular interactions and for the high-molecular weight compounds to sorption on the experimental apparatus. Acetone injected continuously for 32 days into an outdoor model stream did not degrade microbially, contrary to expectations based on laboratory studies. Possible explanations include a nitrate limitation and a limited residence time in the model stream.

REPORTS PUBLISHED:

Rathbun, R. E., and Tai, D. Y., 1987, Vapor pressures and gas-film coefficients for ketones: Chemosphere, v. 16, no. 1, p. 69-78.

Rathbun, R. E., and Tai, D. Y., 1987, Volatilization of ethylene dibromide from water: Environmental Science and Technology, v. 21, no. 3, p. 248-252.

SR074 FLUVIAL PROCESSES

TITLE: Fluvial Processes and River Mechanics

PROJECT NUMBER: SR 83-074

LOCATION: Topical Research

PROJECT CHIEF: Chen, Cheng-lung

HEADQUARTERS OFFICE: NSTL, MS

PROBLEM: The inability to account fully for the causes, occurrences, and mechanisms of catastrophic hydrologic events, such as flash floods, dam breaks, and mudflows (or mudslides) resulting from torrential rainstorms, earthquakes, or volcano eruptions, may be attributed in part to the deficiencies or incompleteness of existing mathematical relationships between the relevant processes and channel response. Many unresolved problems in fluvial mechanics result from inadequate understanding of the multiplicity and interaction of fluvial processes. Some existing relations are inadequate because the solutions represent approximations only. The complexity of the problem has been characterized by intractability to the conventional approaches based on the classical theories and principles of mechanics. For example, the capability to determine whether a hillslope of river channel is susceptible to changes in river form and when and where such changes might occur, does not exist presently. Debris of varying size accompanies flash floods, but the laws governing sediment transport (in particular, mudflows) are not defined adequately to evaluate the effect of such transport. Infiltration from snow melt significantly may affect hillslope responses to stream flow and sediment transport. There are very few investigations dealing with these effects and such cases require elucidation.

OBJECTIVE: (1) Define more fully the various fluvial processes on hillslopes and (or) in river channels, and evaluate the rate of river-form change in response to the hydrologic disturbances caused by torrential rainstorms, earthquakes, or volcano eruptions; (2) modify or generalize existing mathematical relationships (models) to describe more accurately the process-response relationships; (3) formulate rheological relationships for various soils and highly-concentrated sediment-water mixtures involved in such model; (4) using such relationships in conjunction with available field and laboratory data, build, calibrate, verify, and apply mathematical models for flash floods, dam breaks, and mudflows; and (5) ultimately, use these models to evaluate potential hazards that may result from such catastrophic events.

APPROACH: Assess the validity and applicability of existing relationships between various processes and channel responses, such as those related to rainfall, infiltration, snow melt, runoff, and sediment movement on hillslopes and (or) in river channels. Modify or generalize existing mathematical relationships (or models) so that they will become more representative under a wider spectrum of field conditions. Formulate rheological equations for various soils and highly concentrated sediment-water mixtures, and determine the values of specific parameters using available field and laboratory data. Design and construct a conveyor-belt type flume in a hydraulic laboratory to study the mechanism and the rheological properties of a mudflow which propagates with a bore. Devise mathematical models for flash floods, dam breaks, and mudflows; test adequacy of the models with digital computers, using optimum numerical schemes. Verify the models using actual events.

PROGRESS: Debris-flow research has continued both in theoretical and experimental aspects. Major tasks in progress are: (1) the development of a generally applicable macroscopic (continuum-mechanics-based) model for describing the rheological properties of various sediment-water mixtures; (2) the formulation of a general hydraulics-based routing model for simulating an unsteady debris flow at various stages, namely from its initiation to termination, as well as two transitions in the sedimentation process, namely from landslide to debris flow and then from debris flow to bed-load transport; and (3) the development of an experimental debris-flow research facility for evaluating the rheological parameters and material constants of prototype debris flow. Significant results obtained from efforts made in the first and second tasks have been the formulation of a generalized viscoplastic fluid (GVF) model and the subsequent development of a general routing model based on the GVF model. Two pieces of equipment have resulted from an effort made in the third task: a "ring-shear" type apparatus procured from Japan and a "conveyor-belt" type flume built at the Gulf Coast Hydroscience Center. Both apparatus and flume have been shipped to the University of California at Berkeley for performing the third task under a joint research contract between the USGS and the University of California at Berkeley. A number of papers have been prepared to address some critical issues in debris-flow research and their possible resolutions. Other problems on related topics such as dam-break floods have also been investigated and significant findings reported.

REPORTS PUBLISHED:

Chen, C. L., 1986, Viscoplastic fluid model for debris flow routing, in Proceedings of the Water Forum '86: Long Beach, Calif., American Society of Civil Engineers, p. 10-18.

WR064 ICE MODELING AND REMOTE SENSING

TITLE: Polar Ice Remote Sensing

PROJECT NUMBER: WR 70-064

LOCATION: Arctic Ocean

PROJECT CHIEF: Campbell, William J.

HEADQUARTERS OFFICE: Tacoma, WA

PROBLEM: Variations of the major components of the cryosphere--snow packs, sea ice, and ice sheets--and their role in the hydrologic cycle, both worldwide and regional, essentially are unknown. Two major technological advances that have occurred in the last decade now make it possible to attack this problem: (1) Active and passive microwave sensors in space permit observation of many key cryospheric parameters on global scales in time intervals as short as two days; (2) coupled atmosphere-sea ice-ocean numerical models make it possible to use these space microwave data to perform cause and effect simulation of cryospheric variations.

OBJECTIVE: (1) Numerically model the Arctic and Antarctic sea-ice covers and ice sheets for a variety of different rheological assumptions; (2) to acquire data to test the numerical models of the Arctic and Antarctic ice sheets and ice packs by participating directly in remote-sensing and surfacetruth experiments and from remote-sensing polar-orbiting satellites; (3) investigate the dynamics and thermodynamics of the upper ocean and their relation to the ice thickness, to obtain results to be applied to the sea-ice cover models; (4) to construct multi-dimensional, time-dependent models of glacier flow and ice-sheet flow and test them with observations of glaciers; and (5) investigate the use of satellite passive microwave data for snow water quivalent mapping.

APPROACH: (1) Initiate a Sea Ice Sheet Program with the U.S. National Aeronautics and Space Administration (NASA) involving a three-level approach with simultaneous ice observations by satellite, aircraft, and surface teams. (Indirect NASA support to this project is expected to total at least 1.3 million annually: 70 percent in field programs with NASA aircraft, 20 percent in data processing, and 10 percent in computer support. Indirect French space agency support will be 1.1 million annually); (2) participate in the design of microwave sensors for satellite missions and in the subsequent analysis and use of the data; (3) participate in the planning and performance of aircraft remote sensing missions; (4) participate in surface-truth experiments on snow packs, sea ice, and ice sheets; and (5) develop models for sea ice, glacier, and ice sheet dynamics.

PROGRESS: Organized an international MIZEX (Marginal Ice Zone Experiment) Workshop at the project offices in Tacoma. Prepared eight MIZEX papers for Journal of Geophysical Research and Science. Continued joint USGS/CNES (French Space Agency) research program on sea ice and ocean microwave remote sensing using both Seasat and MIZEX data processed at and with CNES funding of $750,000. Continued joint U.S. Geological Survey, National Aeronautics and Space Administration, and National Oceanic and Atmospheric Administration snowpack microwave remote sensing program in the Colorado Basin using scanning multichannel radiometer (SMMR) satellite data, and aircraft and surface data. Conducted a Snow Microwave Workshop and a USGS Glacier modelling workshop at the Tacoma office. Organized and participated in an expedition to Greenland as part of the USGS Icesheet Radar Sounding program.

REPORTS PUBLISHED:

Johannessen, O. M., Horn, D. A., and others, 1986, Marginal Ice Zone Experiment East 83/84--The summer marginal ice zone program in the Fram Strait/Greenland Sea: EOS, v. 67, no. 23, p. 513-517.

Johannessen, O. M., Johannessen, J. A., Svendsen, E., Shuchman, R. A., Campbell, W. J., and Josberger, E., 1987, Ice edge eddies in the Farm Strait Marginal Ice Zone: Science, v. 236, p. 427-429.

Mognard, N. M., Campbell, W. J., Cheney, R. E., Marsh, J. G., and Ross, D. B., 1986, Southern ocean waves and winds derived from Seasat altimeter measurements, in Phillips, O. M., and Hasselmann, K., eds., Wave dynamics and radio probing of the ocean surface: Plenum Publishing, p. 479-489.

Parkinson, C. L., Comiso, J. C., Zwally, H. J., Cavalieri, D. J., Gloersen, P., and Campbell, W. J., 1987, Arctic sea ice, 1973-1976--satellite passive microwave observations: National Aeronautics and Space Administration Special Publication 489, 296 p.

Shuchman, R. A., Burns, B., Campbell, W. J., Johannessen, O. M., Josberger, E. G., and Manley, T., 1987, Remote sensing of the Fram Strait Marginal Ice Zone: Science, v. 236, p. 429-432.

WR140 ESTUARY HYDRODYNAMICS

TITLE: Hydrodynamics and Mathematical Modeling of Circulation and Transport Phenomena in a Tidal Estuary

PROJECT NUMBER: WR 76-140

LOCATION: San Francisco Bay area

PROJECT CHIEF: Cheng, Ralph T.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: The ecosystem of a tide-affected estuary consists of an extremely complicated balance of natural processes. Some of the basic characteristics of such a system (the San Francisco Bay) are not well understood. Comprehensive description of the hydrodynamics and the related transport processes is lacking. Better understanding of the effects of interactions among natural processes and human activities on this system requires advances in basic science and in its application to applied problems. Circulation in a tidal estuary is in response to tides, inflow of fresh water, wind, and gravity and density stratification. Topography of the estuary basin, air-water interaction, turbulent mixing, viscous resistance at the bottom, and rotational effects of the earth, together with the previously mentioned driving forces, constitute a very complicated balance that conserves mass, momentum, and energy in the system.

