CHARACTERIZATION OF FLOW AND TRANSPORT PROCESSES IN SOILS AT DIFFERENT SCALES (W-188)

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WESTERN REGIONAL RESEARCH PROJECT W-188

PROJECT NUMBER: W-188

TITLE: CHARACTERIZATION OF FLOW AND TRANSPORT PROCESSES IN SOILS AT DIFFERENT SCALES

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STATEMENT OF PROBLEM:

A major problem that recurs throughout the geophysical sciences is the interpolation (disaggregation) and extrapolation (aggregation) of flow or transport processes and their measurement across a range of spatial or temporal scales. Such difficulty arises, for example, when field-scale behavior must be determined from experimental data collected from a limited number of small-scale field plots. The scaling problem can not merely be solved by simple consideration of the differences in space or time scale, for several reasons. First, spatial and temporal variability in the properties of the transport medium creates uncertainties when changing from one scale of observation to another. Second, many of the processes of interest in geophysics and vadose zone hydrology are highly nonlinear. Consequently, the averaging of processes determined from discrete small-scale samples may not reflect the true behavior of the larger structure. Hence, there is a pressing need for sophisticated information mapping or upscaling procedures that will allow us to move from one domain of interest to another while retaining the true properties of the medium at each scale. This scale-transfer problem needs to be solved to improve the prediction of coupled fluxes of heat and moisture across the land surface and to establish scale-appropriate parameters to describe the behavior of contaminant plumes in soils at the field scale. The key question that must be answered to make the extrapolation correctly is how the problem of soil heterogeneity at different spatial and temporal scales affects the prediction, measurement, and management of flow and transport processes (e.g. water, heat, chemicals) into and through the vadose zone and underlying ground water.

The members of this regional research committee have developed world-renowned expertise in the modeling and measurement of flow and transport in soils. They will apply this expertise in the new project to specifically address the problem of scaling soil processes and observations in the presence of variability so that the information can be transferred to larger space or time frames. By collaborating in a set of theoretical and experimental studies conducted at different spatial scales, the participants in the new regional research project will provide new information that will vastly improve the understanding of how to interpret measurements and process studies so that their information content can be transferred to the larger domain of practical application.

JUSTIFICATION:

Unquestionably, our society has negatively impacted the quantity and quality of its soil, water and air resources. Chemical pollution generated by agricultural, industrial and municipal activities has contaminated soil and groundwater and surface water systems worldwide. Hence, water quality remains among the top research priority areas nationally and internationally. Global warming is believed to be caused primarily by an increase of carbon dioxide emissions (Barnola et al., 1987) by fossil fuel burning and increasing deforestation (Woodwell, 1989), in addition to the manmade production of chlorofluorocarbons (CFC's, Miller, 1997), which are also believed to be responsible for formation of the ozone hole. (Rowland and Molina, 1994).

Scientists are becoming increasingly aware that soil is a critically important component of the earth's biosphere, not only because of its food production function, but also as the safe-keeper of local, regional, and global environmental quality (Doran and Parkin, 1994). For example, it is believed that management strategies in the unsaturated soil zone will offer the best opportunities for preventing or limiting pollution, or for remediation of ongoing pollution problems. This is so, because chemical residence times in groundwater aquifers can range from years to thousands of years, so that once contaminants have entered the groundwater, pollution is essentially irreversible in many cases. Therefore, prevention or remediation of soil and groundwater contamination starts with proper management of the unsaturated zone (van Genuchten, 1994).

A major problem that is recurring in soil and hydrological sciences is the representation of flow and transport processes in the presence of large soil spatial and temporal variability at a scale larger than the one in which observations and property measurements are made. This scale-transfer problem must be solved to effectively describe the coupled fluxes of heat and moisture across large land surface elements, and to establish appropriate soil parameters for use in describing the behavior of pollutant plumes at the field or basin scale. The increasing awareness that scale issues are at the heart of many hydrologic problems arises because different processes may be dominant at different spatial or temporal scales. For example, the mathematical models of flow and transport processes that best represent behavior in unsaturated soil at the field scale may not be appropriate descriptions of the same processes at the larger watershed scale. Theories that have been developed to make the transition from one domain to another include upscaling or aggregation from small to large scales and dis-aggregation (downscaling) from large to small-scale processes. These theories include both deterministic and stochastic approaches, each of which maintain soil spatial heterogeneity. As remote sensing techniques to estimate large-scale soil parameters, and in situ measurement techniques to obtain point-scale soil information are developed, analysis and data assimilation techniques such as GIS and geostatistical tools are of critical importance to integrate scale-dependent soil physical processes. Specifically, for the application of general circulation models (GCM's), modeling of land surface processes and their spatial variability is essential at grids of about $10^4 – 10^5$ km^2. Soil surface processes define the lower boundary condition for these models, but soil scientists in general have difficulty in providing the relevant soil information at this large scale. We need to understand to what extent small-scale measurements provide information about large-scale flow and transport processes. Moreover, we must define the appropriate measurement techniques and the type of field experiments needed to characterize field-scale hydraulic and transport properties.

Fractal mathematics has been applied in the last decade to analyze scale-dependent flow properties and processes, providing both detailed property variations and rules for averaging and upscaling. In soil science, fractal analysis has mainly focused on particle size and aggregate size scaling. In contrast, the subsurface hydrology community has mostly applied fractal models to the much larger field scale. This apparent discrepancy in scales is surprising, given that the soil science community has long recognized the need to extend its point scale measurements to the field and catchment scale.

The members of this regional research committee will use their broad range of expertise in the modeling and measurement of flow and transport processes to improve our understanding of the scale-dependency of these processes. Specifically, analytical and computer modeling tools will be developed in conjunction with specific experimental techniques that will use site-specific information to produce large-scale characterization of flow and transport fluxes. The Western Region is dominated by arid and semi-arid climates, which may create climate-specific problems in the study of scale-dependent flow processes. For example, as pointed out by Tyler et al. (1998), soils in arid climates can be extremely dry, a condition causing extremely large variability in soil properties and flow and transport rates, including the occurrence of preferential flow if rainfall does occur. Moreover, arid soils are usually underlain by deep vadose zones, in which the dominant flow and transport mechanism is by vapor flow. On the other hand, surface processes in some parts of the region may be dominated by hill-slope hydrology. Hence, different approaches may be needed to characterize large-scale flow and transport processes within the Western U.S. The study of flow and transport, their relationships and scale-dependency is immense and requires the fullest participation of all members.

The regional effort of the researchers in this project is consistent with the highest national research priorities of the USDA, including the protection of the quality of surface and ground waters. Specifically, the USDA-CSRS National Research Initiative on Water Resources Assessment and Protection includes a specific research area on 'The development of new technologies to more effectively reduce or eliminate the movement of agricultural chemicals to surface and groundwaters'. It specifically calls for the development of instrumental and analytical techniques to optimize management practices, which account for soil spatial variability across landscapes and watersheds.

Unquestionably, the effective study of larger-scale flow processes requires integration of hydrological with soil physical principles at the soil-atmosphere interface and the coupling of surface with subsurface flow processes. Hence, the regional project provides a unique opportunity to continue developing vadose zone hydrology, thereby providing a bridge between the surface hydrologic and soil physical sciences. It is strongly believed that this integration of sciences, as defined in vadose zone hydrology, will create the optimal framework to improve our understanding of the coupled land surface-atmospheric processes and will lead to solutions of large-scale pollutant transport problems through the subsurface as well.

The benefits of the proposed joint research in the Regional Project will be an improved understanding of the scaling relationships of both flow and transport processes in inherently spatially-variable soils. Integrated computer and analytical modeling tools will be developed to better manage water quality of surface waters, soil water, and groundwater, specifically caused by non-point pollution from agricultural practices. In addition, the proposed project will facilitate collaborative research between soil physical and hydrological scientists, which in the longer term will benefit both the scientific community and the public. Finally, the analytical, experimental and modeling tools developed will improve land management and water use practices and policies affecting water quality and availability.

RELATED CURRENT AND PREVIOUS WORK:

Many of the experimental research efforts in the past decades on flow and transport processes in field soils are attributed to the seminal studies of Nielsen et al. (1973) and Biggar and Nielsen (1976), both of whom were members of Western Regional Research Project W-155. Their research produced several new directions in soil science (Mulla et al., 1998). Their findings stimulated the transition in solute transport research from an emphasis on the laboratory to field-scale experimentation, and brought to light the inherent field soil heterogeneity, and its tremendous influence on field-scale flow and transport. In addition, their papers suggested applying stochastic approaches to describe field-scale water and solute fluxes.

In previous W-155 projects, large-scale field experiments were established to test theories of water (Hills et al., 1991) and solute transport (Schulin et al., 1987; Ghodrathi and Jury, 1990). These field experiments confirmed that soil heterogeneity controlled large-scale flow and transport, including preferential flow, and confirmed the difficulty of applying deterministic modeling to predict field-scale transport processes. Hence, stochastic approaches were developed, which can characterize field-scale transport using scaling (Bresler and Dagan, 1981), Monte-Carlo analysis (Amoozegar-Fard et al., 1982), stochastic-convective stream tube modeling (Dagan and Bresler, 1979; Jury et al., 1986; Jury and Roth, 1990; Toride and Leij, 1996) and stochastic-continuum modeling using an ensemble-averaged transport equation with parameters described by random functions (Russo and Dagan, 1991). Prediction of large-scale flow problems has followed similar lines, with initial attempts to characterize flow regimes by deterministic modeling. Although studies such as that of Hills et al. (1991) showed a qualitatively acceptable comparison between field-measured and predicted water contents using the deterministic approach, other studies have shown the need for either distributed physically-based modeling (Loague and Kyriakidis, 1997) or stochastic modeling (Famigllietti and Wood, 1994) at the watershed scale. However, flow or transport processes have been shown to be scale-dependent, hence requiring scale-dependent parameterizations. For example, Merz and Plate (1997) pointed out the difficulty of applying scale-effective soil parameter values for scale-dependent processes. The scale-dependency of water flow through porous systems was also discussed by Dooge (1997), who hypothesizes that physical laws such as the Navier-Stokes and Darcy equations are appropriate only for specific spatial scales.

The general theme of the previous 5-year W-188 project addressed the improved characterization and quantification of flow and transport processes in soils, which focused on the development of new approaches, instrumentation and data analysis methodologies to characterize spatial and temporal variability of field soils. Hence, new experimental methodologies were developed that, in combination with large-scale measurements, process-based modeling and data analysis techniques provide the integral framework to study and analyze scaling laws across spatial-temporal scales. New, improved experimental and data analysis approaches include measurements of soil moisture, soil water potential, heat transport, infiltration and solute breakthrough, application of geostatistical and modeling techniques to characterize field-scale transport, the use of pedotransfer functions and neural network procedures, and improved inverse parameter procedures for estimation for the unsaturated hydraulic parameters. These methodologies, including remote sensing techniques, will be applied to improve soil water management practices to reduce erosion and improve surface and ground water quality.

In addition to the current regional project, which addresses specifically the development and evaluation of new instrumentation, techniques need to be developed that are specifically applicable to soil measurements across spatial scales. The revised objectives of this regional project will address this issue, and seek out methodologies and data analysis techniques that will allow extrapolation of local-scale parameters and processes to larger spatial scales in the landscape, such as agricultural fields and watersheds.

