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Challenges and Opportunities in Porous Media Multiphase Flow and Contaminant Transport Research

International Conference in honor of "Rien" van Genuchten on the occasion of his 80th birthday

May 7-9, 2025

Federal University of Rio de Janeiro (UFRJ)
Rio de Janeiro, Brazil

The abstracts are listed alphabetically in terms of the last name of the first author of the presentations. Page numbers where the abstracts are provided are also listed. Both short and extended abstracts are included in the list.

Using HYDRUS to Optimize Soil Mounds for Efficient Irrigation in Date Palm Orchards

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Date palms are high-value traditional fruit trees widely cultivated in arid regions due to their resilience to harsh climatic conditions and saline soils. In the hyper-arid Arava Valley of Israel, date palm cultivation depends on high-frequency irrigation with saline groundwater (~ 3 dS/m) from local aquifers. Large volumes of irrigation are necessary to meet crop water demands and leach salts below the root zone. However, this practice has led to environmental challenges, with some farmers reporting poor drainage, resulting in puddles that hinder agricultural machinery and create mosquito habitats. To address these issues, farmers have adopted the practice of building soil mounds around date palm trees to improve infiltration and salt leaching.

This study aimed to optimize the geometry and soil hydraulic properties of these mounds by combining field measurements with a calibrated HYDRUS numerical model. In our experimental setup, soil mounds approximately 60 cm in height and 200 cm in diameter were constructed around date palm trees. Each mound had a distinct sand-to-compost ratio: 100-0, 75-25, 55-45, 25-7 and 0-100. A network of sensors, including TDR, tensiometers, and suction cups, was installed at different depths within the mounds and local soil to continuously monitor soil conditions. Sensitivity analysis using the HYDRUS model identified key parameters influencing infiltration rates and salt leaching efficiency.

Results showed that compost-based mounds retained higher soil moisture compared to sand mounds. Notably, the mound with a balanced ratio (55-45) exhibited ponding conditions in the field. Compost-dominant mounds (0-100 and 75-25) maintained stable electrical conductivity (EC) levels of approximately 5 dS/m. On the other hand, sand-dominant mounds (100-0, 75-25) showed greater EC fluctuations ranging from 2.5 to 3.5 dS/m, indicating variable salt concentrations. The calibrated HYDRUS model demonstrated high accuracy in predicting soil water content across different sand-to-compost ratios, with a low RMSE of 0.011 to 0.016 cm^3/cm^3.

Sensitivity analysis revealed that the saturated hydraulic conductivity (Ks) was the most influential parameter. Numerical optimization indicated that mounds with 100-0 and 75-25 maximized infiltration while retaining sufficient moisture for root water uptake. Therefore, using a calibrated HYDRUS model to optimize soil mound design with appropriate dimensions and sand-to-compost ratios can enhance infiltration, salt leaching, and water retention in date palm cultivation, thereby improving the efficiency of high-frequency irrigation.

A Novel Application of HYDRUS-1D: Modeling Overland Solute Transport During Furrow Fertigation

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Accurate simulation of solute transport in surface irrigation systems is essential for optimizing fertigation practices and minimizing nutrient losses. The HYDRUS-1D model has become a popular tool to simulate subsurface water flow and solute transport. However, there is no study that has assessed the ability of HYDRUS-1D to simulate solute transport solely in surface flow of furrow irrigation operations. The novelty of this study is to demonstrate that the HYDRUS-1D accurately characterizes breakthrough curves using reasonable assumptions and correctly adapting their parameters, while neglecting interactions with subsurface conditions. In this study, we used the software to fit the nitrate transport in overland water flow during furrow fertigation, using experimental data from the literature.

The model was adapted to represent furrows as saturated, open-surface flow domains, and parameterized using an average (or effective) fluid velocity and longitudinal dispersivity, which were optimized through inverse modeling. The HYDRUS-1D model produced good agreement with observed nitrate concentrations with high coefficients of determination ($0.80 \le R^2 \le 0.93$) and Nash-Sutcliffe efficiencies ($0.79 \le NSE \le 0.93$), and low root mean square errors (RMSE) ranging from 20.3 to 50.1 mg/L across various irrigation methods, including conventional, alternate, and fixed furrow irrigation. Additionally, measured water advance times were successfully estimated using concepts of optimal paths from percolation theory.

Results revealed that the flow velocity and dispersivity were strongly influenced by irrigation strategy and timing, with alternate furrow systems exhibiting lower solute mobility. Despite its original design for subsurface applications, HYDRUS-1D was capable to accurately simulate solute transport in furrow surface flow when appropriately adapted. The modeling approach offers a practical framework for evaluating and improving fertigation strategies in surface irrigation systems.

Statistical Characterization of Solute Transport in Heterogeneous Aquifers: Implications for Groundwater Risk Assessment

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Quantifying the risks posed by toxic chemicals in groundwater remains a complex and pressing challenge, particularly due to the inherent heterogeneity of subsurface formations. Variability in hydraulic conductivity and its spatial correlation structure plays a pivotal role in determining solute plume dispersion and travel time estimates - both of which are fundamental to accurate risk assessment. Compounding this complexity is the limited availability of high-resolution data, constrained by financial and logistical challenges, which often results in incomplete site characterization. As a result, predictions of solute transport are inherently uncertain, necessitating the adoption of probabilistic modeling approaches.

In this talk, I will present a summary of key stochastic methods employed to characterize transport in heterogeneous aquifers. I will highlight the critical influence of characteristic length scales, connectivity and degrees of heterogeneity on solute concentration uncertainty and large-scale dispersive behavior, with the goal of informing more reliable risk assessment and management strategies.

Lattice Boltzmann Multicomponent-Multiscale Modeling for Fluid Flow through Porous Media

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Modeling multiscale transport phenomena for multiphase and multicomponent fluids in porous media is a challenging task, both for predicting real engineering applications and for developing consistent theoretical formulations. Due to the complex pore structure of various porous media (such as rock samples (Neto et al., 2015; Nagata et al., 2023; Vidal et al., 2024) and biological materials (Claro et al., 2023)) pore diameters can range from the nanometer scale up to centimeters. In larger geological formations, including rhizosphere (Schnepf et al., 2022; Claro et al., 2023), aquifers (Ferreira Campos Morato Filpi et al., 2023) and oil reservoirs (Wang et al., 2023), pore diameters may extend from the nanometer scale to meters, especially where geological fractures are present. With advances in X-ray tomography since the 1950s, spanning microtomography, synchrotron light sources, nanotomography, and fourth-generation synchrotron beam-lines, we can now obtain time-resolved experimental results of transport phenomena across different scales (Claro et al., 2023). However, in these X-ray experiments, image sizes are constrained by the detector, making it difficult to capture the range of length scales needed to fully characterize heterogeneity across multiple scales. Consequently, numerical approaches that utilize image data from these tests while coupling different scales are a promising alternative for predicting multiscale behaviors.

Since its development, the lattice Boltzmann method (LBM) has proven to be an excellent tool for simulating multiphase/multicomponent fluid flows through porous media. Rooted in the kinetic theory of particles, the method effectively models the interactions at fluid interfaces between different phases. The discrete formulation of the lattice Boltzmann method, based on the processes of collision and streaming, enables the straightforward implementation of bound- ary conditions, making it particularly suitable for representing fluid flow in complex geometries. This capability is crucial for accurately modeling intricate solid structures, such as 3D micro- tomography images of porous media. Moreover, the LBM framework offers a high degree of parallelization on both CPUs and GPUs, allowing for near-perfect scalability in well-parallelized codes.

However, in the LBM literature, the multiphase/multicomponent multiscale approaches (Spaid and Phelan Jr, 1998; McDonald and Turner, 2015; Pereira, 2016; Zalzale et al., 2016; Ning et al., 2019; An et al., 2020; Lautenschlaeger et al., 2022; Liu et al., 2024) usually keep the fluid segregation term within the porous-continuous media (PCM), thereby clearly identifying the immiscible fluid interface. This aspect eliminates the relative permeability resistance and the capillary pressure effects during fluid-fluid displacement, making it solely dependent on absolute permeability.

Therefore, the present work proposes a multiscale multicomponent modeling by incorporating the non-linearity of relative permeability resulting from fluid–fluid interactions within the PCM region. To achieve this, the study combines pore-scale immiscible flow, represented by the Navier-Stokes equations, with the Buckley–Leverett equation to describe the non-linear mass balance of the two components. Additionally, the generalized porous continuous Navier-Stokes equation proposed by Nithiarasu et al. (1997) is employed to account for the momentum balance. By integrating these equations, the present work provides a comprehensive framework for modeling the PCM region, effectively capturing both mass and momentum dynamics influenced by non-linear relative permeability (described by Lomeland et al. (2005) correlation) and capillary pressure effects (described by Van Genuchten (1980)).

References:

An, S., Y. Zhan, J. Yao, H.W. Yu, V. Niasar, A greyscale volumetric lattice Boltzmann method for upscaling pore-scale two-phase flow, Advances in Water Resources 144 (2020) 103711.

Claro, P.I., E.P. Borges, G.R. Schleder, N.L. Archilha, A. Pinto, M. Carvalho, C.E. Driemeier, A. Fazzio, R.F. Gouveia, From micro-to nano-and time-resolved x-ray computed tomography: Bio-based applications, synchrotron capabilities, and data-driven processing, Applied Physics Reviews 10 (2023).

Ferreira Campos Morato Filpi, T.C., P.H. Ferreira Galvão, L. da Rocha Santos, C. de Vasconcelos Müller Athayde, A. Bahniuk Rumbelsperger, L.F. Cury, G. Barbosa Athayde, Permeability scale effect analyzed in high resolution in brazilian neoproterozoic karst aquifer, Environmental Earth Sciences 82 (2023) 57.

Lautenschlaeger, M.P., J. Weinmiller, B. Kellers, T. Danner, A. Latz, Homogenized lattice Boltzmann model for simulating multi-phase flows in heterogeneous porous media, Advances in Water Resources 170 (2022) 104320.

Liu, Y., J. Feng, J. Min, X. Zhang, Homogenized color-gradient lattice Boltzmann model for immiscible two-phase flow in multiscale porous media, Journal of Applied Physics 135 (2024).

Lomeland, F., E. Ebeltoft, W.H. Thomas, A new versatile relative permeability correlation, in: International symposium of the society of core analysts, Toronto, Canada, 112, 2005.

McDonald, P., M. Turner, Combining effective media and multi-phase methods of lattice Boltzmann modelling for the characterisation of liquid-vapour dynamics in multi-length scale heterogeneous structural materials, Modelling and Simulation in Materials Science and Engineering 24 (2015) 015010.

Nagata, R., P.J. Dos Reis, C.R. Appoloni, Multi-scale approach to assess total porosity and pore size in four different kinds of carbonate rocks, Micron 164 (2023) 103385.

Neto, I.A.L., R.M. Misságia, M.A. Ceia, N.L. Archilha, C. Hollis, Evaluation of carbonate pore system under texture control for prediction of microporosity aspect ratio and shear wave velocity, Sedimentary geology 323 (2015) 43–65.

Ning, Y., C. Wei, G. Qin, A unified grayscale lattice Boltzmann model for multiphase fluid flow in vuggy carbonates, Advances in Water Resources 124 (2019) 68–83.

Nithiarasu, P., K. Seetharamu, T. Sundararajan, Natural convective heat transfer in a fluid saturated variable porosity medium, International Journal of Heat and Mass Transfer 40 (1997) 3955–3967.

Pereira, G.G. Grayscale lattice Boltzmann model for multiphase heterogeneous flow through porous media, Physical Review E 93 (2016) 063301.

Schnepf, A., A. Carminati, M.A. Ahmed, M. Ani, P. Benard, J. Bentz, M. Bonkowski, M. Knott, D. Diehl, P. Duddek, et al., Linking rhizosphere processes across scales: Opinion, Plant and Soil 478 (2022) 5–42.

Spaid, M.A., F.R. Phelan Jr, Modeling void formation dynamics in fibrous porous media with the lattice Boltzmann method, Composites Part A: Applied Science and Manufacturing 29 (1998) 749–755.

van Genuchten, M.Th., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Science Society of America Journal 44 (1980) 892–898.

Vidal, A.D., A.P. M. Neta, J. de Castro Vargas Fernandes, L.C. Medeiros, C.E.M. dos Anjos, R. Surmas, A.G. Evsukoff, Multi-resolution x-ray micro-computed tomography images of carbonate rocks from Brazilian pre-salt, Scientific Data 11 (2024) 1361.

Wang, S., F. Chen, Y.-S. Wu, H. Nasrabadi, The potential of hydrogen storage in depleted unconventional gas reservoirs: A multiscale modeling study, International Journal of Hydrogen Energy 48 (2023) 16007–16019.

Zalzale, M., M. Ramaioli, K. Scrivener, P. McDonald, Gray free-energy multiphase lattice Boltzmann model with effective transport and wetting properties, Physical Review E 94 (2016) 053301.

Improving the Tension and Pressure Extractor Moisture Retention Curve Method by Implementing the HydraProbe Soil Sensor in Soil Cores

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The moisture retention curve (MRC) has fundamental applications in several branches of science and engineering, including irrigation research, plant and soil studies, food security, site assessment for construction projects, landfill and wastewater monitoring, flood warning systems, landslide and wildfire risk assessment, water resources monitoring, oil and mining projects, and more. The MRC depicts the relation between volumetric water content (percentage) and water potential (unit of pressure) of a soil. Some important parameters that can be obtained from the MRC are the saturation point, field capacity, available and unavailable water, the water holding capacity, and permanent wilting point.

The Richards and van Genuchten equations describe water movement and the relation between water content and the unsaturated hydraulic conductivity curves based on several parameters of a soil mostly derived from the moisture retention curve. SoilMoisture's "Lab Setup" has been for several decades to obtain the MRC for soils around the world.

Also popularly used is the Stevens HydraProbe soil sensor, which measures soil temperature, soil moisture, soil electrical conductivity and the complex dielectric permittivity. In order to improve soil moisture measurements and to finetune the calibration of the HydraProbe unit, undisturbed or constructed soil cores can be contained using a metal ring with a fixture to hold the HydraProbe in place in the sample. A mesh on the bottom allows for the exchange of water in and out of the soil sample during the various target pressures. The resulting system, called the "Travel Assembly, can be placed on a low-tension table and in pressure extractors going up to 1500 kPa, while being portable enough to weigh on a balance. The Travel Assembly thus allows users to collect a full suite of pressure data for a soil sample in a single fixture that can travel between the balance and the extractor with a soil sensor in the sample. This "setup has broad implications because with the HydraProbe one can directly obtain not only unsaturated hydraulic heads and unsaturated hydraulic conductivities, but also highly accurate soil moisture measurements.

Six samples of a Columbia silt loam Alfisol were placed in the Travel Assembly and evaluated at saturation and 10 pressures ranging from 0.01 to 2 Bar. The technique was perfected to generate a soil water retention curve with minimal error. To saturate the soil core, each Travel Assembly (containing soil) was placed in a dedicated Saturation Pan. After reaching the saturation point, the water content of the saturated sample was calculated from the empty weight of the Travel Assembly (not containing the soil sample), the weight of the Saturation Pan, the weight of water outside of the Sample Ring, and the dry weight of the soil sample (measured during the last step after obtaining all other datapoints).
To obtain each datapoint of the moisture retention curve at tensions lower than 15 kPa, the soil core was saturated, then placed on a Sandbox Tension Table. Tensions were applied

using a hanging water column setup. A half-bar ceramic tension table plus a hanging water column were used to apply tensions between 150 to 50 kPa. For pressure levels between 50 kPa and 1500 kPa (the permanent wilting point), a 15-bar pressure vessel was used. Pressures were supplied using a nitrogen tank and regulated and stabilized using a precision double-regulating pressure stabilizer. Moisture contents of the samples were measured using the HydraProbe sensor every minute during the tension/pressure application campaigns. The data were collected via a Steelhead data logger and then communicated to the Skyview360 web interface.

The improved system showed several advantages over the conventional MRC measurement system. Adding a HydraProbe to the system made it possible to measure real-time moisture contents of the soil samples, which helped to obtain a more effective troubleshooting process. The HydraProbe also made it possible to calculate (and predict) the equilibrium time and the moisture content at the equilibrium point. The volumetric moisture content of soil cores at different moisture tensions were determined using the gravimetric method (weighing the samples). This provided an opportunity to compare the HydraProbe readings with the measured moisture contents at several moisture levels, which made it possible to finetune the calibration of HydraProbes for specific soil samples. The fine-tuned calibration table of the moisture content associated with water potential per each data point enables HydraProbe to accurately estimate the soil water potential in the field.

Analyzing Macro- and Microporosity with MicroCT Images for Improving NMR and Resistivity Interpretations

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Acquiring 3D μCT images with a resolution of up to 8 microns per voxel on core samples 1.5 inches in diameter has become a standard practice in rock characterization. The high-resolution of this approach enables the identification of macropores with radii exceeding 4 microns. Image segmentations, performed using either manually defined threshold or automatic methods such as Otsu's algorithm, generate a binary representation that distinguishes macropores from the surrounding matrix. However, many carbonate core samples exhibit significant microporosity below the 8-micron resolution threshold, which remains undetected in μCT images. Despite its dependence on pore connectivity, microporosity significantly influences electrical properties and nuclear magnetic resonance (NMR) responses. One of the primary challenges in interpreting NMR data in carbonates is the effect of diffusive coupling between micro- and macropores, which alters the decay rate of polarized hydrogen protons, thereby complicating the differentiation between macro- and micropores in the T_2 distribution. Regarding electrical properties, microporosity can lead to low cementation index (m) values, which substantially impact reservoir oil calculations.

This study analyzed five carbonate core samples from the Morro do Chaves formation in the SE-AL basin, an analogy to the pre-salt reservoirs in Brazil. The samples underwent μCT imaging, NMR analysis, and laboratory gas porosimetry (*RCAL*). To enhance microporosity identification in μCT images, the Density Equation, also known as the 'Law of Mixtures', was applied, using μCT voxel values as proxies for the apparent density. Since the 1.5-inch diameter core samples were subjected to *RCAL* analysis to obtain experimental porosity values before subsequently acquiring images on the μCT, the Density Equation can be expressed as

$$CT_{\emptyset} = \frac{CT_{Matrix} - CT_{Average}}{CT_{Matrix} - CT_{Fluid}}$$

where $CT_{\emptyset}$ represents the porosity obtained from *RCAL*, while $CT_{Average}$ is the mean voxel value core image. If CT_{Matrix} is known, CT_{Fluid} can be determined, and vice-versa. Once one or both values are established through histogram analysis of the μCT values, voxel-specific porosity can be calculated using

$$Voxel_{\emptyset} = \frac{CT_{Matrix} - CT_{Voxel}}{CT_{Matrix} - CT_{Fluid}}$$

Assuming spherical pores, a voxel containing a sphere with a diameter equal to its voxel size would theoretically exhibit a porosity of 53%. Thus, voxels exceeding this porosity threshold can be classified as macroporous. Conversely, microporous voxels can be identified based on the assumption that spherical pores maintain good hydraulic conductivity when their porosity equals or exceeds 33%. This criterion facilitates the identification of well-connected micropores, enabling further analysis through NMR random walk models or electrical conductivity models.

This study provides a quantitative framework for integrating μCT imaging with *RCAL* and NMR techniques, enhancing microporosity characterization of carbonate reservoirs. The methodology improves the reliability of permeability estimations and electrical property assessments, leading to more accurate reservoir evaluations.

Reference:

Ramakrishnan, T.S., R. Ramamoorthy, E. Fordham, L. Schwartz, M. Herron, N. Saito, and A. Rabaute. 2001. A Model-Based Interpretation Methodology for Evaluating Carbonate Reservoirs. SPE Annual Technical Conference and Exhibition, Sep 30 – Oct 3, SPE71704.

Extended Simplified Evaporation Method (XSEM) to Determine Soil Hydraulic Properties Across the Full Moisture Range

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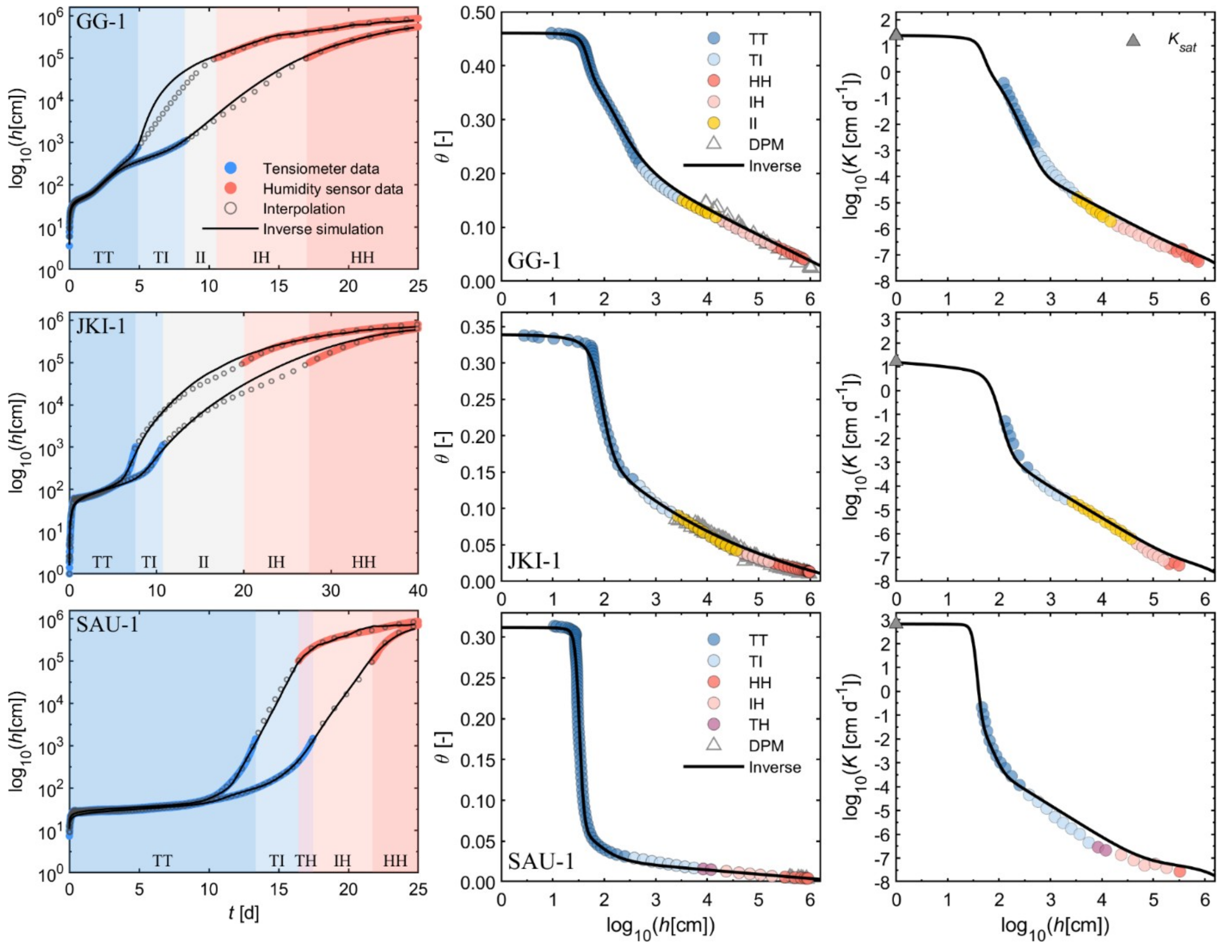
The Simplified Evaporation Method (SEM), as implemented in the commercial product HYPROP™, is widely used to determine the water retention curve (WRC) and hydraulic conductivity curve (HCC) of soil samples. However, its application has traditionally been limited to the suction range measurable by tensiometers. This study introduces the eXtended Simplified Evaporation Method (XSEM), which integrates humidity sensors into the SEM setup to measure soil water potential. By interpolating suction data between the two sensor technologies, XSEM provides a quasi-continuous suction time series from full saturation to air dryness. Combined with measured weight changes, this enables seamless determination of soil hydraulic properties (SHP) from wet conditions to air dryness.

We tested XSEM on three soils with widely differing textures, using two replicates per type. The WRC data obtained in the dry range were compared to measurements from the WP4C™ dew point method (DPM), while SHP results were validated against inverse modeling. Our findings demonstrate that XSEM accurately determines SHP across the full moisture range in a single experiment, with minor biases observed in specific suction ranges for sandy soils. Additional advantages of XSEM include (i) a fully automated protocol with straightforward calculations, (ii) simplified WRC determination beyond suctions of 1 MPa compared to DPM, and (iii) high-resolution data outputs.

Extending soil hydraulic property determination into the dry moisture range improves assessments of film and vapor flow contributions to HCC, which dominate at low soil water contents. This advancement benefits applications such as soil water and solute flux modeling under diverse climatic conditions, salinization risk assessment, and moisture characterization in porous building materials.



Left column: Measured and interpolated suction data from XSEM experiments for the first replicate samples of silt loam (GG-1), sandy loam (JKI-1), and sand (SAU-1) (top to bottom). Shaded regions indicate suction data grouped into six categories based on the measurement type: T (tensiometer), I (interpolation), and H (humidity sensor). Middle column: Resulting water retention curves (WRC), with color-coded data corresponding to the underlying suction measurement types at the lower and upper measurement positions. Additionally, DPM retention curve data (gray triangles) and SHP functions from inverse modeling are shown for comparison. Right column: Same as the middle column but for the hydraulic conductivity curve (HCC), with added saturated conductivity measurements (gray triangles).

Reference:

Bosse, J., S.C. Iden, W. Durner, M. Sut-Lohmann, and A. Peters (2025): Extending the measurement range of the simplified evaporation method using humidity sensors. Submitted to *Vadose Zone Journal*, revised manuscript under review.

MRI Insights into Fow Processes within an REV

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Advanced simulation models for unsaturated water flow and solute transport in the vadose zone are based on the principles of continuum mechanics and energy concepts, expressed through the total matric potential. For soil water flow, the classical Richards' equation (RE) is employed. In this framework, pore geometry and driving force mechanisms are incorporated implicitly through the definition of hydraulic properties, averaged over a representative elementary volume (REV), assuming a continuous medium on a macroscopic scale. In reality, flow processes arise at the microscale within the REV. Measured soil hydraulic properties, such as the retention curve and hydraulic conductivity function, represent averaged values over the sample used. But what happens at the microscale within REV?