OBJECTIVE: Understand the processes and rates by which water, solute, and other organisms interact to assist quantification of the relative importance of river inflow, winds, tides, and other dynamic forces which act on the estuary system, and develop and verify conceptual and numerical models of these interactions.

APPROACH: Construct simple model that preserves the most important features of the hydrodynamic characteristics. Improve this computer program to bring secondary mechanisms into the model. Collecting hydrodynamic data, to provide information for use in calibration of the mathematical model, and other information, such as meteorological data. Modify modeling concepts and measurement techniques to permit most effective construction and use of the model.

PROGRESS: An interagency modeling group for San Francisco Bay was formed in 1985. The participating agencies include the Department of Water Resources, State of California, Bureau of Reclamation, Fish and Games, and California District Office, and U.S. Geological Survey, among others. This interagency modeling group has been proven to be an effective mechanism through which collaboration on research among various government agencies is carried out. Basic research continued on the subject of Lagrangian aspects of circulation properties in estuaries. By following a Lagrangian point of

view, it has been shown that the Lagrangian residual circulation, not the Eulerian residual circulation determines the transport of solutes in estuaries over an intertidal time scale (see Feng, Cheng, and Xi, 1986). Following the same line of thinking, computational methods can be formulated by taking advantage of the Lagrangian nature of the physical processes. By following a Lagrangian point of view with the aid of Eulerian computational grids, computational methods have been developed based on combined Eulerian-Lagrangian Methods (ELM). This approach is general and is particularly relevant to all water resources problems (surface water, ground water, transport of solutes) for which the flow processes are convection dominated. Preliminary results are very encouraging.

REPORTS PUBLISHED:

Cheng, R. T., Feng, Shizua, and Xi, Pangen, 1986, On Lagrangian residual ellipse, in van de Kreeke, J., ed., Physics of shallow estuaries and bays: New York, Springer-Verlag, p. 102-113.

Feng, Shizua, Cheng, R. T., and Xi, Pangen, 1986, On tide-induced Lagrangian residual current and residual transport--part I, Lagrangian residual current: Water Resources Research, v. 22, no. 12, p. 1623-1634.

Feng, Shizua, Cheng, R. T., and Xi, Pangen, 1986, On tide-induced Lagrangian residual current and residual transport--part II, residual transport with applications in South San Francisco Bay, Calif.: Water Resources Research, v. 22, no. 12, p. 1635-1646.

Smith, L. H., and Cheng, R. T., 1987, Tidal and tidally averaged circulation characteristics of Suisun Bay, Calif.: Water Resources Research, v. 23, no. 1, p. 143-155.

WR156 POLARIS OPERATIONS

TITLE: Research Vessel Polaris Operations in San Francisco Bay and Adjacent Coastal Ocean

PROJECT NUMBER: WR 77-156

LOCATION: Topical Research

PROJECT CHIEF: Conomos, T. John

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: A stable moving platform is needed to house at least ten scientists throughout the year (for periods of weeks) so that large volumes of complex and continuous data can be carefully and rapidly collected and precisely measured and analyzed immediately after collection.

OBJECTIVE: Provide scientific platform (research vessel) for estuarine studies, platform functions and measurement, collection, and subsequent analysis of geological, chemical, physical, and biological data throughout the year for extended time periods.

APPROACH: Provide support for research vessel including operating support for dockage fees, boat maintenance, diesel fuel and food for crew.

PROGRESS: Provided research vessel support for several projects whose research is directed in San Francisco Bay and other Pacific Coast estuarine systems.

WR175 ALASKA GLACIOLOGY

TITLE: Alaska Glaciology

PROJECT NUMBER: WR 66-175

LOCATION: Alaska Statewide

PROJECT CHIEF: Mayo, Lawrence R.

HEADQUARTERS OFFICE: Fairbanks, AK

PROBLEM: Glaciers produce 25 to 50 percent of the river runoff and the highest flood runoff in Alaska. Glaciers comprise the largest freshwater storage system in Alaska and also in the world, and change rapidly with small changes in climate. The basic stability and instability mechanisms of glacier flow and glacier hydrology are poorly understood or, as yet, undiscovered. Verification of hypotheses is slow because continuous high quality data of climate, glacier-mass exchange, glacier-flow behavior, and glacier hydrology are limited to short time periods at a few glaciers in Alaska. As a result, a proven conceptualization of the processes is inadequate, and predictive models are either nonexistent or generally inadequate to assess even simple problems such as predicting the effect of a 1 degree Celsius warming of the climate.

OBJECTIVE: (1) Measure and analyze mountain climate and glacier processes to verify or discover cause-and-effect relationships and determine response characteristics of glacier-related hydrologic systems; (2) study regimes of glaciers that present specific types of hazards or benefits; (3) understand the complete cycle of glacier behavior, advise of specific hazards, assess glaciers as a resource, and develop and use methods of prediction of glacier behavior; and (4) assess the importance of Alaskan glaciers to interpretation of climate.

APPROACH: Maintain instrumentation at several glaciers of different climate areas to obtain continuous measurements of high-altitude climate, snow and ice balance, and glacier flow. Analyze baseline data; develop new techniques in glaciology; conduct research studies at hazardous surging glaciers, ice-dammed lakes, calving glaciers, and other glaciers as needed, to obtain new knowledge of these hazards; and develop new scientific knowledge of glaciological principles and processes. Develop numerical models relating climate to glacier balance, glacier flow, and glacier runoff.

PROGRESS: Determined a method to estimate runoff rate from glaciers in Alaska using information shown on topographic maps. Calculated the amount of water that refreezes within glaciers. Analyzed the rapid advance of the Hubbard Glacier which dammed Russell Fiord and advised U.S. Forest Service and people of Yakutat about the impacts to expect.

REPORTS PUBLISHED:

Mayo, L. R., 1986, Annual runoff rate from glaciers in Alaska; a model using the altitude of glacier mass balance equilibrium: American Water Resources Association, p. 509-517.

Benson, C. S., Harrison, W. D., Gosink, J., Bowling, S., Mayo, L. R., and Trabant, D. C., 1986, Workshop on Alaskan Hydrology--problems related to glacierized basins, final report: University of Alaska, Geophysical Institute Report UAG-R (306), 106 p.

Benson, C. S., Harrison, W. D., Gosink, J., Bowling, S., Mayo, L. R., and Trabant, D. C., 1986, The role of glacierized basins in Alaskan hydrology, in Kane, D. L., ed., Symposium--Cold Regions Hydrology: American Water Resources Association, p. 471-483.

WR183 ANALYSIS AND MODELING OF TRANSPORT PROC

TITLE: Analysis and Modeling of Conservative and Nonconservative Transport Processes

PROJECT NUMBER: WR 83-183

LOCATION: Central California, Southeastern Alaska

PROJECT CHIEF: Walters, Roy A.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: The biological and chemical characteristics of aquatic environments depend upon a generally complicated balance of physical, chemical, and biological processes. An understanding of transport processes, including both advection and mixing is basic to describing these characteristics for a given water body; these processes depend heavily on the mass, momentum, and energy transfers at boundaries and the internal response of the system. Many of these transfers and responses are poorly understood and the interaction between man's activities and the natural processes is uncertain.

OBJECTIVE: (1) Understand the physical processes responsible for the transport of conservative and nonconservative solutes of biological and chemical importance; and (2) develop conceptual statistical, and numerical models of these processes through the use of time series analysis and other methods.

APPROACH: Use both data analysis and numerical models as diagnostic tools. The data analysis includes, but is not limited to, the application of digital filters to examine daily the seasonal time-scale phenomena, spectral analysis, empirical orthogonal function analysis, and multiple regressions. The numerical models include both box and finite element models in one, two, and three dimensions.

PROGRESS: Analysis of current meter, sea level, and salinity data has led to an improved understanding of circulation and mixing at both tidal and low-frequency time scales for San Francisco Bay. Development of finite-element tidal and residual circulation models has allowed quantitative estimates of rates of physical processes, and residence times. Interdisciplinary studies include development of an ecosystem model for south San Francisco Bay, time-series analysis of glacier speed with respect to perturbations in sea level at the terminus, an oceanographic investigation of subglacial outflow of fresh water into an unusual Alaskan fjord, and an investigation of the variations in glacial mass balance in relation to large-scale climatic influences.

REPORTS PUBLISHED:

Walters, R. A., and Dunlap, W. W., in press, Analysis of time series for glacier speed, Columbia Glacier, Alaska: Journal of Geophysical Research, 24 p.

Walters, R. A., 1986, A finite-element model for tidal and residual circulation: Communications in Applied Numerical Methods, v. 2, p. 393-398.

WR187 FLOW AND GEOCHEMICAL INTERACTIONS

TITLE: Coupled Transport and Geochemical Processes Determining the Fate of Chemicals in Surface Waters

PROJECT NUMBER: WR 84-187

LOCATION: Topical Research

PROJECT CHIEF: Bencala, Kenneth E.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Chemicals introduced into a stream react in response to a variety of homogeneous and heterogeneous geochemical processes. Transport characteristics of these chemicals are affected by such processes and biota may be influenced. The interactions are both physical and chemical, and occur over a wide range of time and distance scales. Although individual processes may be well understood, the coupling of the processes is not. The ability to quantify the interactions is very limited. The combined transport and geochemical processes determine the fate of chemicals naturally present in the environment as well as those introduced by anthropogenic activities.

OBJECTIVE: (1) Improve knowledge of the mechanisms of solute transport in streams; (2) develop experimental field techniques and mechanistic formulations of reactive transport for solute-solid interaction; (3) develop solute-transport models which are consistent with the availability of parametric field information and field verification data to aid in our ability to interpret and quantify processes; and (4) as the need arises, develop techniques for parameter estimation and model verification.

APPROACH: Analyze data from detailed dynamic field experiments. Work in pristine and acid-impacted streams. Concentrate on: (1) Development of experimental field techniques; (2) development of conservative simulations to quantify hydrologic processes, and (3) development of reactive simulation codes to quantify specific geochemical interactions. Work in the mountain-watershed environment. Study headwater streams because they form the 'boundary conditions' for larger stream systems and thus collectively influence regional water quality. Cooperate with other scientists interested in quantifying transport interactions in stream ecosystems.

