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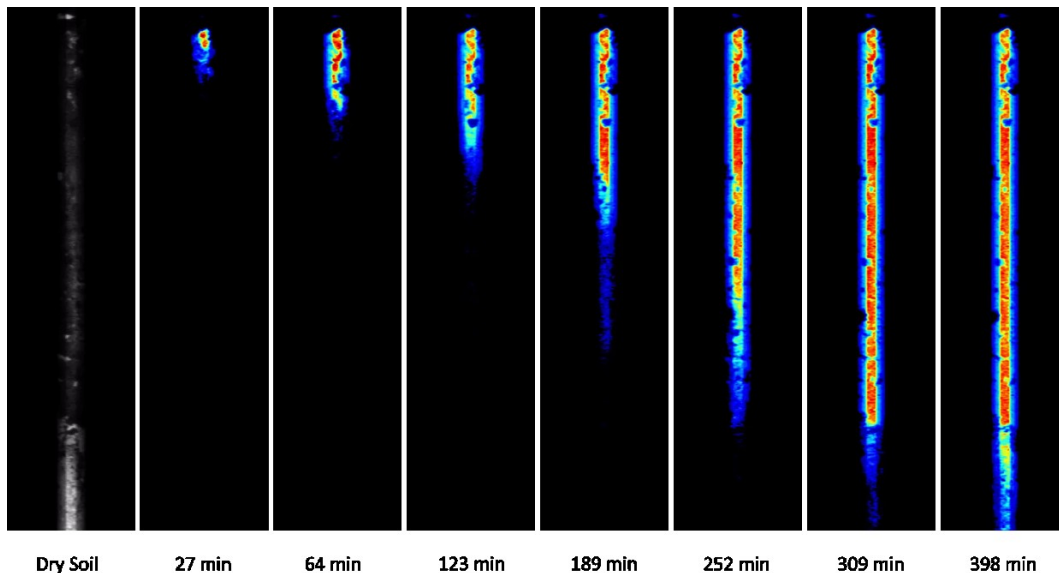
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Non-destructive imaging of a liquid moving through porous media using a Computer Tomography Scanner

A new capability for SRNL was developed to study fluid mechanics by passing a tracer through porous media within an X-ray Computed Tomography Scanner. This new capability will enhance SRNL's ability to describe the movement of liquids as they pass through glass, cement, fractured rock or soil.



Awards and Recognition

"SRNL Team Successfully Completes CT Scanner Project with Clemson University." Jamaica Jimerson. **SRNL News**. Savannah River National Laboratory. 4 Aug 2020, Web, Accessed 6 Aug 2020. srnl.srs.gov/srnlweb/blog/2020/08/04/srnl-team-successfully-completes-ct-scanner-project-with-clemson-university/

Intellectual Property Review

None

SRNL Legal Signature

Signature

Date

Non-destructive imaging of a liquid moving through porous media using a Computed Tomography Scanner

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Project Type: Seedling

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The most common approach used by modelers to describe movement of liquids through a porous solid, such as cement, sediment, or glass, is to assume a uniform flow rate, such as a Darcy Flux or a diffusion constant. However, this convenient simplification is problematic because in many cases it ignores the presence of fractures and macropores, which commonly dominate water flow and contaminant transport. For this reason, it is common that such modeling results do not reflect the multi-modal flow detected in laboratory and field studies. The objective of this seedling study was to develop a new capability for SRNL to track liquid moving through micro-(matrix-) and macro-flow using an X-ray Computed

Topography (CT) Scanner. 4-dimensional animated renditions were created that permitted quantifying traditional matrix flow and macropore flow. These animations were modelled using a public domain software, HYDRUS 1-D, describing one dimension, dual-porosity and dual-permeability processes. This new capability provides a proof of concept for reducing model uncertainty applicable to waste disposal risk calculations, environmental remediation, and waste form development when describing the movement of liquids as they pass through glass, cement, fractured rock, or soil.

FY2020 Objectives

- Develop a new capability for SRNL to study fluid mechanics by passing a non-radiological tracer through porous media within a CT scanner.
- Conduct an experiment within the CT scanner of water moving through a dry core of SRS vadose zone sediment containing a wide range of pores, including micropores (μm diameter) and macropores (mm diameter).
- Use existing software to create animations from the >500 X-ray scans collected during the experiment.
- Model the results using a model that accounts for varying size pores.