Several regional projects focus on water quality related issues. Regional projects W-82, W-128, W-170, W-184, and W-190 focus on water conservation and quality, management of salts and toxic trace elements, and micro-irrigation water management. Regional projects NC-157, NC-174, NC-218, NE-132, and S-275 primarily evaluate farm and soil management practices. Yet there is little or no duplication of these projects with W-188. The only regional project that studies the variation of soil properties across the landscape is S-257 (Classifying soils for solute transport as affected by soil properties and landscape position). Participants of S-257 focus solely on the development of a soil classification system, linking mapped soil properties to solute transport properties. Since the second research objective of W-188 includes the measurement of local-scale transport across the landscape, some duplication is likely. Nevertheless, the main effort of S-257 is on the development of a soil classification system for estimation of solute transport rates using standard soil physical and chemical measurement techniques, whereas the W-188 project is focused on investigations of scale-dependent flow and transport processes, including the development of scale-appropriate experimental methodologies.

Relationships between flow and transport processes across spatial and temporal scales in soils are needed to manage water and chemicals in agriculture, to manage waste disposal sites, and to quantify soil moisture changes in the near surface. Experimental data and simulation models will be applied at a variety of spatial scales, intended to solve both basic and applied problems, including processes from the point (plot, field) to the basin (watershed, region) scale. The revised W-188 project will use the results of previous regional projects to seek these relationships and their uncertainty between local scale and basin-scale flow and transport processes. The development of remote sensing methodologies and its application to large-scale soil physical processes might be the key for extrapolation of field data to larger spatial scales (Sposito and Reginato, 1992). Methodologies that can accommodate these developments are inverse methods for parameter optimization of hydrological and subsurface flow and transport processes, the utilization of geostatistics to match remote sensing information with ground truth measurements, and fractal mathematics to include spatial variability in transport models across spatial scales.

OBJECTIVES:

1. To study relationships between flow and transport properties or processes and the spatial and temporal scales at which these are observed;

2. To develop and evaluate instrumentation and methods of analysis for characterization of flow and transport at different scales; and

3. To apply scale-appropriate methodologies for the management of soil and water resources.

PROCEDURES:

The revised project will be conducted at a variety of experimental and theoretical scales, highlighted by selected ongoing field studies that will provide the large-scale perspective of our project theme. Collaboration will occur in a variety of ways, notably through joint participation in the selected field studies, sharing of information obtained, and comparison of experimental and theoretical approaches obtained in separate investigations of similar phenomena but at different scales. Although the proposed regional research will include other research sites as well, the five common field studies listed below have been developed during the past 5 years, and consequently are the logical joint research sites for the proposed research.

The first site is the Maricopa site (Arizona). This is a well-instrumented 50 m x 50 m plot, that can be irrigated at a precisely controlled water application rate. Tracers can be added to the irrigation water at different times. A large amount of data has been collected during the past two years on water movement and solute transport to the groundwater.

The site is uniquely suitable for the study of scaling relationships between the point and field plot scale. Collected data will be available for detailed modeling. Additionally, the site is excellent for testing of additional monitoring techniques.

The second site is the Southern Great Plains Hydrology Experiment (SGP97) in Oklahoma, which was sponsored by NASA. Many local soil physical, hydraulic and thermal data were collected (California-USSL) across the SGP region to find relationships between point and pixel-scale measurements and processes. Consequently, a great deal of data is already available to study scale issues of space-time dynamics of soil moisture and temperature and to improve hydrologic predictions using remote sensing and ground truth data collection.

The third selected collaborative research site includes many agricultural fields across the San Joaquin Valley, near Firebaugh, CA. This regional project (California-USSL and California-Davis) specifically addresses the influence of reduced availability of irrigation water on drainage water quality and the regional salt balance. Moreover, data will be collected and a regional model will be developed to quantify the economic, environmental and social impacts of reductions in surface irrigation water supply to the region.

The Oakes Irrigation Test Area (OITA) was selected as the fourth research site (North Dakota). This 2000 ha site has been used for the past 10 years to conduct field-scale research, specifically addressing water quality (nitrogen) impacts of irrigated cropping systems. The site includes groundwater-monitoring wells, instrumented tile drains, and heavily instrumented in-situ lysimeters. LandSat images are collected on a bi-annual basis to study relationships between soil and irrigation water management practices and crop yield. In addition to the information already obtained, the site is available for further instrumentation and analysis of remote sensing data.

The final selected field research project is truly regional, since it involves the instrumentation and monitoring of landfill sites across the western United States (DRI, Nevada). This so-called Alternative Cover Assessment Program (ACAP) was initiated by U.S. EPA to apply innovative alternatives for landfill cover designs.

In addition to these five selected research sites, the following objectives will be addressed at other experimental locations as well.

1. To study relationships between flow and transport properties or processes and the spatial and temporal scales at which these are observed.

In essence, both deterministic and stochastic modeling approaches are available to characterize flow and transport mechanisms. However, these methods are limited because of the enormous amount of data required to characterize flow and solute transport at increasing spatial scales. Rather than increasing data collection efforts at a rate proportional to the physical size of the flow system, upscaling can be accomplished more efficiently, assuming that flow processes at the smaller scale are identical to those of the larger spatial scale. However, little information is available on the relationships between the various moments of the flow and transport parameters between spatial scales, as well as their dependency on the initial and boundary conditions of the flow system. Notwithstanding, Kabat et al. (1997) showed that the Darcy-Richards equation was scale-invariant, and concluded that effective soil hydraulic properties could successfully describe area-average evaporative and soil moisture fluxes at the 10-100 km^2 scale, provided that the averaged area contained a single soil type only. This was concluded with the understanding that the estimated effective properties are merely calibration parameters, which do not necessarily have the physical meaning implied by application of the Darcy flow equation. Other approaches include simplifications towards conceptual characterization of the most controlling parameters and processes only, as in simplified distributed modeling (Grayson et al., 1997; Duffy, 1996; Famiglietti and Wood, 1994), where soil heterogeneity is maintained using the representative elementary area (REA) approach.

The influence of soil heterogeneity on flow and transport at different spatial and temporal scales will be investigated using carefully designed experiments involving both local and aggregated soil measurements for a multitude of initial and boundary conditions. Specifically, both experimental and theoretical approaches will be applied to better understand the scale-dependency of the controlling flow and transport parameters, such as the soil water retention and unsaturated hydraulic conductivity and solute transport parameters.

Most theoretical and modeling approaches will use field experimental data from any of the selected field sites to investigate possible scaling relationships. Geostatistical techniques will be applied by Arizona in collaboration with Illinois, Iowa, Minnesota, North Dakota and Wyoming to study the effects of sample support relative to domain size on upscaling and downscaling of remote sensing and soil physical data. Colorado will use field observations of water and solute movement to study the effect of measurement method, support scale and parameter averaging on the accuracy of solute transport modeling. Similar statistical and fractal scaling methods will be developed by ARS-Colorado for the characterization and prediction of space-time patterns of hydrologic processes on the watershed scale, using both field plot and gauged watershed data. Kansas will focus on the characterization of near-surface soil moisture dynamics at a variety of spatial and temporal scales, using the heat-pulse technique (Campbell et al., 1991; Tarara and Ham, 1997) to obtain spatially-distributed surface soil water content measurements. Field soil moisture data in Kansas and at the other identified common field sites will be selected to identify appropriate upscaling techniques. An experimental data set will be analyzed at California-USSL to study the spatial and temporal dynamics of water and heat and their coupled transport across the land surface-atmosphere boundary at the field scale.

Research groups participating in the project will carry out a variety of solute transport studies at various spatial scales. The specific objective of these transport experiments is to determine if and when observations from small-scale experiments can be applied to large-scale soil systems. For example, Washington and Delaware will collectively conduct column studies, testing the presence of scaling relationships of effective sorption and transport properties of chemicals and microorganisms using soil columns of different sizes. Both Illinois and PNNL-Washington will conduct detailed field studies to identify the required small-scale features of flow (PNNL) and transport (Illinois) for large-scale predictions, using geostatistical indicator and conditional simulations. Tile drain studies will be carried out at Iowa, Iowa-ARS and California-USSL to predict solute transport from application of multiple tracers at the field scale, using detailed field measurements of soil hydraulic and solute transport properties, including considerations of preferential movement of water and dissolved solutes through soil macropores. Researchers in California-Berkeley and Washington will study the effect of surface soil topography on the control of water flow and solute transport on hillslopes.

Although significant advances have been made by members of this regional project to better understand the fundamental mechanisms of preferential flow (California-USSL, New Mexico-NM Tech), questions on its importance and description across spatial scales remain to be answered. Investigators at California-Riverside and Washington-PNNL in collaboration with Oregon, California-Berkeley and Nevada will test experimental protocols and unstable flow models at various research sites within the regional project. A central field study in Riverside will be used to monitor the relationship between water flow characteristics during infiltration and redistribution on the initiation and propagation of preferential flow events at the wetting front. A variety of small-scale instruments for monitoring water and chemical characteristics developed within the regional project will be tested at this site.

Project members will also specifically study the influence of scale on soil hydraulic properties. For example, California-Davis will test the lognormal pore-size distribution model (Kosugi and Hopmans, 1998) for its suitability to characterize soil hydraulic heterogeneity for increasing spatial scale, using mean pore size and variance parameters. California-Davis will apply volume-averaging techniques to compute hydraulic conductivity directly from pore geometry considerations, solving the Stokes equation and closure problem. Wyoming will specifically develop scale-dependent relationships of soil hydraulic properties, and study the impact of scale-dependent soil hydraulic properties on water flow and chemical transport in heterogeneous soils. Field experiments will be conducted for determining in situ hydraulic properties of soils using different size tension infiltrometers. Subsequently, a database of spatially variable soil physical and hydraulic properties will be developed to study scale-dependency, spatial variability, and heterogeneity of soil hydraulic properties. Modeling and parameter optimization techniques will be further developed by investigators of California-USSL to determine scale-appropriate soil hydraulic and transport properties.

With harvesting machinery equipped with yield monitors, the resulting images of spatially distributed yield in agricultural fields provide a unique opportunity to compare averaging and spatial analysis techniques. Kansas and Colorado-ARS will investigate scale effects on the temporal and spatial variability of crop yield data on the field and farm scale. The influence of soil, climate, and landscape position on temporally and spatially variable crop yields will be investigated at Iowa-ARS. Yield patterns in a long-term 16-ha field will be analyzed using cluster and multivariate analysis to determine relationships to physical, chemical, and biological soil properties, landscape/hydraulic characteristics, and remotely sensed soil and canopy data. The interaction of soil, climate, and plant processes will be modeled to test their effects on the dynamic nature of yield variability.

2. To develop and evaluate instrumentation and methods of analysis for characterization of flow and transport at different scales.

Notwithstanding the accomplishments of the previous W-188 project in developing new instrumentation and data analysis techniques to characterize soil properties affecting flow and solute transport and their variation, continued innovative and collaborative efforts are needed to improve the understanding of scale-dependent soil physical processes as outlined in objective one. It is intuitively clear that the soil moisture content near the surface is a dominant factor controlling near-surface hydrological processes. Hence, investigators will focus on the measurement and analysis of soil moisture dynamics at various spatial and temporal scales.