PROGRESS: Small scale spatial and temporal variations of stream chemistry were studied in the naturally acidic Snake River. The results emphasize the importance of reconnaissance sampling over a range of process scales in establishing monitoring programs for studies of upland watersheds. Field studies were conducted in St. Kevin Gulch, a stream in the upper Arkansas River Basin near Leadville, Colo., to determine the magnitude for metal source and removal processes in this toxic mine drainage. Field experiments documented rapid exchange of solutes between differing chemical environments in the stream and subsurface gravel zones of Little Lost Man Creek, Calif.

REPORTS PUBLISHED:

Zellweger, G. W., Kennedy, V. C., Bencala, K. E., Avanzino, R. J., Jackman, A. P., and Triska, F. J., 1986, Data on the solute concentration within the subsurface flows of Little Lost Man Creek in response to a transport experiment, Redwood National Park, northwest California: U.S. Geological Survey Open-File Report 86-403W, 72 p.

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WATER CHEMISTRY

CR046 ORGANIC HYDROGEOCHEMISTRY

TITLE: Origin, Characterization, and Quantification of Natural Organic Solutes in Water

PROJECT NUMBER: CR 68-046

LOCATION: Topical Research

PROJECT CHIEF: Malcolm, Ronald L.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: More than 90 percent of the organic solutes in water are of natural origin; yet, little is known about the chemistry or source of these organic materials. However, these substances are known to complex trace metals, to transport pesticides, to be precursors of carcinogen compounds upon chlorination, and to be a food source for aquatic organisms. These processes need further clarification and quantification.

OBJECTIVE: (1) Identify and quantify organic solutes that affect water-quality processes; (2) measure the amount of different organic solutes in various hydrologic environments; (3) understand the origin, structure, and reactivity of aquatic humic substances; (4) predict the processes that affect the fate and movement of organic solutes in surface and subsurface environments; and (5) determine the effect of natural organic solutes in water purification: reverse osmosis, chlorination, activated charcoal, and ozonation.

APPROACH: (1) Conduct intensive stream sampling of the Yampa, Ohio, Missouri, and Ogeechee Rivers to determine climatic, geologic, and seasonal variations in natural organic substances; (2) characterize organic matter from water, soils, and plants in wetland environments to determine origin and source; (3) cooperate with other researchers and District personnel in programs that emphase organic-contaminant movement in ground water; and (4) predict the amount and variety of chlorinated compounds in water from the characterization of natural organic matter.

PROGRESS: A large part of the time was spent writing and reviewing the many scientific reports completed by the research project. Stream and lake humic substances were isolated from several sites in Norway. The suite of Norwegian samples and the humic isolates from the Pacific Ocean have been characterized by liquid and solid-state carbon-13 nuclear magnetic resonance spectroscopy, elemental analysis, infrared spectroscopy, pyrolysis-mass spectroscopy, and various methods for molecular weight.

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CR132 ORGANIC POLYELECTROLYTES

TITLE: Behavior of Natural Polyelectrolytes in Water

PROJECT NUMBER: CR 68-132

LOCATION: Topical Research

PROJECT CHIEF: Wershaw, Robert L.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: Natural organic polyelectrolytes are highly active materials that are present in practically all natural water systems. They interact with both organic and inorganic pollutants and nutrients, influencing, and in many instances, controlling the toxicity, rate of movement, persistence and rate of degradation of the pollutants and nutrients in aquatic environments. Detailed knowledge of the chemistry of natural organic polyelectrolytes is of primary importance in understanding the chemical changes that affect all components of natural water systems. Organic polyelectrolytes are partially eliminated from drinking water by coagulation and chlorination; however, the products of chlorination are not known. Both natural and synthetic organic compounds are present in all natural waters. Some of these compounds are toxic or mutagenic; therefore, it is important that they be identified and quantified in surface and ground water and in precipitation. Many organic substances are difficult to ionize in the source of a mass spectrometer because of this thermal instability, involatility, molecular size, or their polar nature. Ionization of these types of compounds can be achieved by using the recently developed Fast Atom Bombardment (FAB) ion source. This ion source sputters ions representative of the molecule at ambient temperatures. In addition, molecular structural information is produced.

OBJECTIVE: (1) Isolate the various organic polyelectrolytes present in natural water systems; (2) determine the physical and chemical properties of the most abundant organic polyelectrolytes; (3) elucidate the mechanisms of interaction of pollutants with natural organic polyelectrolytes; (4) determine types of chemical compounds that result from the chlorination of natural polyelectrolytes; (5) characterize the effect of organic polyelectrolytes on the chemical speciation of major cations (Na, Ca, K) and trace metals (Cu and Fe) in water; (6) develop nuclear magnetic resonance spectroscopy methods for the characterization of humic materials; (7) develop mass spectrometric methods for the analysis of organic compounds in natural waters; (8) determine and characterize organic pollutants in ground water and precipitation; (9) characterize the interaction of organic pollutants from precipitation with soil systems; (10) optimize operating parameters of the FAB source; (11) investigate various substrates for sample introduction; (12) study effects of different neutral bombardment atoms; and (13) characterize spectra obtained for various compound functionalities.

APPROACH: (1) Isolate chemically unique polyelectrolyte fractions by using column chromatography, electrophoresis, and other techniques; (2) determine the physical and chemical properties of the fractions by using small angle x-ray scattering, ultracentrifugation, and atomic, molecular, and magnetic spectroscopy; (3) use carefully characterized organic polyelectrolyte fractions in experiments designed to elucidate the sorption and solubilization reaction of pollutants and nutrients with natural organic polyelectrolytes; (4) characterize behavior of aquatic fulvic acid as an electrolyte by potentiometric titration; (5) characterize of effect of fulvic acid on activity of Na, K, and Ca by dialysis and specific-ion-electrode measurements; (6) characterize effect of major cations on the complexation of Cu by fulvic acid by potentiometric titrations that measure cupric ion activity and by ultraviolet-titrations that measure absorbance of the charge-transfer band associated with Cu-fulvic acid complex; (7) evaluate the effect of fulvic acid on the activities of major cations and trace metals in different aquatic environments by chemical equilibria calculations and analysis of field samples; (8) isolate organic pollutants from water systems; (9) identify and quantitate these pollutants; (10) identify important operating parameters of the FAB source; (11) select plausible sample substrates and investigate their effects on different compound types; and (12) optimize source parameters with respect to (a) compound functionality; (b) different bombardment atoms; and (c) different substrate materials.

PROGRESS: (1) The humic acid from a tropical podzolic soil from the Amazon Basin of Brazil was extracted and fractionated. Although the fractionation pattern was similar to that obtained from humic acids from temperature climates, the Nuclear Magnetic Resonance (NMR) spectrum of some of the fractions were different; these results apparently indicate a much different source for the carbohydrates in the soil. (2) Working with Dr. J. A. Marinsky of the State University of New York at Buffalo in an attempt to fit measured acid-base titration data of humic substances to a generalized physical chemical model of humic substances, the micelle model of humic materials proposed by Wershaw and mathematical model which Marinsky has used to describe his titration data were found to lead to the same results. (3) A symposium on the NMR spectroscopy of humic substances and coals was organized for the regional American Chemical Society meeting in June of 1986 and a book resulting from the meeting was completed. (4) A study of the molecular weight distributions of humic acid fractions by field flow fractionation was initiated in cooperation with Dr. Ronald Beckett of the Water Studies Centre of Chisholm Institute of Technology, Australia; results indicate that each of the fractions has a distinctive molecular weight distribution. (5) A comprehensive set of NMR analyses of lake, stream, swamp, bog, and marine fulvic and humic acids was completed. This study, the most detailed set of structural analyses ever performed on aquatic humic substances, concluded that most freshwater fulvic and humic acids are very similar to one another from one environment to another, with some subtle differences in concentrations of weakly acidic versus strongly acidic hydroxyl groups, but that major differences exist between freshwater

and marine fulvic acids. (6) Carbon-13 NMR has been used to identify detergents from a contaminated ground water. (7) The non-volatile hydrophobic and hydrophilic organic acids from a contaminated ground water have been isolated and characterized by carbon-13 NMR. This study is the first to isolate the non-volatile organic acids resulting from the degradation of crude oil, and has provided new information on the mechanistic chemistry of the degradation of crude oil in the subsurface. (8) Preliminary results have been obtained in a comprehensive evaluation of advanced one and two dimensional NMR of humic substances. (9) Preliminary results from a study of the organic acids present in the DOC plume down-gradient of the oil spill at Bemidji, Minn., indicate that there is a complex mixture of organic acids and that the aromatic and isoparaffinic compounds of the oil were selectively preserved as the carboxylic acids. (10) A molecular weight study of aquatic fulvic acids has been completed. (11) Work has commenced on the isolation and characterization of hydrophilic organic acids from natural waters.

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CR199 CHEMISTRY OF SEDIMENT SURFACES

TITLE: Water Chemistry of Sediment Surface Coatings

PROJECT NUMBER: CR 76-199

LOCATION: Topical Research

PROJECT CHIEF: Goldberg, Marvin C.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Local chemical composition of natural waters is heavily influenced by sediment surface reactions. Because of sorption phenomena on sediment surfaces, sediments carry larger concentrations of many materials, such as trace metals, pesticides, salts, than water does. The sorbed species may move in either direction across the solid-liquid interface in response to changes in chemical potential set up on either side of the interface. Sediment act as sources, sinks and carriers of a variety of chemical species; to understand the processes controlling a main source of materials that enter and exit water systems, the variety of reactions that govern the distribution of chemical species between the solid and liquid phases must be understood. The solid phase acquires coatings as a consequence of its prior reactive history; these coatings are an important characteristic in determining the current surface chemical reactivity. An understanding of the coating process, chemical composition of the coating, and chemical reactivity of the coatings when exposed to various bulk water compositions is a prerequisite for definition, prediction, and perhaps manipulation of water quality.

OBJECTIVE: (1) Examine natural sediment surfaces to elucidate their surface chemical composition so that the rate-determining sorption processes that occur on these surfaces are described for various particle coatings; (2) correlate these sorption reactions with specific molecular species that reside on the surface; and (3) examine the chemical processes by which sediment coatings are formed and determine the nature of the bonding between coatings and sediment surfaces.