Introduction

The most common approach used by modelers to describe movement of liquids through a porous solid, such as cement, sediment, or glass, is to assume a uniform flow rate, such as a Darcy Flux or a diffusion constant.¹ However, this convenient simplification is problematic because it ignores the presence of fractures and macropores, which, when present, can dominate water flow and contaminant transport. For this reason, it is more common than not that such modeling results do not reflect the multi-modal flow detected in actual field studies. There have been several approaches for the *in-situ* detection of liquid movement through porous media, including Nuclear Magnetic Resonance², CT scanning³, and synchrotron-based micro-CT scanning⁴. The objective of this project was to develop a new capability for SRNL to study fluid mechanics by passing a non-radiological tracer, sodium iodide, through porous media within a CT scanner. An important attribute of this particular scanner owned by the Imaging

Robotics and Rad Systems group is its large size (60 x 60 cm), which is sufficiently large to capture large scale flow features, including fracture flow. Presently this CT scanner is set up to create 3-D renditions of solids. We established a capability that will permit setting up flow experiments within the scanner booth to capture 4-D renditions of the liquid as it passes through the porous media.

Approach

A SRS vadose sediment was packed in a plexiglass core (25-cm L x 3-cm D). It was slowly saturated with water, then placed in a 60 °C oven to dry, creating micropores, macropores, and cracks. As such this is a disturbed sediment core in which the sediment structure was artificially created to insure a wide range of pore sizes for ease of detection. A peristaltic pump was used to introduce a 0.32 molar sodium iodide solution into the top of the sediment core drip at a rate of 0.149 mL/min (Fig. 1). The iodide in this influent solution acted as a tracer that was readily detectable by X-rays. Prior to initiating the experiment, the CT scanner (781-A 420 kV X-ray Booth) was calibrated, which involved taking X-ray images of a moistened sediment core to measure the source to detector distance, the object to detector distance, the detector centerline row, the center of rotation, and effective pixel size based. During the experiment,