MRI visualization of a fully controlled process of water flow through a small soil sample of coarse sandy loam over time revealed a gradual shift in flow mechanisms at the microscopic scale. Initially, ponded infiltration was dominated by rapid gravity flow. Over time, the influence of capillary forces became apparent, gradually reducing the volume of preferentially moving water. Preferential flow paths developed immediately, while slow matrix flow transiently developed later. The most likely reason, which was also detected in later experiments, is the redistribution of the encapsulated residual air. Initially, small pores were blocked by trapped air due to gravity flow. Later, capillary forces - albeit at low velocities - pushed small bubbles of air out of the pore entrances. Over time, the residual air coalesced into larger bubbles that further impeded the fast flow. As a consequence, in a subsequent infiltration experiment under full saturation, the so-called "steady-state" flow rate was significantly lower than in the initial run.

These findings highlight the impact of preferential flow closely connected with flow instability, phenomena not considered in the classical RE approach. This raises doubts about the quality of routinely measured hydraulic conductivities. Similar effects were observed in experiments across various scales and soil types.

Revival of Analytical and Hybrid Methods for Flow and Transport in Porous Media: The van Genuchten Legacy

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Analytical heat and mass diffusion theory was mostly established along the 20th century, particularly within its first seven decades, till the boom of the computer era, then dividing attention with advancements on numerical methods for partial differential equations, that today form the basis of the simulation arsenal in modern engineering practice. Martinus van Genuchten was one of the great names in analytical diffusion theory in porous media along this vibrant period, with numerous important contributions.

The integral transform method is a well-known analytical methodology for the exact solution of linear partial differential equations in mathematical physics, with roots on the separation of variables approach proposed by Fourier, in the first half of the 19th century, on its extension introduced in the work of Koshlyakov, in the first half of the 20th century, and followed by the extension and unification advanced by Luikov, Olçer, Ozisik, and Mikhailov, among others. This approach was progressively generalized under a more flexible hybrid numerical-analytical structure, known as the Generalized Integral Transform Technique (GITT), which includes all the analytical steps inherent to the classical method, but allow for a flexibilization in the numerical solution of the resulting coupled transformed ordinary differential systems.

Since the 1980´s, this computational-analytical methodology was consistently advanced to handle different classes of problems in heat and fluid flow, previously only solvable by purely discrete approaches, offering relative advantages in terms of accuracy, robustness, and computational effort, at the price of further analytical involvement. It has been frequently adopted as a benchmarking tool, besides being quite useful as a computational tool on itself in CPU-intensive tasks, such as in inverse problem analysis, optimization, and stochastic simulations.

With the participation and complicity of Dr. van Genuchten, GITT has been extensively employed in transport phenomena in porous media along the years. The present lecture provides a review on the revival and growth of this analytic-based methodology, focusing on recent progresses on both fundamentals and applications. Future research needs and extension possibilities are then briefly described.

Multiscale Modeling of Heterogeneous Porous Media: Challenges and Applications in Energy, Agriculture and Sustainability

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Modeling heterogeneous porous media is one of the most significant challenges when simulating phenomena involving fluid flow, mass transport, chemical reactions, and heat exchange in natural and artificial systems. This challenge occurs in multiple disciplines, such as in petroleum engineering, agriculture, hydrogeology, the environmental sciences, and civil and biomedical engineering. The structural heterogeneity and anisotropy of porous media studied in these disciplines often require multiscale approaches capable of connecting phenomena that occur from the pore scale to field scale, to allow a more accurate and efficient representation of effective properties and relevant dynamic processes.

In the oil industry, for example, formations such as those in the pre-salt have high structural complexity, with micro and macro heterogeneities that strongly influence the behavior of multiphase flows. At the pore scale, the challenge lies in realistic representations of complex geometries and in the simulation of phenomena such as capillarity, hysteresis, and relative mobility. Microtomography and numerical methods (e.g., pore network models, lattice-Boltzmann approaches, and finite volumes methods involving unstructured meshes) are employed to extract fundamental parameters that feed scale models from plugs. These, in turn, are used in laboratory test simulations (e.g., coreflooding) to infer properties such as relative permeability and capillary pressure curves. At this scale, modeling techniques that incorporate pore scale phenomena into the continuum scale are applied (e.g., integral transform technique and/or numerical simulations).

Unfortunately, many of these parameters are not directly observable and present significant spatial variability. In this context, inverse methods for estimating these parameters play a fundamental role by allowing the estimation of properties of complex porous media based on experimental data, such as time series of pressure, saturation, and production. By adjusting models so that their results approximate those of experimental or field measurements, inverse methods become essential in the calibration of multiscale models, thereby allowing them to more faithfully represent real phenomena.

Inverse approaches are particularly valuable when performing upscaling because when transposing information from the microstructure to larger scales, there is inevitably a loss of details that affect the overall behavior of the system. They help to compensate for this information loss by adjusting multiscale models to maintain their adherence to observations. With this, it is possible to significantly reduce the uncertainties associated with effective properties used in engineering simulations.

At the well scale, conventional tests often do not adequately capture the effects of macro heterogeneities such as fractures, vugs, and high-permeability lenses. Multiscale models, calibrated by inverse methods, allow us to represent these effects consistently, thus improving the interpretation of pressure tests and the prediction of well performance. At the field scale, the combined use of multiscale modeling and inverse methods enables the analysis of connectivity between wells, the extent of drainage, and the effectiveness of techniques such as alternating water and gas injection (WAG), in addition to allowing the evaluation of the uncertainty associated with tracer tests and development strategies.

Outside the energy sector, the challenges and solutions provided by multiscale modeling associated with inverse methods are equally relevant. In agriculture, for example, soils are highly heterogeneous porous media whose structure directly influences water retention, nutrient distribution, and irrigation efficiency. Multiscale models calibrated with field data may adequately represent the interaction between roots, soil particles, and water flow, thereby potentially optimizing the use of water resources and agricultural productivity. In hydrology, aquifers and unsaturated zones have complex geological structures that affect contaminants' transport and groundwater recharge. Inverse methods are fundamental to identifying the spatial distribution of hydraulic conductivity and calibrating regional models that integrate the dynamics of surface and subsurface flows.

Within the context of decarbonization, carbon capture and storage (CCS) processes involve the injection of CO_2 into deep geological reservoirs. The effectiveness and safety of these processes depend on the ability to predict the behavior of injected gas over decades, which is only feasible with the use of well-calibrated multiscale models. Integration with inverse methods allows inferring the movement of CO_2 from seismic, pressure, and tracer monitoring data, leading to a more robust technical basis for environmental assessment and regulation.

With recent advances in computational science, inverse methods are being enriched by machine learning techniques, hybrid physical-data models, and Bayesian approaches. These approaches enable probabilistic estimates and explicit quantification of uncertainties, which is particularly important in systems with data scarcity, high variability, or having noise in the measurements. These modern tools make model calibration more reliable by increasing their predictive capacity and practical usefulness.

In summary, multiscale modeling of heterogeneous porous media, combined with inverse methods for parameter estimation, represents an essential scientific and technological frontier for understanding and controlling complex processes in multiple areas of knowledge. Its continuous development contributes decisively to reducing uncertainties, improving natural resource management, and consolidating sustainable solutions in energy, agriculture, hydrology, and climate mitigation.

Advances in Rock Typing Using Versatile Multi-Scale Micro-CT as an Addition to Conventional (Medical) CT Scans

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Rock typing is a crucial step in reservoir characterization for oil recovery and carbon capture and storage (CCS), enabling the division of the reservoir into flow units that serve as key inputs for multi-scale reservoir models. Conventional rock typing relies on well-logging data (e.g., gamma and resistivity) combined with laboratory-derived porosity and permeability measurements from core plugs. However, rock heterogeneity often leads to discrepancies between log-based and laboratory results, causing over- or underestimation permeability.

Medical computed tomography (CT) has traditionally been used to investigate these mismatches by identifying which dataset is more reliable. However, its limited resolution often fails to reveal the underlying causes of discrepancies or validate the accuracy of conventional methods (Withers et al., 2021).

In this study, we present a multi-scale micro-CT workflow capable of scanning full cores at approximately ten times the resolution of medical CT, while also enabling high-resolution zoom scans on specific regions of interest. This non-destructive approach provides detailed insights into laminations, heterogeneity, and large-scale structures while also capturing grain- and pore-scale features without labor-intensive sampling (Bultreys et al., 2016). By selectively scanning key areas, we demonstrate how the presence or absence of cement influences permeability discrepancies, offering a clearer understanding of log and core data deviations. This methodology enhances current rock typing practices by improving data reliability, optimizing core plug selection, and increasing overall workflow efficiency.

References:

Bultreys, T., W. De Boever, V. Cnudde. 2016. Imaging and image-based fluid transport modeling at the pore scale in geological materials: A practical introduction to the current state-of-the-art. Earth-Science Reviews. https://doi.org/10.1016/j.earscirev.2016.02.001

Withers, P.J., C. Bouman, S. Carmignato, V. Cnudde, D. Grimaldi, C.K. Hagen, E, Maire, M. Manley, A. Du Plesses, S.R. Stock. 2021. Xray computed tomography. Nature Reviews Methods Primers, 1, 18. https://doi.org/10.1038/s43586-021-00015-4

A Robust Variant of the van Genuchten Curve and an Associated Conductivity Curve: Theory, Parameter Fitting, and Performance

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Ippisch et al. (2006) modified the original soil water retention curve (SWRC) of van Genuchten (1980) by introducing a non-zero air-entry value. Rossi and Nimmo (1994) removed the asymptotic residual water content of the SWRC of Brooks and Corey (1964) by a logarithmic dry branch that reaches zero water content at a finite matric potential. We applied that approach to the SWRC of Ippisch et al. (2006). The resulting SWRC has a finite integral, which is a physical necessity (Fuentes et al., 1991), and a zero derivative at saturation, which guarantees that the associated hydraulic conductivity curve (UHCC) is well-behaved near saturation (Durner, 1994; Madi et al., 2018). The latest version of our curve (de Rooij, 2022) allows the matric potential at oven dryness to be fitted independently, which is beneficial if dry-range data points are unreliable or missing. Interestingly, parameter α (L^{-1}), which scaled the matric potential in the original curve, is a true shape factor in our curve, capable of gradually shifting the SWRC from a sigmoidal to a power-law shape as its value increases. Numerical simulations with the original curve, the modification by Ippisch et al. (2006), and our curve, showed that the latter resulted in faster and more robust model runs (de Rooij et al., 2021). The fluxes generated by the original curve and ours appeared more plausible than those based on the SWRC of Ippisch et al. (2006).

Liquid soil water can reside in capillaries as free water, and in films as adsorbed water. Water vapor resides in the gas-filled pore space. De Rooij (2024a) found that arithmetic, harmonic, and geometric averages of the conductivities of these domains are fundamentally unable to capture the effect on the UHCC of the size, configuration, and interactions of the three domains. Compared to straightforward addition of the domain conductivities, averaging mostly did not significantly improve fits to data. Fits of the various UHCCs for different combinations of fitted and fixed parameters revealed some evidence of overparameterization. We therefore developed a more parsimonious junction model that attributes all liquid water to either capillaries or films, depending on the matric potential (de Rooij, 2025). Because the liquid domain and the vapor domain will often be continuous, we added the equivalent vapor conductivity to the resulting liquid-water conductivity. We fitted the additive UHCC model, our junction model, and Kosugi's (1999) generalization of Mualem's (1976) UHCC, which assumes all liquid water to reside in capillaries. The additivity model had one parameter more than the other two. Test simulations crashed the most for the additivity model. The effect of the vapor conductivity on the water fluxes was negligible, even for a semi-arid climate (Nambiar and de Rooij, 2025).

Open-source codes to fit the parameters of the new SWRC and the various UHCC models are available on Zenodo, complete with User Manuals and example input and output files. The codes generate parameter values and their statistics, correlation and covariance matrices, and tables of the resulting SWRC and UHCC (de Rooij, 2024b,c).

References:

Brooks, R.H., and Corey, A.T. 1964. Hydraulic properties of porous media. Colorado State Univ., Hydrology Paper No. 3.

de Rooij, G.H. 2022. Technical note: A sigmoidal soil water retention curve without asymptote that is robust when dry-range data are unavailable. Hydrol. Earth Syst. Sci., 26, 5849-5858. doi: 10.5194/hess-26-5849-2022.

de Rooij, G.H. 2024a. Averaging or adding domain conductivities to calculate the unsaturated soil hydraulic conductivity. Vadose Zone J. e20329. doi: 10.1002/vzj2.20329.

de Rooij, G. 2024b. Fitting the parameters of the RIA parameterization of the soil water retention curve (2.0). Zenodo. doi: 10.5218/zenodo.6491978.

de Rooij, G. 2024c. Fitting the junction model and other models for the unsaturated soil hydraulic conductivity curve: KRIAfitter. Zenodo. doi: 10.5218/zenodo.14047942.

de Rooij, G.H. 2025. Fitting the junction model and other parameterizations for the unsaturated hydraulic conductivity curve: KRIAfitter version 1.0. Preprint EGUsphere. doi: 10.5194/egusphere-2024-3487.

de Rooij, G.H., Mai, J., and Madi, R. 2021. Sigmoidal water retention function with improved behavior in dry and wet soils. Hydrol. Earth Syst. Sci., 25, 983-1007. doi: 10.5194/hess-25-983-2021.

Durner, W. 1994. Hydraulic conductivity estimation for soils with heterogeneous pore structure. Water Resour Res. 30, 211-223. doi: 10.1029/93WR02676.

Fuentes, C., Haverkamp, R., Parlange, J.Y., Brutsaert, W., Zayani, K., and Vachaud, G. 1991. Constraints on parameters in three soil-water capillary retention functions. Transport in Porous Media 6: 445-449. doi: 10.1007/BF00136351.

Ippisch, O., Vogel, H.-J., and Bastian, P. 2006. Validity limits for the van Genuchten-Mualem model and implications for parameter estimation and numerical simulation. Adv. Water Resources 29: 1780-1789. doi: 10.1016/j.advwatres.2005.12.011.

Kosugi, K. 1999. General model for unsaturated hydraulic conductivity for soils with lognormal pore-size distribution. Soil Sci. Soc. Am. J. 63, 270-277. doi: 10.2136/sssal1999.03615995006300020003x.

Madi, R., de Rooij, G.H., Mielenz, H., and Mai, J. 2018. Parametric soil water retention models: a critical evaluation of expressions for the full moisture range. Hydrol. Earth Syst. Sci., 22, 1193-1219. doi: 10.5194/hess-22-1193-2018.

Mualem, Y. 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resour. Res. 12: 513-521. doi: 10.1029/WR012i003p00513.

Nambiar, A., and de Rooij, G.H. 2025. Evaluating unsaturated hydraulic conductivity models for diverse soils and climates: a functional comparison of additive, junction, and Kosugi parameterizations. Preprint EGUsphere. doi: 10.5194/egusphere-2025-412.

Rossi, C., and Nimmo, J. 1994. Modeling of soil water retention from saturation to oven-dryness. Water Resour. Res. 30: 701-708. doi: 10.1029/93WR03238.

van Genuchten, M.T. 1980. A closed-form equation for predicting the unsaturated hydraulic conductivity for unsaturated soils. Soil Sci. Soc. Am. J. 44, 892-898. doi: 10.2136/sssal1980.03615995004400050002x.

Plant Available Water:
Proposal for a Flux-Based Approach

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Plant available water (PAW) is a vital parameter across agronomy, ecology, and hydrology, serving diverse and essential functions in each field. In agronomy, PAW is a key indicator of soil suitability for crop growth and biomass production, guiding decisions on crop selection, irrigation scheduling, and overall farm management. It supports the design of efficient irrigation projects, ensuring that crops receive an adequate amount of water. Ecologically, PAW is essential to describe the hydrological functioning of ecosystems as it influences plant species distribution, survival, and competition. In arid and semi-arid environments, understanding PAW can explain vegetation patterns and plant resilience. Additionally, hydrological and crop models rely on PAW to simulate soil water balance components, crucial for predicting water availability, evapotranspiration, and crop yield under varying climatic and soil conditions.

Traditionally, PAW is divided into total available water (TAW) and readily available water (RAW). TAW is defined as the difference between soil water content at field capacity (FC), which is the upper limit of water storage after excess water has drained, and the wilting point (WP) where plants can no longer extract water. RAW, a subset of TAW, represents the water available to plants between FC and a "limiting point" (LP), beyond which water uptake becomes progressively restricted, leading to plant stress. However, determining FC, LP, and WP accurately remains a challenge due to soil heterogeneity and the dynamic nature of plant- soil interactions. These thresholds are often based on static laboratory measurements that may not reflect real-world conditions, introducing uncertainties in PAW estimation.

This study proposes a novel, process-based approach to improve the prediction of these critical thresholds. Field capacity is estimated by simulating an internal drainage experiment, excluding evapotranspiration, to capture the soil's equilibrium water content when a predefined minimal drainage rate is reached. The limiting point and wilting point are determined using MFLUX, a process-based root water uptake model that simulates how plants extract water from the soil under different moisture conditions. By incorporating hydraulic parameters specific to Brazilian soils, this approach accounts for the diverse soil textures and structures found across the region, improving the accuracy of PAW predictions.

The results offer valuable insights into plant-soil-water interactions, bridging gaps between theoretical modeling and practical application, as more accurate PAW estimates support better-informed decisions in irrigation planning, yield forecasting, and ecosystem management.

Analysis of Soil Water and Soil Aeration Corequisites for Plant Growth

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Plant-available water and diffusion-controlled soil aeration are two fundamental requirements for successful plant growth. These prerequisites have generally been assessed independently in relation to plant growth, with limited focus on their complimentary and competing behaviour in a soil-water matrix. In this study, we leveraged the power of complex numbers to represent soil-water (as the real component) and soil-air (as the imaginary component) as the orthogonal counterparts in a unified framework. The new corequisite index constitutes a soil-water component defined based field capacity and permanent wilting point, and a soil-air component defined based on critical soil-gas diffusivity.

To calibrate model parameters, we used soil-water characteristic (SWC) measurements in vadose soil profiles (0 - 60 cm depth) from 48 replicate sites. Results revealed that the corequisite index, with its magnitude (0.5 – 1) and corequisite angle (0 to 30º) in the given range, provided the best combined soil water and aeration status for the selected soil. The majority of the selected soils were affected by insufficient aeration (gas diffusivity < 0.01) when at field capacity (drained to - 10 kPa), requiring the soils to further loose water (- 50 to - 100 kPa) to satisfy the corequisites.

The derived soil aeration parameters showed promising relationships with measurable soil physical properties. We further recommend adopting a 15% volumetric soil air content as a general threshold for minimum soil aeration in the absence of measured soil-gas diffusivity data.

Should Soil Structure Dynamics be Included in Modeling Variable-Saturated Water Flow?

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Soil texture and soil structure regulate many critical soil processes, such as the movement of water, air, and nutrients as well as their availability for plants. These processes, in turn, affect essential soil functions, including food and biomass production, water storage and purification, and the provision of a biological habitat. Soil texture, determined by the relative proportions of sand, silt, and clay particles, is generally considered a stable property that does not change significantly over time. In contrast, soil structure, referring to the 3D arrangement of soil constituents (minerals, organic matter, void spaces, etc.), can change over time on both short-term and long-term scales.

Various factors which affect the spatial arrangement:

- Short-term (seasonal) changes driven by
    - Abiotic processes (e.g., freezing and thawing, wetting and drying, physico--chemical degradation)
    - Biological processes (e.g., root growth and degradation, earthworm activity)
    - Human-induced changes (e.g., crop rotation, tillage practices)
- Long-term changes due to different carbon inputs, land use change, crop rotation, or soil management operations

These changes result in temporal variations in the soil's ability to retain and conduct water, but also in the reactivity of the soils. In recent years, researchers started to quantify the changes in soil structure and it has been hypothesized that soil structure affects the wet range of the water retention curve and hydraulic conductivity curve. However, the existing experimental data on the topic is limited and the multitude of this effect is not well understood.

In this contribution, we present evidence showing that, for an agricultural loamy soil under diverse tillage management operation, soil hydraulic properties vary not only for different management operations but also evolve over a season. The magnitude of these seasonal changes is in turn dependent on the intensity of tillage. We also discuss the conditions under which these changes become significant and when they should be incorporated into models of variably saturated water flow in soils.

Influence of Inlet-End Diffusers Under Heterogeneous Conditions in 3D SCAL Models

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Core flooding tests are essential tools for characterizing multiphase flow in porous media, providing key parameters such as capillary pressure, relative permeability, and wettability, which are critical for forecasting reservoir performance. By subjecting an outcrop rock sample to a controlled flow rate, these tests facilitate the assessment of permeability and saturation under conditions that approximate those of a petroleum reservoir. These tests measure the pressure differential across the core, the cumulative oil production, and saturation profiles, either at discrete points or continuously along the core. In unsteady-state core-flooding tests, estimating relative permeability and quantifying its associated uncertainties usually requires a numerical optimization approach.

However, the modeling of the inlet diffuser structure has not yet been thoroughly addressed in existing studies. Most existing models are one-dimensional or assume homogeneous injection at the inlet face of the rock, thereby neglecting the potential influence of the diffuser on key flow variables. In this context, the present study aims to model three-dimensional unsteady-state core-flooding tests incorporating various types of complex injection diffusers homogeneous injection diffuser, central point, half-moon down, half moon-up, star, spiral and concentric patterns based on configurations commonly used in laboratory settings. Simulations are conducted using the CMG® IMEX software, which employs the Black-Oil model, for both homogeneous and synthetic heterogeneous cases. Pressure differential and oil production curves are obtained, along with saturation profiles along the core. The results are then compared against a reference case that assumes a homogeneously distributed inlet diffuser.

Regarding the injection layer, it can be inferred that the diffuser with the most uniform water distribution on the inlet face was the concentric one, exhibiting the most symmetric distribution. This was followed by the star-pattern diffuser, which appears to generate the highest differential pressure. Evaluating the overall performance of the diffusers, it is observed that their relevance should not be underestimated regarding the quantification of uncertainties in rock and rock-fluid properties. Failure to accurately represent these complex diffusers may mischaracterize the actual water advancement in the core, making it impossible to properly represent the dynamics of the simulation.

Assessment of Experimental Uncertainty Impact on Capillary Pressure Determination via the Centrifuge Technique

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Since Hassler and Brunner (1945) introduced the centrifuge as an alternative to capillary pressure measurement, the technique has evolved and become more popular. Centrifuge methods have been used to determine the first drainage curve (McPhee et al., 2015), the imbibition curve for coreflooding support (Berg et al., 2021; Maas et al., 2019), and the USBM wettability index (Anderson, 1986).

The centrifuge technique is known for its necessity of inversion from average to inlet face saturations (Forbes, 1994). Figure 1 shows the relationship between average ($\overline{S_w}$) and local (S_w) water saturation for the first drainage case.

$$\overline{S_w} = \frac{1}{(r_2 - r_1)} \int_{r_1}^{r_2} S_w(r)dr \tag{1}$$

where $\overline{S_w}$ is the average water saturation, r_1 and r_2 are the distances from the axis of rotation and the sample ends, and $S_w(r)$ is the local saturation, a function of position r.

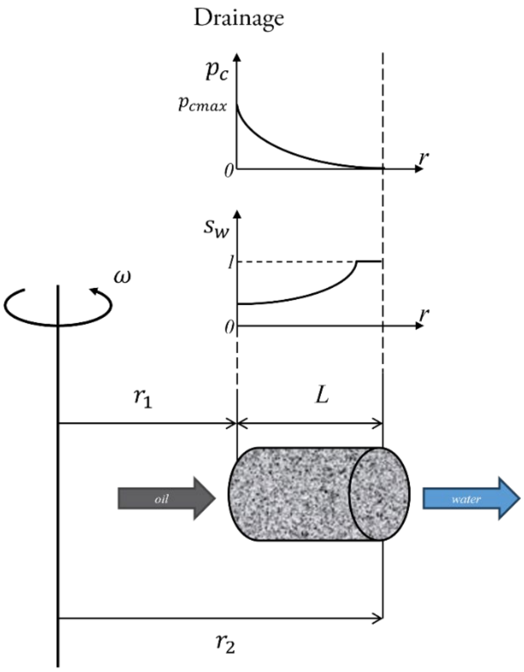

Figure 1. Schematic of drainage in a centrifuge. Adapted from Albuquerque *et al.* (2018).

Several techniques have been tested to solve Eq. (1). Forbes (1997) surveyed the techniques and found that Forbes's second solution and an inverse approach using cubic splines best represented the synthetic data he used. In the present work, an inverse approach using van Genuchten's equation (1980) is used to assess the technique's sensibility to experimental noise. In this approach, Eq. (1) is modified to obtain S_w as a function of P_c to give Eqs. (2) and (3), with van Genuchten's original equation given by Eqs. (4) and (5):

$$\overline{S_w}(p_{cmax}) = \frac{1+\sqrt{1-B}}{2}\int_0^1 \frac{S_w(xp_{cmax})}{\sqrt{1-Bx}}dx \quad (2)$$

$$B = 1 - \left(\frac{r_1}{r_2}\right)^2 \quad (3)$$

$$S_{wd} = \left[\frac{1}{1+(\alpha P_c)^n}\right]^m \quad (4)$$

$$S_{wd} = \frac{S_w - S_{wi}}{1 - S_{wi}} \quad (5)$$

Aiming to control the ground truth solution, synthetic data were used to evaluate the noise level's impact on the local saturation recovery. The noise levels introduced in the centrifuge's volume readings were 0.05, 0.10, 0.25, and 0.50 cm³. This range goes from the automated centrifuge reading (0.05 cm³) to the operator visual reading (0.50 cm³). Local saturations were recovered using the Markov Chain Monte Carlo method. The posterior distribution of the parameters was used to assess the uncertainty and determine the 95% confidence interval. We also compared the use of uninformative and informative priors in recovering the ground truth data.

Figure 2 presents the recovered P_c curves for the different error levels using uninformative priors. From this it is possible to conclude that the increase in noise makes the predictions more uncertain and that only the low errors (0.05 and 0.10 cm³) result in usable curves.

Figure 3 further shows a comparison between uninformative and informative priors for the 0.25 cm³ case. From Figure 3 we conclude that prior knowledge of S_{wi} and P_d can significantly reduce the uncertainty and improve the accuracy of the estimates. The proposed technique using the van Genuchten equation and Markov Chain Monte Carlo method proved to reliably recover the P_c curve for noise levels up to 0.25 cm³ when informative priors are used.