APPROACH: Use spectroscopic methods, mainly Fourier transform infrared spectoscopy, Laser Ramam spectroscopy, and three-dimensional fluorescence spectroscopy, to determine the surface chemical composition of natural and prepared sediment coatings. Obtain supplemental information on the surface composition with Auger and Low Electron Excitation spectroscopy. Examine a natural sediment-water system containing Gibbsite or Geothite type coatings. Simultaneously, synthesize laboratory coatings of the same materials. Study the sorption reactions of materials to understand the surface-bonding mechanism of the coating and of the sorbing material, the surface chemical reactivity to these species, and the speciation of each sorbed component. Characterize fluorescence organic surface coatings and micelles in natural

water samples to evaluate the sorption influence of these materials on local water composition. Conduct studies jointly with the Louisiana District and other research projects to obtain information needed to define the role of some of the bottom coatings on the uptake and release of elements held on the sediment surfaces in Lake Bruin, to use three-dimensional fluorescence spectroscopy to characterize natural organic coatings as an aid in understanding very low dissolved solute waters, and to use three-dimensional fluoresecence spectroscopy to obtain definitive information on humic acid fraction patterns and augment studies of the formation of charge-transfer complexes.

PROGRESS: PS < Abiotic photolytic processes that are operative in natural aquatic systems were investigated with special emphasis on understanding the mechanisms of the reactions. Photolysis for the goethite-ligand system initiates a photoredox reaction producing iron 2 and simultaneously oxidizes the adsorbed organic ligand. Adsorption takes place on three different types of sites and is very pH sensitive so that our mechanisms include site sorption, surface area of the lithologic substrate, number of binding sites, types of binding sites, as well as hydroxyl ion concentration and concentration of the adsorbate. Photolysis of monocarboxylates, such as benzoic acid, when adsorbed to crystalline iron oxides, produces a hydroxy radical from secondary photolysis of Fe^{+2} in solution. This reacts with crystalline iron to yield more reduced Fe^{+2} in solution. Because of this reaction, the rate of iron dissolution for these materials is more than indicated by the lyotropic series of iron production. Crystalline iron dissolution is enhanced by the presence of the hydroxyl radical; conversely, it was found that amorphous iron dissolution is enhanced in the absence of hydroxyl radical or organic reducing agents. Amino acids were found to photolytically react when adsorbed to goethite in water suspensions. The reaction mechanism is comprised of 19 single step reactions which in summary describe the reduction of lattice Fe(III) to solution Fe^{+2} and the concurrent formation of a carboxyl radical on the amino acid which rapidly oxidizes to CO_2. All 19 radical reaction sequences were mathematically evaluated as to their role in the overall reaction by listing each kinetic step in the form of a differential equation and a computer model developed. Fractionated humic materials that were separated on the basis of hydrophilicity and proton affinity were examined by fluorescence spectroscopy. It was found that the Hydrophobic Humic Strong Acid (HHSA) had an aqueous equivalent sphere volume of 9800 cm^3, volumes of the other fractions in cm^3 were: The Hydrophilic Acid (HA), 4000; Hydrophobic Humic Weak Acid (HHWA), 3600; Hydrophobic Strong Acid (HSA), 3350; Hydrophobic Weak Acid (HWA), 3000; Hydrophobic Neutral (HN), 1300. Aqueous shape factors were as follows: HHSA- spherical; HA- spherical; HHWA- very aspherical; HSA- almost spherical, there was a slight asphericity; HWA- slight asphericity; HN- spherical.

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CR223 TRANSURANIUM RESEARCH

TITLE: Transuranium Research

PROJECT NUMBER: CR 77-223

LOCATION: Topical Research

PROJECT CHIEF: Cleveland, Jesse M.

HEADQUARTERS OFFICE: Lakewood, CO

PROBLEM: Information is very limited on the speciation (oxidation state, hydrolysis, rate of formation and stability of complexes with natural organic and inorganic substances) of plutonium and other transuranium elements in ground waters. These speciation data are vital to the accurate prediction of solubilization, transport, and distribution of these long-lived radioactive elements from radioactive-waste repositories over the long term.

OBJECTIVE: Define the chemical and physical speciation and the chemical and hydrologic behavior of transuranium elements (primarily plutonium) in contaminated ground waters.

APPROACH: Obtain contaminated ground waters from shallow land radioactive waste-disposal sites, or from laboratory-leaching experiments on candidate solid-waste forms with actual ground waters from relevant geologic formations, or from direct addition of radioactive solutions to ground waters. Determine speciation of the plutonium by the following procedures: (1) Establish presence of colloids by sequential sub-micron filtration; (2) determine oxidation state distribution extraction and carrier precipitation; (3) establish presence and identity of complexes with natural organic and inorganic substances by ion exchange and other techniques, and determine stability of such complexes if warranted; and (4) in the case of contaminated ground waters prepared by leaching experiments, repeat steps 1-3 using solutions prepared from different ground waters and at various leaching times, temperatures, pH values, and dissolved oxygen concentrations.

PROGRESS: Analysis and interpretation have been completed, and a paper has been written describing speciation of plutonium, neptunium, and americium in twelve ground waters that have possible relevance to nuclear waste disposal and two surface waters that were selected because of their chemical interest. Based on these results, which showed the strong influence of the redox properties of ground waters on plutonium speciation, a potentiostat-galvanostat has been acquired and preliminary studies have been initiated to determine plutonium speciation as a function of the potential applied on the ground water by the potentiostat-galvanostat. In support of this study, a rapid simple procedure for separating the four common oxidation states of plutonium by thenoyltrifluoroacetic acid (TTA) extraction has been developed. Scouting experiments have indicated that actinide elements form complexes with sulfite

ions, as indicated by color changes. The same color change is observed with thiosulfate, but not with sulfate, suggesting the possible existence of complexes with metal-sulfur bonds. To investigate this surprising possibility, two studies are underway, one on the kinetics of reduction of hexavalent actinides by sulfite ion, and another to determine the stability constants of sulfite complexes of trivalent actinides.

CR275 ORG. GEOCHEM OF GROUND WATER

TITLE: Organic Geochemistry of Ground Water; Interstial, and Pore Waters - the Effects of Pollution

PROJECT NUMBER: CR 82-275

LOCATION: Topical Research

PROJECT CHIEF: Thurman, Earl M.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: Hazardous wastes, both liquid and solid, contaminate ground water and soil interstial waters throughout the nation. These wastes decompose both chemically and biologically; the result is a different waste product that is chemically stable and mobile in ground and soil waters. The waste product is a high molecular-weight organic acid, a product of anaerobic decomposition. These polymeric substances contain pollutants within their structure, carry or complex simple organic compounds and trace metals, and may be toxic in themselves. Because they do not extract into organic solvents, they are not analyzed by conventional methods, such as gas chromatography, and little is known of their structure, chemistry, and toxicity. Yet, they make up 50 percent of organic wastes from solid-waste disposal and, perhaps, 25 percent of organic wastes from liquid disposal.

OBJECTIVE: (1) Characterize the polymeric substances in contaminated ground water and compare with natural substances, both structure and reactivity; (2) determine their biologic toxicity and their hazardous nature; (3) understand their function in transport of simple pollutants in ground and soil interstial waters, and (4) model their role in the toxicity and movement of hazardous wastes.

APPROACH: (1) After carefully selecting a waste disposal site, characterize high molecular weight organic wastes by conventional methods including: elemental analysis, molecular weight, and functional group analysis; (2) determine toxicity of the polymeric substances by Ames testing and compare with natural polymeric material; (3) measure the ability of the polymeric organic matter to complex simple pollutants and trace metals; and (4) model and coordinate results with scientists working on simple organic pollutants and ground water flow in the Hazardous Waste Program.

PROGRESS: The Organic Geochemistry of Ground Water Project is actively working on organic and inorganic chemistry of a sewage contaminated aquifer at Cape Code, Mass. The structure of alkyl benzene sulfonates (ABS), linear alkyl sulfonate (LAS), and nonionic surfactants have been identified using ^{13}C-nuclear magnetic resonance (^{13}C-NMR) spectrometry and used these compounds as time markers in the ground water. We also have identified many volatile and semi-volatile contaminants in the ground water and modelled their transport with a template program. We also have used the carbon content of the aquifer solids and the Kow of the compounds to predict their mobility in ground water.

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CR278 TRANSPORT OF HAZARDOUS WASTES

TITLE: Origin, Fate, and Transport of Hazardous Wastes in the Sub-Surface Environment

PROJECT NUMBER: CR 83-278

LOCATION: Topical Research

PROJECT CHIEF: Pereira, Wilfred E.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: A large number of hazardous organic compounds derived from industrial, agricultural, and domestic sources has become a major problem in the management of ground-water quality. The problem is further compounded by the complex physico-chemical behavior of organic contaminants and a lack of knowledge of fundamental processes governing their fate and transport in the subsurface environment. Organic compounds that pose the greatest threat to the quality of ground-water resources are those that are relatively soluble, nonvolatile, and refractory. New analytical techniques are needed to determine these refractory organic compounds in complex mixtures so that information on their origin, fate and transport in the subsurface environment can be obtained.

OBJECTIVE: (1) Develop new analytical methods for the determination of selected refractory organic compounds in ground-water and aquifer materials; (2) investigate new instrumentation for the determination of selected organic compounds in complex matrices; (3) describe the organic geochemistry of ground-water systems; (4) study movement and fate of organic compounds in ground water; and (5) develop chemical criteria for assessing environmental impact of hazardous organic compounds on ground-water quality.

APPROACH: (1) Study ground-water and aquifer-materials samples from a coal tar disposal site in St. Louis Park, Minnesota; (2) evaluate isolation procedures involving "state-of-the-art" techniques such as solvent extractions, preconcentrations, and resin absorption; (3) Use low- and high-resolution mass spectrometry, and ancilliary techniques such as infrared spectrometry, and HPLC (high pressure liquid chromatography) with both ultraviolet and fluorescence detectors to definitively characterize organic compounds; and (4) study microbiological degradation and metabolic pathways of selected pollutants, and characterize intermediates and end products of microbial transformations.