Present theory and applications of remote sensing have tremendous potential to understand large-scale hydrological processes such as runoff, infiltration and evapotranspiration, and their spatial distribution and scale-dependency. Moreover, the monitoring of temporal changes in soil moisture by remote sensing may provide the required soil information to estimate upscaled soil hydraulic parameters such as the saturated hydraulic conductivity or unsaturated hydraulic parameters (Jackson et al., 1988). An excellent example of such an application was presented by Feddes et al. (1993), who showed that remote sensing of soil surface temperature and soil moisture combined may provide the essential information to estimate effective soil hydraulic parameters at the catchment scale. The work of Ahuja et al. (1993) support this potential application of remote sensing, and showed that spatial variations in surface soil moisture can be related to spatial variations in effective values of soil profile saturated hydraulic conductivity. Complementary techniques specifically applicable for soil moisture measurements at different spatial scales are surface electrical measurements (Banton et al., 1997; Hendrickx et al., 1992), and ground-penetrating radar (Chanzy et al., 1996).

Supporting data assimilation techniques include the analysis of relationships between soil properties using indirect methods, such as linear regression analysis, pedotransfer functions and neural networks (van Genuchten et al., 1992, Schaap et al., 1998; van Genuchten et al., 1992). As an example, Salvucci (1998) found simple power law relationships between Miller and Miller scaling factors and soil surface soil moisture for both soil infiltration and evaporation. Other data analysis methodologies include the scaling of field soil water regime (Nielsen et al., 1998), and state-space approaches (Nielsen et al., 1994).

Especially useful in the linking of soil properties and processes between different scales is the theory of fractal analysis, which has been applied to study the evolution of drainage networks and landscapes (Rodriguez-Iturbe et al., 1994). The linking of spatial scales is accomplished by the apparent spatial structure of soil properties, which is characterized by power laws. For example, various studies (Zhang et al., 1990; Kamgar et al., 1993; Rodriguez-Iturbe et al., 1995) have shown a linear relationship between the variance of soil moisture and observation area when presented on a log-log plot.

Inverse procedures offer an additional powerful methodology to estimate flow and transport properties across spatial and temporal scales. Earlier applications were limited to the coupling of parameter optimization with analytical solutions of laboratory data. However, as numerical models become increasingly sophisticated and powerful, inverse methods become applicable to field data as well, no longer limited by the physical dimensions of the field or type of imposed boundary conditions. Inverse methods may prove to be very appropriate for estimating regional-scale effective soil hydraulic parameters, either by manipulating in-situ measurement of the hydraulic properties (Kabat et al., 1997), or by using remotely-sensed measurements of soil surface water content (Feddes et al., 1993).

In the past five years, members of W-188 have made significant progress in the development, testing and application of various soil moisture measurement devices, especially using Time Domain Reflectometry (TDR). Future efforts will be focused on accurate and economical methods of measurement of soil surface moisture dynamics to evaluate temporal and spatial scaling relationships. Both California-Davis and Texas will develop stand-alone solar-powered TDR systems (Frueh and Hopmans, 1997; Evett, 1998) to investigate soil water balances of various crops in spatially-variable agricultural fields. Collaborative work will continue between Montana and Utah to quantify the temperature influence on TDR-measured bulk dielectric constant (Wraith and Or 1999; Or and Wraith 1999). This will provide practical correction factors for measured soil water content using TDR, and will lead to improved understanding of solid-water interactions at multiple scales. Both research groups will collaborate to evaluate a new method for estimating specific surface area of soils based on measured thermodielectric responses to temperature perturbations (Wraith and Or 1998). Potential applications to map soil texture using remote sensing (e.g., SAR) will be investigated. TDR (soil water content) and heat dissipation sensors (soil water potential) are refined and improved for site-specific calibration at the various selected research sites by Utah-Campbell Sci, in collaboration with Utah, Arizona and Nevada

Kansas and Iowa will continue to develop and evaluate the heat pulse method for the combined measurement of surface soil water content and thermal properties (Kluitenberg and Philip, 1999). This relatively new technique is particular useful for measurements of mass and energy balances at the soil-atmosphere interface, and is of large significance with regard to providing ground truth data for remote sensing experiments. Moreover, Iowa will continue to develop the thermo-TDR probe for simultaneous determination of soil water content, bulk density and bulk electrical conductivity. Especially exciting is the proposed experimental work to use a modified heat pulse probe to measure water flow velocities in soils. Both Iowa and Kansas are experimenting collectively to refine the methodology, allowing the estimation of water fluxes at the soil-atmosphere interface as well as in deep vadose zones near the groundwater table. Since a flux measure is the true integrated variable, this development will allow spatial and temporal analysis of flow and transport processes across spatial scales. Berkeley will compare fiber optic sensors and to directly measure soil solute content with other in situ sensors such as TDR and miniature solution samplers in collaboration with Riverside, and recommend proper solute measurement tools for specific measurement scales.

Equally exciting is the development and application of sensors for measuring soil water potentials and fluxes in deep vadose zones, so that much improved water and contaminant flux estimates towards the groundwater table can be determined. This is especially important for the estimation of recharge fluxes to deep water tables in the arid and semi-arid regions of the western US, as well as for the monitoring of contaminant fluxes below hazardous waste disposal sites. Both members at Washington-PPNL and Idaho-INEEL continue to design and evaluate vadose zone monitoring instruments to measure soil water content, soil-water potential, contaminant concentrations and fluxes that are specifically suitable for depths of up to 100 m below the land surface. These and other sensors, such as borehole radar and electrical tomography will be evaluated at other research sites as well, such as the Maricopa (Arizona) and the Hanford site (Washington-PNNL). Experimental data will be used by various W-188 members for model testing and verification, such as by Washington and INEEL where members will integrate vadose zone with groundwater modeling, specifically to investigate surface water-groundwater interactions at the regional scale (Washington) and to predict contaminant transport below hazardous waste sites (INEEL).

As indicated in objective one, paramount to an improved understanding of flow and transport across spatial scales is a better description of the scale-dependency of soil hydraulic and transport properties. Washington will apply the UFA Method (Conca and Wright, 1998; Nimmo et al., 1987)) to determine intrinsic permeability, diffusion coefficient, electrical conductivity, vapor diffusivity, retardation factor, dispersivity and thermal conductivity of spatially-variable soils. Research at California-Davis and California-USSL will continue to develop inverse methods (Eching and Hopmans, 1994; Inoue et al., 1998; Simunek and van Genuchten) to determine scale-appropriate soil hydraulic properties, and solute sampling techniques will be developed that provide scale-dependent solute transport parameters. Based on the field experimental and stochastic simulation data, Wyoming will develop infiltration models to characterize infiltration processes (Zhang, 1997a) and methodologies to determine hydraulic properties (Zhang, 1997b, 1998) in heterogeneous soils. Fractal and geostatistical analyses and other upscaling methods will be used to develop scale-dependent relationships of hydraulic and transport properties (Zhang, 1997c, Kravchenko and Zhang, 1998). Stochastic modeling approaches will be designed to study the impact of scale-dependent hydraulic and chemical heterogeneities on transport processes. Research at Iowa-ARS and Washington will continue to develop simple tracer methods, including dye tracers, for determining the parameters of the mobile/immobile transport model. Methods will be applied to a number of soils under different tillage and crop rotations to characterize the temporal and spatial nature of these parameters.

Evaluation of soil measurements and processes across scales requires appropriate analytical tools. Members of the project will continue to investigate inverse methods to estimate soil thermal, solute and hydraulic properties. Colorado, will apply structural identification in combination with numerical simulations and experimental studies, to estimate soil physical properties without a priori assumptions to the functional forms of the property of interest. Parameter optimization methods will be applied by members in California-USSL for the rapid and cost-effective measurement of hysteretic soil hydraulic properties using the newly-developed HYDRUS-1D code (Simunek et al. 1998). Geostatistical tools that characterize variability structures and employ multiple sample supports will be developed and evaluated by Colorado. Similar techniques in combination with the association rule mining method will be investigated by North Dakota to determine the presence of relationships between spectral properties as obtained from remote sensing (infrared) and ground truth observations (yield). Using data from SGP97, members of California-USSL will develop a hierarchical set of neural network pedotransfer functions, so that soil hydraulic properties such as soil water retention and unsaturated hydraulic conductivity can be estimated for large areas using limited sets of predictors, preferable those already available, e.g., soil survey data. Also Washington-PNNL will apply pedotransfer functions to relate soil particle size distribution to hydraulic properties for sediments in deep vadose zones that are difficult to collect nondestructively.

3. To apply scale-appropriate methodologies for the management of soil and water resources.

As more spatially distributed data becomes available, there is a concomitant need for alternative data analysis techniques to present the intricate relationships of spatial scale and soil heterogeneity on large-scale flow and transport. It is here that geographical information systems (GIS) are increasingly applied in surface and subsurface flow and transport modeling issues. As an example, Mohanty and van Genuchten (1996) describe an integrated conceptual framework for the prediction of basin-scale solute loading rates through the vadose zone, coupling GIS with a flow and transport model, a soil database management system and a geostatistical software package. Continued development of integrated data management systems is needed as a practical tool for large-scale soil water management, as well as for the aggregation of local soil hydraulic soil information to the pixel scale used by remote sensing instrumentation. At California-USSL an integrated GIS-based system will be developed that couples the modeling of local-scale processes with databases of soil taxonomic data and data analysis schemes. At California-Davis, an integrated spatially and temporally distributed agro-economic model of the Firebaugh Zipcode area in California using economic and hydrologic submodels will be developed. This model will be used to quantify the economic, environmental and social impact of reductions in surface irrigation water supply in this mostly agricultural area. Using GIS, remote-sensing data will be integrated with crop growth, vadose zone and groundwater flow and transport models to organize and communicate the findings. Project members in Washington will combine GIS with stochastic modeling techniques to describe flow and contaminant transport at the land surface and the subsurface at the watershed scale. GIS techniques will be used to describe the deterministic component of soil spatial variability within subunits of a watershed, whereas stochastic analysis will be applied to simulate random components of flow and transport within the hydrologic subunits of the specific watershed.

The scaling laws of Miller and Miller (1956) were used by Kabat et al. (1997) and Hopmans and Stricker (1989) to determine effective soil hydraulic properties and to estimate the spatial distribution of water balance fluxes at the watershed scale. Other approaches to determine the scale-dependent soil water flow and transport properties include the direct or indirect estimation of the effective properties by measurement of integrated boundary conditions. For example, Eching et al. (1994) estimated field-representative hydraulic functions using inverse modeling with field drainage flow rate serving as the lower boundary condition for the Richards flow equation applied at the field-scale, whereas Mohanty et al. (1998) tested whether tile drain breakthrough can be used to obtain field-representative effective flow and transport properties. As another example, Szilagyi et al. (1998) successfully estimated catchment-scale saturated hydraulic conductivity utilizing stream flow recession hydrographs. To estimate field-representative infiltration parameters, Shepard et al. (1993) used the time advance of water in furrow-irrigated fields. In all these studies, field-integrated flow measures were applied to infer the scale-approporiate effective flow or transport properties. Using a similar modeling approach, Desbarats (1998) determined scale-appropriate soil water retention and unsaturated hydraulic conductivity functions from three-dimensional modeling of steady-state infiltration, from which the domain-average water content, soil water potential and unsaturated hydraulic conductivity values (equal to steady-state infiltration rate) were computed.