References:

Albuquerque, M. R., Eler, F. M., Camargo, H. V. R., Compan, A. L. M., Cruz, D. A., & Pedreira, C. E. (2018). Estimation of capillary pressure curves from centrifuge measurements using inverse methods. Rio Oil & Gas Conference, 19, 1–10. https://biblioteca.ibp.org.br/riooilegas/pt-BR/search/38799

Anderson, W. G. (1986). Wettability Literature Survey, Part 2: Wettability Measurement. Journal of Petroleum Technology, 38(11), 1246–1262. https://doi.org/10.2118/13933-PA

Berg, S., Unsal, E., & Dijk, H. (2021). Non-uniqueness and uncertainty quantification of relative permeability measurements by inverse modeling. Computers and Geotechnics, 132, 103964. https://doi.org/10.1016/j.compgeo.2020.103964

Forbes, P. (1994). Simple And Accurate Methods for Converting Centrifuge Data Into Drainage And Imbibition Capillary Pressure Curves. The Log Analyst, 35(04). https://onepetro.org/petrophysics/article/170846/Simple-And-Accurate-Methods-For-Converting

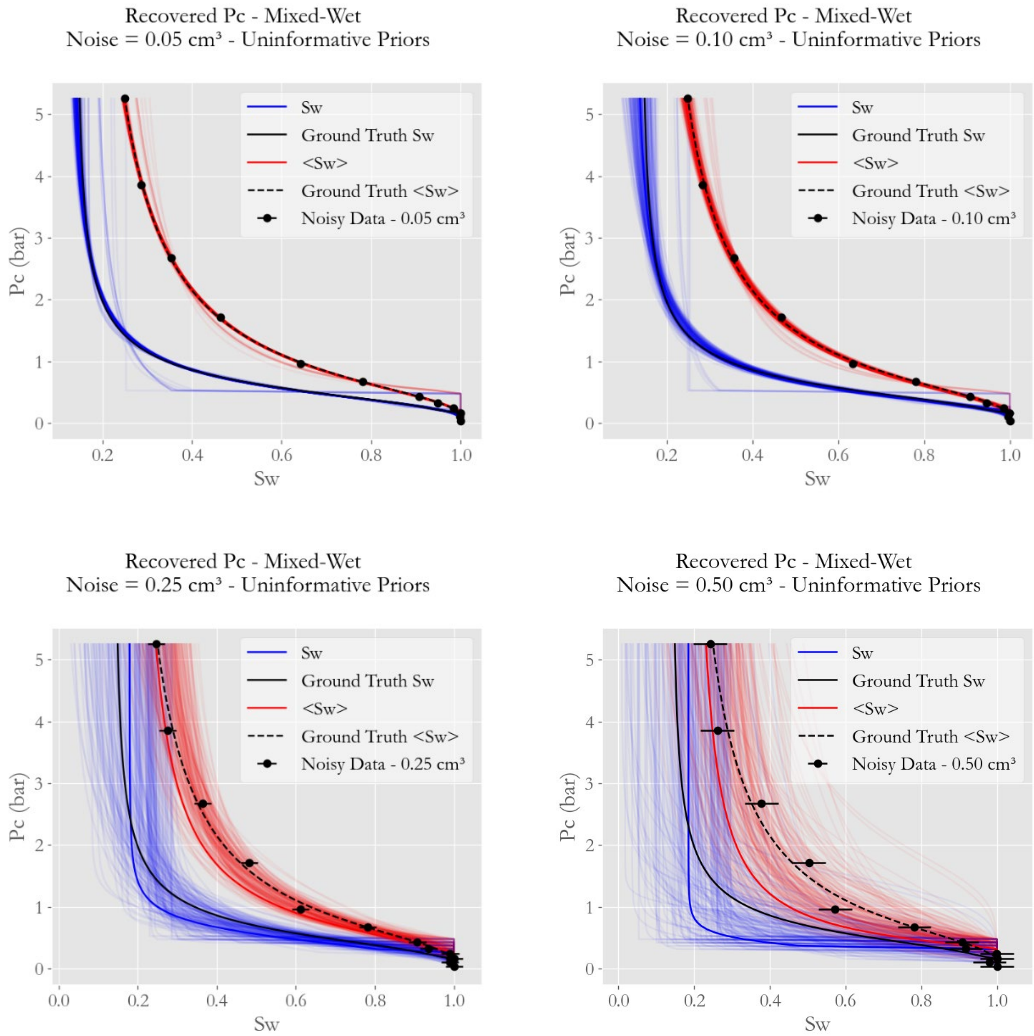

Figure 2. Recovered P_c curves for different error levels using uninformative priors.

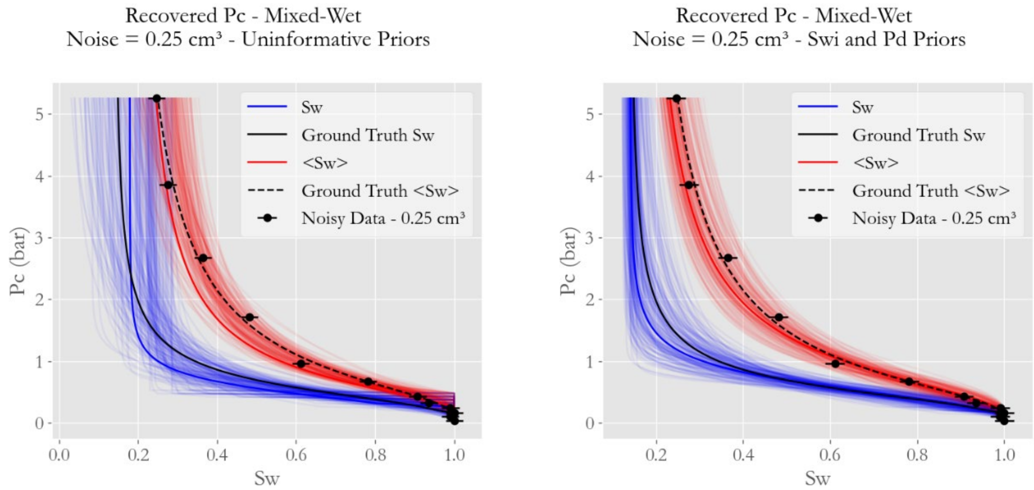

Figure 3. Comparison between the use of uninformative and informative priors for a noise level of 0.25 cm³.

Hassler, G. L., & Brunner, E. (1945). Measurement of Capillary Pressures in Small Core Samples. Transactions of the AIME, 160(01), 114–123. https://doi.org/10.2118/945114-G

Maas, J. G., Springer, N., & Hebing, A. (2019, August). Defining a sample heterogeneity cut-off value to obtain representative Special Core Analysis (SCAL) measurements. International Symposium of the Society of Core Analysts, Pau, France. https://jgmaas.com/SCA/2019/SCA2019-024.pdf

McPhee, C., Reed, J., & Zubizarreta, I. (2015). Core analysis: A best practice guide. Elsevier.

van Genuchten, M. Th. (1980). A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. Soil Science Society of America Journal, 44(5), 892–898. https://doi.org/10.2136/sssaj1980.03615995004400050002x

Relative Permeability Uncertainty Quantification and Reduction in Coreflooding Experiments

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Relative permeability is an essential parameter in reservoir simulations (Zargar & Thakur, 2022). Its applications include aquifer management, fossil fuel exploration, carbon capture, storage, and utilization, among others (Berg et al., 2021b). Relative permeabilities are usually determined via inverse modeling of coreflooding experiments. Although this is standard industry practice, Berg et al. demonstrated how prone the inverse modeling is to non-uniqueness and uncertainties (2021a). Eler et al. (2024) demonstrated how the uncertainty at the laboratory scale can impact the reservoir simulations. In this work, we propose the addition of a capillary pressure constraint in the inverse modeling workflow, which can reduce uncertainty and non-uniqueness of relative permeability determined via coreflooding experiments. This restriction was tested using synthetic data (ground truth is known) for oil-water relative permeability experiments in both steady and unsteady states.

Random noise was added to the synthetic data to avoid committing the inverse crime (Wirgin, 2004). The LET (Lomeland et al., 2005) correlation was used to parameterize the relative permeabilities, and the imbibition capillary pressure was informed. The relative permeability was recovered using both least squares and Monte Carlo via Markov Chain. The posterior distribution of the parameters was used to assess the uncertainty and determine the 95% confidence interval. Three wettability cases were evaluated, and the additional constraint improved the estimation of the relative permeability for water, oil, and mixed-wet cases. The estimation quality was measured by the Hausdorff Distance (Taha & Hanbury, 2015) between the estimated and the true relative permeabilities and water fractional flow curves. Table 1 exemplifies the Hausdorff Distances for the mixed-wet case in the steady-state experiment.

Table 1. Comparison of the Hausdorff Distance between the true and the recovered curves using the standard and the proposed techniques for the mixed-wet steady-state experiment.

	Hausdorff Distance	
Curve	**Standard Technique**	**Additional Capillary Restriction**
Water Relative Permeability	0.07	0.03
Oil Relative Permeability	0.14	0.13
Water Fractional Flow	0.11	0.04

For the water-wet unsteady-state experiment, it is also possible to observe the narrowing of the confidence interval (Figure 1) and the reduction of the non-gaussian distributions (Figure 2), both indicating a decrease of the non-uniqueness of the solution and the reduction of the uncertainty of the estimation.

As demonstrated by Hausdorff Distance and the posterior distributions, the additional restriction proposed in this work proved itself as an efficient method to improve the obtention of relative permeability by the inverse modeling of coreflooding experiments.

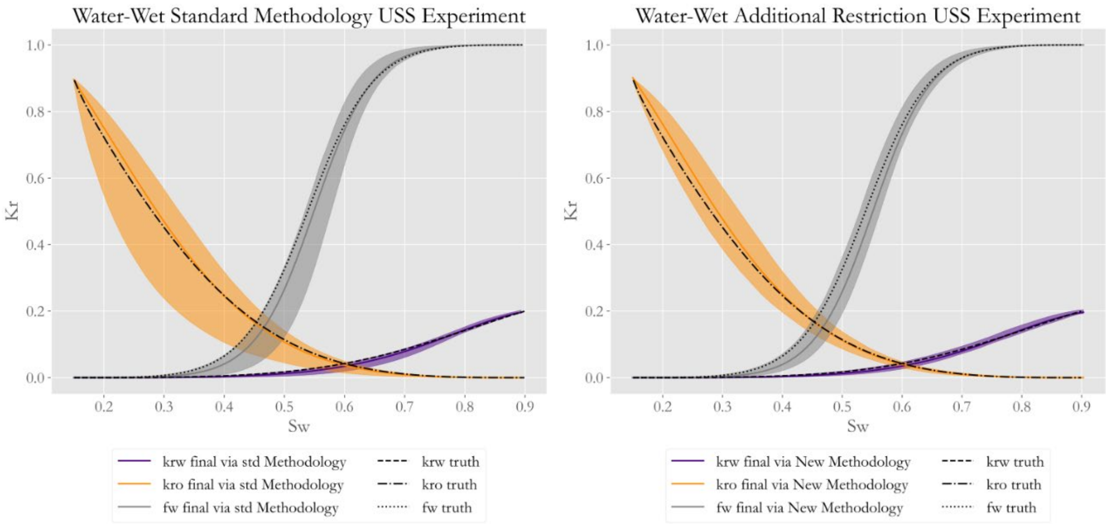

Figure 1. Reduction in the confidence interval by using the additional capillary pressure restriction for the water-wet unsteady-state experiment.

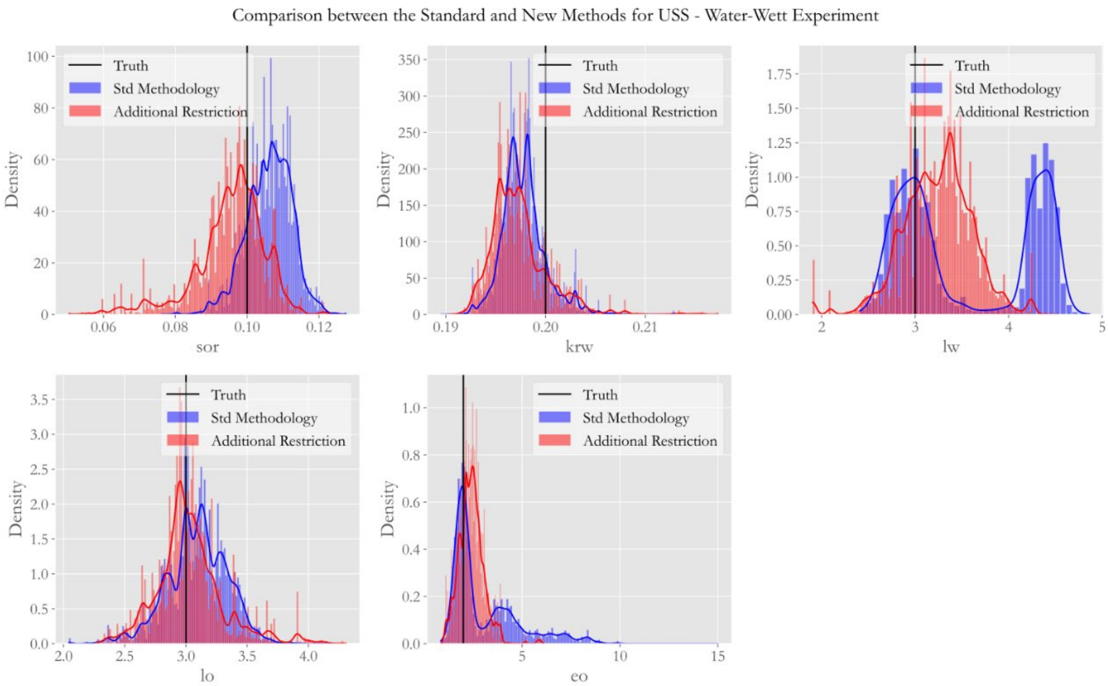

Figure 2. Improvement in parameter estimation by using the additional capillary pressure restriction for the water-wet unsteady-state experiment. The parameter l_w, for example, is estimated with two modes using the standard technique.

References:

Berg, S., Unsal, E., & Dijk, H. (2021a). Non-uniqueness and uncertainty quantification of relative permeability measurements by inverse modelling. Computers and Geotechnics, 132, 103964. https://doi.org/10.1016/j.compgeo.2020.103964

Berg, S., Unsal, E., & Dijk, H. (2021b). Sensitivity and Uncertainty Analysis for Parameterization of Multiphase Flow Models. Transport in Porous Media, 140(1), 27–57. https://doi.org/10.1007/s11242-021-01576-4

Eler, F. M., Júnior, C. R. C., Camargo, H. V. R., & Couto, P. (2024). Impacts of Laboratory Data Uncertainty on the Reservoir Scale. 781–795. https://doi.org/10.48072/2525-7579.roge.2024.2658

Lomeland, F., Ebeltoft, E., & Thomas, W. H. (2005, October). A New Versatile Relative Permeability Correlation. International Symposium of the Society of Core Analysts, Toronto, Canada. https://jgmaas.com/SCA/2005/SCA2005-32.pdf

Taha, A. A., & Hanbury, A. (2015). An Efficient Algorithm for Calculating the Exact Hausdorff Distance. IEEE Transactions on Pattern Analysis and Machine Intelligence, 37(11), 2153–2163. https://doi.org/10.1109/TPAMI.2015.2408351

Wirgin, A. (2004). The inverse crime. https://doi.org/10.48550/ARXIV.MATH-PH/0401050

Zargar, Z., & Thakur, G. C. (2022). Importance of reservoir simulation and early reservoir management for successful field development—Case study. Energy Reports, 8, 5038–5052. https://doi.org/10.1016/j.egyr.2022.03.189

A Systematic Global Recharacterization Method for Reservoir Fluids in Compositional Simulations

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This work presents a systematic global recharacterization method for reservoir fluids in compositional simulations, addressing the challenge of reducing the number of components used in complex hydrocarbon mixtures. Compositional reservoir simulations generally have high computational costs, as the complexity increases proportionally to the number of components in the modeled mixture. To mitigate this limitation, component lumping methods are employed, creating pseudo-components from heavy fractions such as C6+ or C7+, while maintaining the necessary accuracy to adequately represent phase behavior. The proposed method in this work uses Lage's (2007) methodology to recharacterize C6+ or C7+ fractions in complex mixtures, eliminating the need for further adjustments to the equation of state (EoS) parameters.

The main focus is the application of the Quadrature Method of Moments (QMOM) to calculate pseudo-components, ensuring that the new components preserve the key properties of the original fractions. Additionally, the method allows the creation of new discrete distributions, approximating the heavy fractions of the original mixture without relying on additional experimental data or EoS reoptimization. The article compares phase simulation and compositional reservoir simulation results using both original and recharacterized fluid compositions, focusing on parameters such as compressibility factor, vapor fraction, and composition errors. The proposed methodology outperforms other global lumping methods, such as Alavian et al. (2014) [2], both in terms of accuracy and computational efficiency. The study highlights that Lage's (2007) method maintains accuracy while significantly reducing the number of components, effectively representing the C^{6+} or C^{7+} fractions by only three or four pseudo-components.

Results demonstrate that the proposed method provides a robust alternative for compositional characterization, eliminating the need to group critical components such as carbon dioxide (CO_2), methane (CH_4), and ethane (C_2H_6), which are essential for accurately predicting reservoir fluid behavior in gas injection and enhanced oil recovery scenarios. Quantitative error analysis of the simulations reveals that the proposed methodology can accurately reproduce the original phase diagrams with low errors in vapor fraction prediction and phase composition. This study also shows how the application of this methodology accelerates compositional simulations, making them up to 7.5 times faster than using the original compositions, without compromising accuracy.

Therefore, the proposed global recharacterization method can be successfully applied to a wide range of reservoir engineering scenarios, where reducing simulation time and maintaining accuracy are crucial. The authors conclude that the proposed recharacterization is an effective tool to reduce the complexity of thermodynamic models in reservoir simulations, offering a cost-effective and reliable alternative to optimize compositional simulation performance. This advancement has potential applications in projects involving enhanced oil recovery, carbon capture and storage, and other industrial processes related to complex reservoir fluids.

References:

Lage, Paulo L.C., 2007. The quadrature method of moments for continuous thermodynamics. Comput. Chem. Eng. (ISSN: 0098-1354) 31 (7), 782–799. http://dx.doi.org/10.1016/j.compchemeng.2006.08.005, https://www.sciencedirect.com/science/article/pii/S0098135406002146.

Alavian, Sayyed Ahmad, Whitson, Curtis Hays, Martinsen, Sissel O., 2014. Global component lumping for EOS calculations. In: SPE Annual Technical Conference and Exhibition, All Days: SPE–170912–MS. http://dx.doi.org/10.2118/170912-MS.

The Nature and Extent of Bomb Tritium Remaining in Deep Vadose Zones: A Synthesis, Prognosis, and Way Forward

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Tritium in deep vadose zones has long served as a valuable tracer for estimating groundwater recharge, yet its broader utility is limited by uncertainties about where and for how long it can be effectively applied. In this study, we synthesized 44 tritium profiles from 17 globally distributed sites with vadose zone thicknesses ranging from 12 to 624 m. Using transport models, we determined that 26 of the 44 soil profiles, primarily from China, Australia, the United States, South Africa, and Senegal, retain sufficiently high tritium levels to remain useful for an additional 6 to 83 years.

To extend these findings, we developed a statistical model that leverages outputs from a hydrological model to predict broader applicability of the tritium tracing method. Global-scale implementation, excluding Antarctica and Greenland, suggests that approximately 20% of Earth's land surface could still benefit from tritium-based techniques over the coming decades. Details are by Huang et al. (2024).

Looking ahead, we propose several ways to enhance and prolong the usefulness of tritium as a tracer, including targeted sampling strategies (where the bomb signal may still likely exist), refined transport modeling, and integrative approaches that combine tritium data with other hydrological and geochemical tracers. Together, these efforts can help researchers and water managers better characterize, predict, and safeguard critical groundwater resources.

Reference:

Huang, Y., J. Evaristo, Z. Li, K.P. Chun, E.H. Sutanudjaja, M.B. Cardenas, M.F.P. Bierkens, J.W. Kirchner, and M.Th. van Genuchten. 2024. The nature and extent of bomb tritium remaining in deep vadose zone: A synthesis and prognosis. Vadose Zone Journal. doi.org/10.1002/vzj2.20304

Modeling Soil Salinity in Mangrove Swamp Rice Production Systems of Guinea Bissau, West Africa

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Mangrove swamp rice production (MSRP) systems are of fundamental importance for the livelihoods of populations in West Africa and for food security. However, these systems face increasing challenges due to their dependence on rainfall to maintain feasible salinity levels for rice production during the growing season. This study examines the dynamics of soil water and salinity using field observations collected from four different MSRP sites in Guinea-Bissau, along with simulations using the HYDRUS-1D model. Model simulations were valuable in identifying the main factors influencing soil salinity levels during the study period, while the soil water balance helped estimate the relative impacts on crop yields.

Several rainfall and groundwater depth scenarios were also considered to identify the key factors contributing to soil salinity at the study sites. Seasonal rainfall amount and distribution, groundwater depth, and groundwater quality were found to be the most significant factors impacting soil salinity and crop yields at the different study sites. The modelled scenarios also provided insights into effective management strategies for coping with soil salinization, particularly by assessing where and when growing longer, more productive crop varieties is feasible, or where cultivating salt-tolerant crop varieties is necessary.

The maintenance of dikes and other drainage structures was also critical for maintaining minimum rice growth conditions. The findings of this study support agricultural water management in MSRP systems in Guinea-Bissau, but on their own, they cannot overcome the significant yield gap these areas face compared to other rice production regions worldwide.

REV Analysis Through Morphological Young–Laplace Numerical Method

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Carbonate reservoirs in Brazil's pre-salt formations present a formidable challenge in reservoir characterization due to their highly heterogeneous porous structure, where multiple pore types such as intragranular, intergranular, moldic, fenestral, vuggy, channel, and fractures can coexist. These varied pore networks span scales from 10^{-3} to 10^4 micrometers (Soete et al., 2017), substantially increasing the representative elementary volume (REV) required to capture key petrophysical properties, notably permeability (Jouini et al., 2014). Recent advances in digital rock physics, particularly through μCT imaging and high-performance computations, have significantly improved the ability to characterize these complex pore systems (Neumann et al., 2021). However, existing approaches often face limitations, such as insufficient resolution that excludes smaller pores from analysis or domain sizes too small for highly heterogeneous samples (Islam et al., 2018), which can lead to an underestimation of the true REV.

In this study we propose a methodology for determining the REV properties of digital rock images by combining a morphological Young–Laplace numerical method (Zabot et al., 2024) with capillary pressure–saturation curve fitting using the van Genuchten (1980) correlation. Our hierarchical approach integrates both deterministic and statistical assessments of porous media properties, beginning with the average pore diameter and culminating in the evaluation of residual saturations and capillary pressure curves. This procedure leverages binarized 3D μCT images from publicly accessible databases, providing a systematic framework that mitigates the pitfalls of heterogeneity in the sample distribution. Implemented within the LBPM framework (McClure et al., 2021), our methodology offers a more robust and automated approach for determining the REV, ultimately enhancing the reliability of reservoir rock assessments.

References:

Islam, A., S. Chevalier, M. Sassi, Structural characterization and numerical simulations of flow properties of standard and reservoir carbonate rocks using micro-tomography, Computers & Geosciences 113 (2018) 14–22.

Jouini, M., S. Vega, A. Alratrout, Numerical estimation of carbonate rock properties using multiscale images, Geophysical Prospecting 63 (2014).

McClure, J. E., Z. Li, M. Berrill, T. Ramstad, The lbpm software package for simulating multiphase flow on digital images of porous rocks, Computational Geosciences 25 (2021) 871–895.

Neumann, R.F., M. Barsi-Andreeta, E. Lucas-Oliveira, H. Barbalho, W.A. Trevizan, T.J. Bonagamba, M.B. Steiner, High accuracy capillary network representation in digital rock reveals permeability scaling functions, Scientific Reports 11 (2021).

Soete, J., S. Claes, H. Claes, N. Janssens, V. Cnudde, M. Huysmans, R. Swennen, et al., Lattice Boltzmann simulations of fluid flow in continental carbonate reservoir rocks and in upscaled rock models generated with multiple-point geostatistics, Geofluids 2017 (2017).

van Genuchten, M.Th. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Science Society of America Journal 44 (1980) 892–898.

Zabot, A.M., M.A. Camargo, F.G. Wolf, D.N. Siebert, R. Surmas, L.O.E. dos Santos, T.R. Ferreira, F.A.M. Cássaro, L.F. Pires, A unified algorithm for the Young–Laplace method applied to porous media, Brazilian Journal of Physics 54 (2024).

Characterization of Macropore-Matrix Mass Exchange for Modeling Preferential Flow and Soil Hydromechanics in the Drilosphere

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The macropore-matrix mass transfer of water and solutes is largely controlling non-equilibrium-type of preferential flow in structured soil. In a two-domain model approach, which assumes a network of macropores embedded in the soil matrix, the mass transfer term parameters reflect effects of local properties such as the macropore fraction and geometry, and properties at macropore walls such as permeability and sorptivity. In case of coatings along fractures or linings along worm burrows, these properties differ from those of the bulk soil with respect to texture, organic matter, bulk density, and porosity. The local coating properties can affect the macropore-matrix mass exchange with respect to hydraulic, mechanic, bio-geo-chemical, and other processes. Clayey aggregate skins, for example, can restrict water exchange; solutes may become adsorbed along macropore surfaces.

Still relatively little is known of hydro-mechanic dynamics and how to experimentally determine or upscale local mass transfer information to the scale of the soil volume. Previous work included field and lab percolation and infiltration experiments using bromide, Brilliant Blue, iodide, and Na-Fluorescein to identify the preferential flow paths and determine mass exchange parameters. It seemed that preferential transport of reactive solutes depended strongly on the geometry and properties at flow path surfaces. More recent approaches included coupled hydromechanic soil dynamics focusing on the drilosphere with the surrounding matrix that is a macropore-matrix system created by vertically burrowing anecic earthworms. For such samples, changes in local 3D water content and solid phase distributions were observed using combined X-ray and Neutron beam computed tomography (at ILL Grenoble). By using a semi-membrane inside the biopore to control osmotic pressure at the biopore surface, exchange flow in both directions could be imitated. Data revealed sorptivity and permeability dynamics resulting from swelling and shrinkage of the pore network between pore wall surface, coating, and surrounding matrix. Here, the coating presented a stiffer structure than the matrix, displaying smaller plastic deformation.