PROGRESS: Geochemical studies were conducted to better understand the movement and fate of polynuclear-azaheterocyclic compounds, or azaarenes, in aquifers contaminated by wood-treatment chemicals. Two- and three-ring azaarenes and their oxygenated and methylated derivatives were identified in ground water by gas chromatography-mass spectrometry. The presence of oxygenated azaarenes in anaerobic zones of ground water suggested that these compounds probably were microbial-transformation products. Laboratory anaerobic-degradation studies were designed to investigate metabolic pathways of azaarenes. Microbial metabolic-transformation products of quinoline, isoquinoline, and 4-methylquinoline identified in laboratory anaerobic cultures were identical to those detected in contaminated ground water at two hazardous-waste sites. Microbial N-, C-, and O-methylation reactions were reported for the first time, and partial metabolic pathways were elucidated. Distributions of azaarenes in anaerobic zones of ground water indicated that two-ring azaarenes are degraded by indigeneous microorganisms. Oxygenated derivatives of azaarenes are more water soluble, mobile, and biorefractory than parent azaarenes; hence, they are more persistent in contaminated aquifers. Mechanistic studies using $H_2{}^{18}O$ demonstrated that under aerobic and anaerobic conditions, the oxygen atom of water is enzymatically incorporated, as hydroxyl, into the quinoline molecule. Haloarenes derived from anthropogenic activities were identified and quantitated in bed sediments of the Calcasieu River. In waters of high salinity and conductivity, the water solubility of these compounds is decreased and hence their partition coefficients are significantly increased, resulting in a "salting-out" effect. Therefore, these sediments serve as a major sink for the haloarenes. The "salting-out" effect observed for the haloarenes indicates the importance of estuarine sediments in determining the geochemical transport and fate of hydrophobic organic pollutants. Haloarene isomers are differentially sorbed on suspended and bed sediments during transport in the Calcasieu River. Sorption/desorption processes at the sediment-water interface affect the distribution of haloarene isomers, resulting in a "chromatographic effect." Studies of distributions of halogenated organic compounds in different compartments of the Calcasieu River estuary (biota, bottom, and suspended sediments and the water column) suggested that contaminant distributions in biota, suspended sediments and the water column were closer to equilibrium than contaminant distributions between biota, bottom sediments, and the water column. Bioconcentration factors were determined and found to be in reasonable agreement with literature values. Equilibrium distribution patterns provide a useful basis for assessing the impact of system dynamics on fate and transport of halogenated organic compounds in estuarine systems.

REPORTS PUBLISHED:

Pereira, W. E., Rostad, C. E., Updegraff, D. M., and Bennett, J. L., 1987, Fate and movement of azaarenes and their anaerobic biotransformation products in an aquifer contaminated by wood-treatment chemicals: International Journal of Environmental Toxicology and Chemistry, v. 6, p. 163-176.

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CR282 ANALYTICAL CHEMISTRY OF INORGANICS

TITLE: Research in the Analytical Determination of Inorganic Constituents in Water and Water Related Materials

PROJECT NUMBER: CR 83-282

LOCATION: Topical Research

PROJECT CHIEF: Taylor, Howard E.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: The determination of inorganic constituents in water and water-related materials (that is, suspended matter, bottom sediment, and so forth) in a sensitive, accurate and efficient manner, requires highly sophisticated analytical methods and plays a significant role in the study of water quality and environmental chemistry. These methods employ instrumentation based on physical and chemical properties and phenomena. The solution of analysis problems (sensitivity, selectivity, interference effects, data collection/reduction and system automation) often requires the design and construction of suitable laboratory and field instrumentation and apparatus. The study of specialized analytical problems, such as chemical speciation, also requires unique approaches. In addition, the adaptation of analytical chemistry technology to the solution of specific environmental chemistry and water quality hydrologically related problems requires an extensive research and development effort both in the laboratory and the field.

OBJECTIVE: (1) Investigate new concepts and approaches to the analysis of inorganic constituents in water with an emphasis on trace metals; (2) formulate methods and procedures for utilization of new field and laboratory techniques and instrumentation; (3) study specific water quality and environmental chemistry problems; (4) participate in water disciplinary research programs; and (5) provide consultation to other projects and programs in the U.S. Geological Survey.

APPROACH: (1) Maintain a periodic review of pertinent scientific literature, and communicate frequently with colleagues and consultants who are involved in similar research and development programs; (2) identify areas where improvement of existing technology can offer extended analysis capability and efficiency; (3) design and perform laboratory and field experiments that will elucidate the significance of parametric variations in water quality and environmental chemistry using statistical and factorial techniques to optimize and evaluate parametric factors; (4) prepare definitive reports and publications outlining the research findings and interpretation of data from water quality and environmental chemistry studies.

PROGRESS: (1) Studies on the occurrence and distribution of trace metals in pristine lakes (Fremont & New Fork, Wyoming and Emerald Lake, Sequoia National Park) continued, and preliminary evaluations of important geochemical and atmospheric (acid rain) inputs were made. (2) Development of technology for the direct measurement of ultra-trace (nanogram/liter) concentrations of constituents in hydrologic systems by inductively-coupled plasma mass spectrometry continued. Techniques were pioneered for the measurement of stable isotope ratios of selected heavy metals at trace (microgram/liter) concentration levels in natural waters and for absolute quantitation by stable isotope dilution analyses. (3) Research on the use of osmosis and reverse osmosis techniques for preconcentrating heavy metals in highly dilute hydrologic systems prior to chemical analysis began. Apparatus was designed and fabricated for the effective utilization of this approach for preconcentration of heavy metals in rainwater. (4) The use of chelating ion exchange resins to collect and concentrate trace metals from atmospheric precipitation was evaluated and found suitable for field studies. (5) Filters from snow cores from the Cascade/Sierra Nevada Mountains, primarily sampled for solute chemistry, were being studied to determine the distribution and chemical nature of particulates. (6) Research on the measurement of time-resolved ultraviolet absorption spectra from thermally vaporized organic compounds was completed. A unique approach using multi-wavelength photodiode array detection with an electrothermal graphite furnace atomizer was studied. (7) Research was performed on the development of a technique suitable for measurement of field alkalinity using a micro-computer-controlled coulometric titration. (8) Collaborative research with the Geological Survey of Israel was performed to characterize the trace metal chemical composition of highly saline waters and brines.

REPORTS PUBLISHED:

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CR283 SORPTION AND PARTITION PHENOMENA

TITLE: Environmental Dynamics of Persistent Organic Compounds

PROJECT NUMBER: CR 83-283

LOCATION: Topical Research

PROJECT CHIEF: Chiou, Cary T.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: Many persistent organic compounds are hazardous to environmental health. The transport characteristics of the compounds across environmental phases are only qualitatively understood. Quantitation of process rates and partition constants of organic pollutants in air, water, soil, and biota is an important step in defining the level of contaminants in environmental media and the pathway of chemical exposure to man.

OBJECTIVE: Delineate and quantitate the processes affecting the movement and distribution of persistent organic solutes in environmental systems. Specifically (1) determine the sorptive capacity of soil and sediment from air and water; (2) specify the roles of soil, sediment organic matter, mineral components, and moisture content on the sorption process; and (3) establish the physical basis of bioaccumulation of organic solutes from water.

APPROACH: Conduct laboratory experiments to determine the sorption of various organic compounds initially from water; consider thermodynamic properties of the compounds and soil constituents in analyzing data. Determine sorption from the vapor phase to illustrate the effect of soil moisture content on sorptive process and capacity. Measure and interpret the partition coefficients of solutes between liquid and water. Collaborate with other researchers to relate laboratory findings with field data from hazardous waste sites.

PROGRESS: (1) Sorption of vapors of benzene, trichloroethylene, and water by various types of organoclays, and sorption of benzene and trichloroethylene from water on these organoclays were investigated to examine the sorption characteristics as influenced by clay, organic constituents and water present in the organoclays. Results show that certain organic ligands (for example, tetramethyl ammonium groups) strongly modify the clay surface, making it less susceptible to water competition in adsorption of organic solutes. By contrast, long-chain organic ligands attached to clay behave more like a partition phase for organic solutes. (2) Soil samples from a trichloroethylene-contaminated site in New Jersey were used to determine their sorption capacities for water and TCE (trichloroethylene). The water uptake capacity was compared to the field moisture content to determine the degree of water saturation needed to characterize TCE sorption by soil. TCE sorption by soil as a function of humidity also was studied in the laboratory, to determine a reference to characterize field TCE uptake by subsurface soils whose moisture contents may vary with season.

(3) Many synthetic detergents at below critical-micelle-concentrations (CMC) were found to be very effective in enhancing the solubility of DDT in water. The magnitude of the effect was largely related to the size and structure of the nonpolar hydrocarbon moiety in detergent molecules. The nonpolar moiety having large branch and (or) aromatic groups appear to be most effective. Further testing is being made.

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CR285 COMPREHENSIVE ORGANIC ANALYSIS OF WATER

TITLE: Comprehensive Organic Analysis of Water

PROJECT NUMBER: CR 84-285

LOCATION: Topical Research

PROJECT CHIEF: Leenheer, Jerry A.

HEADQUARTERS OFFICE: Arvada, CO

PROBLEM: The structures and concentrations of natural organic solutes, which comprise most of the DOC (dissolved organic carbon), are very poorly defined. A better knowledge of natural DOC in water is essential to advancement of many diverse sciences, such as geochemistry, aquatic biology, soil science, and even atmospheric chemistry involving carbon-cycle research. The Water Resources Division is conducting significant research on the nature of humic substances in water which comprise about one-half the DOC, but a comprehensive study of the entire suite of organic substances comprising DOC is lacking.

OBJECTIVE: (1) Make comprehensive organic analyses of various surface-water samples, that is "state-of-the-art" organic analyses on as many components of DOC as possible within the time and resource limitations of the project; (2) develop chromatographic methods for DOC separations; and (3) define the chemical, biologic, and hydrologic processes that lead to DOC in water, as the components of DOC are defined chemically.