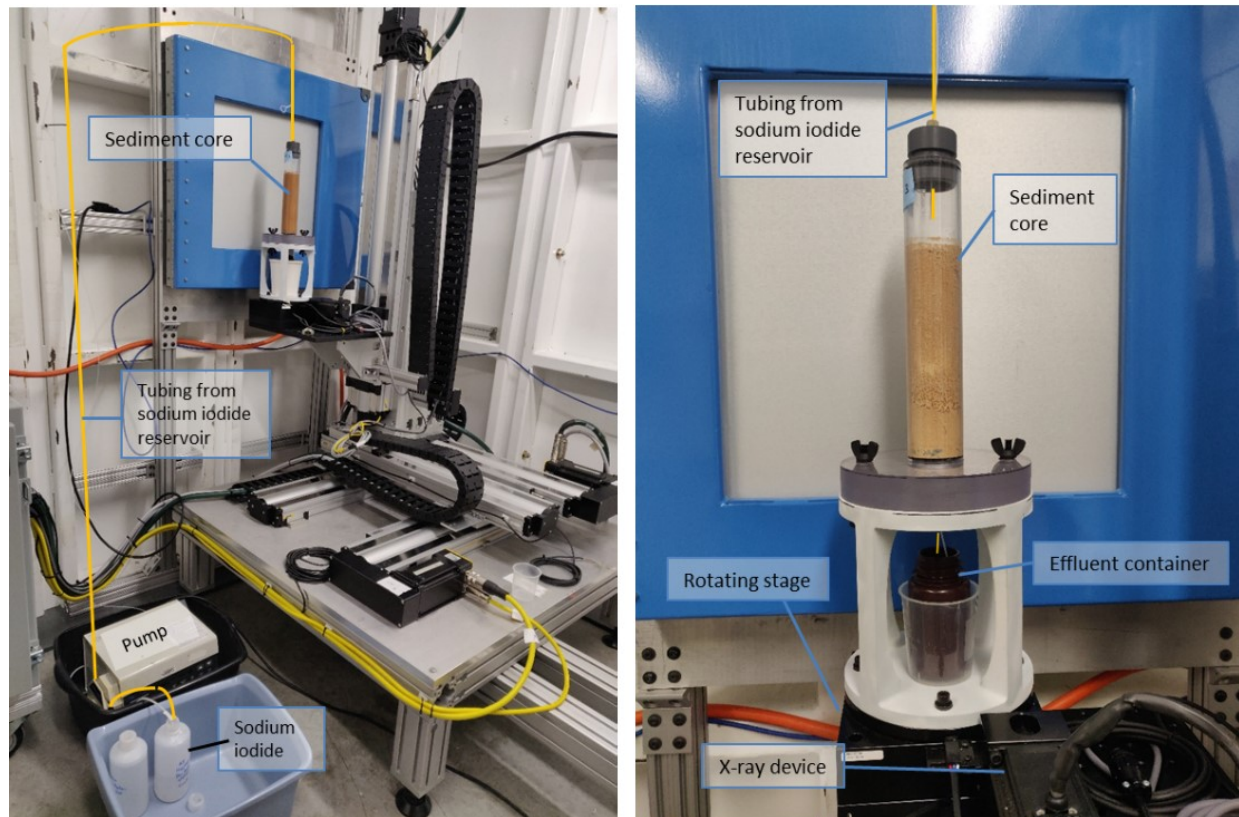


Figure 1. (Left) Set up within the CT scanner booth during the flow experiment of water (with sodium iodide added as X-ray tracer) slowly introduced into a dry sediment. **(Right)** Close up of the sediment core assembly on the rotating stage.

CT scan acquisitions were set for an exposure time of 0.45 sec, tube voltage of 400 kV and tube current of 8 mA while the sediment core rotated 360 degrees. The flow experiment continued until the entire core was saturated with water, resulting in a flow rate of 58.36 mL over 393 minutes or 0.149 mL/min.

After the experiment, existing CT scanning software was used to compile various sets of scans into 4-D rendering of the water (more specifically the iodide) moving through the sediment core. The voxel size of the CT reconstructions was 0.1mm x 0.1 mm x 0.1 mm. The data generated from these experiments were later modelled using a public domain software, HYDRUS-1D⁵, to describe one dimension, dual-porosity and dual-permeability processes.

Results/Discussion

After completing the experiment, the data was compiled in a manner that permitted examining the core from any perspective, e.g., from top to bottom or longitudinally. Furthermore, animations were created that enhanced visualization of the data and accessing key time steps. Figure 2 provides an example of the resulting data, showing the dry sediment core at the start of the experiment (Figure 2, Left) and then a series of time steps during the experiment. After 7 minutes it is possible to see the moisture entering the core, as depicted by the light blue. By 27 minutes, close examination indicates the presence of some ponding on the soil surface, which was not intended to occur. By 45 minutes, the front progressed down the column in the shape of an upside down 'U,' suggesting that the plexiglass surface of the core was creating an experimental artifact, which is always carefully monitored during these types of experiments. It is not until 142 minutes, that the macropore on the left side of the core starts to fill up. It is important to note that the front of the matrix (micropores) advanced ahead of that of the macropores. This is consistent with well-established theory for these experimental conditions. The implications of this observation are that the presence of macropores in unsaturated sediment cores do not fill first, thereby by-passing the slower matrix flow. Once the macropores fill, they transmit greater fluxes of water than the matrix. At 252 minutes, the existence of the macropore at about 100 mm depth appears to be creating a type of capillary break, not permitting moisture to move left and below the macropore. Again, this is consistent with theory that predicts that finer pores fill first, and not until the water potential is sufficiently high, will it be able to enter the larger pore. By 309 minutes, the moisture front initially reaches the bottom of the column. By the end of the experiment, 398 minutes, the moisture front across the entire core cross-section had reached the bottom of the core. It is also note-worthy, that a similar height of ponding occurred throughout the study.