In an attempt to upscale local properties, a discrete element model (DEM) was constructed to imitate an aggregated soil of known bulk and aggregate densities including a finer-textured coating. The pore scale mechanical parameters were obtained using macroscopic strain versus pressure head relations from observed bulk soil deformation data during drainage. After parameterization, a two-phase pore-scale finite volumes model coupled to discrete element (DEM-2PFV) model was used to simulate the hydro-mechanic processes in the drilosphere during stepwise drainage. The resulting water retention functions spanned across the inspected specific volumes. To incorporate this dynamics into flow model simulations, soil structural deformation must be accounted for using a shrinkage curve or constitutive relation, alongside with hydraulic properties that link specific volumes to water content or pressure head. Such coupled DEM-2PFV modeling and CT-based experiments can contribute to the development of mechanistic modes of mass transfer and preferential flow in structured soil.

Solving New Digital Rock Challenges with van Genuchten's Equation

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Digital rock analysis (DRA) is a powerful tool to evaluate complex rock samples which can be an aquifer, a CO_2 storage or a hydrocarbon reservoir [1]. Different modeling techniques to solve the single and multiphase fluid flow in complex rock porous systems have been applied recently, with some emphasis given to Pore Network Model (PNM) [2] and Lattice Boltzmann Method (LBM) [3]. In order to properly represents the result from the pore-scale simulations, it is necessary to evaluate the Representative Elementary Volume (REV), which can be defined as the volume of a sample capable of capturing a representative quantity of its heterogeneity.

Since the REV evaluation depends on the property to be evaluated, several different studies have been conducted to explore REV based on single-phase fluid [4, 5] as well as multiphase flow studies [6, 7]. Regular laboratory samples range from few to several centimeters, with 1.5 inches diameter samples the most common ones for special core analysis (SCAL) studies. In this sense, recent DRA studies focused on PNM developments to properly evaluates the dynamics of single-phase fluid flow in heterogeneous carbonate rocks [8, 9], including evaluation of sub-resolution porosity [10] which also can be impacted by REV evaluation based on the resolution of micro-computed tomographyimages.

However, due to the highly interested in multiphase flow in porous media and digital SCAL tests, ongoing research focuses on refining techniques to identify two-phase flow REV properties from digital rock images by coupling a morphological Young–Laplace numerical approach [11] with capillary pressure–saturation curve fitting employed by the van Genuchten [12] correlation. This insight is vital for understanding multiscale mass transport. At the same time, REV-scale capillary pressure data are being utilized in lattice Boltzmann multiscale-multicomponent modeling to capture the non-linear behavior of relative permeability and capillary pressure resulting from fluid–fluid interactions in gray porous media (porous-continuous media), ensuring accurate and robust computational simulations. This study presents these new digital rock challenges that can be solved based on van Genuchten's equation [12].

References:

[1] M.J. Blunt. Multiphase Flow in Permeable Media: A Pore-Scale Perspective. Cambridge University Press(2017).

[2] A. Raoof; H.M. Nick; S.M., Hassanizadeh; C.J. Spiers. Poreflow: a complex pore-network model for simulation of reactive transport in variably saturated porous media. Computers & Geosciences 61: 160-174 (2013).

[3] T. Bultreys; W. de Boever; V. Cnudde. Imaging and image-based fluid transport modeling at the pore scale geological materials: a practical introduction to the current state-of-the-art. Earth-Science Reviews 155: 93-128 (2016).

[4] B. Vik, E. Bastesen; A. Skauge. Evaluation of representative elementary volume for a vuggy carbonate rock – Part I: Porosity, permeability, and dispersivity. Journal of Petroleum Science and Engineering, 112, 36-47 (2013).

[5] W.G.A.L. Silva; E.H. Rios; F.O. Hoerlle; E.M.B.D Pontedeiro; L.F. Borghi; J.L.D. Alves; P. Couto. Representative elementary volume of a region of interest of a heterogeneous carbonate rock using x-ray computed microtomography and numerical simulation. Revista Brasileira de Geofísica, 36, p. 1 (2018).

[6] B. Vik, E. Bastesen; A. Skauge. Evaluation of representative elementary volume for a

vuggy carbonate rock; Part II: Two-phase flow. Journal of Petroleum Science and Engineering, 112, pp. 48-60 (2013).
[7] S. An, Y. Zhan, J. Yao, H.W.Yu, V. Niasar, A greyscale volumetric lattice boltzmann method for upscaling pore-scale two-phase flow, Advances in Water Resources 144 (2020).
[8] W. Godoy; E. M. Pontedeiro; F. Hoerlle; A. Raoof; M. Th. van Genuchten; J. Santiago; P. Couto. Computational and experimental pore-scale studies of a carbonate rock sample. Journal of Hydrology and Hydromechanics, v. 67, p. 372-383 (2019).
[9] E.M. Pontedeiro, M.Th. van Genuchten, W. Godoy, M.G. Ramirez, C.M.P. Vaz, S. Crestana, M.C.O. Lima, P. Couto, S. Jian. Multiscale pore-network reconstruction of a fine-textured heterogeneous soil, Vadose Zone Journal, 10.1002/vzj2.20354, 23, 4, (2024).
[10] W. Godoy; E.M. Pontedeiro; R.A.B.R. Barros; E.T. de Vries; A. Raoof; M.Th. van Genuchten; P. Couto. Modeling sub-resolution porosity of a heterogeneous carbonate rock sample. Vadose Zone Journal, 23 (2024).
[11] A.M. Zabot, M.A. Camargo, F.G. Wolf, D.N. Siebert, R. Surmas, L.O.E. dos Santos, T.R. Ferreira, F.A.M. Cássaro, L.F. Pires, A unified algorithm for the Young–Laplace method applied to porous media, Brazilian Journal of Physics 54 (2024).
[12] M.Th. van Genuchten, A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Science Society of America Journal 44, 892–898 (1980).

Water Retention Curves of Sandy Soils in Northern Poland

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Understanding soil hydraulic properties, including the soil water retention curve (SWRC), which defines the relationship between soil water potential and water content, is essential in various fields such as agriculture, hydrology, and civil and environmental engineering. Moreover, in shallow, sandy aquifers common in post-glacial regions of Northern Europe and North America, an accurate characterization of SWRC plays a crucial role in assessing groundwater recharge and the susceptibility of these areas to contamination.

This study evaluates different approaches for describing the hydraulic properties of sandy soil samples collected from young glacial deposits in northern Poland. To estimate SWRC, three analytical models were applied: the classical van Genuchten (VG) model, its modified version incorporating the Campbell and Shiozawa function for adsorbed water (CS-VG), and the Brunswick model (BW-VG), which integrates both SWRC and the hydraulic conductivity curve (HCC) across the entire range of soil saturation. Additionally, the parameters of the BW-VGM-PTF model were determined based on the standard van Genuchten-Mualem (VGM) model parameters and pedotransfer functions (PTFs) developed by Weber et al. (2022).

The study also explores the feasibility of determining SWRC based on fundamental soil physical characteristics, such as particle size distribution. To this end, three variants of the Arya and Paris (1981) model (AP1, AP2, AP3) were examined, along with a scaled version of the Mohammadi and Vanclooster (MVS) method and the Chang and Cheng (2018) (CC) method. The latter two approaches specifically aim to improve the representation of SWRC in the low-water content range. All methods were calibrated using drainage experiments conducted with a sand box and a kaolin-sand box apparatus from Eijkelkamp. These devices enabled the determination of SWRC in the wet range, providing a foundation for further analyses and comparisons.

This work has been (partly) funded by National Center for Research and Development (NCBR, Poland) as part of EU Water4All project: WATER4ALL/I/37/AQUIGROW/2024 and the EU Horizon project SOILPROM (grant 101156589, soilprom.eu).

Water Distribution in Soil Pores: Predicted via the Young–Laplace Equation vs. Observed via X-Ray MCT

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Understanding functioning and diversity of microbial communities in soils at pore scale is impossible without a reliable model of water distribution within the pore network. This is particularly true for understanding the relationships between redox-dependent bio-geochemical reactions and spatial/temporal distributions of gas and liquids in soil pores.

The objective of this work was to compare water distribution within soil pores as determined by the Young-Laplace equation vs. its direct observations. The young-Laplace equation relates the capillary pressure to the radii of water menisci in capillary systems and commonly used in mercury porosimetry. We applied it to pore-size distributions obtained from monochromatic scanning of intact soil cores via X-ray computed micro-tomography (mCT), while observations of actual spatial distribution of liquids within soil pores of the same samples were obtained via a dual-monochromatic X-ray mCT.

Calculations and observations were performed at 5 levels of water saturation in intact cores of sandy loam, loamy sand, loam and silt loam soils. Image analysis showed that the total number of disconnected water bodies (referred hereafter as water fragments) decreased, while mean fragment volumes and connectivity among the fragments increased with increasing pore saturation. Deviations between the Young–Laplace predictions and the observed distributions varied with soil texture and water content level, yet the predictions and observations generally followed the same trends. However, the Young–Laplace equation overestimated the number of water fragments and underestimated their average volumes and connectivity at pore saturation below ~ 70% of pore volume detectable at X-ray CT images.

Celebrating Rien van Genuchten: A Life of Science, Mentorship, and Impact

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This presentation celebrates the extraordinary journey of Dr. Martinus Theodorus (Rien) van Genuchten—renowned soil physicist, pioneering hydrologist, and mentor to generations. From his humble beginnings on a Dutch family farm to becoming a globally respected scientist, Rien's career has been shaped by curiosity, collaboration, serving the community, and an unwavering commitment to solving some of the most critical challenges in water flow and contaminant transport. Through academic positions in the U.S., Brazil, and the Netherlands, and foundational work underlying models of flow and transport in the vadose zone, his contributions transformed soil physics. Beyond science, Rien is a beloved colleague, teacher, friend, and grandfather—an inspiration to all who know him. This presentation reflects on his life, scientific impact, and the human values he embodies.

The HPx Tool for Geochemical and Coupled Reactive Transport Simulations for Engineered and Environmental Porous Systems

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HPx refers to a modeling framework in which flow and transport solvers (HYDRUS-1D/2D/3D or MT3D-USGS) are coupled with geochemical solvers (PHREEQC, ORCHESTRA) for geochemical (with PHREEQC if there is no transport involved) and coupled reactive transport simulations. The framework has some advanced options compared to, for example, default PHREEQC, including: (i) Inline variables in the input file for which actual values are inserted in the input during runtime. The value itself can be defined in different ways, including the option to change it during runtime. (ii) An alternative scripting language to the embedded BASIC interpreter in PHREEQC using a more modern form of the BASIC-like language. Embedded Python scripts form a second alternative. (iii) An advanced way for graphical output using the open software gnuplot.

A new graphical interface for geochemical calculations (HPGeochemistry) was developed, providing the HPx framework with increased flexibility, reuse, and reproducibility of models and simulations organized in managed projects. Basic tools are, amongst others, user-defined input tables and modules. The real power of HPx is in its interaction with flow and transport solvers, which creates advanced reactive transport codes. For example, HPx is coupled with the HYDRUS family of codes for water flow, heat transport, and solute transport in variably saturated conditions for up to three-dimensional problems. Another example is HPx coupling with the MT3D-USGS code for studies in hydrogeological environments.

The HPx framework allows for a smooth integration of geochemical models developed in HPGeochemistry in the coupled reactive transport simulations. Examples are available for complex models for redox chains, organic matter degradation and transport, sorption modeling on organic matter, cement chemistry, etc. The reactive transport models have been applied in agricultural applications, contamination studies, evaluating consequences of climate change such as acidification of acid sulfate soils under prolonged drought conditions, and studies on the geochemical evolution of (radioactive) waste repositories.

Nitrogen Dynamics in Hyporheic Zones: Interactions Among Porous Media Flow, Reactive Nutrient Transport and Biofilm Growth

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The hyporheic zone serves as a natural biogeochemical reactor, playing a pivotal role in mitigating nitrogen pollution through attenuation and removal processes. Sediment heterogeneity leads to microscale variations in flow dynamics, redox conditions, and microbial communities. Microbial bioclogging alters flow patterns, redox states, and nutrient transport, yet most studies assume a continuous medium with constant permeability, overlooking these effects. This study employs microfluidic and flume experiments to monitor bioclogging-induced changes in flow, biofilm dynamics, permeability, and microbial communities. A new multi-process coupled model is developed under sediment heterogeneity at different scale (pore network, flow tube, dune) to assess bioclogging impacts on flow patterns, redox conditions, and nitrogen transport.

Results show that biofilm growth significantly intensifies the non-uniformity of microscale water flow, gradually transitioning from dispersed flow to preferential flow. The oxygen-rich zone in the hyporheic zone gradually shrinks with biofilm growth, while the anoxic zone expands. When nutrients are abundant and convection dominates in the hyporheic zone, anoxic microzones can develop sustainably; otherwise, they exist only during the early or middle stages of biofilm growth. In heterogeneous riverbeds, biofilm promotes coarse-grained structures to not only transport substances but also possess strong denitrification potential, becoming a significant source of N_2O. A new Damköhler number is proposed to identify whether the hyporheic zone acts as a source or sink of N_2O.

River scouring and particulate organic carbon deposition respectively reduce and enhance the denitrification capacity of the hyporheic zone. The spatial distribution of biogeochemical reaction hotspots does not completely overlap with the surface water-groundwater mixing zone, and variations in the mixing zone size significantly affect nitrate (NO_3^-) removal. The heterogeneity of sediment has little effect on the nitrate removal capacity of a hyporheic zone, while neglecting microbial spatiotemporal heterogeneity can severely underestimate denitrification capacity. The findings of this project provide significant theoretical support for watershed nitrogen pollution prevention, control, and remediation.

References

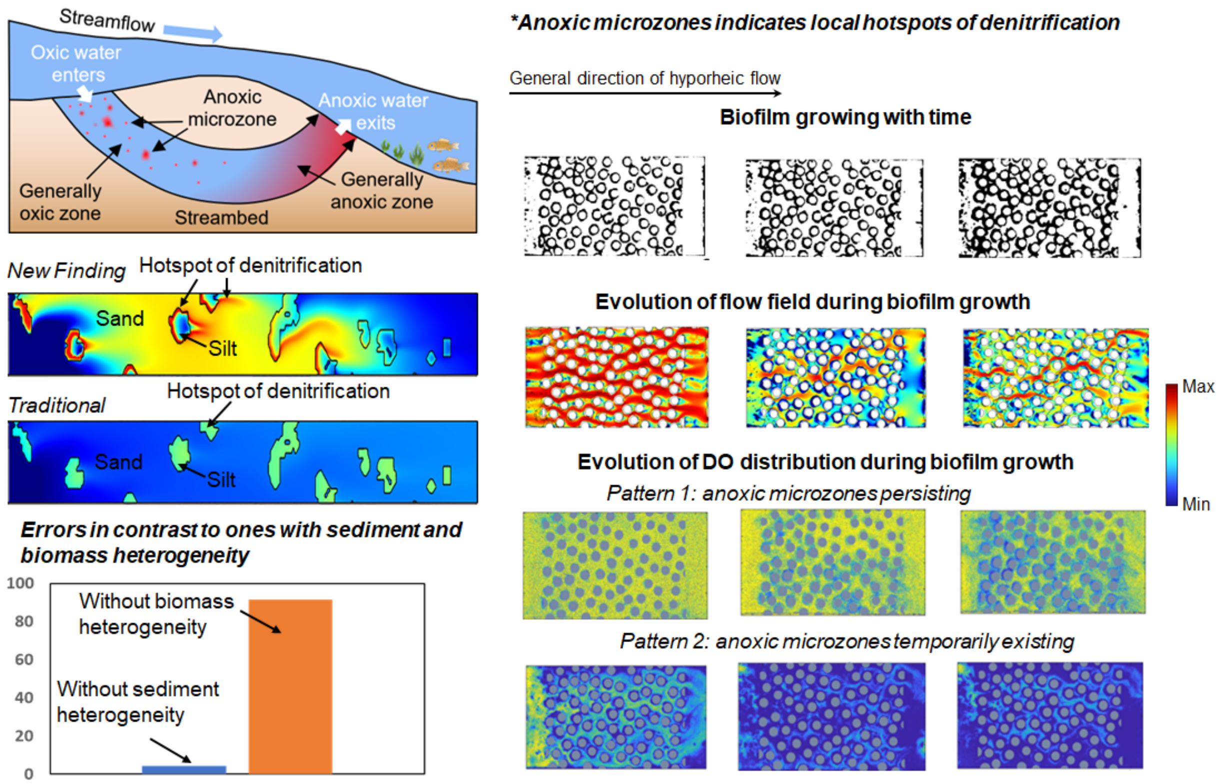
Ping, X., Y. Xian, M. Jin. 2022. Influence of bedform migration on nitrate reduction in hyporheic zones of heterogeneous sediments, Water Resources Research, 58(11): e2022WR033258.

Ping, X., Y. Xian, M. Jin. 2023. Effect of particulate organic carbon deposition on nitrate reduction in the hyporheic zone, Water Resources Research, 59(7): e2022WR034253.

Xian, Y., M. Jin, H. Zhan, X. Liang. 2022. Permeable biofilms can support persistent hyporheic anoxic microzones, Geophysical Research Letters, 49(14): e2021GL096948.

Xian, Y. Z. Wen, M. Jin, X. Liang, H. Jakada. 2023. Groundwater-borne nitrate removal within heterogeneous sediments under interactions between hydraulics, nutrients, and biofilms, Journal of Hydrology, 616: 128777.

Zhang, Z., Y. Xian, X. Ping, M. Jin, H. Guo. 2024. Effect of microbial growth and electron competition on nitrous oxide source and sink function of hyporheic zones, Journal of Hydrology, 638: 131585.



Analytical and HYDRUS Modeling of 2D Heat Conduction in the Design of the Optimal Locus - Shape of Galleries/Subterranean Holes: Lobachevskii's Geophysical Legacy for Solving Inverse Problems Revisited

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Heat flow from subterranean galleries, under the lysimetric station at Moscow State University (see the photo in Fig.1 and Umarova et al., 2021) is modeled analytically with the help of the theory of holomorphic function, and numerically. Heat fluxes from/into such galleries (tunnels, bunkers, etc.) are important for controlling and optimizing temperature regimes (cooling or heating of galleries' interior). The studied gallery traverses an array of bunkers (concrete-lined and earth-filled), about 1.75 m deep. The annual average air temperature swing in Moscow is about 35 C, while inside the gallery this variability is attenuated, as firstly measured by Lobachevskii and modeled using Fourier analysis, based on experimental data in deep shafts in Kazan, two centuries earlier.

First, we retrieved the thermographs from soil thermometers buried at five depths (0-60 cm) in the near-gallery soil. Using Wolfram's (1991) *Mathematica* we realized the Horton et al.(1983) algorithms for solving the inverse problem of assessing the thermal diffusivity and, therefore the conductivity, □, from analytical cyclo-stationary solutions to a parabolic 1-D transient heat conduction equation (see e.g. Danilaev, 2001). We also did a sensitivity analysis, considering a more general PDE of convective heat transfer, with an annually averaged infiltration rate coined into the velocity term in the PDE. After this, for 2D steady-state heat conduction we solved the following two isoperimetric optimization problems (see Fig.2a, the right half, G_z, of the gallery):

Given

- the cross-sectional area of the gallery,
- the in-gallery, surface and neutral layer temperatures, T_{tu} , T_s, and T_n ($T_{tu}>T_n>T_s$),
- the depth, d_n, of the neutral layer at a given locus d_r,

Determine:

A) the locus, d_r, of the gallery's centre of a given width,$2L$, and height, d, such that the heat losses, Q (both ascending and descending) from the gallery are minimal, and.
B) the dyad (L,d), which minimizes Q at a given locus d_r.

From the Weierstrass extreme value theorem, both problems A) and B) have a global and unique minimum. For finding these minima and the potential nontrivial local extrema (minima and maxima) we used:

I) The method of conformal mapping, and
II) HYDRUS2D

For method I) we employed the Schwartz-Christoffel formula, *viz.* we mapped both G_z and the heptagon G_w (Fig. 2b) in the complex potential plane onto a reference half-plane G_ζ (Fig. 2c). For method II), we solved the Laplace equation in the horizontal plane by considering a fully-saturated Darcian seepage (Fig. 3). The topology of heat flow (e.g. the isotherms, thermal gradients, isotachs) are similar to what was found for confined groundwater flow (Ilyinsky and Kacimov, 1992) and unsaturated 2-D infiltration-induced flow (Kacimov et al., 2022a,b). For example, the heat line $S_1S_2S_3$ in Fig. 3 is a separatrix, which demarcates three subzones of G_Z: ascending heat flux from the neutral horizon to the soil surface, descending and ascending fluxes from the gallery. At the stagnation point S_2 on the neutral line, the heat line is not perpendicular to the isotherm but makes angles $\pi/4$ with it.

Fig.1 Gallery under the lysimeter station at Moscow State University, Russia

Our computations showed that Problems A) and B) do not have local extrema. The results of our modeling can be used for design of various types of subsurface structures and as isoperimetric estimates-inequalities (see e.g. Polya and Szegö, 1951) for solving most complex inverse geophysical problems, *videlicet*, identification of subsurface “objects”, rather than simpler problems of coefficients’ reconstruction in PDEs.

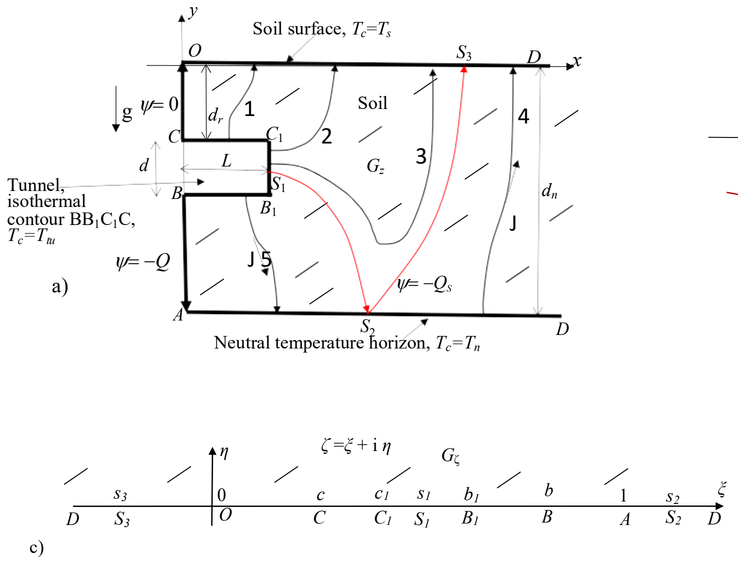

Fig. 2. Cross-section of heat conduction domain a), polygon in the complex potential plane b), reference plane c).

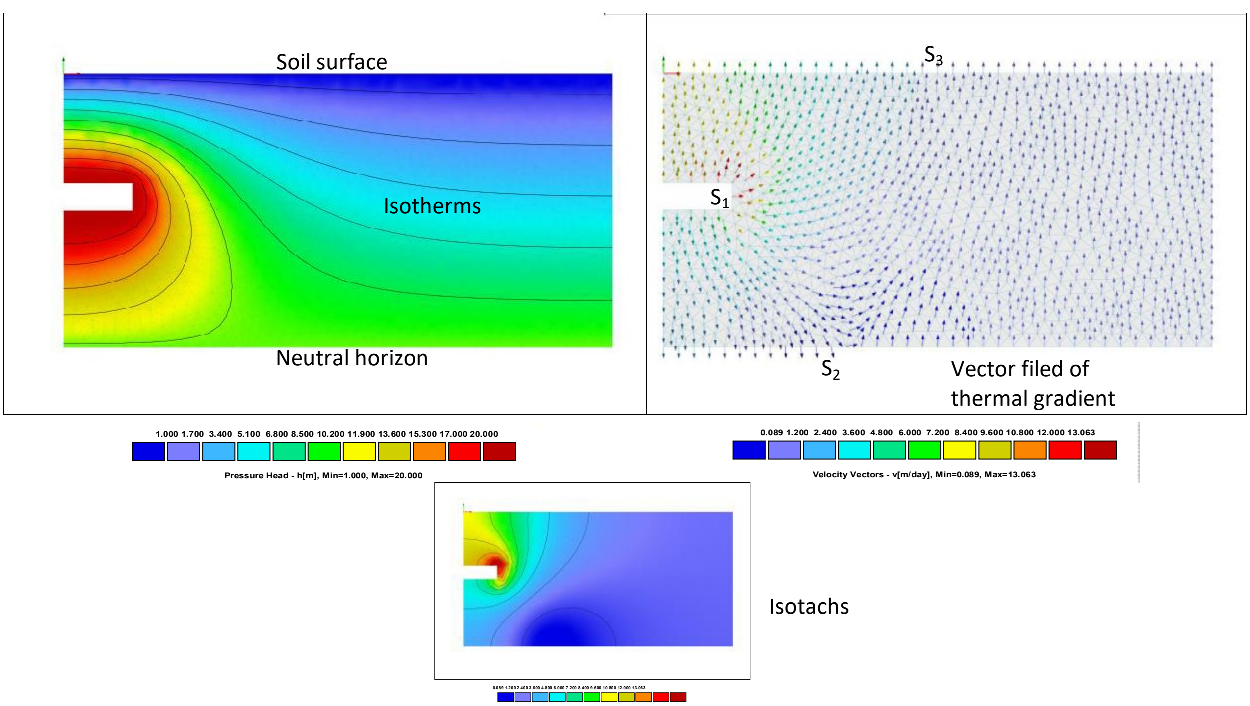

Fig. 3. HYDRUS 2D computations (isotherms/isobars, thermal/hydraulic gradient, and isotachs).

References:

Danilaev, P.G.E., 2001. Coefficient Inverse Problems for Parabolic Type Equations and Their Application. VSP, Utrecht.

Horton, R., Wierenga, P.J. and Nielsen, D.R., 1983. Evaluation of methods for determining the apparent thermal diffusivity of soil near the surface. Soil Science Society of America Journal, 47(1), 25-32.