APPROACH: Field study sites with specific types of organic inputs to DOC have been selected. Algal inputs will be characterized in fresh water (Island Lake, Nebraska) and saline water (Big Soda Lake, Nevada). Terrestrial vegetative contributions to DOC will be studied in the Suwanee River in southern Georgia in a subtropical environment, and in the Yukon River of Alaska in an arctic environment. The effect of salmon migration and die-off in arctic streams upon DOC will also be studied. A few hundred gallons of water will be processed in a mobile field laboratory at each site to isolate several grams of DOC for subsequent characterization. Chromatographic techniques to separate DOC into its constituent compounds will be developed, and the compounds will be structurally determined by various spectrometric techniques.

PROGRESS: A two-stage fractionation scheme based on normal-phase chromatography on silica gel was developed to fractionate the Suwannee River fulvic acid into 31 fractions. Chemical characterization of the fractions show great diversity in chemical characteristics, especially acid-group content, of these subfractions of fulvic acid. Humic and fulvic acid was isolated from the Calcasieu River in Louisiana, and a study with Cary Chiou showed this fulvic acid was five times as active for contaminant partitioning behavior than Suwannee River humic substances. An average structural model constructed for

Calcasieu River humic substances indicated differences in aliphatic hydrocarbon structure and carboxyl-group content may be responsible for increased contaminant-partitioning activity. Most of the chapters for the 17-chapter Water Supply Paper "Suwannee River Fulvic Acid: Interactions, properties and Proposed Structures" have been submitted for Director's approval.

REPORTS PUBLISHED:

Leenheer, J. A., and Noyes, T. I., 1986, Effects of organic wastes on water quality from processing of oil shale from the Green River Formation, Colorado, Utah, and Wyoming: U.S. Geological Survey Professional Paper 1338, 56 p.

Leenheer, J. A., Brown, P. A., and Stiles, E. A., 1987, Isolation of non-volatile, organic solutes from natural waters by zeotrophic distillation of water from N,N- dimethylforamide: Analytical Chemistry, v. 59, p. 1313-1319.

Zepp, R. G., Brown, A. M., Hoigne, J., and Leenheer, J. A., 1987, Photoproduction of hydrated electrons from natural organic solutes in aquatic environments: Environmental Science and Technology, v. 21, p. 485-489.

CR296 Colloid Geochemistry

TITLE: Colloid Geochemistry and Transport Research

PROJECT NUMBER: CR 86-296

LOCATION: Central Colorado

PROJECT CHIEF: Rees, Terry F.

HEADQUATER OFFICE: Denver, CO

PROBLEM: In recent years there has been a growing realization that many organic substances, hazardous materials, heavy metals and radioactiive substances are present in natural waters not as dissolved species, but in association with dispersed microparticulates (colloids). Consequently, an additional mechanism for the transport of these substances is the movement of colloidal materials through the geosphere to the accessible environment. A limited amount is known about the nature of indigenous colloids in surface and ground waters. Similarly, knowledge is limited concerning the interactions of dissolved species with these indigenous colloids. The parameters which control the movement of colloids through different types of aquifers has never been systematically investigated. Because of these three deficiencies, it is impossible to assess the possible importance of colloid-controlled migration of hazardous substances.

OBJECTIVE: (1) Develop a better understanding of the parameters which affect the movement of colloidal materials in surface and ground-water systems; (2) utilizing survey techniques, determine the types of indigenous colloids in a variety of surface and ground waters; (3) study size distributions and surface characteristics; (4) investigate parameters controlling sorption of materials onto colloids; (5) study the parameters which control the movement of colloids in surface and ground-water aquifers; and (6) using these studies, assess the role of colloid-controlled migration of hazardous substances.

APPROACH: (1) Development methods. When possible, modify techniques used in biochemistry, surface chemistry and industrial colloid technology to meet the needs of geochemical investigations. Where this approach does not work, develop new techniques, instruments and procedures. (2) Collect samples from representative aquifer types and surface water to determine the nature of colloidal materials naturally present. Characterize the colloids using ultrafiltration, ultracentrifugation, and photon scattering procedures to determine the physical characteristics (size, shape, and density). Determine the chemical form by standard analytical procedures. Determine surface characteristics by electrokinetic techniques. Determine correlations between water-aquifer type and types of colloids present. (3) Conduct studies to determine the parameters that control the movement of colloids in natural water systems.

Assess the effect of particle size and surface charge characteristics. Study the role of complexation and sorption onto different geologic media. (4) Develop computer models to describe and predict the migration of colloidal materials through ground-water systems.

PROGRESS: Field investigations were begun at the Bemidji, Minn., Pensacola, Fla., Whitewood Creek, S. Dak., and the Upper Arkansas River, Colo., sites. At the Bemidji site, evidence for stable microemulsion formation was developed. Apparently, the organic acids that are microbiologically produced at the site have sufficient surface activity to stabilize the microemulsions. The clays at this site also show significant alteration within the contaminant plume. Two technical talks were given at national meetings about these preliminary findings. First year efforts at Whitewood Creek identified three candidate sites where colloid transport may be occurring. Two of these sites are seeps where ground water has percolated through the tailings to the surface. At one of these sites, colloids were identified using SEM/EDX which contain significant concentrations of arsenic. Preliminary results were presented at a meeting of the American Chemical Society (ACS). A data report has been prepared for the Open-File series, and a paper will be published in a proceedings volume for the ACS meeting. Several sites were identified on the upper Arkansas River where geochemical precipitation is generating significant populations of colloidal iron which may contain other heavy metals. An instrument was developed by project personnel that will allow colloids be sized in-situ without the need to pump a sample to the surface; this down-hole analyzer will be field tested during summer 1987. Project personnel also organized a very successful symposium on Colloid Controlled Migration of Pollutants. A symposium volume is being produced.

REPORTS PUBLISHED:

Rees, T. F., and Ranville, J. F., in press, Colloids in seeps and springs along Whitewood Creek, in Goddard, K., ed., U.S. Geological Survey Applied Research Studies of the Cheyenne River System, S. Dak.: U.S. Geological Survey Open-File Report 87-4051.

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Ranville, J. F., and Rees, T. F., in press, Influence of colloidal particles on the geochemistry of Whitewood Creek, S. Dak.--a preliminary investigation, in Rees, T. F., ed., Colloid controlled migration of pollutants: Washington, D.C., American Chemical Society.

WR036 UNSATURATED ZONE SOLUTES

TITLE: Factors Determining Solute Transfer in the Unsaturated Zone

PROJECT NUMBER: WR 68-036

LOCATION: Topical Research

PROJECT CHIEF: James, Ronald V.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Quality of ground and surface waters often is influenced significantly by chemical and solute-dispersion processes of the unsaturated zone. Frequently, these influences are impossible to predict because the effects of certain relevant, unsaturated zone factors (for example, changes in water content or in the nature of solid surfaces) are understood imperfectly and because the current transport-modelling methods may not be well adapted to the situations encountered in practice. As a result, it may be impossible to assess properly the availability of a given water resource, and to predict the impact of certain human activities and of management upon such availability.

OBJECTIVE: Develop and test theories and mathematical models of reacting-solute transport to enhance the usefulness of such theories and models for assessing the impact of solute transport in the unsaturated zone on water resources and environment quality. Include in the study chemical reactions involving radioactive nuclides as well as reactions of certain solutes found in industrial and agricultural effluents. Develop mathematical models aimed at managing subsurface water quality.

APPROACH: Considering the special conditions encountered in the unsaturated zone, develop new mathematical models, predicting transport of reacting solutes through porous media or at media boundaries. Use theory, numerical methods and controlled experiments. Utilize the interaction between theory and experiment for enhancing the understanding of processes involved. Stress unidirectional transport. Study water-saturated systems with slow, steady water flows and a single, essentially equilibrium-controlled chemical reaction; study steady but unsaturated flows, paying special attention to the influence of water content on chemical and disperion parameters; and study fast, perhaps transient flows and chemical kinetics influences and interactions among several reactions. Develop ground-water pollutant management models that combine numerical-simulation models and management techniques such as linear programming. Initially focus on pollutant-source management in transient one-dimensional systems with linear chemistry. Subsequently, investigate pollutant-source management in two-dimensions with non-linear one-component chemical systems. Use existing simulation models and management models to enhance joint management and simulation capabilities.

PROGRESS: The study of solute transport in unsaturated laboratory columns of Delhi sand continued. The miscible displacement of strontium by calcium yielded the following results: (1) Not all of the strontium initially present in the soil was displaced; (2) the strontium profile depth was found to be less than expected from the initial steady-state concentration of strontium and the concentration of calcium in the displacing solution; and (3) apparent dispersion coefficients for strontium are larger than those for chloride in corresponding experiments. Evaluation of short, off-the-shelf chromatography columns continued with the objective of finding one or more that yield a theoretical response for miscible displacement experiments.

REPORTS PUBLISHED:

James, Ronald V., and Rubin, Jacob, 1986, Transport of chloride ion in a water-unsaturated soil exhibiting anion exclusion: Soil Science Society of America Journal, v. 50, no. 5, p. 1142-1149.

WR065 SOLUTE PARTITIONING

TITLE: Partitioning of Solutes between Solid and Aqueous Phases

PROJECT NUMBER: WR 70-065

LOCATION: Topical Research

PROJECT CHIEF: Davis, James A., III

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: When solutes are introduced into a ground-water system, or into surface waters, physiochemical reactions may occur between the dissolved solutes and native solid materials. Detailed knowledge of the chemical reactions that occur at solid surfaces is required to assess the impact of such inputs on water quality. In addition, the geochemical cycling of some trace elements may be controlled by the distribution between solid and aqueous phases. A fundamental understanding of the surface-chemistry reactions is needed to incorporate a mathematical description of these processes into chemical equilibrium and solute transport models.

OBJECTIVE: (1) Study the adsorption behavior of inorganic and organic solutes on particulate materials that are important in natural systems, including aluminosilicate minerals, model colloids, such as hydrous oxides of aluminum, silicon, iron, or manganese, and solids of biogenic origin; (2) derive stability constants for the partitioning of solutes between a particular solid surface and the aqueous phase and understand the mechanisms of surface bonding from a theoretical perspective, including electrical double layer theory; and (3) generate a surface-stability constant data base that is compatible with existing computer models of chemical equilibrium and that could be used in the field evaluation of solute transport models.

