Modeling Platform as an Innovation Playground for Advances in Characterization and Remediation of Contaminated Sites

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November 22, 2022

Abstract

The importance of water supplies cannot be overstated, yet contaminant monitoring and management have not seen strong innovation in information and computing technologies (ICT) such as internet-of-things (IoT), big data, arti>cial intelligence (AI) and numerical modelling. As a water risk, regulated contaminated sites are unique in that they have owners with obligation and cost responsibility, creating conditions that traditionally drive technology innovation. As contaminated site management moves toward risk management rather than resource intensive remediation, ICT technologies will be increasingly applied. A high subsurface complexity, varying land and local weather conditions, however, strongly impact contaminant fate and transport to make each site unique. Site uniqueness means that development of innovation is slow to occur due to lack of scale economic bene>ts. For this reason, a key technology suited for early adoption is reactive transport modeling (RTM). Such modelling can be coupled with diverse compute technologies (e.g. Steefel et al. 2021) supporting long term site modeling for climate change. In this presentation, we explore a modeling platform for data-driven RTM. The work draws from extensive research efforts on quantitative, process-based approaches and measurement methods that span multiple disciplines (e.g. Sookhak Lari et al. 2019). Challenges and limitations of such an RTM platform are discussed, considering: 1) complexity levels, modularity, and computational requirements; 2) existing models; 3) adaptiveness to sitespeci> c data and predictive analytics; 4) upscaling of pore-scale processes; 5) platform Rexibility to account for natural depletion processes (e.g. variably saturated media; microbial dynamics; heat transport; contaminant distribution); 6) platform and model operations to handle in situ remedial activities (e.g. point injections; surface cover / solarization; phytoremediation); 7) use of intelligent systems to provide select model parameters from existing big data sets. An RTM platform is an innovation that has many bene>ts, providing a ‘digital twin’ for contaminated site decision making and an ‘innovation playground’ for novel characterization and remediation techniques.

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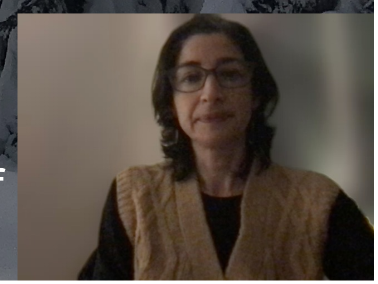
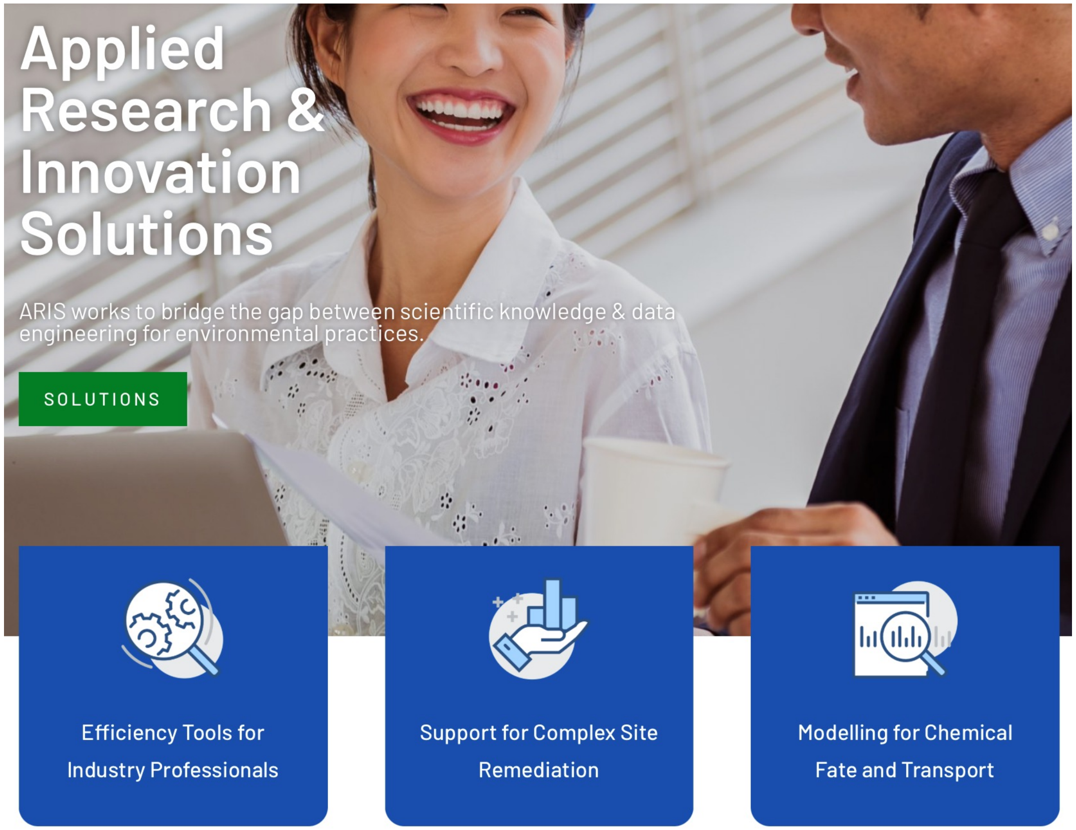
Parisa Jourabchi and Caitlin Brandon