Ilyinsky, N.B. and Kacimov, A.R., 1992. Analytical estimation of ground-water flow around cutoff walls and into interceptor trenches. Ground Water, 30, 901- 907.

Kacimov, A., Obnosov, Yu.V. and Šimůnek, J., 2022a. Seepage to staggered tunnels and subterranean cavities: analytical and HYDRUS modeling. Advances in Water Resources, 164, 104182.

Kacimov, A., Obnosov, Yu., V. and Šimůnek, J., 2022b. Subterranean holes in the arid vadose zone as perturbations of descending pore water fluxes: J. R. Philip's legacy revisited. Abstracts of the International Conference “Water Resources Management and Sustainability: Solutions for Arid Regions”, Dubai, March 22-24, 2022. p. 46-49. Edited by M.Sherif, M.A.Faiz and A. Sefelnasr.

Polya, G. and Szegö, G., 1951. Isoperimetric Inequalities in Mathematical Physics. Princeton University Press, Princeton.

Umarova, A.B., Arkhangelskaya, T.A., Kokoreva, A.A., Ezhelev, Z.S., Shnyrev, N.A., Kolupaeva, V.N., Ivanova, T.V. and Shishkin, K.V., 2021. Long-term research on physical properties of soils in the MSU large lysimeters: main results for the first 60 years (1961–2021). Moscow University Soil Science Bulletin, 76, 95-110.

Wolfram, S., 1991. Mathematica. A System for Doing Mathematics by Computer. Addison-Wesley, Redwood City.

The Potential of Micropollutants in Irrigation Water to Contaminate Soil and Groundwater

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Agricultural soils can be contaminated by various organic micropollutants. Common micropollutants are various pesticides used for plant protection and weed reduction, and their metabolites. Another source of contamination can be irrigation water. In areas with a shortage of water, treated wastewater that may contain, for example, pharmaceuticals, hormones, personal care products and various industrial chemicals, can be used directly for irrigation. However, even river water, which is often used for irrigation, can be contaminated by compounds in wastewater discharged into rivers, runoff from agricultural or urban land, etc. The occurrence of compounds in the soil or their leaching from the soil and migration into groundwater depends on climatic conditions, the properties of the vadose zone environment and the behavior of compounds, i.e. their sorption into soils and sediments and stability in the soil-water environment.

Our study first focused on the occurrence of organic micropollutants in various matrices (surface and groundwater, soils and plants) in areas intensively irrigated with river water. Six compounds were selected from a wide range of diverse compounds identified: 1,3-diphenylguanidine, triethyl citrate, napthalene-2-sulfonic acid, benzo(d)thiazole-2-sulfonic acid, 4-acetamidoantipyrine, and 6:2 fluorinated telomer sulfonate. The compounds were selected considering the likely source, i.e., contaminated surface water, the limited or no information on the behavior of the compounds in the environment, and the form of the molecules. Since these compounds were found in the environment, they are relatively stable. Their sorption in soil should be significantly diversely influenced by their different dissociation, i.e. either the negative or positive charge of their molecules.

Our study further focused on the potential of the selected compounds to accumulate in soil or contaminate groundwater. To find out the influence of various soil properties on their sorption in soil, standard sorption experiments were performed for each of the compounds and 16 representative soils of the Czech Republic. Freundlich sorption isotherms were then calculated for each compound and soil, which describe the equilibrium between the concentration in solution and the concentration sorbed on soil particles.

Correlations between the Freundlich sorption coefficient (K_F), obtained for the average exponent n for the various compounds, and the soil properties were subsequently evaluated. The largest sorption was found for 1,3-diphenylguanidine followed by triethyl citrate, 4-acetamidoantipyrine, 6:2 fluorinated telomer sulfonate, benzo(d)thiazole-2-sulfonic acid, and napthalene-2-sulfonic acid. While the sorption of the first three was controlled by the cation exchange capacity or clay content, the sorption of the remaining ones correlated with the organic carbon content or potential wettability index. Multiple linear regressions were also used to derive equations for predicting K_F values using the properties of tested soils.

The resulting equations and maps of soil properties were used to predict the K_F distributions within the irrigated areas, and subsequently to delineate classes of compounds' mobility in the soil environment. Finaly, specific groundwater vulnerability maps for each compound were obtained by combining the DRASTIC vulnerability index, mobility index and stability index.

Acknowledgement:

The work was supported by the Ministry of Agriculture of the Czech Republic, Project No. QK23020018 and QL24010384.

Behavior of Selected Micropollutants Originating from Treated Wastewater and Sewage Sludge in the Soil-Water-Plant System

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Treated wastewater and sludge from wastewater treatment plants (WWTPs) can be contaminated by various organic micropollutants. These compounds can contaminate soils, plants and even groundwater if treated wastewater is used for irrigation or if stabilized sewage sludge is used for soil amendment. To assess the behavior of selected micropollutants (mainly pharmaceuticals) in soil-water-plant system, nine raised beds were installed in March 2021 near the outlet channel in WWTP for České Budějovice in the Czech Republic (Kodešová et al., 2024). Two beds contain soil taken from the surface horizon of the Arenosol Epieuric and seven beds contain soil from the surface horizon of the Haplic Cambisol. In 2021, either corn or a mixture of different vegetables (lettuce, onions, carrots) were grown in the beds.

Four treatments were carried out for maize grown in the Cambisol beds: A. irrigation with tap water (control); B. irrigation with wastewater; C. application of composted sewage sludge; and D. application of sewage sludge. Three treatments A, B and C were suggested for vegetables grown in the Cambisol beds and two treatments A and B for vegetables in the Arenosol beds. In 2022, two different mixtures of vegetables were grown in these beds. Potatoes, soybeans, and beans were planted in originally maize beds. Kohlrabi, parsley, radishes, and brussels sprouts were planted in the original vegetable beds.

Composition and average concentrations of compounds in wastewater measured in 2022 were like those in 2021. Similarly, composition and concentrations of compounds in sludge and composted sludge measured in 2022 were like those in 2021. While less compounds leaked from the beds in 2022 than in 2021, a larger spectrum of compounds was quantified in soils in 2022 than in 2021. Taken up and mobile compounds in plants were mostly accumulated in plant leaves. Concentrations were usually much higher than in other plant tissues. In addition, some compounds, such as carbamazepine, can be metabolized by plants and thus their metabolites were also found in leaves. Mostly no compounds were quantified in fruits (e.g., soybean pods). Compounds of low mobility (due to high sorption in soil and onto plant cells) remained in soil and belowground plant tissues.

The highest (but low) concentrations were typically found in the periderm of carrot and parsley roots, followed by concentrations in the phloem and xylem. Low concentrations were recorded on the surface of potato tubers but not inside. Different behavior has been found for sertraline, which despite its high sorption in soil, can be taken up by plants, transported within plants and accumulated in leaves (potato). The behavior of compounds in the soil-water-plant system can be simulated (Brunetti et al., 2023). However, the models require many parameters, which is a challenging task. To interpret the observed data with a mathematical model, it will be necessary to obtain further information about the behavior of individual compounds under controlled laboratory conditions.

Acknowledgement:

The work was supported by the Ministry of Agriculture of the Czech Republic, Projects No. QK21020080, QK23020018, and QL24010384.

References:

Brunetti, G., Kodešová, R., Švecová, H., Fér, M., Nikodem, A., Klement, A., Grabic, R., Šimůnek, J. 2022. A novel multiscale biophysical model to predict the fate of ionizable compounds in the soil-plant continuum. Journal of Hazardous Materials, 423, 127008.

Kodešová, R., Švecová, H., Klement, A., Fér, M., Nikodem, A., Fedorova, G., Rieznyk, O., Kočárek, M., Sadchenko, A., Chroňáková, A., Grabic, R. 2024. Contamination of water, soil, and plants by micropollutants from reclaimed wastewater and sludge from a wastewater treatment plant. Science of the Total Environment, 907, 167965.

Spontaneous Imbibition and Multiphase Flow Behavior in a Pre-Salt Rock: Insights from Time-Resolved X-Ray Microtomography

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This study investigates spontaneous imbibition in a coquina, a carbonate rock from Brazil's pre-salt reservoir facies, to enhance understanding of multiphase flow in porous media. By employing time-resolved X-ray microtomography, we monitored fluid displacement and its distribution at the pore scale throughout various stages of oil production, under different saturation conditions: dry, water-saturated, oil-aged, and in contact with recovery water. Micro-CT images were segmented at each condition and time step to analyze porosity profiles, fluid saturations, and phase occupancy maps (Figure 1).

A contact angle test was conducted on the oil-aged sample immersed in formation brine to validate observations related to reservoir condition restoration. Initially, the aging process resulted in an oil-wet condition, but over time spontaneous imbibition indicated over time a shift toward neutral or water-wet conditions. The wettability alteration was confirmed by water occupancy profiles within the pore space.

This study also revealed a preferential pathway for fluid flow, thus improving our understanding of multiphase displacement in carbonate formations. The interaction of viscous and capillary forces was found to play a crucial role since oil stored in nanopores and micropores could not be recovered with the brine, suggesting that the extracted oil originated from macropores and mesopores. These findings contribute to a better understanding of fluid dynamics in pre-salt carbonate reservoirs, offering valuable insights for optimizing oil recovery strategies.

Acknowledgements

This research was carried out in association with an ongoing R&D project registered as ANP no 23020-1, "Caracterização Experimental, Modelagem e Otimização de Processos de Injeção de Água Alternada Com Gás – WAG-EX Fase II" (UFRJ/Shell Brasil/ANP), sponsored by Shell Brasil Petróleo Ltda under the ANP R&D levy as "Compromisso de Investimentos com Pesquisa e Desenvolvimento. The authors would like to acknowledge the support of the Human Resources Program of the National Agency of Petroleum, Natural Gas, and Biofuels – PRH-ANP, supported with resources from the investment of qualified oil companies under the R&D Clause of ANP Resolution No. 50/2015. This study was also financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior, Brasil (CAPES), Finance Code 001. The authors also acknowledge partial support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico, Brasil (CNPq), through research productivity grant 310291/2022-4.

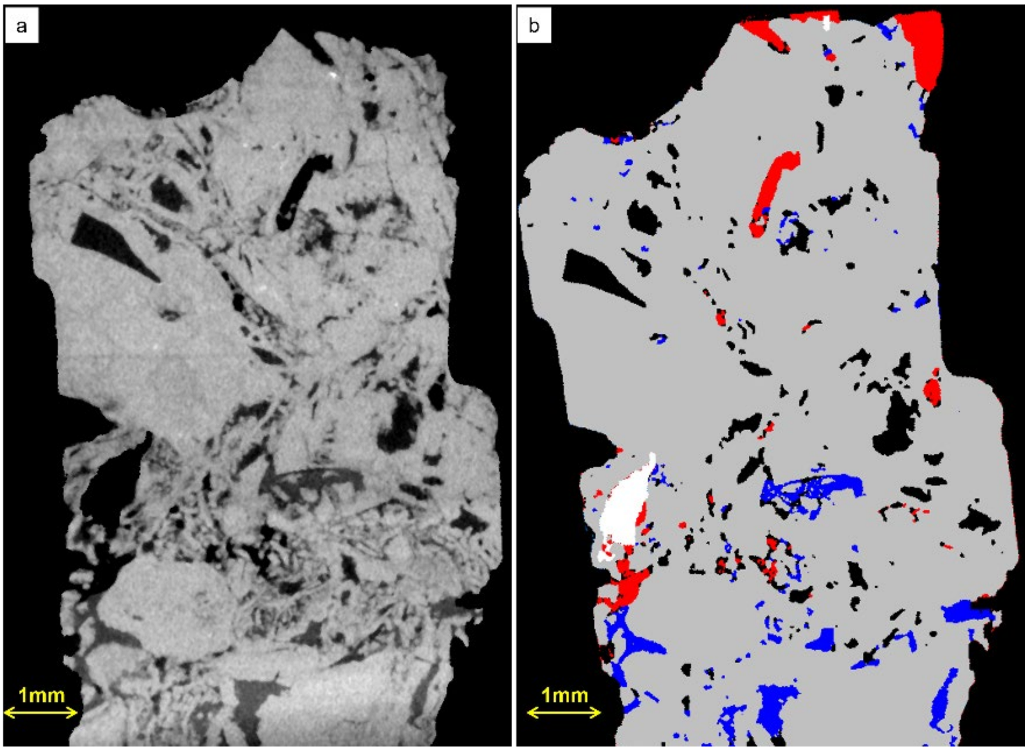

Figure 1. a) MicroCT slice of the miniplug with 9 µm as a voxel size (XZ coordinate). The yellow dashed circle highlights the empty pore (air inside); the blue dashed circle highlights the pore filled with oil and, the red dashed circle highlights the pore filled with doped brine; b) Segmented slice of the miniplug. Colored parts of the pores represent fluid saturation, while air is colored black

Correcting the Micro-Continuum Model for Simulation of the Absolute Permeability of Rocks

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Micro-continuum (MC) models are versatile tools for flow simulation in porous media at different length scales. One application is the determination of absolute permeability from direct numerical simulation (DNS) in computational domains built from μCT images (Soulaine, 2024). Compared to traditional DNS methods, MC models have the advantage of allowing the simulation of pore-scale processes on simple Cartesian meshes, being the most viable DNS method for reactive transport with mineral dissolution reactions where the porous space is evolving during the process, once it does not require complex re-meshing strategies such as those needed to solve conservation equations in the fluid domain (Soulaine et al., 2017; Maes et al., 2022). Previous studies demonstrate the ability of the MC model to describe complex phenomena at the pore scale (Carrillo et al., 2020; Yang et al., 2021; Soulaine, 2024). Still, these studies used very fine meshes, which are not always applicable in pore-scale simulations on domains built from μCT images of rocks. In the present study, we present two corrections to the micro-continuum model to accurately simulate single-phase flow in porous media on coarse meshes: including the second Brinkman term to the averaged momentum balance equation and discretizing the gradients of this term using the Gaussian scheme with a harmonic interpolation.

To verify the impact of the proposed corrections, we compared the velocity and absolute permeability profiles obtained by numerical simulation using the corrected and uncorrected MC model with those obtained by simulations of the Navier-Stokes model in different 2D and 3D porous media, including domains constructed from μCT images of sandstone and carbonate rocks. Considering all DNS on coarse meshes, the uncorrected MC model presented errors of up to 54.2% in the absolute permeability, which were reduced to a maximum of 4.3% using the corrected MC model. We verified that the accuracy obtained with the corrected MC model using coarse meshes was similar to the uncorrected MC model on very fine meshes. For simulations in a two-dimensional bed of particles, this resulted in a speedup of 8483. Therefore, accurate flow simulations on meshes obtained from μCT images of rocks, which are usually coarse, require the corrected micro-continuum model.

References:

Carrillo, F.J., Bourg, I.C., Soulaine, C.: Multiphase flow modeling in multiscale porous media: an open-source micro-continuum approach. Journal of Computational Physics: X 8, 100073 (2020).

Maes, J., Soulaine, C., Menke, H.P.: Improved volume-of-solid formulations for micro-continuum simulation of mineral dissolution at the pore-scale. Frontiers in Earth Science 10, 917931 (2022).

Soulaine, C., Roman, S., Kovscek, A., Tchelepi, H.A.: Mineral dissolution and wormholing from a pore-scale perspective. Journal of Fluid Mechanics 827, 457–483 (2017).

Soulaine, C.: Micro-continuum modeling: An hybrid-scale approach for solving coupled processes in porous media. Water Resources Research 60(2), 2023–035908 (2024).

Yang, F., Stack, A.G., Starchenko, V.: Micro-continuum approach for mineral precipitation. Scientific Reports 11(1), 3495 (2021).

Developing a simplified landslide alert model for Petrópolis, Brazil, using HYDRUS-1D

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The increase in soil pore pressure due to rainfall infiltration is a triggering factor for landslides. Some countries use soil water balance models in their Landslide Early Warning Systems (LEWSs) to identify the soil saturation level and the precipitation threshold, capable of triggering such events. In Brazil, in the Quitandinha neighborhood of Petrópolis, RJ, there is a high frequency of landslides. This work proposes a simplified model for regional landslide alerts, evaluating the linearity trend between accumulated simulated infiltration and accumulated precipitation in locations close to landslide areas, from September to December 2021.

Infiltrations were simulated using HYDRUS-1D (PC-progress, 2025) at two locations: a forest area and an urbanized area, both close to a landslide location. The event of December 18, 2021, as recorded by civil defense and the media, served as a reference for the simulation, which started in September (dry month) and extended for three consecutive rainy months. Precipitation data from the Rua Amazonas station (code 2243433), from the National Center for Monitoring and Alerts for Natural Disasters (CEMADEN), were used, and soil parameters were obtained through field and laboratory tests, including the aturated hydraulic conductivity (Ksat) at three depths, up to 1.70 m.

Result were validated with volumetric moisture data from the EnviroSCAN probe (CEMADEN, 2024). The results revealed a linear trend between accumulated simulated infiltration and accumulated precipitation, up to the landslide date, in the two locations analyzed. The research continues, evaluating whether this linearity is repeated in other points of the water basin, enabling the creation of a simple model to estimate landslide probability, based only on infiltration and precipitation data. The method is expected to be promising for a simplified alert system and a better understanding of the causes of landslides by infiltration. Further research is needed to evaluate the applicability of simulated infiltrations in landslide prediction, the lead time for calculating accumulated values of infiltration and precipitation, and the probability of landslide event estimation.

References:

CEMADEN. 2024 Centro Nacional de Monitoramento e Alertas de Desastres Naturais. Geotechnical Stations. Retrieved on December 2, 2024, from http://www2.cemaden.gov.br/mapainterativo/# (in Portuguese).

PC-progress. 2025. HYDRUS-1D. Retrieved on February 3, 2024, from https://www.pc-progress.com/en/Default.aspx?hydrus-1d.

Characterizing Large-Scale Preferential Flow Across Continental United States

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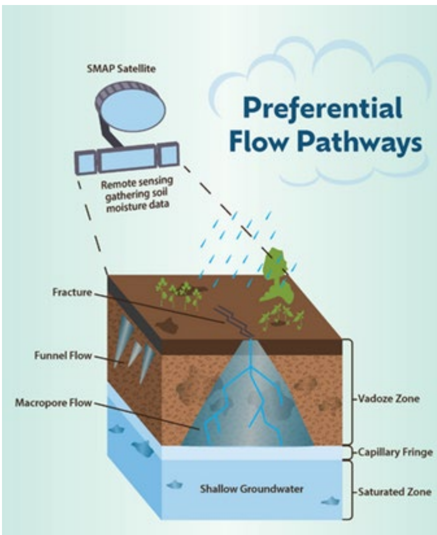

In this presentation, we will summarize a study related to preferential flow (PF) (*Kocian and Mohanty, Vadose Zone Journal Special issue, 2024, Honoring the legacy of Rien van Genuchten*). Preferential flow at large scales is critical for improving land management and groundwater (GW) quality. However, limited knowledge of this process, due to soil surface heterogeneity and observational constraints, hampers progress. In this study, we propose estimating effective PF at remote sensing footprint scale (4 – 9 km) by examining its impact on soil moisture (SM) distribution and shallow GW (SGW) table fluctuations (depth ≤ 5 m).

Effective PF encompasses macropore, funnel, and finger flow pathways influencing SGW table fluctuations. We compiled daily SGW observations (2019-2021) from 19 continental US (CONUS) sites through USGS. Using inverse modeling in HYDRUS-1D, SGW data, and CHIRPS precipitation data, we inversely estimated soil hydraulic parameters of the dual porosity model (DPM) simulating vertical flow from soil surface to subsurface. Effective PF presence was inferred using three criteria: (1) daily precipitation ≥ the site-specific average across multiple (calibration) years, (2) daily observed SGW table increase, and (3) daily difference between observed and DPM simulated SGW tables ≤ 50% of the site-specific RMSE.

Leveraging optimized DPM parameters and associated soil texture, classified PF events, and Soil Moisture Active Passive (SMAP L3E) satellite-based SM, a Random Forest algorithm with 10-fold cross validation predicted large-scale effective PF events. Results indicate seasonal dependence, with spring having the highest occurrence of PF events. The Random Forest model achieved 98% accuracy in predicting large-scale PF events, with SMAP SM and saturated hydraulic conductivity (Ks) among the 4 most impactful variables. Our approach provides a soil hydraulic property, site characteristic, soil texture and remote sensing based generalized tool to analyze large-scale effective PF.

Modelling the Effects of Compaction on Soil Water Retention and Infiltration

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This paper reports on the development, validation and application of two numerical approaches for determining the effect of compaction on the soil water retention curve (WRC). The proposed approaches satisfactorily expanded the applicability of the van Genuchten (1980) model. The WRC of a wide range of soil types and textural classes used for arable cropping in the US and Australia with different levels of compaction (no compaction, and 10%, 20% and 30% increases in soil bulk density) was estimated using the van Genuchten-Mualem (VG) model. The VG water retention parameters of non-compacted soils were obtained first by fitting measured soil hydraulic data. To construct the WRC of the compacted soils, gravimetric values of the permanent wilting point (θ_{gw}, 1500 kPa) and the residual water content (θ_{gr}) were assumed to remain unchanged with compaction.

The VG parameter α and exponent η after compaction were estimated using two approaches. In Approach 1, α and η were estimated from saturation, the permanent wilting point, and the residual water content. In Approach 2, the value of η was assumed to remain unchanged with compaction, which allowed α to be determined immediately from the VG equation. Approach 2 provided a better agreement with measured data than Approach 1; however, both numerical approaches yielded satisfactory solutions and may be used with confidence. The effects of compaction on the saturated hydraulic conductivity (K_s) were predicted using semi-theoretical approaches and the VG-WRC function. HYDRUS-1D was further used to simulate vertical infiltration into a single-layered soil profile to determine the impact of compaction on the infiltration characteristics of the soils used in our analyses.

Across all soils, results showed that a 10%–30% increase in soil bulk density, due to compaction, reduced cumulative infiltration (I_c) at time $T = T_{final}$ (steady-state) by about 25 to 94%, and the available water storage capacity by 3 to 94%, depending upon soil type and textural class. Adoption of mechanisation systems that mitigate (e.g., low-ground pressure systems), or possibly avoid (e.g., controlled traffic farming) soil damage due to compaction is a pre-requisite for improving water-use efficiency. Quantification of the benefits of compaction avoidance, in terms of improved infiltration, soil water retention and water-use efficiency, as well as better predictions of the hydrology of compacted soils, may be possible through the application of the models reported in this study.

Improving Infiltration Modeling in the National Water Model

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The National Water Model (NWM) is a computational hydrology tool developed by the National Oceanic and Atmospheric Administration, National Weather Service (NIAA-NWS) The model was developed to facilitate the prediction of the hydrology at the fine scale across the entire continental U.S., Hawaii, southern Alaska, and U.S. territories. Currently the model makes predictions at 2.7 million river reach locations on a continuous basis. Of interest is the ability to predict flood and potential inundation (flooding) of land parcels, and also to predict streamflows during drought periods. There is also interest in being able to predict water quality parameters for these flows.

To make the model run efficiently on a large number of grid cells or geographical locations, it is necessary to have an efficient means of predicting infiltration at each grid cell. Due to the large number of grid cells, the prediction method needs to be computationally efficient. One approach is to solve the classical Richards equation using numerical methods, such as is done by the HYDRUS 1-D model. The shortcoming is that numerical solutions of the Richards equation with fine vertical discretizations is computationally demanding and in some cases does not converge. The current NWM uses the Noah-MP land surface scheme, which solves the moisture content form of Richards equation on a coarse discretization, necessitating the use of an empirical land-surface runoff partitioning function. An alternative approach is to solve the flow equations using a Green-Ampt formulation. Such a formulation is well-established to be efficient computationally, but in the past the equation has been applied only to individual infiltration events and has neglected the effect of water redistribution following infiltration, while also neglecting the effect of a water table at depth, and evaporative uptake of water.

A new formulation of the Green-Ampt approach has been developed, referred to as LGARTO (Layered Green-Ampt with Redistribution with Talbot-Ogden groundwater bi-directional coupling). This formulation facilitates modeling the processes of infiltration, redistribution, and evaporation/evapotranspiration; it also accounts for a water table at depth. Tests were done of LGARTO against field observations and HYDRUS-1D. This presentation will outline some background about the NWM, and will provide important details of the LGARTO solution with example simulations of infiltration events. The topic of this presentation is the focus of a project funded by NOAA through the CIROH (Cooperative Institute for Research to Operations in Hydrology) program.

An Updated Version of the Hydrophysical Database for Brazilian Soils: Perspective for Generating Maps of Soil Hydraulic Properties

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Soil hydraulic properties, such as water retention and hydraulic conductivity, play a fundamental role in soil modeling studies and technical applications. Efforts to compile comprehensive datasets related to soil hydraulic properties have been underway. The Hydrophysical Database for Brazilian Soils (HYBRAS, Ottoni et al., 2018) represented a significant effort in consolidating soil hydrophysical data for Brazilian tropical soils. However, there is still a lack of data to cover the whole Brazilian territory, which prevents the development of soil hydraulic properties maps that could be very useful for distributed hydrological and soil modeling.

In this study, we introduced an enhanced and updated version of HYBRAS, referred to as HYBRAS V2, and made a general investigation of its potential for generating maps of hydraulic properties. This dataset is accompanied by general information on sampling locations, including georeferenced coordinates and their accuracy, soil hydrophysical properties, land use and cover, Brazilian soil classes, and applied hydrophysical and chemical measurement methods. The HYBRAS V2 data were subjected to rigorous quality control procedures, including the elimination of duplicated and inconsistent data. Harmonization and consistency were ensured by following standard procedures from literature and expert knowledge. A total of 8,546 records from 225 publications were compiled in HYBRAS V2, representing an increase of 7,471 soil samples concerning the first version. The dataset offers broad national coverage, representing all 26 Brazilian states and the Federal District.

HYBRAS V2 provides data on the 12 textural classes, as well as on the 13 Brazilian soil classes. All 8,546 records in the database include information on sand, silt, and clay contents, with 2,015 providing data on saturated hydraulic conductivity (Ksat). The large number of soil samples also include information on bulk density (7,709) and organic carbon content (5,741). The van Genuchten (VG) model was fitted for 2,732 soil samples, with global root mean squared error values of 0.012 $cm^3.cm^{-3}$. The HYBRAS V2 database employs consistent and well-defined measurement methods for soil properties, with ranges in soil properties broader than those presented in HYBRAS version 1. The Ksat data at the surface (< 30 cm) and subsurface (> 30 cm) depths cover 22 and 16 Brazilian states, respectively, and both datasets showed high spatial resolution (< 100 m) in more than 90% of their respective data.