Various scaling laws will be tested by members at California-USSL and California-Davis, specifically for application to heterogeneous field soils, to be used to describe field and larger-scale transport of water and solutes in deterministic and stochastic modeling approaches. In Idaho-INEEL, field-scale measurements will be incorporated into numerical models to determine the effectiveness of integrated characterization and modeling approaches for predicting contaminant transport below hazardous waste sites. Also Nevada will use numerical simulations to investigate infiltration processes and geochemical reactions in mining waste materials, with an emphasis on the potential use of numerical models to assess environmental impacts of heterogeneous mining wastes. Specifically, dual porosity modeling of the transport processes will be conducted in collaboration with California-USSL. Texas will continue to develop a wireless thermometer system, combined with a scaling analysis of soil surface temperature, allowing the estimation of the energy balance and surface evaporation for large areas from limited surface temperature data (Evett et al., 1994 and 1996; Evett, 1998).

California-Davis will develop and evaluate improved simulation models for transport and transformation of N within the vadose zone and emission of N gases into the atmosphere for various agricultural management scenarios. Ground water contamination by nitrate from agricultural sources is a major problem in many areas of the Western United States. In addition, the emission of N gases from soil such as ammonia, nitric oxide, and nitrous oxide have generally increased due to increased use of N fertilizers and animal manure in intensive cropping systems. Several simulation models of N transport and transformation including those being evaluated by members of this regional project (Ahuja et al., 1991; Schaffer et al., 1991) are available. However, most of the commonly-used models do not consider the transformation processes resulting in production of N gases in sufficient detail to adequately predict the emission of important gases such as nitric oxide and nitrous oxide. Other recently-developed models (Grant et al., 1993a,b) explicitly consider the biochemical processes controlling emission of nitrous oxide but are lacking in their ability to consider transport processes in heterogeneous soils. Investigators will evaluate the existing models in terms of their ability to adequately predict emissions of nitrous oxide from agricultural cropping systems. This effort will be complemented by laboratory and field experiments to understand the soil and environmental factors affecting the emission of nitric oxide from spatially-heterogeneous soils. Nevada is quantifying the role of land use changes and spatial distribution of land use on subsurface nutrient loading in watersheds of Lake Tahoe, CA/NV. Specifically, land use changes along riparian corridors may have significant impacts on nutient loading to the streams and ultimately to Lake Tahoe. Research with California-Davis will focus on quantifying the spatial distribution of base flow inputs and changes associated with various adjacent land use practices.

Much of what is learnt in the revised regional project will be applied to improve agricultural soil and water management practices. North Dakota will develop evapotranspiration-yield relationships as determined from remote sensing experiments, to predict field available water and seasonal water-use at the watershed scale. Montana will extend a satellite-based drought index for weekly updated estimates of location-specific plant-available soil water status. This will be combined with weather forecasts and long-term climate records to provide crop yield forecasts with associated probabilities. The products will be provided online to farmers and ranchers in Montana, with extension to additional states such as North Dakota. Geostatistical approaches evaluated in the second objective will be evaluated by Illinois to determine the appropriate scale required for varying fertilizer applications for site-specific agriculture applications. At Iowa-ARS, spatially and temporally dynamic N-fertilizer programs will be developed and tested to maximize corn yield while minimizing nitrate leaching to subsurface drainage systems. Three approaches will be used – a spatially uniform side-dress program based on a late spring soil nitrate levels, a side-dress program where soil testing is conducted for spatially distinct crop response areas, and a late season real-time on-the-go variable rate side-dress program based on crop canopy reflectance. Economic and environmental impact of each N-management system will be determined by measuring yields, stalk nitrate levels, and nitrate concentrations in subsurface drain tubes. Wyoming will develop a decision support system for agrochemical management to enhance both the agricultural productivity and environmental quality at large scales. The decision support system will integrate soil, chemical, weather and geographical databases with transport and risk analysis models. By analyzing the risk of groundwater contamination under different agricultural management practices, the system will provide an efficient and powerful tool for environmentally sound decision-making. This work will provide a template for other project members.

EXPECTED OUTCOMES:

The proposed regional research is expected to contribute in advancing the understanding of large-scale flow and transport processes, the directing of cutting-edge research to both graduate students and post-doctoral scientists, and the extension of knowledge to different user groups. First and foremost, we expect to publish our results in a wide array of publications, including professional society and extension publications. Through the selection of five joint research sites we anticipate even more collaboration than achieved in previous W-188 projects This will increase our effectiveness in achieving the project objectives. Additionally, the focus of the proposal to integrate soil physical with hydrological processes will stimulate the development and recognition of vadose zone hydrology, thereby making possible the solution of a wide array of complex, multi-disciplinary problems related to the improved and efficient use of our soil and water resources and environmental pollution. Moreover, the emphasis of the proposal on large-scale processes, in combination with remote sensing and GIS techniques will benefit the solution of such problems as well. As in previous regional projects (W-155 and W-188), an international workshop will be organized (Kirkham Conference) to highlight our accomplishments and to provide a benchmark for future research needs.

The problem of characterizing the scale dependence of transport processes and the parameters needed in their characterization is ideally suited to regional research investigation. One of the main reasons why so little progress has been made in the past in this area is because of the enormous amount of effort required to collect and analyze the data needed to develop and test relationships among processes and properties at different scales. Only through the efforts of a large team of investigators looking at a wide range of conditions will we develop the information needed to work confidently at different scales of observation in the variable domain of the vadose zone. We are confident that the project we have designed will meet our objectives and at the same time provide a wealth of new information for both scientists and practitioners interested in large-scale transport processes.

ORGANIZATION:

The regional research technical committee consists of members who represent SAES, USDA-ARS, and other research units. The committee will conduct coordinated regional research under the supervision of an administrative advisor (Dr. G.A. Mitchell) appointed by the SAES directors of the Western region. Participants will use similar methods, shared databases, and centrally developed models, to achieve the project objectives. At the annual meeting of the committee, a chairperson and a secretary will be elected from the participating membership to a one-year term of duty. The chairperson will coordinate the regional research activities, arrange annual meetings, and prepare annual reports in consultation with the committee members, the administrative advisor, and the CSRS representative (Dr. B.L. Schmidt). The secretary will record and distribute the minutes of the annual meeting, perform duties of the chairperson in case of absence, and be promoted to chairperson at the conclusion of the one-year of office. A new secretary will, therefore, be elected annually. The chairperson may appoint members to serve on subcommmittees for technical and administrative duties.

REGIONAL PROJECT TITLE: CHARACTERIZATION OF FLOW AND TRANSPORT PROCESSES IN SOILS AT DIFFERENT SCALES.

Signatures:

Administrative Advisor — Date: 1/13/99

CHAIR, REGIONAL ASSOCIATION OF DIRECTORS — DATE: 3/24/99

Administrator, Cooperative State Research Service — Date

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APPENDIX A: Attachments

REGIONAL PROJECT TITLE: CHARACTERIZATION OF FLOW AND TRANSPORTPROCESSES IN SOILS AT DIFFERENT SCALES

PROJECT LEADERS

LOCATION	PRINCIPAL INVESTIGATORS	AREA OF SPECIALIZATION
A. EXPERIMENT STATIONS:		
Arizona	A.W. Warrick (U of AZ)	In-situ methods, modeling infiltration from permeameters and point sources
	P.J. Wierenga (U of AZ)	Model development and field experimentation
California	J.W. Hopmans (UC-Davis)	Inverse methods, non-invasive measurements, field experimentation, vadose zone hydrology
	D.R. Nielsen (UC-Davis)	Field experimentation, management of soil spatial variation
	D.E. Rolston (UC-Davis)	
	W.A. Jury (UC-Riverside)	Transfer function modeling and field experimentation, in-situ measurements
	L.Wu (UC-Riverside)	Water flow modeling and field experimentation
	M. Ghodrati (UC Berkeley	Characterization of flow and transport
Colorado	G. Butters (CO State U)	Field experimentation, root zone management
Indiana	J. Cushman (Purdue Univ)	Multi-scale stochastic modeling
Illinois	T.R. Ellsworth (U of IL)	Field experimentation, in-situ measurements, mathematical modeling, inverse methods
Iowa	R. Horton (IA State U)	Field measurements, in-situ measurements, coupled heat and transport modeling, site-specific management practices
Kansas	G. Kluitenberg (KS State)	Heat-pulse methodology, field experimentation, spatial data analysis, site-specific management
Minnesota	D.J. Mulla (U of Minnesota)	Transfer function modeling, field experimentation, site-specific measurements
Montana	J. M. Wraith (MT State U)	In-situ measurements, site-specific management Tools, field experimentation

Nevada	S.W. Tyler (U of Reno, DRI)	Fractal models, modeling preferential flow, in-situ measurements, inverse methods
	W.W. Miller (U of Reno)	In-situ measurements
North Dakota	R. Knighton (ND State U)	Field measurements, fractal models, in-situ measurements, site-specific management
Utah	D. Or (Ut State U)	In-situ measurements, pore-scale processes, Upscaling issues, electromagnetic methods
Washington	J. Conca (Wa State U)	Soil characterization
	M. Flury (Wa State U)	Modeling solute transport, in-situ measurements
	J. Wu (Wa State U)	Groundwater modeling, GIS applications
Wyoming	R. Zhang (U WY)	Stochastic modeling, fractal models, in-situ measurements, inverse methods

B. USDA

California	M.Th. van Genuchten (USSL-Riverside)	Preferential flow. field experiments, in-situ measurements, inverse methods, solute management modeling
	P.J. Shouse (USSL-Riverside)	Field measurements with dyes and tracers, in-situ measurements
	F. Leij (USSL-Riverside)	Modeling soil hydraulic conductivity, modeling of water and solute transport
	J. Simunek (USSL-Riverside)	Numerical modeling of soil water and transport, inverse methods
	T. Skaggs (USSL-Riverside)	Stochastic modeling, inverse problems
Colorado	L.R. Ahuja (ARS Great Plains Unit)	Root zone management modeling, field experimentation

	T. Green (ARS Great Plains Unit)	Upscaling issues in soil hydrology
Iowa	D. Jaynes (ARS Tilth Lab)	Solute transport modeling, non-invasive measurements, field experimentation, root zone and site-specific management
Texas	S.R. Evett (ARS CPRL)	Portable TDR, root zone water balance measurements

C. OTHER PARTICIPANTS

Delaware	Y.Jin (U of Delaware)	Experimentation and modeling of contaminants, including microorganisms, fate and transport
Idaho	J.B. Sisson (INEEL)	In-situ measurements and sensor development
	J.M. Hubbell (INEEL)	In-situ measurements and sensor development
	I. Porro (INEEL)	Real time monitoring and characterization
Nevada	G.V. Wilson (DRI)	In-situ monitoring, vadose zone hydrology
New Mexico	J.N. M. Hendrickx (NM Tech)	Modeling preferential flow, field experimentation, non-invasive measurements, remote-sensing, GIS
Utah	J. Bilskie (Campbell Sci)	In-situ measurements, sensor development
Washington	G.W. Gee (Batelle PNNL)	In-situ measurements, solute leaching management and modeling
	M. Rockhold (Batelle)	Inverse methods, models for subsurface leaching Management