ARIS Environmental Ltd.
Vancouver, Canada

AGU Fall Meeting 2021
Emerging Methods for Subsurface Monitoring and Characterization of Contaminated Sites – Session H44C 16 December 2021



ARIS



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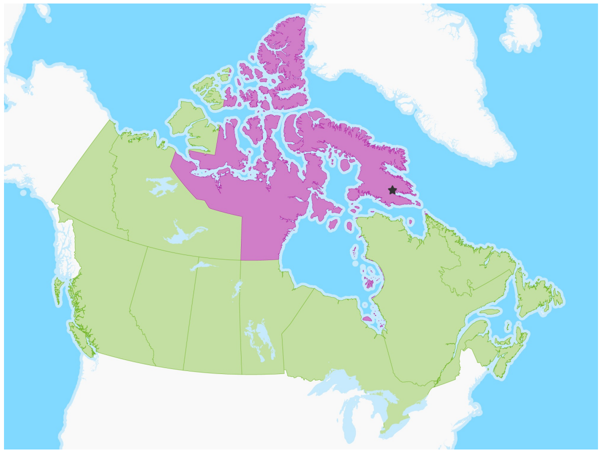
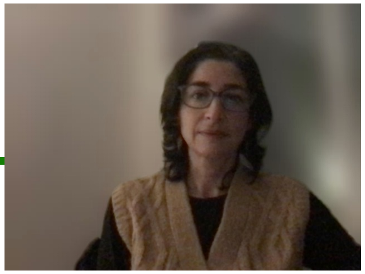
ARIS works to bridge the gap between scientific knowledge & data engineering for environmental practices.

Iqaluit 2021: 8,000 people no drinking water for 2 months (so far)