The VG parameters dataset also presented large representation in the Brazilian territory, with surface and subsurface data covering 24 and 23 states, respectively, with about 85% of their respective data showing high resolution. These results open great opportunity to generate maps of hydraulic properties with resolution up to 100 m in different soil depths. The method to derive those maps (using pedotransfer functions and or geostatistical analysis) with uncertainty estimations is still under investigation. HYBRAS V2 has shown to be representative of a wide range of Brazilian soils, with a high potential to generate hydraulic property maps for the soil profile and many other applications.

Reference:

Ottoni, M.V., T.B. Ottoni Filho, M.G. Schaap, M.L.R.C. Lopes-Assad, and O.C. Rotunno Filho. 2018. Hydrophysical database for Brazilian soils (HYBRAS) and pedotransfer functions for water retention. Vadose Zone Journal 17:170095. doi:10.2136/vzj2017.05.0095.

Soil Pore Space Structural Classification System (SPSCS): I. Theory

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Water, air and solute dynamics in soils is strongly dependent on the soil pore structure. This structure refers to the shape, size, and arrangement of pores, which result from the distribution of the solid soil elements. Its determination is essential in studies of hydrological modeling, climatology, irrigation, drainage, and soil and water conservation. To characterize this structure, different approaches are used, but the lack of a standardized method makes interpretation and comparison of results difficult. The Soil Pore Space Structural Classification System, with the acronym SPSCS, was developed by Ottoni (2017) to promote a quantitative and standardized approach to characterize the soil pore structure.

The SPSCS sytem is based on the volumetric distribution of pore size, at the soil sample level. It has a design partially similar to the Textural Classification System, which considers the particle size distribution. The System has two categorical levels: Order (9) and Sub-Order (4). Therefore, 36 possible structural classes are possible, called Families, which group soils according to their air availability curves, $A_a(s)$, close, with s being suction and A_a (s) the complement of the water retention curve (WRC) to the saturation water content. To specify the Order, the percentages of macro, meso, and microspaces are plotted on a ternary classification diagram, called structural triangle, in which its nine specific subareas will define the Orders.

The Sub-Orders are defined from four variation ranges of the effective porosity values. In these procedures, the van Genuchten WRC equation and an optimization protocol of its parameters are required based on specific WRC data. Within each Family, its theoretical reference soils, called type-soils, are conceived. The distributions of the $A_a(s)$ type-curves of the 36 Families thus allow a global assessment of the porous volumetric structure of the soils, which makes SPSCS a new tool for pedological investigation. It was also demonstrated that SPSCS allows an estimate of the air and water capacities of the type-soils. The application potential of SPSCS will be enhanced if other pedological tools are used, such as mineralogical, textural and pedogenetic information.

Reference:

Ottoni, M.V. 2017. Sistema de Classificação dos Solos baseado na Estrutura do Espaço Poroso. COPPE, Federal University of Rio de Janeiro, UFRJ.

A Soil Shrinkage Model Inspired by van Genuchten's Soil Water Retention Model and Beyond

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Twenty years ago, I was in Kiel as a postdoctoral working in Rainer Horn's Laboratory. At that time, I collected some soil shrinkage data and intended to model them. However, there is no an easily and friendly model. I found that the soil shrinkage curve presents a similar "S" shape but the direction is opposite to the soil water retention curve (SWRC). As inspired by van Genuchten's SWRC model, I developed a new model for the soil shrinkage curve (SSC), which was published in SSSAJ in 2005. After that, I further found that constant loading (like overboard stress) and transient loading impacted soil shrinkage behavior differently. Under transient loading, the soil bulk density will change. The SSCs under different transient loadings (or different bulk densities) are parallel with the same coefficient of linear extensibility (COLE). On the other hand, the SSCs under different constant loading stress converged at zero shrinkage or the dry-end point with load-free soil shrinkage. On the basis of different shrinkage behaviors resulting from the two mechanical stresses, we proposed numerical formulae to illustrate a series of curves for the SSC and load stress relationship (Peng et al., 2009).

Several years later I led my research group working on a Shajiang black soil (Vertisol) which contains up to 20% calcareous concretions (CC) and how to remediate its poor structure. We observed that the increasing CC content reduced the saturated void ratio and COLE but the CC size did not. The shrinkage curves of the CC–soil mixtures were proportional to that of the fine soil, which was modified by the portion of CC volume in the CC–soil mixtures. A new numerical equation based on our shrinkage model was proposed to illustrate the relationship among SSC and CC content (Chen et al., 2022). More or less, these studies have brought me and Rien van Genuchten closer although the physical distance is very far.

Peng and Horn model (2005) for soil shrinkage

$$(\vartheta)=e_{\mathrm{r}} + \frac{e_{\mathrm{s}} - e_{\mathrm{r}}}{[1+(\chi\vartheta)^{-p}]^{q}},\ 0\leq \vartheta\leq \vartheta_{\mathrm{s}}$$

References:

Chen, Y.M., Z.B. Zhang, Z.C. Guo, L. Gao, and X.H. Peng. 2022. Impact of calcareous concretions on soil shrinkage of a Vertisol and their relation model development. Geoderma 420, 115892, https://doi.org/10.1016/j.geoderma.2022.115892.

Peng, X.H., and R. Horn. 2005: Modeling soil shrinkage curve across a wide range of soil types. *Soil Science Society of America Journal*. 69:584-592.

Peng, X.H., J. Dörner, Y. Zhao, and R. Horn. 2009. Shrinkage behavior of transiently- and constantly-loaded soils and its consequences on water release characteristic. European Journal of Soil Science, 60: 681-694.

Modeling Residue Disposal Using the HYDRUS Software

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This paper summarizes studies in which the HYDRUS software was used to investigate the performance of two different waste disposal scenarios in Brazil: One scenario concerns a conventional subsurface permanent disposal installation containing naturally occurring radioactive materials (NORMs) and heavy metals. The second scenario considers the same site, but with the material disposed of only temporarily in a pile.

Residues containing natural U and heavy metals at the site are often being permanently disposed of in an industrial landfill on top of a base of earth material to ensure integrity of the deposit over relatively long geologic times (thousands of years). Brazilian regulations, like those of many other countries, require a performance assessment of the disposal facility using a leaching and off-site transport scenario (the first scenario. We also modeled the temporary disposal of the residues in a pile (positive disposal) for a shorter time period (100 years). The two disposal systems will be modeled using HYDRUS to obtain subsurface residue concentrations and the impact of the disposal on the environment and populations living in the vicinity of the disposal facilities (the critical group).

The first scenario concerned the subsurface transport of radionuclide decay chains (notably the ^{238}U series) leached from a conventional mining installation. The disposal site contained slags having radionuclide concentrations and other chemicals. The disposal system is modeled as a sequency of cells, underlain by a compacted clay layer and covered with soil and natural vegetation from the area. The second application is concerned with the temporary disposal of the residues in an uncovered pile underlain by a same compacted clay later.

We used the HYDRUS-5.04 software package to predict long-term radionuclide transport vertically through both the landfill and the temporary pile, as well as the underlying unsaturated zone, and then laterally in the groundwater system. We assumed that a downgradient well or water stream intercepted groundwater, which was then used as the only source of water for a resident farmer, and that all contaminated water from the well was somehow used in the biosphere. The future impact of the disposal method is analyzed for both scenarios.

Evaluating the Permeability of Carbonate Rocks Using Critical Path Analysis and Combining MICP and NMR Measurements

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Knowledge of the permeability of porous media is crucial to understanding fluid flow in natural and artificial porous materials. The complex nature of pore structure, along with such pore characteristics as the porosity, distribution and especially the pore radii, has been widely discussed because of its direct influence on the permeability. Equations developed to estimate permeability based solely on total porosity often fail to yield satisfactory results for heterogeneous porous media such as carbonate rocks and many soils.

One promising technique is Critical Path Analysis (CPA) as derived from percolation theories. Based on the CPA, flow through a porous medium is controlled by pores whose sizes are greater than some critical value (the critical pore radius), being the smallest radius required to form a conducting sample-spanning cluster. Percolation theory provides a physical basis for the effects of flow interconnectivity in heterogeneous media.

The main objective of this study was to use nuclear magnetic resonance (NMR) and mercury injection capillary pressure (MICP) data to optimize the van Genuchten (VG) hydraulic parameters. The analyzed samples consisted of coquina plugs collected from an onshore well in Brazil. Routine petrophysical and well log data were further used to support the classification of samples into distinct rock types.

In this study we determined the critical pore radius using the critical path analysis. The fluid retention curves were obtained from transversal relaxation time distributions (T_2) of the NMR and MICP experiments, which permitted us to estimate the unsaturated parameters of the van Genuchten equation. The critical radius was obtained using

$$r_c = 0.149\,\alpha m^{1/n}$$

in which α, m and n are the VG hydraulic parameters. Please note that the above equation is formulated in terms of the cgs unit system, with the constant 0.149 having a dimension of L^2. If other units are used for r_c and/or α, the value of 0.149 needs to be adjusted accordingly. We also used a more direct way of estimating the critical radius by considering its value to be at the inflection point of the mercury intrusion curve. The correlation between the percolation radius (instead of the total porosity) and the measured permeability could then be evaluated.

We chose to integrate multiple data sources to support the classification of rock types, thus aiming to improve correlations between the critical radius and the permeability. By defining the critical radius using different methods and grouping results by rock types, the permeability could be assessed through established equations, with the critical radius substituting for total porosity. Finally, the relationship between calculated and measured permeabilities, as well as between the critical radius and the measured permeability by rock type, could be analyzed.

Multiscale Approaches for Upscaling Flow, Transport, and Reaction Parameters in Heterogeneous Porous Media

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This presentation addresses recent advances in multiscale approaches for imaging, characterizing and upscaling flow, transport, and reaction parameters in heterogeneous porous media, with special emphasis on carbonate rocks and structured soils. Understanding the relationship between micro-scale properties and macro-scale behavior remains a fundamental challenge in porous media science, particularly for media with complex pore structures.

We have developed and validated novel methodologies that bridge observations across scales using experimental data and computational modeling, and use pore network modeling techniques to characterize pore structures and predict a complete set of transport properties. In dual-porosity media, we examine the critical impact of aggregate porosity and permeability on solute exchange between mobile and immobile domains, and quantify the relationship between pore-scale properties and the macroscopic mass transfer coefficient. For soil compaction studies, we show how changes in pore body and pore throat size distributions affect the hydraulic conductivity and soil water retention properties.

The developed pore-scale modeling framework, implemented in the PoreFlow and PoreStudio softwares, enables accurate simulation of various flow regimes and provides a foundation for generating constitutive relationships needed in field-scale models. These findings significantly enhance our ability to predict hydraulic and transport properties across scales, with important applications in groundwater remediation, subsurface contaminant transport, and reservoir characterization for geo-energy and carbon sequestration.

Comparison of NMR Log T2 Distributions with Petrographic Image Analysis and Special Core Analysis in Pre-Salt Formations

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Many pre-salt wells have been drilled with Synthetic Oil Base Mud (OBM). The NMR logs run on these wells show a distinct bimodal T_2 distribution, where the OBM filtrate preferentially invades macropores, while micropores remain occupied by capillary formation water. Considering that the Pre-salt formations tend to be oil-wet to neutral-wet one should expect to see the T_2 distribution responding to the surface to volume ratio rather than only to the bulk effect of the OBM filtrate.

To investigate this further, thin-section microphotographs of pre-salt core samples were analyzed using the ImageJ software to create pore-size distributions (PSDs) of visible macropores at a resolution of 8 microns/pixel. The PSDs were then correlated with NMR logs from the same well, 2-ANP-2A-RJS, to determine the effective surface relaxivity parameter (ρ), which relates T_2 to the surface to volume ratio (S/V). For spherical pores, S/V is expressed as 3/radius, and for cylindrical pores, 2/radius, with the numerator often referred to as the Geometric Factor. Image analysis in ImageJ allows the extraction of various measurements such as Ferret Diameter, Minimum Ferret, Perimeter, and Area of detected pores once thresholding is used to distinguish pores from the matrix in the thin sections.

We examined the results from using the Ferret method to calculate an effective pore radius and applying the ratio of Perimeter to Area as a proxy of the surface to volume ratio to correlate with the NMR T_2 distribution. This workflow will be presented in detail. Results corroborate recent findings that, in carbonate formations, the effect of surface roughness on the pores due to calcite crystals increases the effective surface area. Consequently, the ρ value must be adjusted upwards compared to earlier studies in carbonates or, alternatively, the Geometric Factor must be increased from the conventional 3 (for spheres) or 2 (for cylinders). These observations may provide insights for future studies on determining irreducible water saturation and permeability, indicating a potential to enhance the reliability of production estimates.

References:

Straley, C. 1994. Core analysis by low field NMR, SCA Conference

Looyestijn, W. 2019. Practical approach to derive wettability index by NMR in core analysis experiments. Petrophysics, 60 (4).

Coutinho, B. et al. 2024. Integrating statistically significant laboratory information in variable T_2 cut-off logs for NMR interpretation in Pre-salt". SPWLA 65th Annual Logging Symposium, May 18-22, 2024 DOI: 10.30632/SPWLA-2024-0091

Ma, S.M. et al. 2020. Objective driven solid surface roughness characterization for enhanced formation evaluation, SPE 201689-MS, 2020 SPE ATC, October 26-29, Denver, Colorado.

El-Husseiny, A. and R. Knight. 2017. A laboratory study of the link between NMR relaxation data and pore size in carbonate skeletal grains and micrite. Petrophysics, 58(2) 116–12.

Water Monitoring using Hydrological Modeling and Satellites

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This presentation establishes as academic-scientific framework for the evaluation of the hydrometeorological and environmental behavior in catchment areas of the highlands of the state of Rio de Janeiro. The areas cover urban, agricultural and forested regions, notably in the Piabanha river watershed, with potential for extension to the metropolitan area of Rio de Janeiro, based on hydrological studies developed in Brazil for various national river basins, including the Amazon basin.

The perspective is the conception of a water observatory in which basins play the role of a laboratory for developing experiments. We emphasize the use of remote sensing in conjunction with computational numerical models, with a view to the development and evaluation of methodologies and hydrometeorological and atmospheric parameterizations in the river basin scale. Additionally, it is argued that it is essential to articulate obtaining basic field data from in situ monitoring and remote sensing technologies, enabling multidisciplinary studies on modeling of water resources, with emphasis on the physical aspects of the understanding of the hydrological cycle and evaluation of climate change.

The proposed approach is integrated with a social vision of the physical system of the basin, so that updated information can be provided to society. For this very broad perspective, the following issues are highlighted: to develop and implement models to address surface hydrology and groundwater hydrology in order to forecast streamflows and water levels during critical events (flood and drought) in river basins, and to evaluate the use of remote sensing technology in monitoring surface and underground water flows jointly with the use of datasets collected using sensors and in situ measurements.

Soil Pore Space Structural Classification System (SPSCS): Application to Brazilian Latosols

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The porous structure of soils significantly influences water and gas storage and flow, and solute transport. Ottoni (2017) developed the Soil Pore Space Structural Classification System (SPSCS) to provide a quantitative and standardized method for classifying soil pore structure. This system utilizes the similarity of soil air availability curves, defined as the difference between saturated water contents and the water retention curves. Latosols, prevalent in Brazil, are known for their high aggregate stability and water infiltration rates, but require careful management for sustained productivity and conservation. This study applies the SPSCS to a hydrophysical database of 45 Brazilian Latosol samples from the HYBRAS database (Ottoni et al., 2018), examining the relationship between SPSCS structural classes and hydrological functionalities. The database included water retention curves, soil texture, bulk density, and saturated hydraulic conductivity. The majority of samples exhibited fine texture and blocky structure.

The SPSCS classification revealed that 48.9% of the soils fell within the Macro-Mesoporous Order (Order B), followed by the Highly Macroporous Order (Order A) at 22.2%, and the Macroporous Order (Order D) at 14%. These soils generally displayed high effective porosity (EP), defined as the difference between saturated water content and residual water content (θ_r in the van Genuchten equation), ranging from 40% to 60%. Available water content (AW), the difference between volumetric water contents at 33 kPa and 1500 kPa suction, correlated with EP. Soils with low to moderate EP showed corresponding restrictions in AW, while those with high EP exhibited minimal to no AW limitations. EP was categorized as low ($EP \leq 0.20$ $cm^3.cm^{-3}$), moderate ($0.20 < EP \leq 0.40$ $cm^3.cm^{-3}$), high ($0.40 < EP \leq 0.60$ $cm^3.cm^{-3}$), and very high ($EP > 0.60$ $cm^3.cm^{-3}$). AW was classified as low ($AW < 0.06$ cm^3/cm^3), moderate ($0.06 \leq AW \leq 0.12$ cm^3/cm^3), and high ($AW > 0.12$ cm^3/cm^3).

Furthermore, soils with higher microspace (the SPSCS term related to soil microporosity) values, such as those in Orders I, G, and H, tended to have air capacity (AA) limitations ($AA < 0.10$ cm^3/cm^3), where AA is the saturated water content minus water content at 33 kPa suction. Conversely, soils with higher macrospace (the SPSCS term related to soil macroporosity) values, such as those in Orders A, B, and D, showed water capacity limitations ($AW < 0.06$ cm^3/cm^3). Granular soils displayed enhanced water and air capacities compared to blocky soils, likely due to their higher EP. These findings highlight significant variations in soil pore structure among Latosols, despite their morphological homogeneity, impacting air and water capacities. The SPSCS methodology proves to be a valuable tool for assessing soil hydraulic behavior, aiding in informed decision-making within agricultural and environmental contexts.

References:

Ottoni, M.V. 2017. Sistema de Classificação dos Solos baseado na Estrutura do Espaço Poroso, COPPE, Federal University of Rio de Janeiro, UFRJ.

Ottoni, M.V., T.B. Ottoni Filho, M.G. Schaap, M.L.R.C. Lopes-Assad, and O.C. Rotunno Filho. 2018. Hydrophysical database for Brazilian soils (HYBRAS) and pedotransfer functions for water retention. Vadose Zone J. 17:170095. doi:10.2136/vzj2017.05.0095.

Maps of van Genuchten Parameters for the Contiguous USA at 100 m Resolution and Seven Depths: Code Design and Preliminary Results

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Estimates of the van Genuchten (1980, abbreviated as VG) parameters and saturated hydraulic conductivity (K_s) were made for the contiguous USA at a resolution of 100 meters and seven soil depths by combining the SoilGrids+ (SG+) soil property maps of Ramcharan et al., (2018) with the R3H3 member of the Rosetta3 hierarchical pedotransfer functions (PTFs) of Zhang et al. (2017). To this end, we developed multi-threaded code that significantly speeds up computation (up to a factor 25) depending on the level of parallelism. We verified estimates first by calculating simple summary statistics of estimated basic properties of SG+ with actual measured soil properties for 14,113 pedons in the National Cooperative Soil Survey (2023) labsample database (NCSS). Next, we computed summary statistics of PTF-estimated moisture contents for NCSS and SG+ data.

Results show that estimation errors are dominated by intrinsic errors of the PTF, and that (potentially correctable) systematic errors are present in SG+ soil properties and PTF estimates. The resulting hydraulic property maps (see the figure below for an example for K_s) contain well over 750 million points for each of the seven layers and show considerable horizontal and depth variation for each VG parameter and K_s, except the VG "*n*" parameter, which is dominated by values between 1.25 and 1.6.

The hydraulic property maps are 99.9% complete. We demonstrate that plausible profiles and uncertainty information can be generated for virtually each point. The maps are available as two multi-channel GeoTIFF maps per SG+ layer: one with the five hydraulic parameters and one with the corresponding covariances. Total data size is 350 gigabytes, distributed over 14 files. Details of this work can be found in Schaap et al. (2024) which also includes links to open data and code. The reference also includes some guidance how stochastic distributions of estimated VG curves can be generated using the covariance matrices using Python or R languages. Work is underway to improve the current maps with the new NRCS data product SOLUS100.

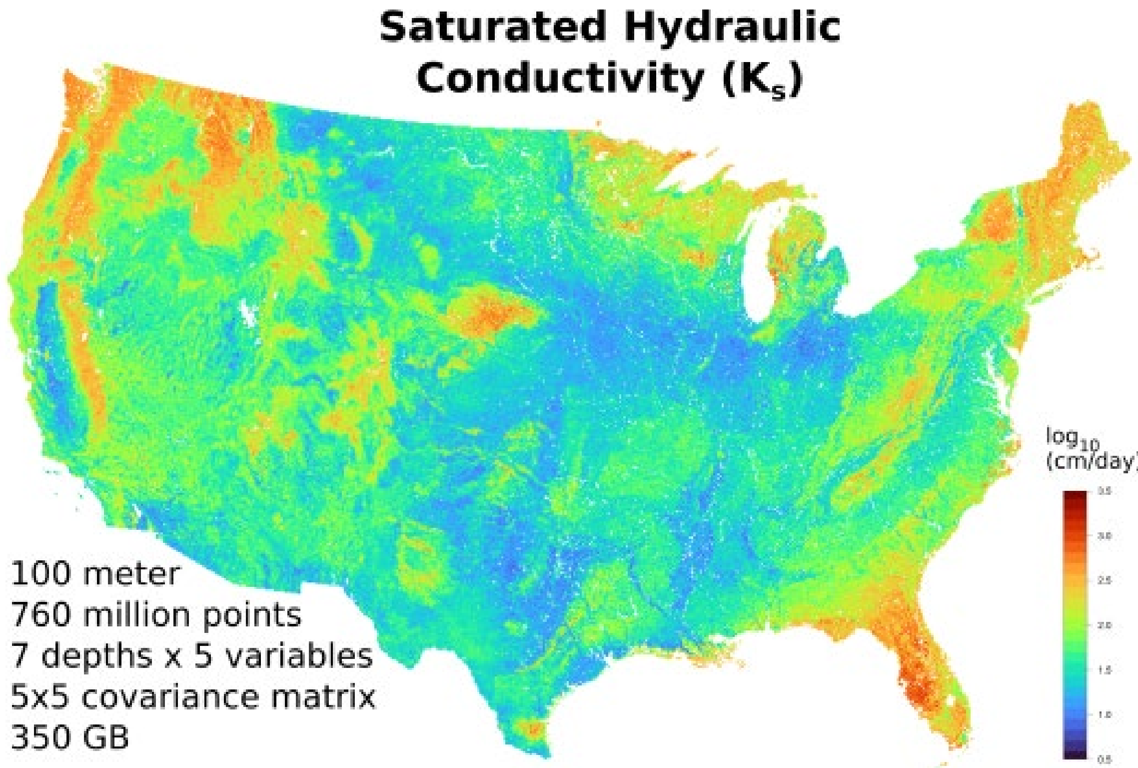
References:

Schaap, M.G, Zhang, Y., and Rasmussen C., 2024. Soil hydraulic property maps for the contiguous USA at 100 meter resolution and seven depths: Code design and preliminary results, Vadose Zone Journal, 2024;e20377. https://doi.org/10.1002/vzj2.20377.
Data are at https://doi.org/10.25422/azu.data.26060383.
Code at https://github.com/mschaap8/ROS_SGplus_VZJ2024.

National Cooperative Soil Survey, 2023. National Cooperative Soil Survey soil characterization database. https://ncsslabdatamart.sc.egov.usda.gov/.

Ramcharan, A., Hengl, T., Nauman, T., Brungard, C., Waltman, S., Wills, S., Thompson, J., 2018. Soil property and class maps of the conterminous United States at 100-meter spatial resolution, Soil Science Society of America Journal, 28 (1): 186-201. DOI: 10.2136/sssaj2017.04.0122

Zhang, Y., Schaap, M.G., 2017. Weighted recalibration of the Rosetta pedotransfer model with improved estimates of hydraulic parameter distributions and summary statistics (Rosetta3), Journal of Hydrology, p. 39-53. doi: 10.1016/j.jhydrol.2017.01.004 https://www.sciencedirect.com/science/article/pii/S0022169417300057.



Map of saturated hydraulic conductivity at 5 cm depth for the contiguous USA. This map shows large-scale variation with high conductivities on coarse materials (orange-red, such as Florida, mountains, glacial sediments) and low conductivities on the fine sediments in the US interior (blue). Actual map holds 49,810 × 31,390 pixels (West–East × North–South) at 100-meter resolution

Required Log Reduction Values of Virus for Groundwater Protection and Potable Reuse of Wastewater

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Two topics are presented: Ground water protection against virus contamination and required Log Reduction Values (LRVs) of virus by advanced wastewater treatment for potable reuse.
In the Netherlands, groundwater needs to be protected against microbial contamination in order not to exceed the 1/10,000 persons/ year infection risk level by potable water consumption (Anonymous, 2005). The distance between a contamination source and the production well (protection zone) allows for pathogen removal by inactivation and attachment to the soil.

A risk analysis (Anonymous, 2020) was conducted encompassing the following items:

1. Vulnerability assessment of the groundwater production sites to pathogen contamination based on the properties affecting pathogen survival in groundwater.
2. Protection zone calculation, using a standard contamination scenario with a LRV of 8.5 log10 in order not to exceed the infection risk level (Schijven et al., 2010).
3. Assessment of contamination within the protection zone, such as ditches, sewage pipes, septic tanks, farms.
4. Quantitative Microbial Risk Analysis (QMRA) for identified contamination sources within the protection zone. If the risk level is too high, the contamination needs to be removed, groundwater discharge needs to be reduced or stopped, or additional water treatment needs to be installed. QMRAwell is a computational tool designed to conduct such as QMRA (https://www.rivm.nl/en/who-collaborating-centre-risk-assessment-of-pathogens-in-food-and-water/tools/qmrawell).
5. Monitoring if the protection zone is larger than the currently protected zone in which case, unidentified contamination sources may be present within the protection zone. The monitoring programme must be executed every 4 years, in which at least 3 samples of 100 litres, if possible 1000 litres, are analysed for the presence of somatic coliphages as proxy for virus transport.