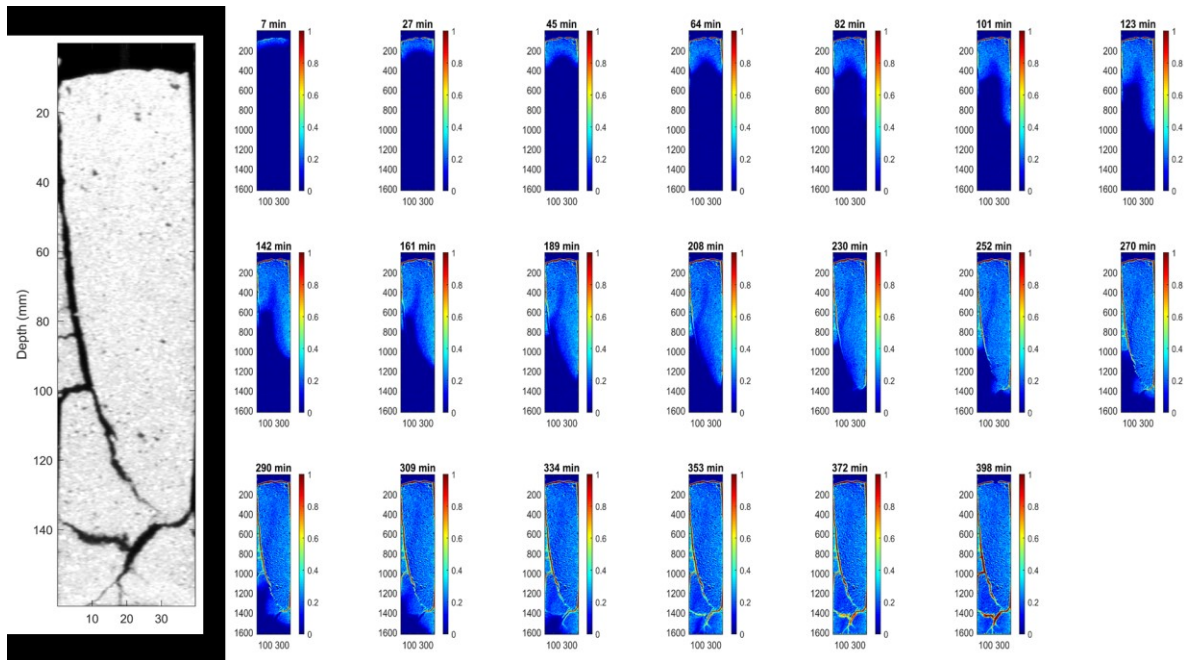


Figure 2 (Left) Dried soil core used at start of experiment with naturally occurring macropores. **(Right)** Progressive time-steps of fractional water content as water is introduced at the top of the column during 398 min experiment.

The averaged water contents of these profiles were estimated for the macropore (Figure 3A), the matrix/micropores (Figure 3b) and for the whole column (Figure 3C). Using HYDRUS-1D, we reproduced