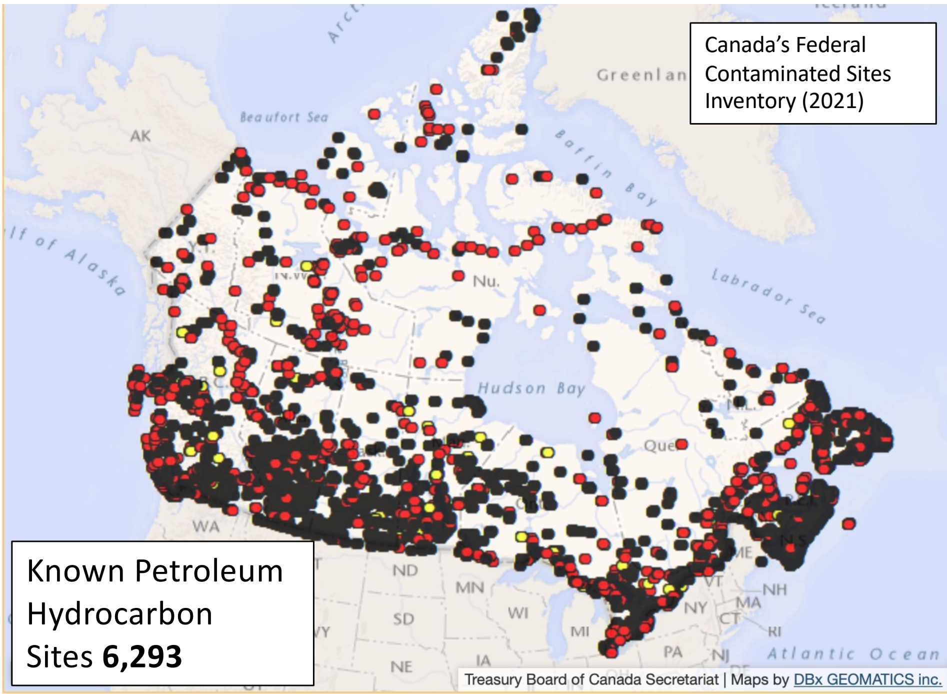


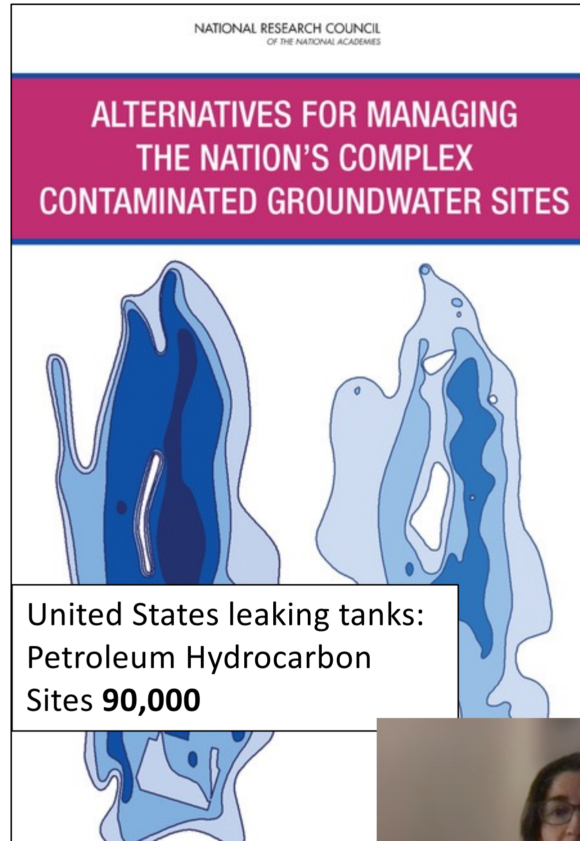
"City of Iqaluit says historical fuel spill likely source of drinking water contamination"

~CBC News October 26 2021

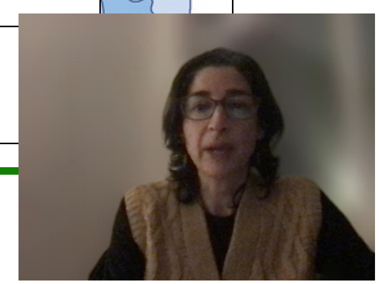


Petroleum Hydrocarbon Sites, North America



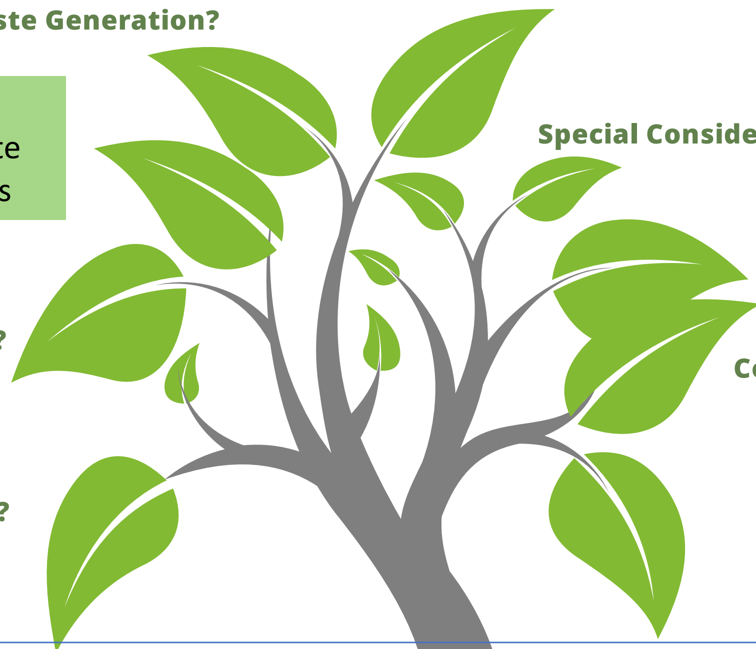


Learn More*: Understanding complex LNAPL sites: Illustrated handbook of LNAPL transport and fate in the subsurface* Tomlinson, D, Rivett, M.O., Wealthall, G.P., and Sweeney, R. (2017) Journal of Environmental Management