Advanced water treatment processes are indispensable to mitigate microbial and chemical contaminants present in recycled waters for potable reuse. Betancourt et al. (2023) analysed samples at three facilities that apply advanced wastewater treatment for eleven different enteric viruses in order to determine their LRVs. In addition, the samples were also analysed for somatic coliphages, male specific phages, pepper mild mottle virus, and crAssphage in order to investigate their potential as process indicators of enteric virus reduction. All viruses were detected by means of digital PCR, except for the somatic coliphages and male specific phages, which were detected by classical plaque counting. Inevitably, after every successive treatment step, relatively more non detects were collected. A major objective of the study was to develop a model to handle censored data to estimate LRVs. In addition, the virus reduction model was applied in a QMRA to evaluate whether the finished water met requirements for potable reuse with regard to exposure to adenovirus, enterovirus and noroviruses GI and GII and to evaluate the phages as indicator for virus reduction. This study provides data for the on-going discussion on required LRVs.

References:

Anonymous, 2020. https://www.ilent.nl/onderwerpen/drinkwater/documenten/publicaties/2020/11/27/richtsnoer-analyse-microbiologische-veiligheid-drinkwater-amvd (in Dutch).

Anonymous, 2005. Ministerie van VROM. Inspectierichtlijn 5318 “Analyse microbiologische veiligheid drinkwater” (in Dutch).

Betancourt, W., 2023. WRF 4955: Indicator Viruses to Confirm Advanced Physical Treatment. The Water Research Foundation.

Schijven, J. F., Hassanizadeh, S. M., the Roda Husman, A. M. (2010). Vulnerability of unconfined aquifers to virus contamination. Water Research, 44(4), 1170-1181.

Development and Optimization of Multimodal Unsaturated Soil Hydraulic Models: Implementation of the Unsatfit Library and its Performance

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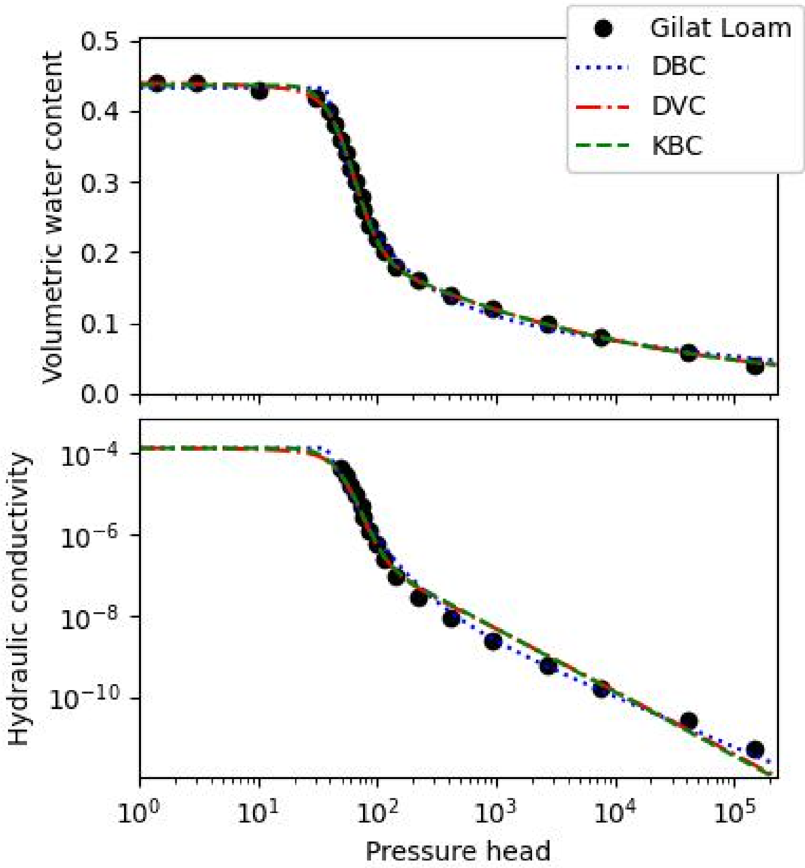
Unimodal functions of the soil hydraulic properties, such as the standard BC (Brooks and Corey, 1964), VG (van Genuchten, 1980), and KO (Kosugi, 1996) models, are inadequate for simulating unsaturated flow in soils with dual- or multi-porosity features. Durner (1994) proposed a multimodal water retention function for these media by linearly combining VG models as sub-retention functions. Our research (Seki et al., 2022) extended Durner's model to incorporate linearly superposed sub-retention functions using any combination of the BC, VG, and KO water retention models. We derived closed-form expressions for the hydraulic conductivity function based on the generalized Mualem model using Priesack and Durner's mathematical approach.

In Seki et al. (2023a) we demonstrated the practical utility of these equations by evaluating three models: the dual-BC-CH (common head) (DBC), dual-VG-CH (DVC), and KO_1BC_2-CH formulations. Testing these models with 20 soils from the UNSODA database showed good agreement with measured water retention and hydraulic conductivity data across a wide range of pressure heads. Parameters were optimized in two steps: first optimizing the water retention parameters, and then the saturated hydraulic conductivity and two parameters (p, q) or (p, r) in the general hydraulic conductivity equation. While traditionally only the tortuosity factor p is optimized with fixed (q, r), sensitivity analyses revealed that optimization of two parameters ($p+r$, qr) is necessary for multimodal models. The attached figures show typical results for one soil (Gilat loam).

A Python library (Unsatfit) was developed to optimize parameters of the different unsaturated soil hydraulic functions. Unsatfit was designed to systematically evaluate various hydraulic models and datasets using different optimization methods, including the selection of constant and initial parameters. The Unsatfit website (https://sekika.github.io/unsatfit/) provides sample codes that demonstrate how to calculate parameters from measured data and to generate the fitted curves by following the same methodology as described in Seki et al. (2023a). Complete documentation is available in Seki (2024a,b).

We also developed a web application (SWRC Fit) that generates Soil Water Retention Curves (SWRC) using various soil hydraulic models from measured data with a single click. SWRC Fit can be downloaded freely from https://purl.org/net/swrc/. This application, based in part on the Unsatfit Python library, simplified the optimization process by eliminating the need to select initial values of the water retention parameters.

The algorithm for fitting the dual-VG model was improved further by Seki et al. (2023b), who for various Japanese soils obtained results that were comparable to global optimization methods.



References:

Brooks, R.H., and Corey, A.T. 1964. Hydraulic properties of porous media. Hydrology Papers 3. Colorado State University, Fort Collins, CO, USA.

Durner, W. 1994. Hydraulic conductivity estimation for soils with heterogeneous pore structure. Water Resources Research, 30(2): 211-223. https://doi.org/10.1029/93WR02676

Kosugi, K. 1996. Lognormal distribution model for unsaturated soil hydraulic properties. Water Resources Research, 32: 2697-2703. https://doi.org/10.1029/96WR01776

Seki, K., Toride, N. and van Genuchten, M.Th. 2022. Closed-form hydraulic conductivity equations for multimodal unsaturated soil hydraulic properties. Vadose Zone Journal, 21(1): e20168. https://doi.org/10.1002/vzj2.20168

Seki, K., Toride, N. and van Genuchten, M.Th. 2023a. Evaluation of a general model for multimodal unsaturated soil hydraulic properties. Journal of Hydrology and Hydromechanics, 71(1): 22-34. http://dx.doi.org/10.2478/johh-2022-0039

Seki, K., Iwata, Y., Yanai, Y. and Kameyama, K. 2023b. Improved regression of the water retention curve for highly aggregated soils. Toward the automation of parameter determination for dual-van Genuchten models. Journal of the Japanese Society of Soil Physics, 155: 35-44 (in Japanese). https://doi.org/10.34467/jssoilphysics.155.0_35

Seki, K. (2024a): SWRC Fit and unsatfit for parameter determination of unsaturated soil properties. Journal of Toyo University Natural Science, 68: 57-79. https://doi.org/10.34428/0002000817

Seki, K. (2024b): Evaluation of a general model for multimodal unsaturated soil hydraulic properties. Journal of Hydrology and Hydromechanics, 71(1): 22-34. http://dx.doi.org/10.2478/johh-2022-0039

van Genuchten, M. Th. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Science Society of America Journal, 44: 892–898. https://doi.org/10.2136/sssaj1980.03615995004400050002x

Integral Transform Solution for the Three-dimensional Modeling of Aquifer Drawdown and Recovery by Multiple Wells

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A mathematical model is adopted for the transient three-dimensional pumping problem of aquifers with a single fully penetrating vertical well between two parallel streams. The proposed model simulates confined, leaky, or unconfined aquifers in an anisotropic and homogeneous media. In a first proposed approach, a hybrid numerical-analytical solution based on the Generalized Integral Transform Technique (GITT) is obtained. The unconfined case introduces a boundary condition of the fourth kind, which results in a coupled eigenvalue problem, leading to a coupled transformed ordinary differential system, which must be solved numerically.

For this purpose, the reordering scheme of the eigenvalues to accelerate the convergence of the series is simplified by neglecting the coupling term. Subsequently, a model that simulates multiple horizontal and/or vertical wells in a contaminated aquifer recovery process via PAT (Pump-and-Treat), was included in the source term. In this second approach, an eigenfunction expansion was developed to account for the coupled eigenvalues, resulting in a purely analytical solution through the Classical Integral Transform Technique (CITT), when all the PDE terms are integral transformed.

Mathematical formulation:

The dimensionless model that describes the three-dimensional pressure distribution $h(x,y,z,t)$ varying in the direction of the sinks located at points $(x_{0,i}, y_{0,i})$ in Vertical Multiwells (VMw) or Radial Collector Multiwells (RCMw) is expressed as:

$$\frac{\partial h}{\partial t}=\frac{\partial^2 h}{\partial x^2}+k_y\frac{\partial^2 h}{\partial y^2}+k_z\frac{\partial^2 h}{\partial z^2}+q_i(x,y,z)\ \therefore\ 0<x<w_x;\ 0<y<w_y;\ -1<z<0\ \text{ e } 0<t$$

$$h(x,y,z,0)=h_0(x,y,z)$$

$$\frac{\partial h(0,y,z,t)}{\partial x}-k_1 h(0,y,z,t)=0;\qquad \frac{\partial h(w_x,y,z,t)}{\partial x}+k_2 h(w_x,y,z,t)=0$$

$$\frac{\partial h(x,0,z,t)}{\partial y}=0;\quad \frac{\partial h(x,w_y,z,t)}{\partial y}=0$$

$$\frac{\partial h(x,y,-1,t)}{\partial z}=0\,;\quad \frac{\partial h(x,y,0,t)}{\partial z}+k'h(x,y,0,t)+\frac{\sigma}{k_z}\frac{\partial h(x,y,0,t)}{\partial t}=0$$

where

$$q_i\left(x,y,z,Q_i\right)=\begin{cases}\sum_{i=1}^{Nw}Q_i\delta(x-\bar{x}_{0,i})\delta(y-\bar{y}_{0,i}) & \text{to VMw}\\ \sum_{i=1}^{Nw}Q_i\delta(x-\bar{x}_{0,i})\delta(y-\bar{y}_{0,i})\delta(z+\bar{z}_0) & \text{to RCMw}\end{cases}$$

The source term q_i defines the well at point $(x_{0,i}, y_{0,i})$ with constant pumping rate Q_i, $i=1,2,3\ldots,N_w$, where N_w is wells number, as shown in Fig. 1a for RCMw and Fig. 1b for VMw.

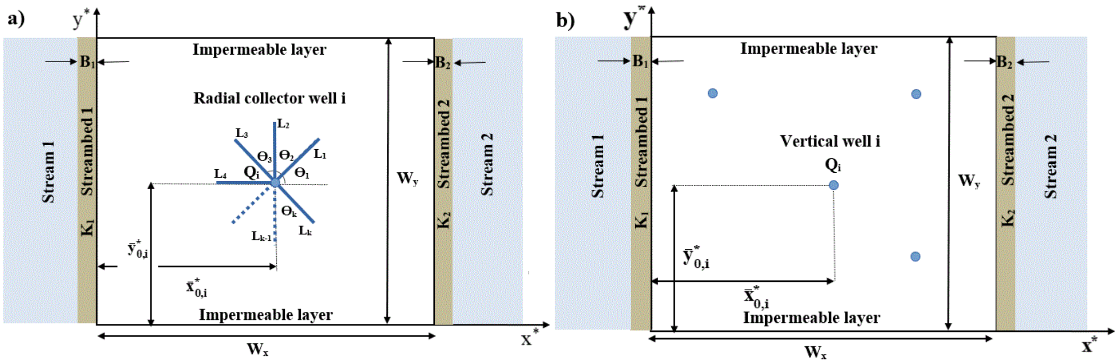

Figure 1. Horizontal (a) and vertical (b) well distributions.

CO_2 Underground Storage: Generalizing Fractional Flow Theory

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Carbon capture and underground storage (CCUS) is a practical approach to combat climate change and global warming. In underground CO_2 sequestration, spontaneous imbibition (SI) plays a key role. Therefore, its accurate modeling and CO_2 plume predictions have been active subjects of research. In this study, we generalized the Buckley-Leverett fractional flow theory by means of Hausdorff fractal derivative in combination with non-Boltzmann transformation ($x \propto t^{\alpha/2}$ in which $0 < \alpha < 2$ is the fractal index). We found that α varied with contact angle, pore space heterogeneity and dynamic viscosity by comparing the proposed model with both experiments and stimulations. We also proposed a dimensionless time to scale the normalized imbibed volume-time data measured on sandstones, diatomite, carbonate, and synthetic porous media. We showed that the non-Boltzmann transformation resulted in a better collapse of the SI data than the Boltzmann transformation ($x \propto t^{0.5}$). More specifically, we found that α ranged from 0.88 to 1.54.

Enhancing Relative Permeability Uncertainty Quantification via Sobol-Based Parameter Reduction in Unsteady-State Core Flooding

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Core flooding experiments offer critical insights into fluid flow behavior in porous media, with the estimation of relative permeability curves being a central objective. In unsteady-state experiments, this often requires solving an inverse problem to estimate multiple parameters, some of which may lack direct physical relevance. To address this challenge, this study employs a Global Sensitivity Analysis (GSA) based on variance decomposition, using the Sobol method to evaluate the influence of each parameter over a predefined range. Oil production, water saturation, and pressure differential responses are analyzed over the simulation period to assess model overparameterization. Results indicate that, for the LET relative permeability model, only a subset of parameters significantly affect water saturation and cumulative oil production. Conversely, pressure differential responses exhibit low first-order sensitivity indices across all parameters, indicating limited sensitivity to single parameter variation.

Based on these findings, a reduced LET model is proposed, retaining only the sensitive parameters within the specified range. This reduction enables simplification of the inverse problem without compromising the accuracy of the model outputs, thereby improving the efficiency of both optimization and uncertainty quantification processes. To present a case study applying these conclusions, it was considered simulations based on the Buckley-Leverett equation for one-dimensional, longitudinal multiphase (water/oil) flow, assuming incompressible fluids and constant water injection. Numerical solutions are obtained via an implicit finite difference method with adaptive time-step control, incorporating the LET model for relative permeability.

A synthetic dataset based on a benchmark case is generated, and parameter estimation and uncertainty quantification are performed using the Markov Chain Monte Carlo (MCMC) method with the Metropolis-Hastings algorithm for both LET model and the proposed reduced model. The results show that both global and local sensitivity analyses agree on the low influence of certain parameters in the relative permeability model. Furthermore, it is observed that parametric reduction increases the influence of the remaining parameters, facilitating their uncertainty quantification.

HYDRUS and its Specialized Modules (Version 5) for Numerical Modeling of Vadose Zone Processes

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Version 5 of HYDRUS resulted from merging earlier versions of HYDRUS-1D (4.x) and HYDRUS (2D/3D) (3.x). This new HYDRUS version simulates variably saturated water flow and transport of multiple solutes in 1D, 2D, and 3D, but also implements the new integrated form of coupling PHREEQC with HYDRUS (HPx) and includes several new modules such as Furrow, PFAS, Particle Tracking, Dynamic Plant Uptake, Cosmic, Stable Isotopes, C-Ride, etc. The new HYDRUS GUI dramatically improves graphical capabilities and extends its compatibility to new Windows-based (e.g., 64-bit) operating systems.

The new modules and capabilities include a) the Particle Tracking module (to calculate soil water's transit times and their frequency distributions), b) the Cosmic module (to calculate cosmic-ray neutron fluxes and to use them to inversely estimate large-scale soil hydraulic properties), c) the Dynamic Plant Uptake (DPU) module (to calculate the translocation and transformation of chemicals in the soil-plant continuum), d) the PFAS module (to consider sorption on the air-water interface and the effects of concentration on viscosity and surface tension, and correspondingly on conductivities and pressure heads), e) the Isotope module (to consider the fate and transport of soil water isotopes with evaporation fractionation, f) the C-Ride module (to consider colloid and colloid-facilitated solute transport), and many other new options and graphical (e.g., two-dimensional *z-t* graphs of main variables) capabilities.

Several nonstandard HYDRUS modules (e.g., accounting for overland flow, freezing/thawing, and alternative root water uptake models) will also be discussed. Several new processes and factors presently being implemented into HYDRUS will be reviewed.

The Legacy of Rien van Genuchten, a Recipient of the 2023 Wolf Prize for Agriculture

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I will discuss Rien's legacy in terms of his scientific contribution to soil physics and vadose zone hydrology and his unprecedented impact on the careers of many contemporary scientists in these research areas. I will also briefly describe the Tel Aviv ceremony where Rien was awarded the Wolf Prize in Agriculture. This prize is considered by many to be the equivalent of the Nobel Prize for the field. Rien was awarded this prize "for his groundbreaking work in understanding water flow and predicting contaminant transport in soils."

To further quote from the Wolf Prize citation: "During his 40-year career, Professor Van Genuchten transformed the broad fields of soil physics and vadose zone hydrology, which are central to modern agricultural operations and climate science. He created a much-needed scientific basis for understanding fluid flow and contaminant transport processes in unsaturated soils, including their interactions with the atmosphere above and groundwater below. Contemporary vadose zone hydrology is unthinkable without his many contributions, which established links between agriculture, soil science, geology, environmental sciences, and civil engineering. Particularly important were his studies on the basic processes governing water and chemical transport in soil systems, with his work on the nonequilibrium transport of agricultural chemicals remaining a landmark. He pioneered the representation of dual-porosity and dual-permeability models considering mobile and immobile liquid regions in unsaturated porous media, derived novel analytical and numerical solutions, and performed some of the most definitive laboratory and field experiments to test the models. His models profoundly improved predictions of complex field phenomena and motivated an avalanche of studies along similar lines to address water and chemical transport in natural soils and rocks. Because of their attractive mathematical properties and their simplicity, the "van Genuchten equations" are now universally used in numerical simulators of subsurface flow and transport processes."

Finally, I will briefly describe the capabilities and applications of the latest Version 5 of the HYDRUS software package, which implements many ideas and theories developed throughout Rien's career.

Application of Superabsorbent Polymers for Water Content Control and Volumetric Stability in Iron Ore

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Excess water content in iron ore compromises transportation and port operations, increasing both logistical and operational costs. The presence of excess water hinders ore handling, stockpiling, and unloading processes. Water content control is particularly challenging due to factors such as weather conditions and the efficiency of drainage systems in stockyards and vessels. Superabsorbent polymers (SAPs) have emerged as a promising solution, as they retain water within their structure and promote an unsaturated state, which can enhance the mechanical behavior of the material during handling and transport.

Four PVC columns, each 1.3 meters high, were assembled and filled with iron ore treated with three different types of SAPs. A control sample was prepared using only water. The ore was compacted to an initial void ratio of 1 (ρ_d = 2.392 g/cm³) and a gravimetric water content of 9%, corresponding to the material's Transportation Moisture Limit (TML). The columns were assembled in segments. After 72 hours, the columns were disassembled, and water content was measured segment by segment. The control sample (water only) exhibited higher density due to the absence of SAPs, which allowed water to drain rapidly, saturating the segments and facilitating volumetric reduction. Consequently, this control column presented a much lower void ratio compared to the others.

The iron ore without SAPs was unable to maintain the intended high void ratio (e = 1), with the column showing a 30% reduction in height compared to those with SAPs. This occurred due to the near-complete saturation of the material. In contrast, the SAP-treated columns rapidly absorbed water, promoting an unsaturated condition. This prevented volume reduction and ensured structural stability of the packed material. SAPs act by retaining water without reducing the overall water content. Figure 1 below illustrates the profiles of saturation and void ratio across the four columns. As shown in Figure 1a, the degree of saturation decreases slightly with height but remains between 40% and 50%. A key observation is that, even at water content equivalent to the TML, the untreated ore underwent volume reduction, reaching a void ratio indicative of saturation.

The results of this study indicate that the use of superabsorbent polymers (SAPs) in iron ore may be a promising technical alternative for water content control during transportation. The application of SAPs allowed the material to remain in an unsaturated state, even when prepared with water content close to the TML, effectively preventing the volume reduction observed in the control sample. This led to greater structural stability of the ore stack and preservation of the target void ratio (e = 1), in contrast to the volume reduction observed in the untreated sample due to saturation. Water retention by SAPs, without removing it from the system, promoted more uniform moisture distribution along the column, avoiding saturation at the base. Therefore, SAPs may enhance logistical efficiency and reduce costs. However, further investigation is needed into the mechanical behavior of SAP-treated materials when subjected to static and cyclic loading conditions.

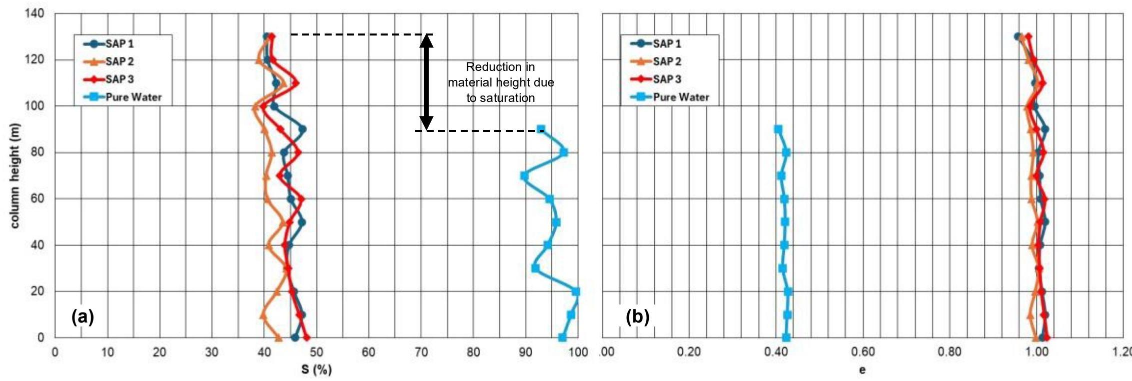

Figure 1. Variation of degree of saturation and void ratio with column height for the ore with and without SAPs.

Open-Access Inventory of Pedotransfer Functions for the Hydraulic Properties of Brazilian Soils

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Pedotransfer functions (PTFs) are essential tools for estimating soil hydraulic properties using more easily available data. Numerous PTFs have been developed to predict field capacity, permanent wilting point, and the soil water retention curve in Brazilian soils. However, these PTFs are scattered across various publications, limiting user access and often prompting the recalibration of new models, sometimes redundantly. This study aimed to create an open-access inventory of Brazilian PTFs for hydraulic properties and provide recommendations for their broad application. We compiled 468 PTFs from publications spanning 1987 to 2023. These were categorized into two groups for statistical analysis: Point-based PTFs (309 models) that estimate water content at field capacity and permanent wilting point, and Parameter-based PTFs (159 models) that predict van Genuchten retention parameters.

Our analysis revealed that multiple linear regression was the dominant approach in developing point-based PTFs, while parameter-based PTFs showed an increasing reliance on machine learning techniques, particularly artificial neural networks. The spatial scale of PTF development varied from state-level to national applications, with state-level models being the most common in both categories. However, very few PTFs were available for the entire country, underscoring the urgent need for nationally applicable models to support soil modeling efforts. In both groups, predictor selection was largely driven by soil physical properties, with particle size distribution being the most frequently used variable. The study identified critical gaps in Brazilian PTF research, including the lack of concise PTF presentation, absence of essential statistical indicators to assess model performance, and insufficient documentation of soil sampling locations used for calibration. These shortcomings highlight the need for improvements in PTF development and reporting.

To enhance the comparability and reproducibility of PTF studies in Brazil, we recommend the standardization of calibration and validation error reporting, as well as greater transparency in model development. Addressing these issues will improve the accessibility, reliability, and applicability of PTFs for diverse soil modeling applications across Brazil.

Rien van Genuchten and Radiological Safety Assessments of Mining Residues in Brazil

Su Jian

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Rien van Genuchten has been closed associated with the activities of radiological safety assessment of mining and milling residues in Brazil in the past two decades. He contributed as a consultant to two projects for radiological safety assessment of uranium mining residues at the INB unit in Caetité, BA, one for a liquid waste pond and the other for solid waste piles. After his retirement from USDA, he participated actively in the radiological safety assessment of the production platform at INB Caetité.

Later, Rien participated in two radiological safety assessment projects of metallurgical slug deposit cells and piles for a Unit of Mineração Taboca in Pirapora de Bom Jesus, SP. He carried out Hydrus simulations for three projects he actively participated in. Rien helped setting up the framework of radiological safety assessments of mining and milling residues, including site characterization, leaching experiments for source term determination, residue and soil sampling, experiments for sorption (Kd) determination, physical characterization of the soil and residue samples, simulation of radionuclides and heavy metal migration in variably-saturated soils, calculation of equivalent doses in critical public, and the final safety assessment.