RESOURCE LISTING

PARTICIPANT	OBJECTIVES 1	2	3	RESOURCES SY	PY	TY
A. SAES						
Arizona SAES						
A.W. Warrick	X	X	X	0.3	0.2	0.1
P.J. Wierenga	X	X	X	0.1	0.1	0.2
W.O. Rasmussen	X	X	X			
California SAES						
J.W. Hopmans	X	X	X	0.3	0.1	0.1
D.R. Nielsen	X	X	X	0.2	0.0	0.0
D.E. Rolston		X	X	0.1	0.0	0.2
W.A. Jury	X	X		0.1	0.1	0.1
L. Wu	X	X	X	0.2	0.1	0.1
M. Ghodrati		X	X	0.2	0.1	0.1
Colorado SAES						
G. Butters	X	X		0.2	0.1	0.0
Indiana SAES						
J. Cushman	X	X		0.2	0.1	0.0
Illinois SAES						
T.R. Ellsworth	X	X	X	0.2	0.1	0.1
Iowa SAES						
R. Horton	X	X		0.2	0.0	0.0
Kansas SAES						
G. Kluitenberg	X	X		0.3	0.5	0.0
Minnesota SAES						
D.J. Mulla	X	X	X	0.2	0.1	0.0
Montana SAES						
J.M. Wraith	X	X	X	0.20	0.0	0.0
Nevada SAES						
S.W. Tyler	X	X	X	0.15	0.0	0.0
W.W. Miller	X	X	X	0.15	0.0	0.0
North Dakota SAES	X	X	X	0.2	0.0	0.2
R. Knighton						

Utah SAES						
D. Or	X	X	X	0.2	0.0	0.0
Washington SAES						
J. Conca		X		0.1	0.0	0.0
M. Flury	X	X		0.3	0.0	0.2
J. Wu	X		X	0.2	0.0	0.0
Wyoming SAES						
R. Zhang	X	X	X	0.2	0.2	0.1
Subtotal				**4.5**	**1.8**	**1.5**
B. USDA-ARS						
California						
M.Th. van Genuchten	X	X	X	0.2	0.0	0.0
P. J. Shouse	X	X	X	0.2	0.0	0.0
F. Leij	X	X	X	0.2	0.0	0.0
J. Simunek	X	X	X	0.2	0.0	0.0
T. Skaggs	X	X	X	0.2	0.0	0.0
Colorado						
L.R. Ahuja	X		X	0.2	0.3	0.3
T.R. Green	X		X	0.3	0.0	0.0
Iowa						
D. Jaynes	X	X	X	0.1	0.1	0.1
Texas						
S.R. Evett		X		0.2	0.0	0.0
Subtotal				**1.8**	**0.4**	**0.4**
C. OTHER PARTICIPANTS						
Idaho						
J.B. Sisson		X		0.2	0.0	0.0
J.M. Hubbell		X		0.2	0.0	0.0
I. Porro		X		0.2	0.0	0.0
Nevada						
G.V. Wilson	X	X	X	0.1	0.0	0.0
New Mexico						
J.N.M. Hendrickx	X	X		0.1	0.1	0.0

Washington							
G.W. Gee	X	X	X		0.1	0.0	0.0
M. Rockhold	X	X	X		0.1	0.0	0.0
Delaware							
Y. Jin	X	X	X		0.2	0.0	0.0
Subtotal					**1.2**	**0.1**	**0.0**
Total				`	**7.5**	**2.3**	**1.9**

SY – Scientific man year (project leader)
PY – Professional support year (task leader)
TY – Technical support year (technician)

CRITICAL REVIEW OF ACCOMPLISHMENTS UNDER REGIONAL RESEARCH PROJECT W-188

October 1, 1994 – September 1999

TITLE: **IMPROVED CHARACTERIZATION AND QUANTIFICATION OF FLOW AND TRANSPORT PROCESSES IN SOILS**

OBJECTIVES:

1. To develop and evaluate new approaches for quantifying the effects of spatial and temporal heterogeneity on water and solute movement in field soils,

2. To develop and evaluate new instrumentation and methods of data analysis for improved characterization of water and solute transport, and

3. To apply existing models and new measurement techniques to improve the management of soil water resources

ACTIVE PERSONNEL AND COOPERATING UNIVERSITIES/AGENCIES

Ahuja, L.R.	USDA, ARS, Ft. Collins, CO
Bilskie, J.R.	Campbell Scientific, Logan, UT
Butters, G.	Colorado State University, Ft. Collins, CO
Cushman, J.H.	Purdue University, W. Lafayette, IN
Ellsworth, T.R.	University of Illinois, Urbana, IL
Flury, M.	Washington State University, Pullman, WA
Gee, G. W.	PNNL-Battelle, Richland, WA
Ghodrati, M.	University of California, Berkeley, CA
Hopmans, J.W.	University of California, Davis, CA
Horton, R.	Iowa State University, Ames, IA
Jaynes, D.B.	National Soil Tilth Lab., Ames, IA
Jin, Y.	University of Delaware, Newark, DE
Jury, W.A.	University of California, Riverside, CA
Kluitenberg, G.J.	Kansas State University, Manhattan, KS
Knighton, R.E.	North Dakota State University, Fargo, ND
Leij, F.J.	USSL, USDA-ARS, Riverside, CA
Levitt, D.	Bechtel NV, Las Vegas, NV
Mulla, D.J.	University of Minnesota, St. Paul, MN
Nielsen, D.R.	University of California, Davis, CA
Or, D.	Utah State University, Logan, UT
Parlange, M.B.	Johns Hopkins University, Baltimore, MD
Rasmussen, W.O.	University of Arizona, Tucson, AZ
Shouse, P.J.	USSL, USDA-ARS, Riverside, CA
Šimunek, J.	USSL, USDA-ARS, Riverside, CA
Sisson, J.B.	Idaho National Eng. Lab, INEEL, Idaho Falls, ID
Sully, M.	Bechtel Nevada Corp., Las Vegas, NV.
Tyler, S.W.	DRI, Univ. of Nevada, Reno, NV
van Genuchten, M. Th.	USDA-ARS, USSL, Riverside, CA
Warrick, A.W.	University of Arizona, Tucson, AZ
Wierenga, P.J.	University of Arizona, Tucson, AZ
Wilson, G.P.	DRI, Las Vegas, NV

Wraith, J.M.	Montana State University, Bozeman, MT
Wu, L.	University of California, Riverside, CA
Zhang, R.	University of Wyoming, Laramie, WY

WORK ACCOMPLISHED UNDER THE ORIGINAL PROJECT OBJECTIVES

During the past five years, W-188 members have made many outstanding scientific contributions as part of this regional research project. For example, W-188 members produced some 300 refereed journal articles, approximately 30 book chapters, several books and edited conference proceedings, a large number of reports and proceedings papers, and two patents. In addition, W-188 members organized and/or participated in a large number of national and international conferences and workshops, were active in several professional societies, served the professional community in other capacities, supervised graduate students, and/or were member of M.S. and Ph.D. thesis committees. These activities reflect the high national and international stature of W-188 members, and the leadership role of this committee with respect to delineating, articulating, and resolving flow and transport issues involving the vadose zone.

This review provides an overview of some of the major accomplishments of W188 during the past five years. Space limitations require that this report is more illustrative than comprehensive. The attached list of publications provide details of the broad array of contributions that have resulted from this project.

The accomplishments below are grouped according to the three project objectives. By their very nature, however, many of the accomplishments overlap and/or touch upon more than one objective. For example, modeling efforts as part of objective 1, and improvements in instrumental techniques and data analyses as part of objective 2, both had considerable bearing upon the design, implementation and interpretation of relevant field experiments. The field experiments in turn provided important feedback for improving the description of the basic flow and transport processes, and for advancing new methods and instrumentation for estimating field-scale soil properties. Also, improved process descriptions and instrumental methods resulting from selected field studies should motivate the formulation and testing of improved management tools and practices under objective 3. This iteration of improving process understanding, modeling, designing new measurement methods and instrumentation, field experimentation and, concurrently, developing improved management tools, has been key to promoting collaboration and productive synergism between W-188 members, each having different expertise, interests and backgrounds.

OBJECTIVE 1: To develop and evaluate new approaches for quantifying the effects of spatial and temporal heterogeneity on water and solute movement in field soils

W-188 contributions under objective 1 include improved tools for modeling field-scale flow and transport processes; various geostatistical, scaling and other methods to deal with field-scale heterogeneity; and improved mathematical descriptions of relevant unsaturated soil-hydraulic and solute transport properties. Aspects related to direct measurement of unsaturated flow and transport parameters are discussed under objective 2.

A large number of models were developed, or considerably improved, for more realistic predictions of water and solute movement into and through the vadose zone. These models involve improved deterministic solutions to the relatively standard Richards equation describing variably-saturated water flow, and the convection-dispersion equation (CDE) describing solute transport, simplified solutions for approximate analysis of specific flow and transport problems, integrated process-based models for a variety of management applications, and deterministic and stochastic formulations addressing soil heterogeneity and preferential flow from widely different perspectives.

W-188 members developed and tested detailed theories describing the simultaneous transfer of heat, water, and inorganic and organic chemicals in porous media. The theory includes four fully-coupled partial differential equations. Heat, water, and inorganic and organic chemicals were shown to move in the presence of temperature, soil water pressure and solute concentration gradients. Field experiments were conducted in several states to test the models, with predicted and observed values showing similar trends. W-188 members also developed a transient three-dimensional root growth and water flow model. The model simulates the effects of soil water status, soil strength and temperature on plant root growth and architecture, and accounts for nutrient uptake and transport. Both passive and active nutrient uptake by roots is considered, as well as zero- and first-order source/sink terms. Root age effects on root water and nutrient uptake activity were also included, as well as the influence of nutrient deficiency and ion toxicity on root growth. The model was constructed in attempts to better characterize plant root systems, their response to a variety of environmental conditions, and their influence of water flow and solute transport in the vadose zone. Model simulations demonstrate that the amount and timing of nitrate fertilizers, as well as root uptake of these fertilizers, affects both the amount and the quality of water leaching from the root zone. Related experimental and modeling studies on root growth and water uptake were conducted in several states.

W-188 members from several locations combined to develop a new generation of windows-based computer software (HYDRUS-1D, HYDRUS-2D) for deterministic modeling of water and solute transport in the one-and multidimensional variably-saturated subsurface systems. For example, HYDRUS-1D may be used to simulate the movement of water, heat and a variety of solute decay chains. The transport equations include provisions for nonlinear and nonequilibrium reactions between the solid and liquid phases of the soil, linear equilibrium reactions between the liquid and gaseous phases, zero-order production and first-order degradation reactions which may occur independently or though coupling of solutes involved in sequential first-order decay reactions. Root growth is simulated by means of logistics functions, and accounts for water and salinity stress in the soil root zone. The software further implements a parameter estimation procedure for inverse estimation of selected flow and transport parameters. Microsoft windows-based Graphical User Interfaces (GUIs) manage the input data required to run HYDRUS, and are used for nodal discretization and editing, parameter allocation, problem execution and visualization of input and output results. A related version additionally accounts for the interception of precipitation or irrigation water by plant roots, and for estimating evapotranspiraton for different agricultural canopies. The codes may be used for a variety of applications in research and management, as well as for class room instruction of flow and transport processes in the vadose zone.

Several more approximate models for water flow, infiltration and solute transport were also derived. For example, W-188 members tested a large number of infiltration models for their ability to fit infiltration data. To account for potential levels of uncertainty, three levels of measurement error were included using a Monte-Carlo analysis. Results show that extending the measurement period provided parameter estimates with higher confidence, and more precise estimates of that confidence. The empirical Horton model resulted in the worst fit due to model bias, while overall the Swartzendruber model was found to the best for most relevant applications. A related analytical study investigated the effect of sloping layers on downward flow in the vadose zone. This study provided better understanding of flow through deep arid soils or buried waste repositories.