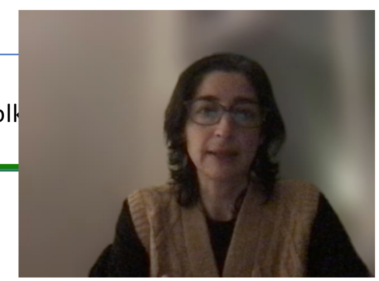


Data Gathering in Remedial Technology Selection

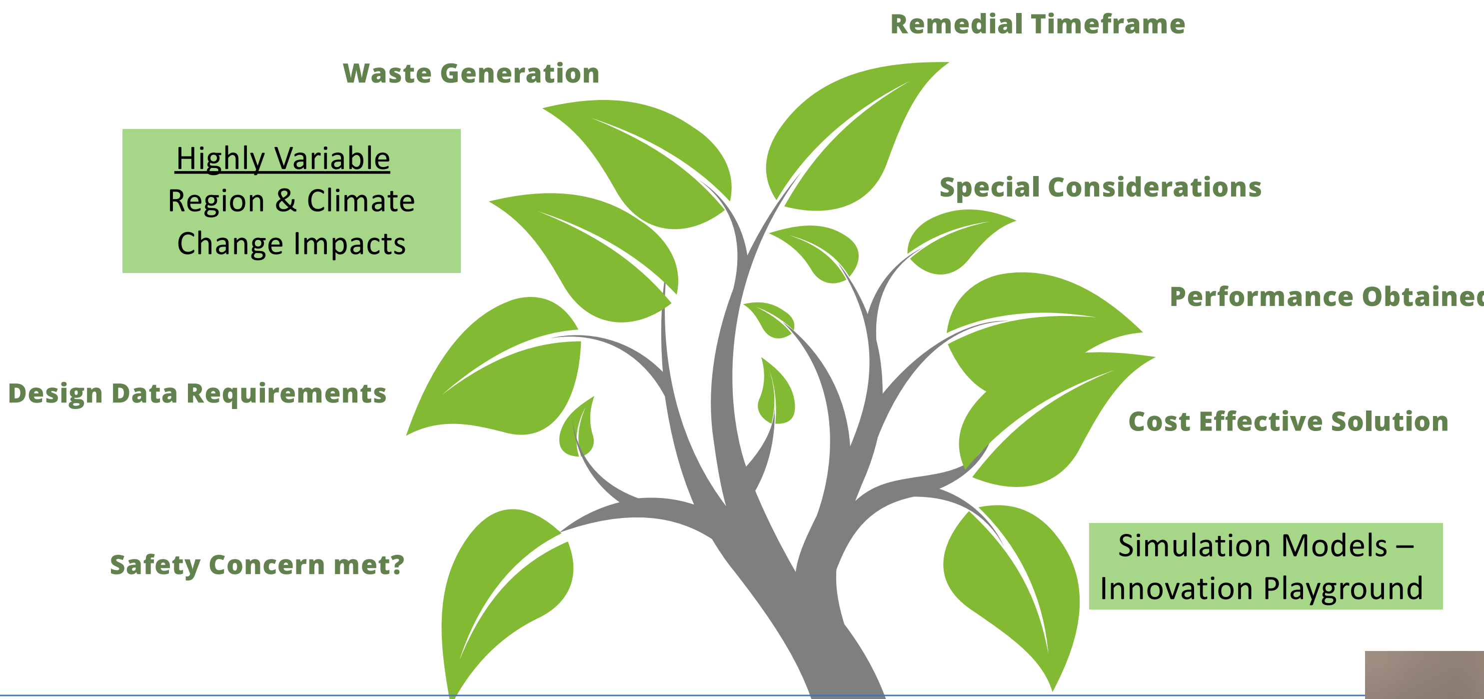
<u>Highly Variable</u>
Region & Climate
Change Impacts



Adapted from Table B of Golder (2021): **Remediation Toolkits**. Toolkit 3: Evaluation of Remediation Technologies for Petroleum Hydrocarbon Sites (April 5, 2021); Toolkit 4: Methods for Sustainable Remediation (April 6, 2021); Principal authors: Ian Hers (Toolk and 4), Parisa Jourabchi (Toolkits 3 and 4), Francois Beaudoin (Toolkit 4) https://csapsociety.bc.ca/csap-toolkits/



Data Gathering in Remedial Technology Selection



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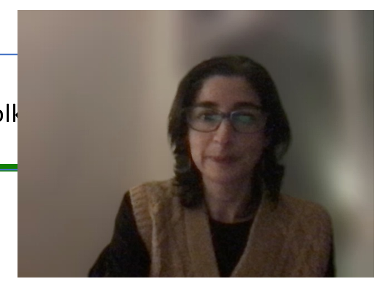


State of Science

High Performance Computing

- MIN3P-HPC: A High-Performance Unstructured Grid Code for Subsurface Flow and Reactive Transport Simulation ~ Su et al. (2020)

Digital Twin

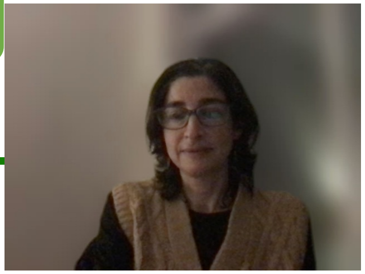
- Towards a digital twin for characterising natural source zone depletion: A feasibility study based on the Bemidji site ~ Lari et al. (2021)

Machine Learning

- On Demand Machine Learning for Multi-Fidelity Biogeochemistry in River Basins Impacted by Climate Extremes ~ Steefel et al. (2021)

Real-time Performance Monitoring

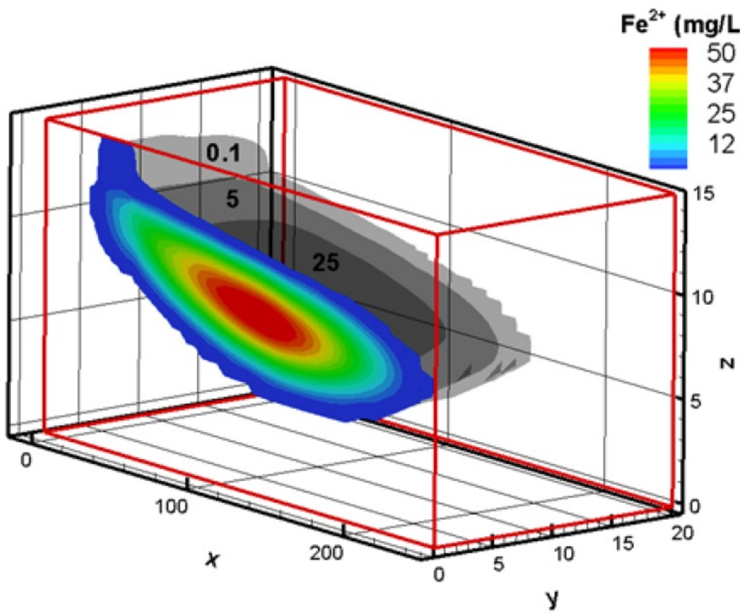
- Real-Time Remediation Performance Monitoring with ORP Sensors ~ Blotevogel et al (2021)