Fate and Transport of Substances Associated with Aerobic and Anaerobic SOM Decomposition in Paddy Soils using the HP1 Program

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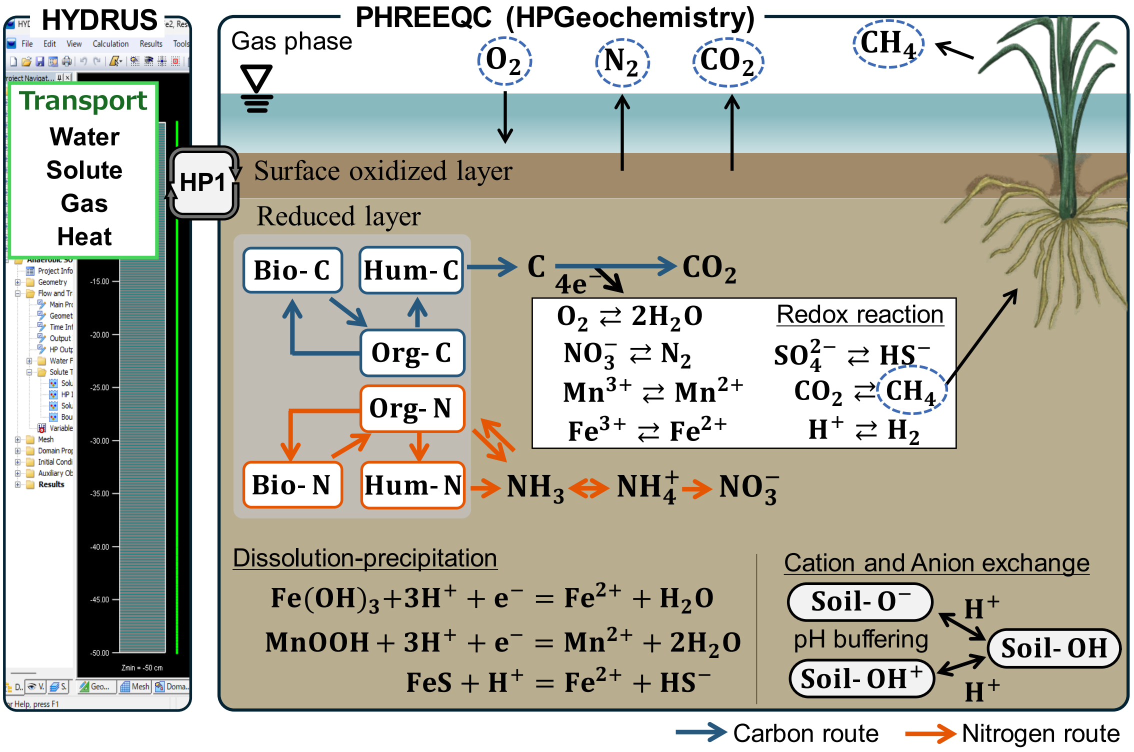
The decomposition of soil organic matter (SOM) and reactive transport of related components are crucial processes for assessing environmental effects. Therefore, a comprehensive understanding of the reaction and transport mechanisms of various components in carbon and nitrogen cycles is necessary. In paddy soils, aerobic and anaerobic layers are formed because of the limited supply of dissolved oxygen from the surface water and its consumption by microbial activity during SOM decomposition. Under anaerobic conditions, microorganisms utilize electron acceptors, such as nitrate, manganese, iron, sulfuric acid, and carbonic acid, for respiration. In addition, the chemical species formed through these redox reactions are absorbed on the soil surface as exchangeable ions. Thus, in paddy soils, each component moves through a complex pathway, undergoing pH- and Eh-dependent transformations, ion exchange, mineral dissolution, and precipitation, as well as other reactions that occur within the interactions between gas, liquid, and solid phases. Given this complexity, it is crucial to develop a process model that integrates knowledge from soil physics, chemistry, and biology, to comprehensively elucidate the reactive transport of various components under mixed aerobic and anaerobic conditions.

The objective of this study was to develop a reactive transport model that describes aerobic and anaerobic SOM decomposition, carbon and nitrogen cycling, cation and anion exchange, mineral dissolution, and precipitation in paddy soils. Model development was carried out using the HP1 program, which couples HYDRUS-1D with PHREEQC. The use of PHREEQC enables the representation of complex biological and chemical reactions in soil, including SOM decomposition, transformations of chemical species, cation and anion exchanges at surface charges, and mineral dissolution reactions, independent of mass-transport calculations. Soil pH buffering is described by surface protonation and deprotonation sites. A numerical experiment was conducted assuming a paddy field with steady saturated water flow and organic matter application. Furthermore, we investigated variations in Eh and pH in the surface oxidized and reduced layers, as well as the temporal changes and concentration distributions of various components. Particular attention was paid to the influence of manganese and iron mineral dissolution and precipitation on hydrogen sulfide and methane formation, emphasizing the interrelationship between the liquid and solid phases.

As a result, we successfully simulated the formation of a surface oxidized layer of approximately 1 cm and a reduced layer, where reduction progressed to methanogenesis. We also evaluated the concentration changes of each component in these layers depending on the Eh, pH, and cation and anion exchange. The dissolution and precipitation of manganese and iron minerals significantly influence both the composition of the liquid-phase solution and the mineral composition of the solid phase. After the iron minerals were depleted, sulfate (SO_4^{2-}) was reduced to hydrogen sulfide (H_2S), producing insoluble ion sulfide (FeS). The precipitation of FeS continued until exchangeable Fe^{2+} was depleted during the sulfate reduction process. Furthermore, carbon dioxide began to reduce to methane at the final stage of sulfate reduction.



The Mobile-Immobile Model for Reactive Transport with Aerobic and Anaerobic SOM Decomposition in Soils Using the HP1 Program

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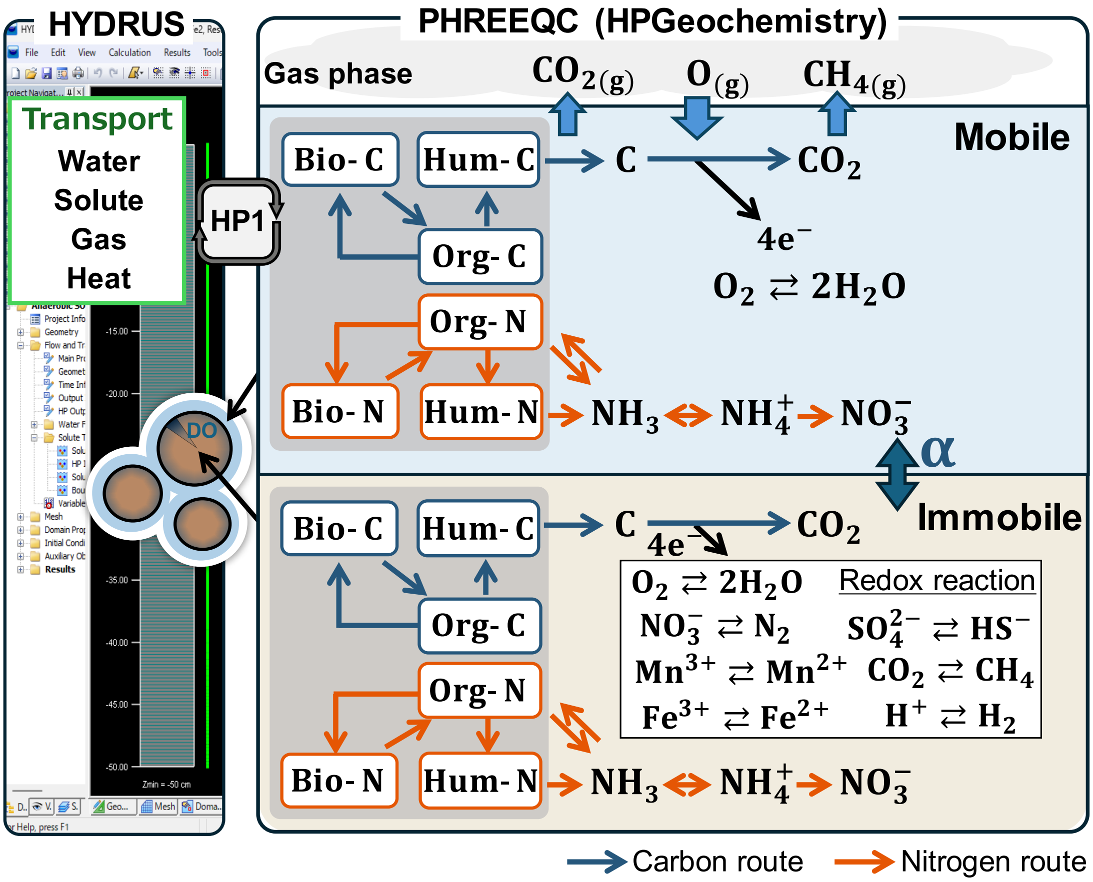
In aggregated soils, relatively rapid water and solute transport occurs in large inter-aggregate pores, whereas water flow within fine intra-aggregate pores is extremely slow, and solute transport is predominantly diffusive. When waterlogged soils drain through inter-aggregate pores, such as puddy soils, oxygen is supplied to the lower layers from the atmosphere by diffusion in the air phase, but the diffusion of dissolved oxygen in the liquid phase into the aggregates is quite slow. When organic matter is decomposed in such a soil complex, anaerobic conditions occur inside the aggregates, where the oxygen supply rate is limited, resulting in microbial distribution and aerobic and anaerobic SOM decomposition depending on the pH and Eh conditions inside and outside the aggregates. In this study, the mobile-immobile model (MIM) was implemented to describe mixed aerobic and anaerobic conditions in aggregated soils. The aerobic/anaerobic SOM decomposition model developed for paddy soils was independently applied to mobile and immobile phases. Soil pH buffering was described by surface protonation and deprotonation sites. All biological and chemical reactions in soil, including SOM decomposition, transformations of chemical species, cation and anion exchange, and mineral dissolution, were described using PHREEQC coupled with HYDRUS-1D using the HP1 program.

A numerical experiment was conducted to demonstrate heterogeneous aerobic and anaerobic SOM decomposition and the related chemical reactions. Organic matter was applied to water-saturated soil with groundwater at a depth of 50 cm, and variations in Eh and pH, reduction reactions, transformation of carbon and nitrogen, cation and anion exchange, and mineral dissolution and precipitation during the drainage process were studied for different immobile fractions, mass exchange rates between mobile and immobile phases, and SOM decomposition rates.

As drainage progresses to groundwater, the water content decreases from the surface layer, and oxygen enters the soil. The Eh in the mobile phase, which is in contact with the air phase, increases, resulting in aerobic decomposition, which consumes oxygen. On the other hand, in the immobile phase, where the oxygen supply is limited, the reduction of the immobile phase proceeds. This reduction in the immobile phase proceeds with a smaller exchange coefficient, resulting in a smaller oxygen supply. Furthermore, the SOM decomposition rate in the immobile phase is a critical factor in determining oxygen consumption and reduction rate in the immobile phase. Methane can be generated in soils that are not fully saturated with water when the Eh level in the immobile phase decreases sufficiently to initiate the reduction of carbon dioxide.


HYDRUS
Transport
Water
Solute
Gas
Heat
HP1
DO
PHREEQC (HPGeochemistry)
Gas phase
$CO_{2(g)}$
$O_{(g)}$
$CH_{4(g)}$
Mobile
Bio- C
Hum- C
Org- C
C
CO_2
$4e^-$
$O_2 \rightleftarrows 2H_2O$
Org- N
Bio- N
Hum- N
NH_3
NH_4^+
NO_3^-
α
Immobile
Bio- C
Hum- C
Org- C
C
CO_2
$4e^-$
Redox reaction
$O_2 \rightleftarrows 2H_2O$
$NO_3^- \rightleftarrows N_2$
$SO_4^{2-} \rightleftarrows HS^-$
$Mn^{3+} \rightleftarrows Mn^{2+}$
$CO_2 \rightleftarrows CH_4$
$Fe^{3+} \rightleftarrows Fe^{2+}$
$H^+ \rightleftarrows H_2$
Org- N
Bio- N
Hum- N
NH_3
NH_4^+
NO_3^-
Carbon route
Nitrogen route

Physical and Hydraulic Properties: A Contrast Between Tropical and Temperate Soils

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Some tropical soils exhibit distinct soil types and characteristics, often shaped by intense weathering processes over millions of years. This leads to a high prevalence of clay-sized particles with a unique mineralogy compared to temperate soils, characterized by a significant percentage of iron (goethite and hematite), aluminium (gibbsite), and silicon (kaolinite) oxides and hydroxides. While expansive clays are present in some tropical soil classes, such as Vertisols, Chernozems, and Luvisols, they are generally less common. The acidic nature and low cation exchange capacity are also typical for large areas of tropical soils.

A defining feature is the abundance of clay-textured soils, particularly in Brazil, where "very clayey" soils are classified as having over 600 g kg-1 clay content. These very clayey soils are less extensive in temperate regions, where silty soils are quite common, a soil textural class less frequent in the tropics, except in soils originating from specific geological formations such as the Içá and Solimões, and in many Gleysols in the Amazonian floodplains. Sandy soils in temperate and tropical regions tend to behave more similarly, especially if the sandy fraction is dominated by quartz particles.

Tropical clayey soils, especially those with well-developed structure, often display unusual hydraulic behaviour. Termed "pseudo-sands," they exhibit high infiltration rates and saturated hydraulic conductivity, sometimes reaching thousands mm day-1. Many have a bimodal pore size distribution, where a large proportion of macropores (including soil cracks) facilitates rapid water infiltration during intense rainfall, reducing runoff and avoiding leaching of the scarce mineral nutrient in the soil matrix. Conversely, the presence of mesopores and micropores leads to reduced unsaturated flow, enabling plant roots to absorb water between rainfall events. The high surface area of these soils, due to the large amount of clay particles, allows the soils to retain substantial volume of water at high potentials (>1500 kPa), resulting in moderate to low water availability for plants.

Accurate description of the soil water retention curve (SWRC), which represents the relationship between volumetric soil water content and soil water pressure head, is crucial for understanding water movement in soils. While the van Genuchten equation is frequently used, it often falls short in soils with a bimodal pore-size distribution, a common characteristic of clayey Ferralsols. To address this, the Durner model, which employs two overlapping van Genuchten functions, is utilized to better represent the complex pore structure. This approach allows for a more accurate SWRC representation, vital for predicting water flow and solute transport, especially near saturation. Furthermore, the complexity of accurately representing hydraulic functions in structured clayey soils like Ferralsols, where standard PTFs may be inadequate, will also be addressed. The discussion will focus tropical soils that occurs in Brazil.

The determination of hydraulic properties is essential in agricultural and environmental research, but these properties are spatially and temporally variable, making reliable soil hydraulic characterization challenging and time-consuming.

Thanks!!! And …

Rien van Genuchten

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The most important message of this presentation is a big thanks. First and foremost a big thanks to the many participants who came to this conference from nearby and faraway, and the many I was fortunate to work with over the years. They all played a role, big and small, in my life and career, the people at Wageningen University, New Mexico State, Princeton, the University of California, the U.S. Salinity Laboratory, Utrecht University and, last but not least, the Federal University of Rio de Janeiro (UFRJ). The many colleagues and coauthors there and elsewhere: from students and beginning scientists to seasoned veterans across geographic, socio-economic, disciplinary and even political boundaries.

I equally thank the many people who helped to organize this conference, especially those within the LASME and LRAP groups of UFRJ such as Elizabeth May Pontedeiro, Su Jian, Paulo Couto Luana Oliveira and many others. I equally appreciated the enormous support by many sponsors listed on the conference website. And my family: My wife Betty May, my children and their partners (Kristy and Mac, Case and Sofie) and my grandchildren (Bo and Alfred).

And…I want to equally stress that more work is needed to safeguard this planet and its inhabitants. We are facing enormous challenges in terms of climate change, extreme weather, lack of fresh water, pollution of our soil, water and air resources with agricultural and engineered contaminants, soil salinization, agricultural production problems, mining and other wastes, urban pollution, biodiversity losses, and seemingly endless socio-economic and political problems worldwide. At the same time, we are fortunate that our understanding of the basic physical and biogeochemical processes of natural and engineered porous media, from the molecular scale to the global scale, has never been better than today. We are witnessing a revolution in terms of increasing our knowledge of these processes, and how to convert this knowledge into practical solutions. That progress is sorely needed in this fast-changing world. My message in this sense is simple: To realize that we are all in this together.

Using Mechanistic Models to Derive Root Water and Solute Uptake Functions and their Parameters

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Flow and transport processes in soil are strongly affected by the uptake of water by plant roots. Where in the soil profile and how much water is extracted is an interplay between meteorological conditions, the distribution of soil water and roots in the soil profile, and the soil and root hydraulic properties. Quantitative assessments of how much and where water is extracted by plant roots is important to assess how much water percolates through the soil and recharges groundwater, how much solutes leach out, and to assess the water status or stress of the vegetation.

Mechanistic models that describe water fluxes and solute transport in the soil-plant system based on physical principles can be used to predict plant water and solute uptake and how it depends on soil and plant properties. The soil-plant system is a hierarchically structured system with structures that exist and influence flow processes at different scales. At each specific scale, the structures can be represented in a spatially explicit way and flow and transport models can be used to relate the spatial arrangement of the elements, which make the structure, and their properties with the flow and transport processes and to derive structure-function relationships. These structure-function relationships can then be used to parameterize models that describe the flow and transport processes at a larger scale using effective properties that are a function of the structure and properties of the smaller scale structural elements.

We show how to use this approach to relate properties of plant cells and tissues, root system hydraulic architecture, and soil hydraulic properties of the rhizosphere, to parameters of functions that describe plant water and solute uptake in the root zone. These functions are used in larger scale models that do not resolve the detailed flow and transport processes within and towards the three-dimensional root architecture. With this approach, properties of the root system and the rhizosphere can be linked to root water and solute uptake functions so that the impact of these properties on water uptake and solute transport can be evaluated.

Commodifying a Carcinogen: Critical Raw Materials from Arsenic-laden Groundwater

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Naturally-occurring arsenic (As) in groundwater has been a global public health concern for decades. Iron-based groundwater treatment is an established approach to safeguard human health from carcinogenic As, but generates concentrated As-rich waste as a by-product that is universally viewed as an environmental and economic burden. However, As is experiencing a renaissance. Multiple regions, including the United States (US) and European Union (EU) have now classified As as a Critical Raw Material (CRM) due to the indispensable use of metallic As(0) in materials needed to transition to clean energy systems, such as batteries and high-speed electronics. Taken together, the requirements to improve As-rich sludge management and create local sources of CRMs reveal a compelling opportunity to redefine carcinogenic As as a commodity.

In this presentation, we will show that As contained in the iron oxide sludge from a variety of As treatment plants can be transformed to pure As(0). The simple two-stage upcycling process consists of extracting As from the solid sludge using alkali solution followed by reductive precipitation of extracted aqueous As via a common sulfur-bearing reductant. In optimal conditions, alkali As extraction using 1 M NaOH released up to >99% As contained in the initial sludge, with the extracted As concentration exceeding 200 mg/L for sludge with the highest As mass fractions (>2.0 g/kg). Selective reduction of the extracted aqueous As yielded pure As(0) precipitates characterized by a highly disordered or amorphous structure, which contrasts with the high crystallinity of commercially available metallic As(0). This difference in structure could favour further processing of upcycled As(0) to form advanced functional materials, such as 2-dimensional arsenene.

The valorization of As-rich groundwater treatment waste has potentially far-reaching implications for groundwater treatment operations and global As(0) supply chains. Through the sale of recovered materials, As waste upcycling might also help improve the challenging economics of water treatment in marginalised regions affected most profoundly by As contamination.

Estimating the Field-Scale Dispersivity of Unsaturated Sediments

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The dispersivity to describe the large-scale transport processes in an aquifer, at field scales of tens or hundreds of meters, may be orders of magnitude larger than those observed in the laboratory (Gelhar, 1993). Consequently, the use of laboratory-scale dispersivities is inappropriate in estimating field-scale solute transport. There is general agreement in hydrology literature that hydraulic conductivity variations induced by field-scale heterogeneities play an important role in field-scale transport processes. However, there does not appear to be a clear consensus about how best to describe such processes quantitatively. Theoretical studies based on the stochastic method suggest that filed-scale dispersivity (aka macrodispersivity) increases with distance from the source, and then increase more slowly farther downgradient, eventually approaching an asymptotic value (Dagan, 1988; Gelhar and Axness, 1983; Gelhar et al., 1979).

Gelhar and Axness (1983) solved the stochastic convection-dispersion equation of solute transport in a statistically heterogeneous porous media. Assuming groundwater flow is two-dimensionally horizontal, they obtained an equation to estimate the maximum or asymptotic value of macrodispersivity for saturated media. Macrodispersivity for unsaturated media has been determined with field experiments (e.g., Butters et al., 1989; Porro et al., 1993; Ward et al., 1998), column experiments (e.g., Maraqa et al., 1997; Nützmann et al., 2002; Padilla et al., 1999), or numerical experiments (e.g., Güven et al., 1984; Rockhold et al., 2016; Rockhold et al., 2015).

In this study, assuming that macrodispersivity reaches a stable asymptotic value when solute travel distance is sufficiently large, an empirical expression for calculating the asymptotic macrodispersivity for unsaturated media was obtained by extending that for the saturated media. Macrodispersivity for unsaturated media is affected by such factors as saturation and the heterogeneity and correlation length of the unsaturated hydraulic conductivity.

References:

Butters, G.L., W.A. Jury and F.F. Ernst. 1989. Field scale transport of bromide in an unsaturated soil: 1. Experimental methodology and results. Water Resour. Res. 25: 1575-1581.

Dagan, G. 1988. Time - dependent macrodispersion for solute transport in anisotropic heterogeneous aquifers. Water Resour. Res. 24: 1491-1500. doi:10.1029/WR024i009p01491.

Gelhar, L.W. 1993. Stochastic Subsurface Hydrology. Prentice Hall, Eaglewood Cliffs, New Jersey.

Gelhar, L.W. and C.L. Axness. 1983. Three-dimensional stochastic analysis of macrodispersion in aquifers. Water Resour. Res. 19: 161-180. doi:10.1029/WR019i001p00161.

Gelhar, L.W., A.L. Gutjahr and R.L. Naff. 1979. Stochastic analysis of macrodispersion in a stratified aquifer. Water Resour. Res. 15: 1387-1397. doi:10.1029/WR015i006p01387.

Güven, O., F.J. Molz and J.G. Melville. 1984. An Analysis of Dispersion in a Stratified Aquifer. Water Resour. Res. 20: 1337-1354.

Maraqa, M.A., R.B. Wallace and T.C. Voice. 1997. Effects of Degree of Water Saturation on Dispersivity and Immobile Water in Sandy Soil Columns. J. Contam. Hydrol. 25: 199-218.

Nützmann, G., S. Maciejewski and K. Joswig. 2002. Estimation of Water Saturation Dependence in Unsaturated Porous Media: Experiments and Modeling Analysis. Adv. Water Resour. 25: 565-576.

Padilla, I.Y., T.-C.J. Yeh and M.H. Conklin. 1999. The Effect of Water Content on Solute Transport in Unsaturated Porous Media. Water Resour. Res. 35: 3303-3313.

Porro, I., P.J. Wierenga and R.G. Hills. 1993. Solute Transport Through Uniform and Layered Soil Columns. Water Resour. Res. 29: 1321-1330.

Rockhold, R.L., Z.F. Zhang and Y. Bott. 2016. Scale-Dependent Solute Dispersion in Variably Saturated Porous Media. Pacific Northwest National Laboratory, PNNL-25146. Richland, Washington. https://www.pnnl.gov/main/publications/external/technical_reports/PNNL-25146.pdf.

Rockhold, R.L., Z.F. Zhang, P.J. Meyer and J.N. Thomle. 2015. Physical, Hydraulic, and Transport Properties of Sediments and Engineered Materials Associated with Hanford Immobilized Low Activity Waste. Pacific Northwest National Laboratory, PNNL-23711. Richland, Washington.

Ward, A.L., R.E. Clayton and J.S. Ritter. 1998. Hanford Low-Activity Tank Waste Performance Assessment Activity: Determination of In Situ Hydraulic Parameters of the Upper Hanford Formation. In Khaleel, Raziuddin FAR-FIELD HYDROLOGY DATA PACKAGE FOR INTEGRATED DISPOSAL FACILITY PERFORMANCE ASSESSMENT. Fluor Government Group, Inc., RPP-20621 Rev. 0. Richland, Washington.

Using Bacillus Subtilis to Guarantee the Safe Utilization of Brackish Water by Improving Soil Physical Properties and Cotton Production

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Brackish water (BW) instead of fresh water (FW) for agricultural irrigation can alleviate water resource shortages in arid regions but also create potential risks such as soil salinization, soil environment deterioration, and crop yield declines. Bacillus subtilis, known for its multifunctional benefits in enhancing soil quality and stimulating crop growth, was selected to be applied in two application rates (0 and 45 kg·ha^{-1}) for cotton production with BW and FW irrigations. The aim was to study the effects of Bacillus subtilis on soil water and salt transport, physical properties, the microbial community and cotton production, and to explore effective ways to promote the safe utilization of BW.

Results indicated that Bacillus subtilis could effectively optimize the water holding characteristics (e.g., soil moisture contents, pore distributions, the water characteristic curve and the water supply capacity) by inhibiting soil salinization and enhancing soil water-stable aggregate (WSA) stability. Consequently, this alleviated water and salt stress of soils, leading to an increased net photosynthetic rate (Pn), more SPAD and biomass, less malondialdehyde (MDA) in cotton leaves, and eventually increased cotton yields and water use efficiencies (WUEs) by 3.33-5.04% and 1.81-7.52%, respectively. Additionally, under Bacillus subtilis application, the structure and functioning of the soil bacterial community was improved. The main soil biomarkers of the FW and BW irrigations were Proteobacteria and Gemmatimonadota, respectively.

Further analysis found that the augmentation of the bacterial community diversity and overall abundance of predominant bacterial phyla, coupled with the function enhancement of amino acid and carbohydrate biosynthesis within the bacterial community, acted as significant driving forces in ameliorating soil physical properties and cotton production. The prediction models of the soil water characteristic curve based on soil salinity and WSA stability, as well as an analysis of the response and correlation degree of research indexes, showed that the positive driving mechanism of Bacillus subtilis enhanced the buffering capacity and resistance of soil physical properties and cotton growth to the adverse effects of BW irrigation, which was conducive to the formation of long-acting protection.

In summary, our results revealed the significant effects of Bacillus subtilis in improving soil physical properties and cotton production, and verified that its application can serve as an effective approach to ensure safe utilization of BW and relieve water resource crisis in arid regions.

Transient Flow Effects on Solute Transport in an Unsaturated Soil

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The influence of flow regime and soil saturation on solute transport processes is significant, yet the associated effects have not been adequately studied. To address this gap, we conducted three sets of solute transport experiments in a sandy soil, complemented by numerical modeling, under both steady-state and dynamic drainage conditions. Results from the steady-state experiments revealed a non-monotonic relationship between the dispersivity and saturation. Both classical advection-dispersion and dual-porosity (mobile-immobile) type transport equations were used to simulate the measurements. The fitted dispersivity-saturation function was subsequently employed in simulations of the transient flow experiments. We will analyze the data also in terms of a dynamic capillary model.