W-188 members also developed an exact solution of the Richards equation for water flow in heterogeneous porous media. The solution technique was based on the exact integral solution for an exponential hydraulic conductivity function. The exact solution was extended to arbitrary hydraulic property functions by approximating these functions with piecewise-linear curve segments and integrating the functions analytically segment by segment. The resulting analytical solution technique is more efficient than standard numerical solutions, and provides a convenient tool to study complex problems of water flow and solute transport in variably saturated, heterogeneous porous media. Possible uses include establishing initial conditions for numerical flow and transport models, estimating effective parameters or upscaling hydraulic properties for large-scale modeling, and calculating travel times or travel time probability density functions for use in stochastic-convective representations of solute transport. The method was used to calculate net infiltration rates through the Hanford site in Washington, and applied to data from Yucca Mountain to analyze flow in layered, unsaturated, fractured rock.

A relatively simple and efficient method was developed to simulate one-, two- and three-dimensional random fields of soil properties. The proposed method used an iterative numerical scheme to solve a stochastic differential equation. Since the procedure requires minimal computer memory and computation time, the method is especially useful for simulating large fields for studying spatial variability and sampling distributions. Besides its efficiency, the procedure also produced accurate realizations of random fields, in terms of mean and covariance of simulations. Covariances or variogram values calculated from the simulated data using the procedure matched the theoretical functions very well, with the simulated mean values being very close to the theoretical mean. Simulations of soil water content in a large field in Wyoming using the proposed technique conditioned with 45 data points compared well with results from kriging using 91 data points

Research as part of this project also focused on estimating surface fluxes into the atmosphere. Turbulent atmospheric mixing above the land surface provides field scale information on the flux of water and other volatiles. The study considerable improved the estimation of surface fluxes by means of similarity models, turbulence dissipation methods, eddy accumulation. Field measurements obtained in the Central Valley and Owens Valley of California demonstrated the utility of the different approaches.

Several W-188 members also investigated virus transport and reactions by means of saturated and unsaturated flow experiments. The transport data, as well as data from batch experiments, were used to develop a model of virus transport and reactions in soil. Results suggest that the interfaces between the solid, liquid, and gaseous phases in soil have the capacity to inactivate viruses. Also, the mechanisms of virus sorption on surfaces appear much more complex than those controlling chemical sorption. Viruses have the capacity to exclude each other from solid surfaces, thereby causing sorption reaches saturation sooner than can be deduced from surface area alone. A major finding of this research was that virus transport cannot be described with the commonly used CDE model. Also, the association of viruses with colloids likely causes increased virus survival, and facilitates rapid virus transport in the subsurface environment.

Preferential flow of water and solutes through the vadose zone is a serious environmental concern, as well as poses tremendous modeling challenges. W-188 members developed several dual-porosity (mobile-immobile) and dual-permeability models to account for preferential flow. For example, a new version of the CXTFIT code was released for evaluating equilibrium and nonequilibrium solute transport in the subsurface, and for estimating selected unknown transport parameters in those models. Several W-188 members cooperated to develop in-situ laboratory and field methods for estimating dual-porosity type nonequilibrium processes. The field method uses a tension infiltrometer to apply a time series of four conservative non-interacting anionic flourobenzoate tracers. After infiltration of the tracers, a soil core is taken below the infiltrometer and the tracers extracted and measured. A log-linear regression method is subsequently used to obtain estimated of both the immobile water content, 2_{im}, and the mass transfer coefficient, ", from the measured tracer concentrations.

W-188 members also cooperated in the development of improved equations for the mass transfer coefficient in a dual-permeability model simulating water and solute movement in macroporous field soils. A new partitioned solution procedure was used to obtain more efficient numerical solutions of this model. Sensitivity analyses with the process-based formulation explained many of the preferential flow features often observed in undisturbed field soils, especially during saturated or near-saturated conditions. The approach is consistent with plot-scale transport experiments which suggest the presence of a medium made up of two (or sometimes more) overlapping continua, one for the bulk soil matrix and one for the macropore region. Fluid and solute mass transfer in and between the two regions in the conceptual model occurs as a function of both pressure and concentration gradients.

Other research focused on geostatisical indicator simulation techniques to interpolate field-measured water contents and hydraulic properties, and the use of a conditional simulation technique, based on similar-media scaling, to estimate hydraulic properties from a set of scale-mean parameters and the initial water content and porosity distributions. An upscaling algorithm was used to determine effective model parameters and comparisons made between measured and predicted values. The overall technique was applied to a large-scale tracer study at the Department of Energy's Hanford Site in Wahsington. During the experiment, water and radioactive tracers were injected in multiple increments at a 4.6 m depth in well-drained, heterogeneous sandy soil. The water plume was monitored using a neutron probe to log profiles from 32 wells arranged radially around the injection well. Comparison of the modeling results with field data were good, indicating that the conditional simulation and upscaling method provides an efficient, systematic means for estimating effective soil hydraulic properties for field-scale modeling purposes.

Other stochastic approaches developed or tested included a first-order reliability method (FORM) as a possible approach for a quantitative analysis of subsurface transport, and a method for simulating water table dynamics in tile-drained fields subject to intermittent precipitation or irrigation. A stochastic state equation for the water table height midway between drain laterals was obtained by adding a random noise term to the deterministic drainage equation. The random term accounted for dynamics not modeled with the deterministic equation, which was based on numerous simplifying assumptions. A continuous-discrete Kalman filter was used to obtain an estimate of the time variation of the water table height, as well as the variance of the estimate. W-188 also successfully developed a stochastic model of wetting front movement through heterogeneous soils using a modified cellular automata approach. In this approach the water pulse is discretisized and the flow of individual water volume elements tracked in response to local moisture conditions. The method allows soil heterogeneity and spatially varying soil properties to be considered.

Direct measurement of the soil hydraulic properties is time-consuming, costly, and often of limited accuracy because of instrumental limitations, the highly nonlinear nature of unsaturated flow, and the general problem of subsurface heterogeneity. To improve indirect estimation methods, W-188 initiated the development of a large international database (UNSODA) of unsaturated soil hydraulic properties. Approximately 1000 data sets representing different soil types from various parts of the world have now been included. UNSODA provides a repository and source of soil hydraulic data for a variety of applications. The data also may be used for evaluating and calibrating statistical pore-size distribution or pore-scale network models predicting the unsaturated hydraulic conductivity from observed soil water retention data, as well as for deriving pedotransfer functions (PTFs) to predict the hydraulic functions from soil texture, bulk density, organic matter content, and other relatively easily measured soils data.

UNSODA and other data were used to evaluate the ability of several previously published PTF's to predict selected soil water retention parameters and the saturated hydraulic conductivity. Existing PTF's were compared with a hierarchical system of neural network models. Neural networks are universal function approximators which should be well suited to related hydraulic properties with the surrogate soil taxonomic data. Uncertainty in the neural network predictions was calculated using bootstrapping to yield probability density functions of the predicted hydraulic parameters. The uncertainty information can be very useful for Monte Carlo simulations, and also provides insight in how existing PTF's can be improved.

In related research, a set of new water retention function was developed to cover water contents from oven dry to saturation. The modified functions used popular retention equations for the main range of water contents, and an adsorption equation for the dry range. The modified functions were combined with Mualem’s conductivity model to generate closed-form analytical expressions for the calculation of unsaturated hydraulic conductivity. W-188 members also developed a procedure to estimate the soil water retention function from soil particle-size distribution data. A relationship between the fractal dimension and the cumulative particle-size distribution was derived and subsequently incorporated into the retention model. Using in-situ and laboratory data, new piecewise-continuous soil water retention and hydraulic conductivity functions were formulated for application to dual-porosity type soils. When incorporated into HYDRUS-2D, the functions successfully predicted the preferential flow of water and dissolved nutrients to tile drains in a flood-irrigated agricultural field in New Mexico.

Finally, W-188 members also examined the roles of adsorption and capillary condensation in variably-saturated porous media. A new model for pore space geometry comprising an angular pore cross section connected to slit-shaped spaces is proposed for a more realistic representation of natural pore spaces. The analyses resulted in relatively simple expressions for relating pore cross-sectional saturation to matric potential. The pore scale model was subsequently upscaled to represent a core-sample scale retention properties. Comparisons of the model with measured retention data yielded favorable results and enabled separation of adsorption and capillary contributions as well as explicit calculations of liquid-vapor interfacial area. Similar work focused also on predictions of the unsaturated hydraulic conductivity.

OBJECTIVE 2. To develop and evaluate new instrumentation and methods of data analysis for improved characterization of water and solute transport

W-188 has made many contribution to the acquisition of new instrumental techniques, as well as more efficient and accurate methods for analyzing laboratory and field data. These contributions, again, are documented in detail in attached publications; only a limited few contributions are highlighted here.

Members of W-188 have long been at the forefront of designing, constructing, calibrating, testing and applying Time Domain Reflectometry (TDR) methods and instrumentation for measuring soil water contents and/or solute concentrations. New probes for soil water content measurements were developed using oscillator circuits that have a sensitivity and spatial response similar to traditional sensors, but are much less expensive and nearly independent of cable length. New Fourier techniques were devised to extract additional information on the frequency dielectric properties from common TDR waveforms. A user manual for the windows-based Win-TDR acquisition and analysis software program (free of charge to interested scientists) was also produced.

Much research was directed to improved calibration of TDR probes. In one study a physically-based calibration method applied to multi-level probes in the field and laboratory yielded standard errors about 0.015 $cm^3\ cm^{-3}$ or smaller for the water content when segment-specific calibrations were carried out. In a related study, three commonly used calibration methods were evaluated to relate the impedance with the solute concentration. Numerical integration of the in-situ observed response to a tracer input function proved to be the most accurate method. Results indicate that long measurement periods are important when following nonequilibrium transport through undisturbed and/or structured soils. Work also focused on the use of TDR in providing real-time estimates of ionic solute distributions in field soils. Field results showed the great promise of TDR for monitoring soil water and fertilizer salt distributions to improve agricultural management.

Another study used TDR and the initial liquid water content to better quantify the contributions of the vapor, liquid, and solid phases to the water content of frozen soils for which conventional TDR calibration curves are inadequate. Results agreed closely with reference data obtained with nuclear magnetic resonance (NMR) for fine-textured soils but not for sandy soils. Studies also focused on the effects of temperature on TDR measured soil water contents. Because TDR is extensively used by scientists and managers, measurement errors resulting from a temperature artifact have substantial practical importance. Experimentation led to a unifying hypothesis and a physical model with correction factors recommended for TDR practitioners. Results also have importance for remote sensing of near-land-surface water content at microwave frequencies, and for other approaches that infer water status based on dielectric constant of porous media.

Encouraged by the success of TDR, studies were conducted to explore the use of other electromagnetic methods for characterizing porous media and its constituents. Results based on transmission line measurements of dielectric properties across a wide band of frequencies (0-18 GHz) provided a quantitative description of bound water on clay surfaces. At the low frequency range (0-MHZ), very large dielectric constants were measured and directly attributable to the presence of macromolecules (e.g., organic matter).