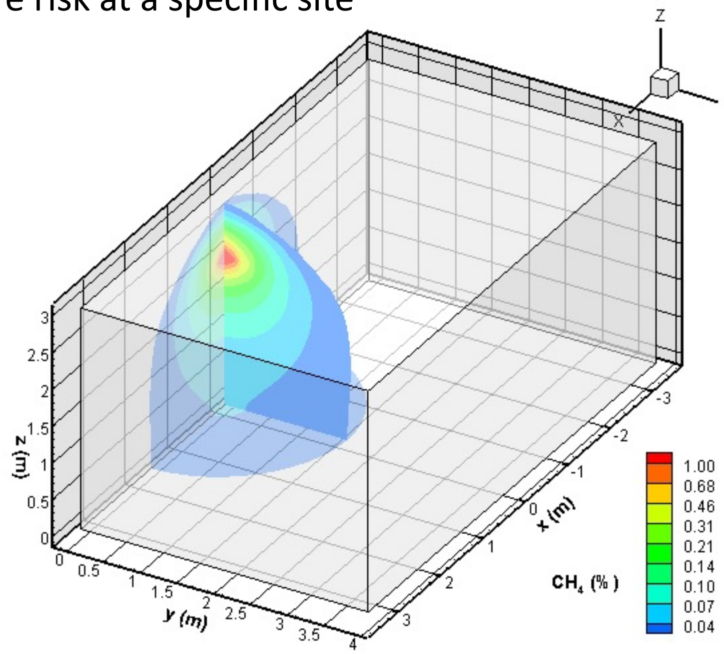


Towards Practice

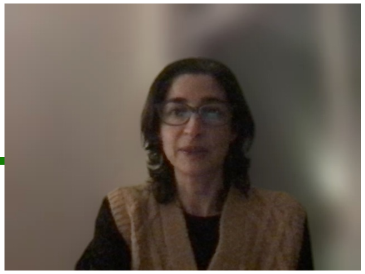
Reactive Transport Models (RTMs)

For understanding of current and future risk at a specific site



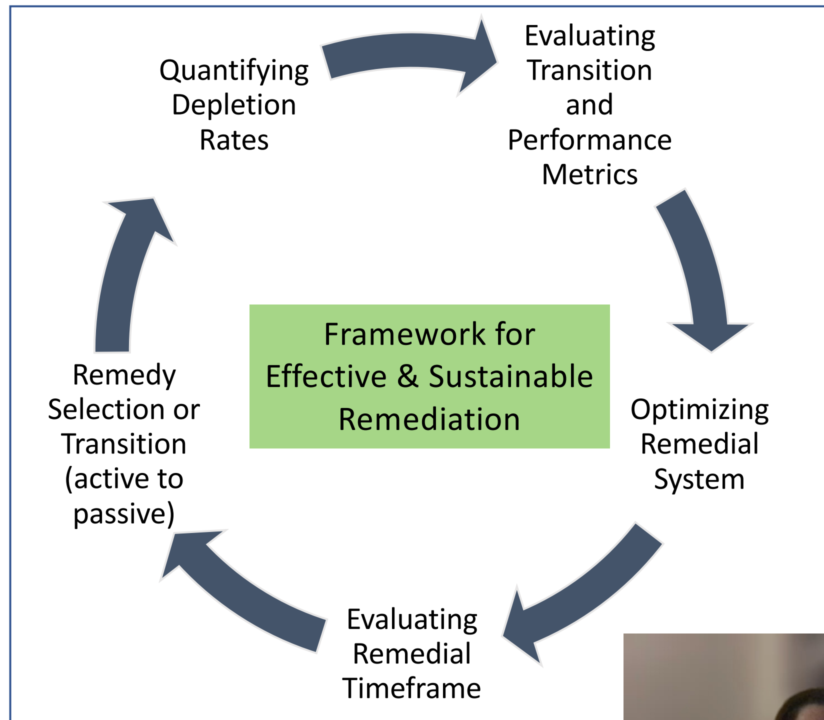


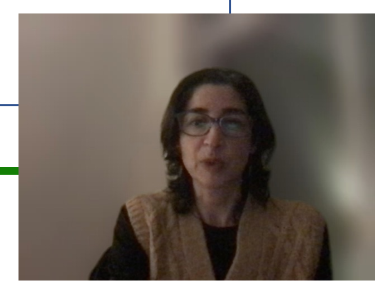
MIN3P Simulations: Jourabchi and Hers (2013) and Jourabchi et al. (2016)



