

# **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
_imunek, 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 400 refereed journal articles, approximately 50 book chapters, several books and edited conference proceedings, a large number of reports and proceedings papers, and three 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 through 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 evapotranspiration 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 be 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 considerably 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,  $\theta_{im}$ , and the mass transfer coefficient,  $\alpha$ , 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 geostatistical 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 discretized 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  $0.015 \text{ cm}^3 \text{ cm}^{-3}$  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  $\mu\text{m}$  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  $\text{cm}/\text{cm}^3$  soil, whereas the CT-measured  $L_v$  was about 76  $\text{cm}/\text{cm}^3$ .

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  $0.02 \text{ m}^3 \text{ m}^{-3}$  and changes in the water content to within  $0.01 \text{ m}^3 \text{ m}^{-3}$ . 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 was 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  $1 \text{ mm}^2$ . 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 procedure 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 estimation 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 and 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 of 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 ( $\delta^{15}\text{N}$ ) 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  $\delta^{15}\text{N}$  remained fairly constant with depth, indicating little denitrification during transport, with little difference between natural and fertilizer sources (0-4). Higher  $\delta^{15}\text{N}$  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.