Considerable progress was made also in the application of electromagnetic induction (EM) methods for water content and solute concentration measurements. EM methods were perfected and used for salinity mapping of riparian areas in New Mexico. A promising inverse method was developed for non-invasive detection of breakthrough curves in the field. Another study used EM to delineate field-scale heterogeneities for implementation of site-specific precision farming. Non-contacting EM was tested as an inexpensive soil mapping aid. EM maps showed good correspondence with soil survey maps. EM data, linked to a global positioning system, were successfully used to map the depth of a clay layer in a field in Iowa. EM data also showed great potential for use as a co-regional variable to predict soil organic carbon content.

X-ray Computed Tomography (CT) is a non-invasive technique that allows for three- dimensional, nondestructive imaging of heterogeneous materials. To date, few investigators have examined the potential of CT in vadose zone studies. A method was devised for measuring the phase-volume fractions in tomographic representations of two-phase (air, water) systems. Another study used CT to quantify plant roots in situ. The stems of the bean plants were excised and their root systems imaged with a high-energy industrial tomography unit (420 kV). Forty individual horizontal tomograms, each 200 µm thick were combined into a 3-D data set for a total rooting depth of 0.8 cm starting at the base of the hypocotyl. This volumetric data set was analyzed for root volume through estimation of relative fractions of root and soil matrix within each voxel for the entire 3-D data set. The rendering of iso-attenuation surfaces illustrated the spatial arrangement of roots with diameters equal and larger than 0.36 mm. Destructive root sampling yielded a root length per unit volume (L_v) between 44 and 60 cm/cm^3 soil, whereas the CT-measured L_v was about 76 cm/cm^3.

Several W-188 members, together with researchers from Australia, combined to develop a much improved dual-probe heat pulse (DPHP) technique for measurement of soil water content and thermal properties. An automated data acquisition system was constructed for simultaneous measurement of 24 DPHP probes. Software was developed for extracting thermal properties from the DPHP data. Comparisons with gravimetric measurements showed that the DPHP sensors measured average water content within about 0.02 $m^3\ m^{-3}$ and changes in the water content to within 0.01 $m^3\ m^{-3}$. W-188 members also developed a thermo-TDR probe to determine soil water content, bulk electrical conductivity, thermal conductivity, heat capacity, and thermal diffusivity of soil simultaneously. The probe provides an opportunity to monitor a range of properties of a given soil volume; TDR is used to determine water content and a heat pulse method for the volumetric heat capacity. An important advantage of the thermo-TDR probe is its ability to determine water content and bulk density changes on the same soil volume.

A new generation of tensiometers wsas developed for measurement of water potentials in soil, gravel and fractured rock.. The new "Portable and Advanced Tensiometer" does not show the strong diurnal fluctuations often seen in conventional tensiometers, are not depth limited, can be used over longer time periods without maintenance, and operate in soil, cobbles, and rock. The precision of the tensiometers was further improved by removing barometric pressure effects.

Several other new measurement techniques and probes were designed, built and/or tested in cooperative W188 research. These include a multi-port soil solution extractor, a new matric-potential TDR-based probe, a fully automated apparatus for measurement of two- and three-fluid (air, oil, water) pressure-saturation and permeability relationships, and various image analysis techniques for field monitoring of mobile dye tracers at spatial resolutions of about 1 mm^2. The latter approach offers unique opportunities for analysis of solute transport patterns in heterogeneous soils.

Another promising new technique is the use of remote fiber optic fluorometry for in-situ measurement of solute transport processes in real time and on a continuous basis. The methodology consists of transmitting a constant beam of light through the input leg of a bifurcated fiber optic miniprobe (3 mm diameter) to a location of interest within the soil matrix. At the probe tip, incoming light interacts with the soil matrix where it is partially absorbed and partially reflected back into the probe. The reflected signal is transmitted through the output leg to a photodetector and quantified. The intensity of the output signal, which is constant under steady conditions, changes when a plume of fluorescent water tracer passes through the soil matrix in front of the probe. This allows in-situ measurement of a solute breakthrough curves at the point of observation in real time. The new system allowed simultaneous measurement of solute BTCs at 20 different points within a soil column.

Several studies focused on improved field research for rapid in-situ measurement of the soil hydraulic properties. In one typical project, a new double-ring tension infiltrometer was developed and field tested on field data in Colorado and Wyoming. The infiltrometer was used for estimating the unsaturated hydraulic conductivity using inverse analysis (discussed further below). A much improved two-term equation for describing three-dimensional infiltration from a disc infiltrometer was developed. The infiltration solution provides an accurate yet simple approach to estimate fluxes from an axisymmetric source by permitting the estimation of the sorptivity and hydraulic conductivity from cumulative infiltration data.

A comprehensive field research project was carried out at the Maricopa Agricultural Center (MAC) in Arizona for the purpose of (1) assessing state-of-the-art monitoring systems that are or could be used at low-level radioactive waste disposal and decommissioned facilities to detect early releases of radio nuclides to the environment, (2) determining how best to implement the monitoring systems; and (3) evaluating relevant strategies for monitoring flow and transport in relatively deep vadose zones. Experiments were conducted at MAC to test a variety of monitoring techniques during two large-scale drip-irrigated infiltration experiments. Water flow was measured with tensiometers, heat dissipation sensors (HDS), electromagnetic induction, and neutron probes. Good agreement between wetting front arrival times measured with HDS probes and tensiometers was found both in the monitoring islands and buried trench.

Other W-188 work focused on the use of inverse methods for estimating the hydraulic properties of variably-saturated media. Many members have long been involved with such inverse methods for a variety of applications. For example, a generalized parameter estimation procedure was developed to evaluate unsaturated soil hydraulic properties from transient one- or multi-dimensional flow experiments in the laboratory or the field. The procedures combines the Levenberg-Marquardt nonlinear parameter estimation method with appropriate, state-of-the-art numerical solutions of the variably-saturated flow equation. The procedure permits measurements other than the infiltration rate to be included in the objective function, as well as optionally a penalty function for the optimized parameters to remain in some feasible region (Bayesian estimation). The software was used to address the problem of optimal sampling design (i.e., selecting the best points in space and time for making measurements) by studying the sensitivity on the objective function to changes in the optimized hydraulic parameters. The method was used to analyze a large number of laboratory and field experiments, including multi-step inflow and outflow experiments, one-and two-rate evaporation experiments, and a multi-step cone penetrometer infiltration experiment. In a related study, an annealing-simplex method was developed to improve the nonlinear parameter estimaiton problem. The method incorporates simulated annealing strategies into a classical downhill simplex method to improve converge and parameter uniqueness irrespective of the assumed initial hydraulic parameters. The annealing procedure has great promise for use in water resource optimization problems that require a robust global search capability.

A closely related inverse parameter estimation study focused on the rate-dependence of unsaturated hydraulic characteristics as determined by laboratory outflow experiments on undisturbed soil samples. A significant effect of the flow rate on both the water retention and the unsaturated hydraulic conductivity function was observed for a sandy soil, but not for a more fine-textured soil. The experiments indicate that it is important to consider the method by which the hydraulic properties of unsaturated soils are determined, thus keeping in mind the purpose of the measurement. Results show that hydraulic parameters obtained under extreme high outflow conditions in the laboratory may not accurately represent relatively slow flow processes as they normally occur in the field. Data from this and other studies indicate that the rate dependency is due to entrapped water occupying dead-end pore space, with the amount of entrapped water increasing with increasing flow rate. Entrapped air also appears to play an important role.

Soil scientists have long addressed the problems of two-phase (air, water) flow in soils. This expertise, with appropriate modifications, is very much applicable also to the more general problem of multi-phase (air, oil, water) flow typical of soil and groundwater contamination by nonaqueous phase liquids (NAPLs) originating from industrial and commercial activities. Several studies were conducted to estimate the permeability and retention properties of multi-fluid systems. Multi-step outflow experiments were carried out using a modified Tempe cell for air-water, oil-water, and air-oil fluid pairs. Results were used to directly estimate capillary pressure and wetting phase permeability functions. The capillary pressure saturation data for each fluid pair were scaled using their interfacial tension values relative to that of air-water, thereby yielding a single capillary pressure curve. The combined relative permeability data coalesced to a single curve, indicating that the relative permeability is a function of the porous medium only. Results also showed that the inverse solution is very sensitive to the hydraulic resistance of ceramic cup of the extraction device.

W-188 members also performed experiments and modeling of the dissolution of light and dense NAPLs in saturated soil columns. In the experiments, NAPL was added at residual saturation to 10-cm columns and leached at high flow rates for several hundred pore volumes. A model which assumes that the NAPL consists of isolated spheres that releases mass by rate-limited dissolution into the water phase was successfully used to model outflow and the final concentrations of NAPL (in experiments where the flow was stopped prior to complete removal) using a value of about 1 mm for the sphere diameter. Research suggests that the NAPL emulsified and traveled as small droplets for short distances in the soil before becoming trapped again.

In a separate study, several W-188 members cooperated to estimate interfacial areas of porous media containing two or three fluids from measured capillary pressure - saturation relationships. A new parametric model was developed for the wetting phase (water) and nonwetting phase (air, oil) constitutive relationships. The dynamics of the air and water phases during the infiltration of water into the unsaturated column was also studied. Analytical two-phase infiltration equations accounting for air compression ahead of the wetting front, air counterflow, and flow hysteresis in the soil were derived on the basis of the Green and Ampt equation. The equations also accounted for the presence of macropores near the soil surface. Experimental testing showed that the equations were reasonably accurate in predicting the infiltration process. The capillary pressure at the wetting front was found to vary between the dynamic water-bubbling an air-bubbling values of the soil.

OBJECTIVE 3. To apply existing models and new measurement techniques to improve the management of soil water resources

Models and tools developed under objectives 1 and 2 have been used in a broad range of practical applications, such as devising agricultural best management practices, salinity assessment, local or regional pollution from pesticide and nitrate leaching, soil reclamation, and pesticide volatilization. A selected few examples are given below.

Integrated models used as part of this regional project included the Root Zone Water Quality Model (RZWQM), HYDRUS-2D, GLEAMS, the multi-component major ion chemistry code UNSATCHEM-2D, and the multiphase, multidimensional STOMP code. Problems addressed with RZWQM included the presence water and chemicals in tile outflows, pesticide fate in soils and runoff; corn root distribution effects on water use, nitrogen leaching, effects of tillage, water stress, residue cover; and swelling-shrinking phenomena; scientists from many states in the Midwest cooperated in this effort. HYDRUS-2D applications involved fertilizer and pesticide transport to tile drains, prediction of the water balance of arid waste disposal sites, capillary barrier performance, methyl-bromide fate and transport, and contaminant transport from a landfill.

W-188 members tested new methods to remotely sense soil water, crop water stress and other crop stress parameters. Satellite images and aerial photos were used to obtain spectral signatures of crop yield, disease occurrence, weed pressure, and insect damage in North Dakota. Farm-scale multispectral aerial photography was employed eight times during the growing season. Flights corresponded to key crop phenological events to gather additional relevant information for crop management practices at finer resolutions. The farm-scale images were used for ground-truthing and subsequent calibration of satellite image features (signatures). On-the-go yield monitors were used in four successive years to measure yield on irrigated corn and potato fields. Correlations of spectral signatures with yield provide a very effective method of estimating nitrogen use on a watershed scale, and concomitant predictions of nitrogen leaching to ground water. A novel system, SMILEY, was developed to access, distribute, and analyze massive amounts of remote sensed data in order to determine the required correlations. The system utilizes state-of-the-art Internet technology and provides a distributed multi-tier client/server architecture for accessing and analyzing remote sensed data.