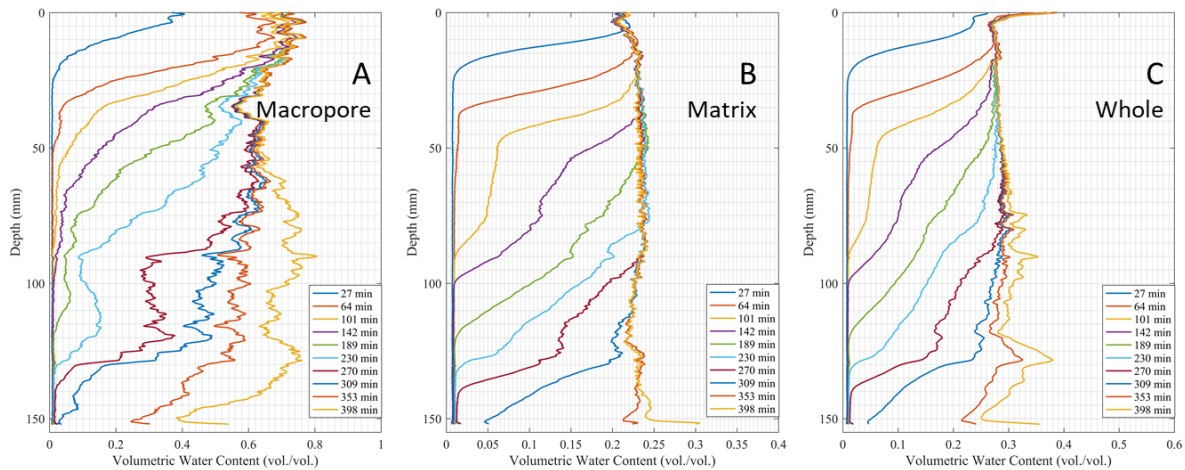


Figure 3. Averaged water contents of these profiles are provided for the macropore (A), the matrix/micropores (B), and for the whole sediment column (C).

the water content profiles in the macropore and matrix domains (data not shown). However, we were unable to adequately reproduce the whole sediment column. This important finding brings into questions the accuracy of averaging flow in systems known to include both macropore and matrix flow. The problem stems from the inability to include geometry-explicit processes, pore-scale processes, in HYDRUS-1D. It is not possible to produce different macropore flow features, such as film flow or capillary bridging, because

they are geometry-implicit processes. Also, HYDRUS-1D assumes capillary dominated Richards equation for the flow physics in macropore domain, which is not conceptually accurate. Thus, currently we are attempting to simulate the flow in macropores in a geometry-explicit 3D software, COMSOL Multiphysics, Ver. 5,⁶ that will enable us to incorporate gravity-viscosity dominated Navier-Stokes equation to demonstrate different macropore flow mechanisms.¹

FY2020 Accomplishments

- **New Capability:** A new capability for SRNL was developed to study fluid mechanics by passing a nonradiological tracer through porous media within a X-ray CT Scanner.
- **Business Development:** Can now write proposals (and manuscript) that include this new capability. This is especially useful in research related to environmental remediation, waste form development, and waste disposal risk calculations for describing the movement of liquids as they pass through glass, cement, fractured rock (e.g., Yucca Mountain) or soil.

Future Directions

- Continue modeling efforts using the geometry-explicit 3D COMSOL Multiphysics software.
- Write manuscript describing these findings.
- Using the information reported here as seed data, write a proposal to vary a series of sediment physics properties in a systematic manner to monitor changes in hydrological properties.

FY 2020 Peer-reviewed/Non-peer reviewed Publications

None

Presentations

None

References

1. Hillel, D., *Introduction to environmental soil physics*. Elsevier: 2003.
2. Gummerson, R.; Hall, C.; Hoff, W.; Hawkes, R.; Holland, G.; Moore, W., Unsaturated water flow within porous materials observed by NMR imaging. *Nature* **1979**, *281* (5726), 56-57.
3. Anderson, S. H.; Wang, H.; Peyton, R. L.; Gantzer, C. J., Estimation of porosity and hydraulic conductivity from X-ray CT-measured solute breakthrough. *Geological Society, London, Special Publications* **2003**, *215* (1), 135-149.
4. Nakashima, Y.; Nakano, T.; Nakamura, K.; Uesugi, K.; Tsuchiyama, A.; Ikeda, S., Three-dimensional diffusion of non-sorbing species in porous sandstone: computer simulation based on X-ray microtomography using synchrotron radiation. *Journal of Contaminant Hydrology* **2004**, *74* (1-4), 253-264.
5. Simunek, J.; van Genuchten, M. T. Hydrus-1D, Version 4.17, Software Package for Simulating the Movement of Water, Heat, and Multiple Solutes in Variably Saturated Media. <https://www.pc-progress.com/en/Default.aspx?hydrus-1d> (accessed 5 April 2020).
6. COMSOL Multiphysics, Ver 5.0. <https://www.comsol.com/> (accessed 2 Feb. 2020).

Acronyms

CT – Computed Tomography

SRNL – Savannah River National Laboratory

SRS – Savannah River Site

Intellectual Property

None

Total Number of Post-Doctoral Researchers

0

Total Number of Student Researchers

Abdullah Al Mamun, Ph.D. candidate, Clemson University. He conducted research on and off site.

External Collaborators (Universities, etc.)

Dr. Brian A. Powell, Professor, Clemson University; joint appointment with SRNL