An Innovation Playground for…

- ❖ Creating sustainable remediation program
  - ❖ minimize usage of limited resources
  - ❖ minimize impact to the environment (e.g. GHG emissions and energy use)
  - ❖ maximize effectiveness in reducing risk and protecting groundwater resources
- ❖ Digital twin for simulation of characterization & remediation technologies
- ❖ Increased resiliency by incorporating climate change projections





Available RTM Tools

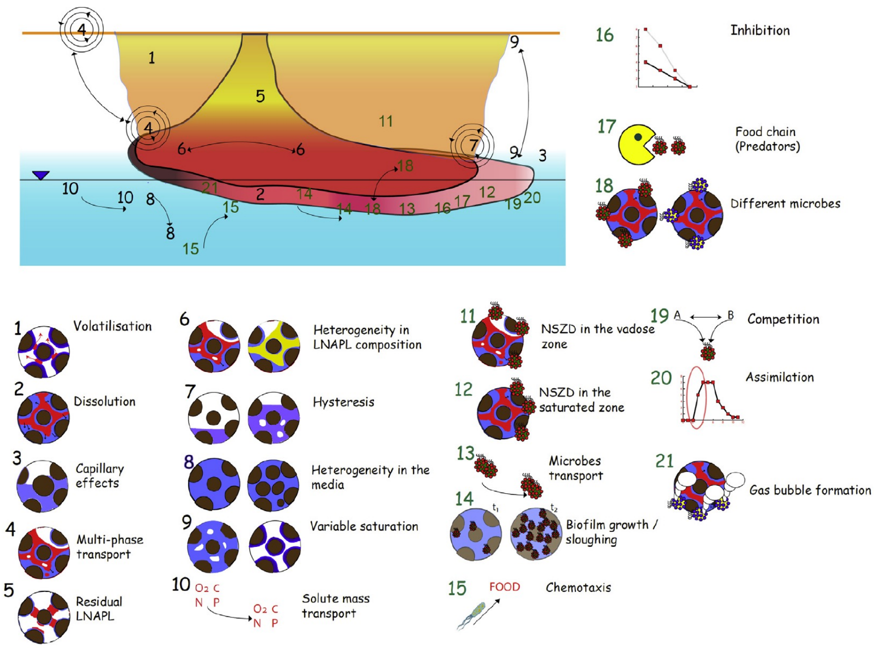


Fig. 1. Some of the major processes and parameters in NSZD.

More than 1 in 3 of the processes identified relate to microbial process for biodegradation of contaminant hydrocarbons

Also required:

Heat generation & conduction (Non-isothermal system)

Flexible platform for simulating in-situ remediation activities

Water Research 157 (2019) 630–646

Contents lists available at ScienceDirect

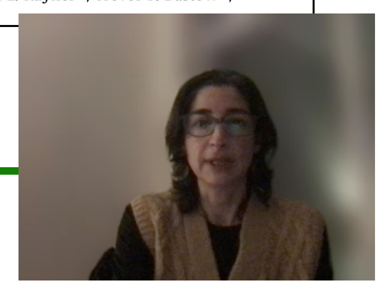
Water Research

journal homepage: www.elsevier.com/locate/watres

Review

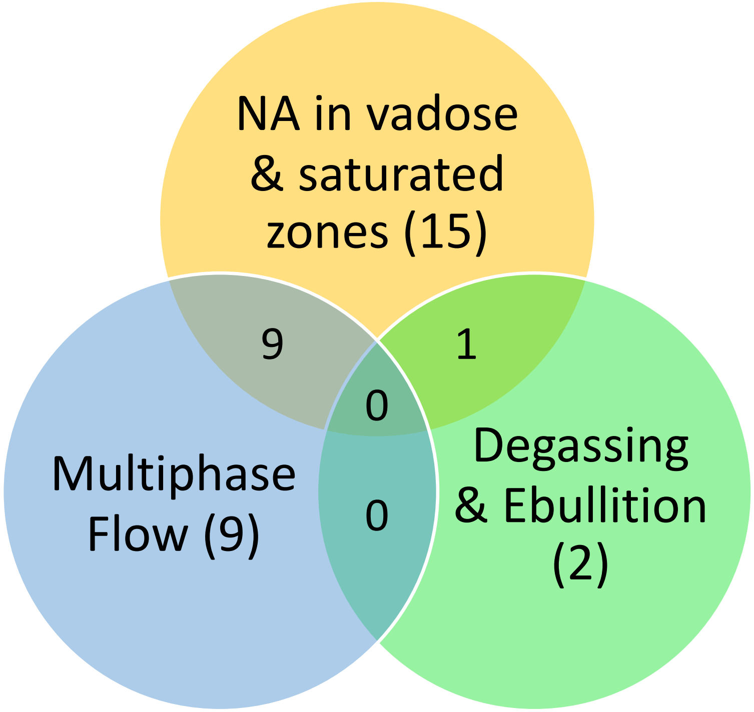
Natural source zone depletion of LNAPL: A critical review supporting modelling approaches