APPROACH: (1) Conduct experiments in the laboratory using physical-chemical techniques to characterize surfaces and to measure adsorption behavior as the type of solute, type of surface, and water composition are varied; (2) use controlled laboratory solutions in both kinetic and equilibrium studies to evaluate the importance of surface reactions for a given solute in a given geochemical environment; (3) develop quantitative phenomenological models to describe observed laboratory results, and predict the behavior of solutes under other experimental conditions with the aid of a computer; and (4) conduct field studies periodically to assess the applicability of the models to natural aqueous systems.

PROGRESS: Research on the partitioning of As between dissolved and particulate phases in Whitewood Creek, S. Dak., was begun (an interdisciplinary study site of the Surface Water Toxics program). The results show that both adsorption and precipitation processes may be important in controlling the dissolved As concentration in the creek. Laboratory experiments were begun to study the sorption behavior of As on iron hydroxide precipitated in artificial stream water. A laboratory study of sequential extraction methods for Se in sediments was begun.

REPORTS PUBLISHED:

Davis, J. A., and Hayes, K. F., 1986, Geochemical processes at mineral surfaces: Washington, D.C., American Chemical Society, 683 p.

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Nolan, K. M., and Fuller, C. C., 1986, Sediment accumulation in San Leandro Bay, Alameda County, Calif., during the 20th Century--a preliminary report: U.S. Geological Survey Water-Resources Investigations Report 86-4057, 25 p.

Chang, C. C. Y., Davis, J. A., and Kuwabara, J. S., 1987, The study of metal ion adsorption at low suspended solid concentrations: Estuarine and Coastal Shelf Science, v. 24, p. 419-424.

Davis, J. A., and Fuller, C. C., 1987, The roles of complexation and adsorption processes in toxic metal transport, in Ragone, S. E., and Sulam, D. J., eds., Program overview and selected papers from the toxic-waste program technical meeting, Tucson, Ariz., March 20-22, 1984: U.S. Geological Survey Open-File Report 86-324, p. 107-116.

WR076 CHEMISTRY OF HYDROSOLIC METALS

TITLE: Chemistry of Hydrosolic Metals and Related Constituents of Natural Water

PROJECT NUMBER: WR 57-076

LOCATION: Nationwide

PROJECT CHIEF: Hem, John D.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Hydrosolic metals are elements that form hydroxides with low solubilities. They may form colloidal suspensions (hydrosols). Some of these elements are toxic and they may interfere in various ways with water use. Understanding the occurrence and behavior of these elements in water is complicated by effects of pH, oxidation and reduction, formation of complex ions, coprecipitation and kinetics. Research results from this project are utilized extensively world-wide for such purposes as education and training of hydrologists and geochemists, design and operation of water wells, water-treatment and waste-disposal processes, mineral prospecting, and improvement of pharmaceutical products.

OBJECTIVE: Define dilute-solution chemistry of elements of interest in sufficient detail to apply findings to natural water systems; the final reports should be useful in predicting the fate of hydrosolic metals and associated substances, either in natural or polluted systems, as guides for designing optimal data collection programs, and as aids in the interpretation of water analyses and related hydrologic data.

APPROACH: Develop a predictive inorganic chemical model for behavior of the element of interest in dilute solution; models are based on chemical thermodynamic data from literature and appropriate laboratory experiments and may postulate either equilibrium closed-system or irreversible open-system conditions. Test models in chemical laboratory experiments and apply to field data to determine applicability. Modify models, as necessary, to allow for kinetic and biochemical factors.

PROGRESS: An open-system titration technique has been developed and applied to evaluate the kinetics and thermodynamics of the formation of microcrystalline gibbsite in unseeded solutions over the pH range 4.75 to 5.40 and at 10°, 25°, and 35° C. The first stages of the reaction produce monomeric and polymeric aluminum hydroxide ions. The rate of polymer formation increases by a factor of about 1,000 when the pH is increased by one unit, and this reaction rate also is strongly temperature dependent. An increase of 10° C in the temperature increases the reaction rate by a factor of about 5. This and other observations indicate the process has high energy barriers. A nearby field site for study of manganese precipitation from the water of a small stream has been found and preliminary work has been done to set up experiments to test theoretical models.

REPORTS PUBLISHED:

May, H. M., Kinniburgh, D. G., Helmke, P. A., and Jackson, M. L., 1986, Aqueous dissolution, solubilities, and thermodynamic stabilities of common aluminosilicate clay minerals--kaolinite and smectites: Geochemica et Cosmochimica Acta, v. 50, p. 1667-1677.

Hem, J. D., Roberson, C. E., and Lind, C. J., in press, Synthesis and stability hetaerolite, $ZnMn_2O_4$, at 25.0° C: Geochemica et Cosmochimica Acta, v. 51.

Lind, C. J., Hem, J. D., and Roberson, C. E., 1987, Reaction products of manganese-bearing waters, in Averett, R. C., and McKnight, D. M., eds., Chemical quality of water and the hydrologic cycle: Chelsea, Mich., Lewis Publishers, p. 271-301.

WR080 GEOCHEMISTRY OF GEOTHERMAL SYSTEMS

TITLE: Geochemical Studies of Geothermal Systems

PROJECT NUMBER: WR 72-080

LOCATION: Topical Research

PROJECT CHIEF: Barnes, Ivan

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Geochemical data are needed for estimating reservoir temperatures, outlining favorable exploration areas, identifying potential pollution problems, and estimating recharge-discharge relations as related to depletion. Corrosion and fouling problems require such data. The carbon dioxide in the steam may be the result of (1) metamorphic reactions or (2) mantle degassing. The chemical and isotopic character of volatiles issuing from volcanoes, such as Mount St. Helens, have not been determined adequately.

OBJECTIVE: Collect and analyze gas, water, and solids for chemical, mineralogic, and isotope data to provide detailed understanding of geothermal systems in both their natural and disturbed states, and of volcanic systems before, during, and after eruptions.

APPROACH: Apply field methods developed for unstable constituents and special sample collection and preservation techniques already in use to prospective geothermal areas and to areas around Mount St. Helens and possible other volcanoes. Analyze data using present and currently developing computer programs.

PROGRESS: Studies of selenium in the San Joaquin Valley, Calif., show that oxidation of pyrite in the arid climate produces $MgSO_4$ hydrates, $Na_2SO_4 \cdot 10H_2O$ and their less hydrated forms, jarosite, alunite, and gypsum, along with konyaite, bloedite, burkeite, and trona. Much the same chemistry in volcanic terrains yields the Na-SO_4 solutions that yield the SO_2 identified in volcanic emanations. SO_2 is not a magmatic gas in terms of direct origin.

WR128 TRACE ELEMENT PARTITIONING

TITLE: Processes and Controls of Trace Element Partitioning in Natural Waters

PROJECT NUMBER: WR 75-128

LOCATION: Topical Research

PROJECT CHIEF: Nordstrom, Darrell K.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: Development of land, water, mineral and energy resources have led to air and water-quality problems that often are caused by unhealthy mobilization of trace and radioactive elements in the environment. Trace contaminants may originate from radioactive-waste disposal, coal and base-metal mining wastes, oil-shale wastes, agricultural activities, and improper land-use development. Efforts to understand and model the trace element chemistry of natural waters are severely hampered by (1) inadequate sampling and analytical procedures, (2) inadequate or unevaluated thermodynamic and electrolyte data needed to calculate the form of dissolved chemical species and saturation states, and (3) inadequate testing of current models against laboratory measurements and well-documented field data.

OBJECTIVE: (1) Investigate methods of analyzing the species form of a trace element in a given water sample; (2) compile and critically evaluate equilibrium constants and related thermodynamic data used to make distribution of species calculations; (3) investigate the reliability of other parameters used in chemical models, especially activity coefficients; and (4) test current chemical models with carefully selected laboratory and field data to determine the range of conditions over which they can be considered reliable.

APPROACH: (1) Investigate ion-selective electrode potentiometry, ion chromatography, and high-sensitivity visible spectrophotometry for measuring specific forms of major and trace elements in natural waters; (2) search literature for thermodynamic data and evaluate for thermodynamic and statistical consistency to update the WATEQF/WATEQ2 data base; and (3) make computations with WATEQ2 under varying conditions of ionic strength, temperature, and composition of mineral solubilities to compare with laboratory and field measurements.

PROGRESS: General consideration of how and to what extent fluid inclusions might leak into granitic groundwater systems has been completed. A remarkable similarity of high Br/Cl ratios in granitic rocks with ratios in deep crystalline rock brines has been found that suggests a similar history. Several programs for the calculation of water-mineral equilibria, including WATEQ2, PHREEQE, and BALANCE, have been converted into versions suitable for personal computers. Arsenic speciation of high arsenic groundwaters from Nevada, a groundwater spring in Oregon, Mono Lake and Coos Bay groundwaters analyses have been successful.

REPORTS PUBLISHED:

Ball, J. W., Nordstrom, D. K., and Zachmann, D. W., 1987, WATEQ4F--A personal computer Fortran translation of the geochemical model WATEQ2 with revised data base: U.S. Geological Survey Open-File Report 87-050, 108 p.

Filipek, L. H., Nordstrom, D. K., and Ficklin, W. H., 1987, Interaction of acid mine drainage with waters and sediments of West Squaw Creek in the West Shasta Mining District, Calif.: Environmental Science Technology, v. 21, p. 388-396.

WR139 GEOCHEMISTRY OF GEOPRESSURED SYSTEMS

TITLE: Geochemistry of Water in Fine Grained Sediments

PROJECT NUMBER: WR 76-139

LOCATION: California, Texas, Oklahoma, Louisiana

PROJECT CHIEF: Kharaka, Yousif K.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: The energy potential of geothermal waters from geopressured systems is enormous. Geochemical data are necessary for delineating favorable exploration areas, estimating the recoverable geothermal resources from a given reservoir, and identifying potential pollution, waste disposal, and corrosion problems.

OBJECTIVE: (1) Study the chemistry and controls on the chemistry of water in geopressured geothermal systems; (2) provide basic data needed to identify potential pollution, waste disposal, and corrosion problems associated with extraction of energy from these systems; and (3) conduct an assessment of geopressured geothermal resources in California.