Localized compaction and doming (LCD) provides a method to alter water flow paths around knife-injected nitrogen fertilizer bands. Reduced water flow through the fertilizer band decreases solute transport and leaching. Small plot lysimeters were used in Iowa to evaluate leaching losses of anionic tracers applied under different management types. Results indicate that leaching indeed can be controlled through this soil management practice. As compared to conventional fertilizer banding, LCD plots showed larger nitrate concentrations in the upper root zone after rainfall, larger corn yields after high rainfall growing seasons, and less chemical in the effluent of field lysimeters

Nitrate contamination of ground water was investigated at a field site in California. Nitrogen isotope ratios (*^{15}N) were measured on nitrate extracted from core samples removed from the surface to the water table below natural, fertilizer, onsite sewage disposal systems, and animal sources located within two alluvial valleys of California. The *^{15}N remained fairly constant with depth, indicating little denitrification during transport, with little difference between natural and fertilizer sources (0-4). Higher *^{15}N levels were found for the animal (8-20) and sewage disposal (2-12). This study showed that nitrogen isotope ratios tend to be site specific and can provide valuable information regarding suspected sources in the vadose zone and in ground water.

The HYDRUS-2D code was used to analyze water and nitrogen transport data collected in a large tile-drained field. A tile drainage system installed in the 60-acre commercial farm provided experimental data on nitrate and pesticide transport rates to shallow groundwater. The data revealed a rapid transport of high concentrations (>50 mg/L) of nitrate from nitrogen fertilizers immediately after an irrigation, followed by a return to background levels (< 5 mg/L) afterwards. There was a similar rapid response in drain flow following water input at the soil surface. These and other observations suggest the presence of preferential flow. New piecewise continuous soil water retention and hydraulic conductivity functions were formulated based on the New Mexico data, as well as data collected at a tile-drained site in Iowa, and incorporated in the HYDRUS-2D code. Numerical simulations using the new functions showed significantly better predictions of the preferential flow rates in the tile drains following rainfall/irrigation events at both sites.

Stochastic techniques were applied to GLEAMS for the purpose of simulating pesticide transport within experimental plots in southern Ohio. Hydraulic parameters were described using random multi-variate normal (MVN) vectors. Simulations of the transport of three commonly used pesticides (alachlor, atrazine and metribuzin) in the root zone were carried using either mean parameter values or probability density functions derived from the MVN vector realizations. Results confirmed that soil spatial heterogeneity significantly affects pesticide transport, and that the probabilistic approach provides better predictions of pesticide transport across the experimental area.

In another project, transfer functions and numerical models were used to simulate pesticide transport under field conditions in Wyoming. Transfer functions were used to predict the average field concentration at different depths, while numerical models were used to simulate various physico-chemical processes in the layered soil, including infiltration due to rainfall and irrigation, evaporation, root uptake, advective transport, dispersion, adsorption, and degradation. While the mathematical models provided reasonable predictions of water flow and solute transport, spatial variability of soil hydraulic properties strongly affected the results.

W-188 members conducted several studies on the transport, degradation and emissions of volatile compounds, including especially Methyl-Bromide (MB) which is a suspected ozone depleter and scheduled for elimination by 2001. Since MB is an important fumigant in the agricultural community (such as for strawberries and almonds), and farmers are concerned about its elimination, a study was conducted to examine processes governing MB emissions under various field conditions. Conventional practices (e.g., tarping a field for 1-2 days) were found to be ineffective. Application of a small irrigation after MB injection and before tarping significantly reduced losses into the atmosphere. Also, conventional tarping was found to be ineffective at preventing methyl bromide losses to the atmosphere, typically allowing about 50-60% to reach the atmosphere. A field plot study was conducted using a new polyethylene tarp that effectively blocked the release of methyl bromide to the atmosphere during preplant fumigation, while at the same time allowing a reduction in the application rate of up to 50% without loss of pest control efficacy. With the reduced loading, the cost of the tarp will not be a factor, thus permitting pest control without releasing ozone-depleting chemicals to the atmosphere. The HYDRUS-2D code was successfully modified used to simulate the complex two-dimensional processes of water flow, heat movement, and vapor-phase transport in tarped MB treated fields.

Leaching of water and solute from highly disturbed lands associated with mining activities can significantly impact surface and groundwater quality. Six-meter long column tracer experiments were conducted in Nevada to determine the transport properties of mine ore subjected to cyanide heap leaching. Cyanide heap leaching of gold ore is commonly used to extract gold from low concentration ore. After extraction, the spent heaps (which may exceed 100 m in height and 100s of hectares of land area) contain large volumes of cyanide laden fluids which must be rinsed to eliminate this contamination. TDR-measured breakthrough curves were fitted best using a mobile-immobile model of solute transport, consistent with both field observations and the large range of particle sizes found for the ore. Results were used to formulate optimal rates and volumes for rinsing the mine tailings of cyanide. In a related study, the soil hydraulic properties of native and reconstructed mine-spoils (strip coal mine in southeastern Montana) were quantified and compared with respect to the behavior of water on reconstructed landscapes. This effort may help in the design of improved soil profiles and topographies when reclaiming severely impacted lands.

W-188 members investigated the effect of land retirement on subsurface flow and solute transport in the western San Joaquin Valley, CA. Land retirement has been adopted as an agricultural management alternative in this area to alleviate problems related to shallow groundwater tables. The essential strategy of land retirement is to cease irrigating lands with poor drainage characteristics and high levels of salt and trace element concentrations. In this study the effect of land retirement on subsurface flow and solute transport was evaluated using an integrated groundwater flow and unsaturated-zone model. Results suggest that retiring a substantial area of land from irrigation will lead to a relatively stable water table situation. However, long-term salt accumulation near the soil surface due to increased upward fluxes of water and solutes may pose serious hazards to the environment and human health.

W-188 members used vapor stripping of chlorinated solvents from contaminant sites. PNNL's STOMP simulation program was used to predict vapor stripping efficiency and the well hydraulics. The procedure depends greatly on the hydraulic conductivity, which was severely reduced at the site because of the low sodium adsorption ratio.. The STOMP code was also used to estimate leakage rates of contaminants from high level radioactive waste tanks, which are covered with gravel. Simulations of the transport of mobile (e.g., H-3, Tc-99, nitrate) and reactive (Cs-137) contaminants were run using STOMP. Effects of leakage rate, recharge rate, preferential flow, and sorption characteristics on transport of contaminants were evaluated for a 50-year period using estimated hydraulic properties and historic and simulated climatic conditions. Over the 50 years of simulation, the volume of water leaching the waste at the highest recharge rate (100 mm/y) was over 20 times the estimated leak volume (nearly 1 M Liters).

W-188 members used computer models to assist the Nuclear Regulatory Commission (NRC) to solve problems related to nuclear water sites. Capillary barriers provide site isolation under a variety of climatic conditions and rainfall scenarios. New developments in similar-media scaling techniques coupled with geostatistical analyses led to the development of a method for conditioning soil hydraulic properties based on their spatial distribution and initial conditions. This method can significantly reduce the uncertainty in predictions of water flow and solute transport in spatially-variable field soils.

Data collected from monitoring of near-surface water balance at an arid site in southern Nevada was used to investigate the applicability of HYDRUS-2D to predict the water balance of an arid landfill site. Two years of water content, water potential and meteorologic data were available for the study. Using only limited soil hydraulic property information and estimated evapotranspiration data, HYDRUS was used in a forward simulation to predict the temporal variation of water content in the upper 200 cm of the profile. Very good agreement was found between predicted and measured water contents when additional phenology data was used about the root distribution and transpiration season of the desert vegetation.

Relatively little data is available on the spatial distribution of soil water under drip irrigation, and how it is affected by root distribution, emitter placement and irrigation amounts. W-188 members hypothesized that variables such as emitter position relative to the active roots as well as irrigation amount and frequency will affect spatial and temporal changes in soil water content as controlled by root water uptake and leaching. A field study was conducted in Arizona to study the soil water regime of a surface drip irrigated almond tree. The experimental site (6.6 m x 4.8 m) was intensively instrumented with tensiometers and neutron probe access tubes to infer the three-dimensional distribution of soil water and root water uptake during the irrigation season. Drainage fluxes were estimated from measured hydraulic head gradients and hydraulic conductivity data. Unsaturated hydraulic conductivities were determined from both in-situ measurements by the instantaneous profile method, and multi-step outflow methods in the laboratory. The water balance results showed that the applied water was not sufficient to match the actual tree water use by evapotranspiration, thus causing soil water depletion around the tree as the irrigation season progressed. Moreover, soil water content data demonstrated temporal changes in the water uptake patterns. The temporal patterns of leaching justifies regular soil water measurements in the design and implementation of drip irrigation systems.

DEGREE TO WHICH OBJECTIVES HAVE BEEN ACCOMPLISHED

The preceding review, and the long list of references, should show that the project objectives have been fully accomplished. Progress in model development has been truly impressive, both in terms of the formulating specialized deterministic and stochastic models addressing particular laboratory- and field-scale flow and transport issues, and in terms of developing integrated process models for application to pertinent environmental and agricultural management problems. Equally impressive has been the broad array of new instrumental methods and methods of analyses devised and implemented as part of this regional research project. Improved TDR equipment, electromagnetic induction, ground-penetrating radar, X-ray computed tomography, heat pulse techniques, remote fiber optic fluometry, novel methods of image analysis, new tensiometric methods, and the use of increasing power inverse modeling procedures are now providing better means for studying and quantifying fundamental underlying water flow and solute transport processes at a hierarchy of spatial scales in both the laboratory and the field. At the same time, advances in remote sensing techniques, geographic information systems, global positioning systems, and comprehensive data assimilation techniques, are providing the tools needed to foster the site-specific management of agricultural systems, the ultimate purpose being to optimize agricultural production without sacrificing the long-term integrity of our soil and water resources.

A LOOK AHEAD

Responsible stewardship of our limited soil, air and water resources, within the context of maintaining agricultural production for an ever increasing world population, is a critical issue that will require increased understanding of the complex factors governing ecosystem behavior, and its response to natural and human activities, at local, regional and global scales. While the current project has provided vastly improved modeling and measurement tools, effective integration and use of these tools at a variety of spatial and time scales remains a challenge.

The overwhelming heterogeneity of the subsurface environment (and the soil surface when viewed from the larger scales) remains at the center of this problem. Needed are improved representations of spatially aggregated flow and transport processes, and/or soil properties, that account for the naturally occurring spatial and temporal variabilities. Disaggregation (or down-scaling) may be similarly needed when dynamic processes or static properties at the larger scale are observed (e.g., through remote sensing), but require translation to smaller (but inherently heterogeneous) subscales if they are to be made useful for, for example, site-specific environmental or farming operations. This scale-transfer problem needs to be solved to improve the prediction of coupled fluxes of heat and moisture across the land surface, and to establish appropriate parameters to describe the behavior of solute transport processes in soils at local (field) or regional (watershed) scales. One important question is how the problem of soil heterogeneity at different spatial and temporal scales will affect the measurement, prediction and management of land surface hydrologic and subsurface flow and transport. As shown in this critical review, W-188 committee members collectively have the expertise in modeling, experimentation and data assimilation techniques to address these scale issues.

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