Kaveh Sookhak Lari [a, b, *], Greg B. Davis [a, c], John L. Rayner [a], Trevor P. Bastow [a], Geoffrey J. Puzon [a]



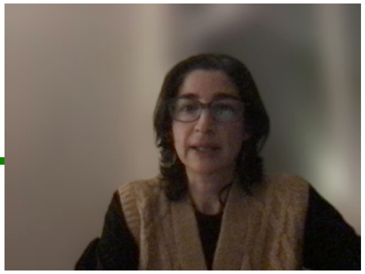
The Challenge

1. Identifying a single model that incorporates all of the relevant processes in saturated and unsaturated zones.
2. Interconnected processes through
   - Infiltration (downward towards water table)
   - Soil gas transport (upwards towards ground surface)
3. LNAPL source zones typically straddle the water table



More collaborative effort needed towards an Innovation Playground

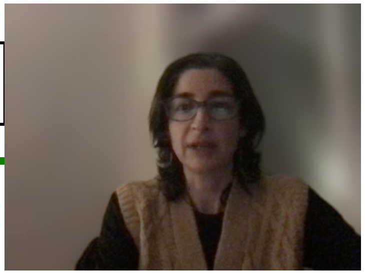
Based on review of 35 RTMs by Lari et al. (2019)



Site Management Process

1. Risk Identification & Evaluation
2. Baseline Assessment
3. Remedy Selection & Implementation
4. Performance Evaluation & Transition Assessment

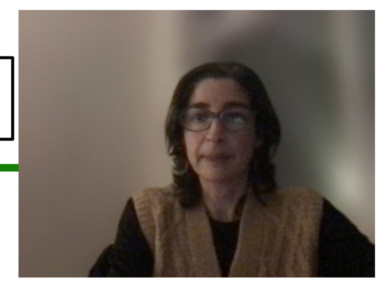
Shell Compendium of Tools and Methods to Support the Optimization and Termination of Active Remediation Systems