APPROACH: (1) Collect water, gas, and rock samples from prospective geopressured systems for chemical, mineralogic, and isotopic analyses; (2) collect data on sand distribution, porosity, temperature, pressure, and water salinity for assessment in California; (3) conduct membrane and water/rock interaction laboratory studies; and (4) use available and planned computer programs to analyze data.

PROGRESS: (1) Formation water from at least two fracture systems in the Cajon Pass's DOSECC well, Calif., were studied. Results show major differences in salinity and chemical composition of waters from fractures separated by less than 250 ft. (2) Major additions to the SOLMNEQ computer program were made, including options for: (a) activity coefficient using Pitzer's equations; (b) surface interactions; (c) dissolution precipitation; (d) gas partitioning. (3) The new SOLMNEQ program was used to study controls on geochemistry of high metal brines. (4) Decarboxylations rates for acetate calculated from field data were found to give half-life values of about 25 million years at 100 °C.

REPORTS PUBLISHED:

Kharaka, Y. K., and Carothers, W. W., 1986, Oxygen and hydrogen isotope geochemistry of deep basin brines: Handbook of Environmental Isotope Geochemistry, v. II, ch. 2, p. 305-360.

Kharaka, Y. K., Law, L. M., Carothers, W. W., and Goerlitz, D. F., 1986, Role of organic species dissolved in formation waters in mineral diagenesis: in Gautier, D., ed., Role of organic matter in mineral diagenesis: Tulsa, Okla., Society of Economic Paleontologists and Mineralogists, Special Report 38, p. 111-122.

WR189 CHEMISTRY OF AQUATIC ORGANIC MATTER

TITLE: Chemistry of Aquatic Organic Matter

PROJECT NUMBER: WR 84-189

LOCATION: Topical Research

PROJECT CHIEF: Goerlitz, Donald F.

HEADQUARTERS OFFICE: Menlo Park, CA

PROBLEM: The intrusion of industrial, agricultural, and domestically produced organic chemicals and wastes into the aquatic environment is a well-known reality and is considered to be one of the most important environmental problems. The widespread finding of these anthroprogenic substances, in addition to naturally occurring organics and their detrimental impact on the Nation's water resources, points to the need to understand how these substances act and react in the environment. Knowledge of transport, persistence, transformation, solubility, sorption, and reaction kinetics is needed to determine the fate of the substances in the hydrosphere.

OBJECTIVE: (1) Identify organic substances associated with the field problem, in aqueous and non-aqueous conditions, sorbed, and in unsaturated atmosphere; (2) chemically determine any biotic or abiotic degradation or transformations occurring in the field; (3) measure sorption and reaction equilibria and rates within the aqueous system and at the water-mineral interface, using both on the observations and laboratory simulations; and (4) determine the behavior of organic solutes and vapors in the unsaturated zone.

APPROACH: (1) Use high performance liquid chromatography, capillary gas chromatography, and computerized gas chromatography mass spectrometry to make qualitative and quantitative organic analyse; (2) do sorption studies using column technology, previously developed in this laboratory; and (3) conduct work at two field study sites on organic wood preservatives, which are groundwater contaminants, and initiate work at two other field study sites where the ground water is contaminated with crude and refined petroleum products.

PROGRESS: Comprehensive analysis for organics in contaminated ground water at Pensacola, Fla., revealed an interesting vertical profile of previously undetected compounds. They are oxidized components of the creosote solutes contaminating the aquifer, and range from simple fatty acids to polynuclear alcohols and ketones. The identities of some of these compounds imply degradation pathways previously not reported. The distribution of the metabolites in the 10 meter vertical sampling depth suggests that both aerobic and anaerobic moderated alterations are controlling the fate of the contaminants in the aquifer. Examination of the same samples by high performance liquid chromatography revealed the presence of additional compounds not detected or identified by gas chromatography mass spectrometry.

REPORTS PUBLISHED:

Franks, B. J., Goerlitz, D. F., and Baedecker, M. J., 1986, Defining a contaminant plume using on-site analytical techniques, in Petroleum hydrocarbons and organic chemicals in ground water: Prevention, Detection, and Restoration Conference, 2nd, Houston, Texas, 1985, p. 265-275.

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Godsy, E. M., and Goerlitz, D. F., 1986, Anaerobic microbial transformations of phenolic and other selected compounds in contaminated ground water at a creosote works, Pensacola, Fla.: U.S. Geological Survey Water-Supply Paper 2285, ch. H, p. 55-58.

Godsy, E. M., Goerlitz, D. F., and Ehrlich, G. G., 1986, The effects of pentachlorophenol on methanogenic fermentation of phenol: Bulletin of Environmental Contamination and Toxicology, v. 36, p. 271-277.

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Appendix I. Research Projects Listed for Each Water Resources Division Region

Appendix II. Project Chiefs of the Water Resources Research Program

PROJECT CHIEF	PROJECT SHORT TITLE	PROJECT NUMBER	PAGE
Andrews, Edmund D.	Hydrological-Biological Interactions	CR273	98
Back, William	Chemical Constituents of Water	NR034	54
Baedecker, Mary Jo	Organic Degradation	NR129	74
Baltzer, Robert A.	Numerical Simulation	NR019	158
Baltzer, Robert A.	Water Qual. Model Devel. and Imple.	NR074	160
Barnes, Ivan	Geochemistry of Geothermal Systems	WR080	217
Bencala, Kenneth E.	Flow and Geochemical Interactions	WR187	182
Benson, Larry V.	Hydrochemistry and Paleoclimatology	CR207	46
Bredehoeft, John D.	Wells-Strain Meters	WR176	142
Bricker, Owen P.	Trace Metals and Nutrients	NR109	70
Brown, Charles E.	Surface Geophysics and Hydrology	NR130	127
Callender, Edward	Sed.-Water Exchange of Nut./Metals	NR065	62
Campbell, William J.	Ice Modeling and Remote Sensing	WR064	173
Carter, Virginia P.	Wetland Studies	NR090	15
Cheng, Ralph T.	Estuary Hydrodynamics	WR140	175
Chiou, Cary T.	Sorption and Partition Phenomena	CR283	205
Claassen, Hans C.	Geochemical Kinetics Studies	CR189	44
Cleveland, Jesse M.	Transuranium Research	CR223	195
Cloern, James E.	Estuarine Plankton Dynamics	WR164	31
Conomos, T. John	Polaris Operations	WR156	177
Constantz, James E.	Temperature Effects, Unsat. Zone	WR193	151
Cooley, Richard L.	Simulation of Subsurface-Water Flow	CR191	115
Coplen, Tyler B.	Isotope Fractionation	NR064	60
Davis, James A., III	Solute Partitioning	WR065	213
DeLong, Lewis L.	Surface-Water Hydraulics	SR029	167
Eberl, Dennis D.	Clay-Water Reactions	CR276	48
Ehrlich, Garry G.	Organic Chemicals in Subsurface	WR068	23
Emmett, William W.	Bedload Transport Research	CR187	94
Feder, Gerald L.	Water Quality and Health	NR132	76
Getzen, Rufus T.	Hydrologic Analysis of Petrofabrics	WR171	141
Glenn, Jerry L.	Estuary Sedimentation/Eutrophication	CR266	96
Goerlitz, Donald F.	Chemistry of Aquatic Organic Matter	WR189	222
Goldberg, Marvin C.	Chemistry of Sediment Surfaces	CR199	192
Gorelick, Steven M.	Models for GW Management	WR178	144

PROJECT CHIEF	PROJECT SHORT TITLE	PROJECT NUMBER	PAGE
Grove, David B.	Ground-Water Quality Modeling	CR085	106
Harvey, Ronald W.	Bacteria-Contaminant Interactions	WR191	39
Herkelrath, William N.	Nonisothermal Multiphase Flow	WR179	146
Hsieh, Paul A.	Hydrology of Fractured Rocks	WR184	150
Hubbell, David W.	Sediment Transport Phenomena	CR098	88
James, Ronald V.	Unsaturated Zone Solutes	WR036	211
Jones, Blair F.	Mineral-Water Interaction in Saline Environments	NR020	52
Kennedy, Vance C.	Solute Transport at Low Flow	WR044	82
Kharaka, Yousif K.	Geochemistry of Geopressured Systems	WR139	220
Kipp, Kenneth L.	Solute-Transport Simulation	CR292	119
Konikow, Leonard F.	Transport Modeling -- Saturated Zone	NR120	125
Kraemer, Thomas F.	Radioisotopes in Ground Water	SR075	80
Kuwabara, James S.	Solute Transport Involving Biota	WR190	37
LaBaugh, James W.	Hydrol-Biol Geochem Interactions	CR293	8
Lai, Vincent C.	Computational Hydraulics	NR096	161
Landa, Edward R.	Uranium Mill Tailings	NR092	64
Landwehr, Jurate M.	Regional Hydrologic Processes	NR133	166
Leavesley, George H.	Rainfall-Runoff Modeling	CR228	154
Leenheer, Jerry A.	Comprehensive Organic Analysis of Water	CR285	207
Leland, Harry V.	Toxic Substances: Aquatic Ecosytems	WR137	27
Lovley, Derek R.	Microbial Geochemical Models	NR136	17
Luoma, Samuel N.	Trace Elements Availability in Sediments	WR125	25
Malcolm, Ronald L.	Organic Hydrogeochemistry	CR046	186
Mariner, Robert H.	Western U.S. Geochemistry	WR165	84
Mayo, Lawrence R.	Alaska Glaciology	WR175	178
Mcknight, Diane M.	Organic-Trace Metal Interactions	CR286	6
Meade, Robert H.	Sediment in Rivers	CR102	90
Moency, Allen F.	Energy Transport in GW	WR127	140
Neuzil, Christopher	Cretaceous Shale Hydrology	NR035	121
Nichols, Frederic H.	Estuarine Benthic Comm. Dynamics	WR192	41
Nordstrom, Darrell K.	Trace Element Partitioning	WR128	218
Olmsted, Franklin H.	Nevada Geothermal	WR082	133
Olmsted, Franklin H.	Geothermal Coordination	WR108	137
Olmsted, Franklin H.	Heat and Mass Transport--Cascades	WR121	138
Oremland, Ronald S.	Microbial Biogeochemistry	WR174	33
Osterkamp, Waite R.	Sediment Impacts from Coal Mining	NR107	103

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