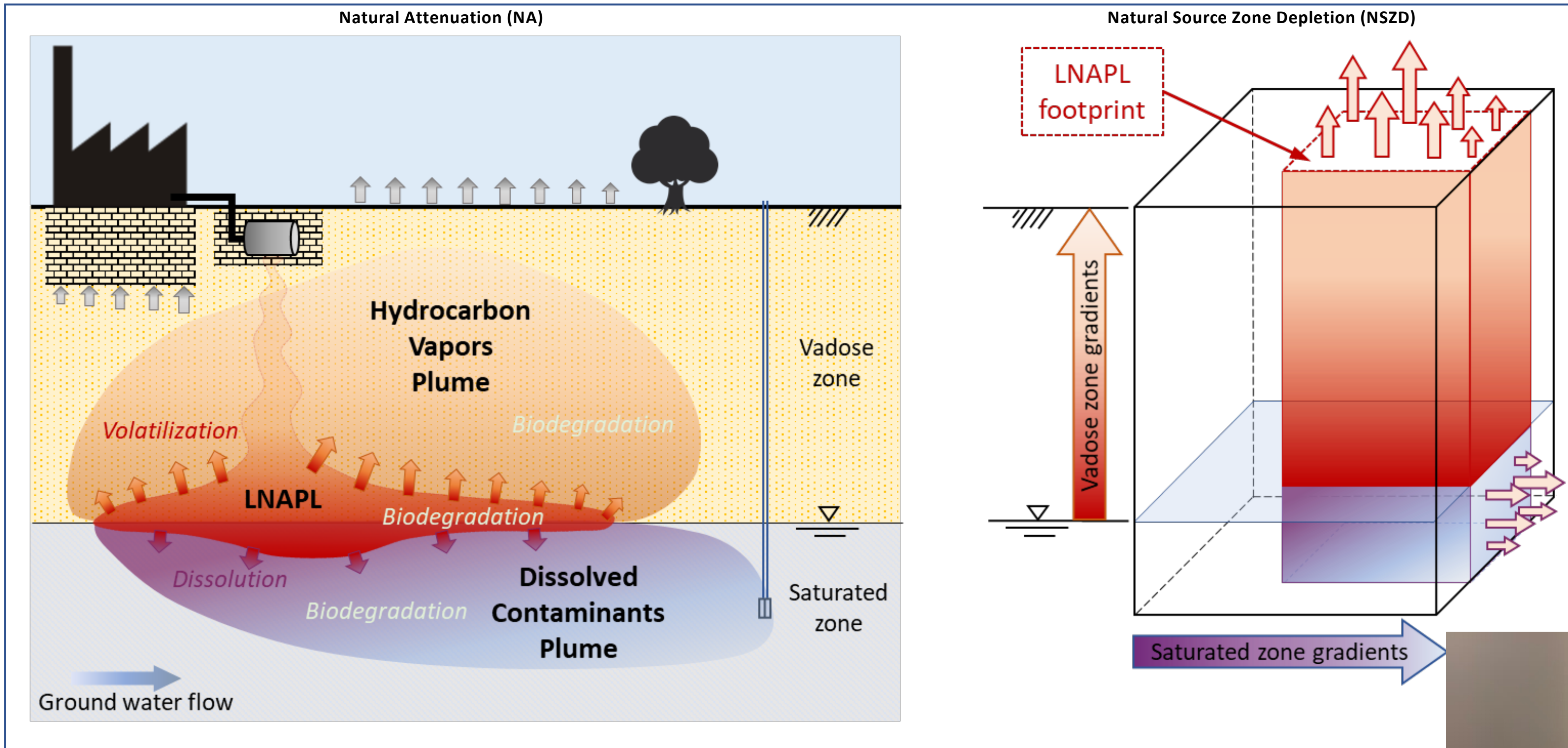
Baseline Assessment

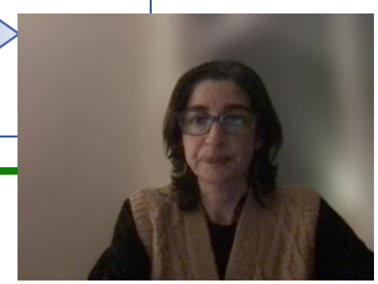
1. Risk Identification & Evaluation
2. Baseline Assessment (Quantifying Natural Attenuation)
3. Remedy Selection & Implementation
4. Performance Evaluation & Transition Assessment

Shell Compendium of Tools and Methods to Support the Optimization and Termination of Active Remediation Systems

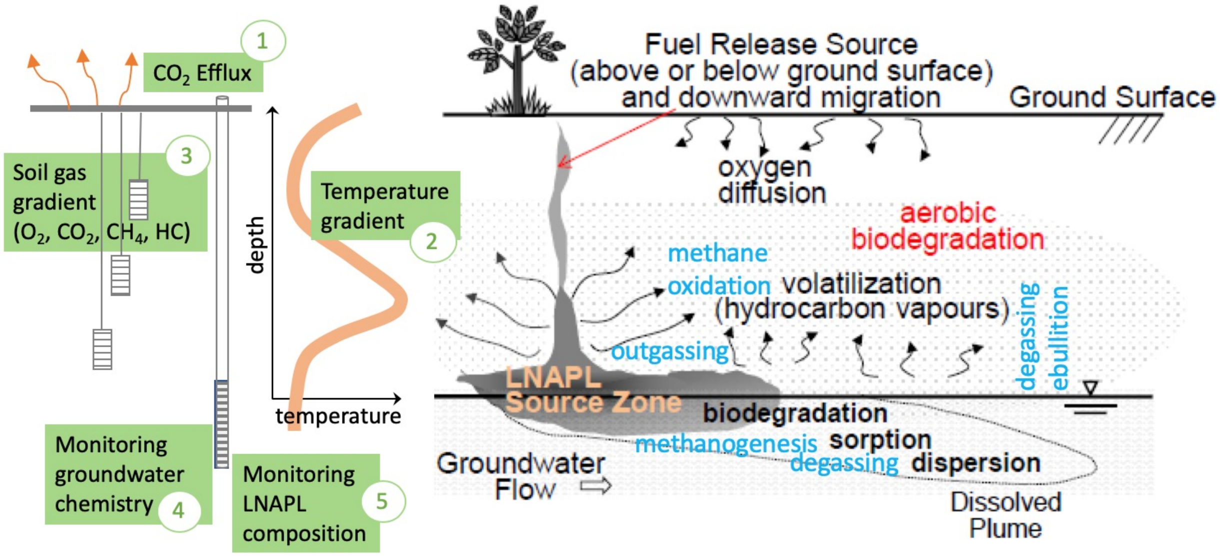


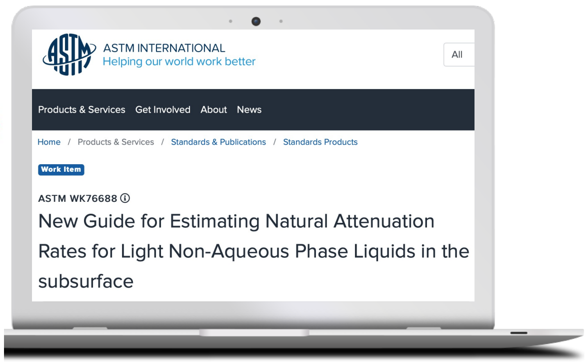
Natural Attenuation & Natural Source Zone Depletion (NSZD)





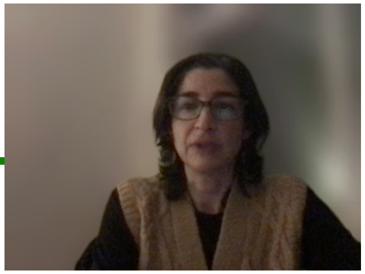
Natural Attenuation Processes & Pathways





https://www.astm.org/workitem-wk76688

For more information, contact parisa@arisenv.ca

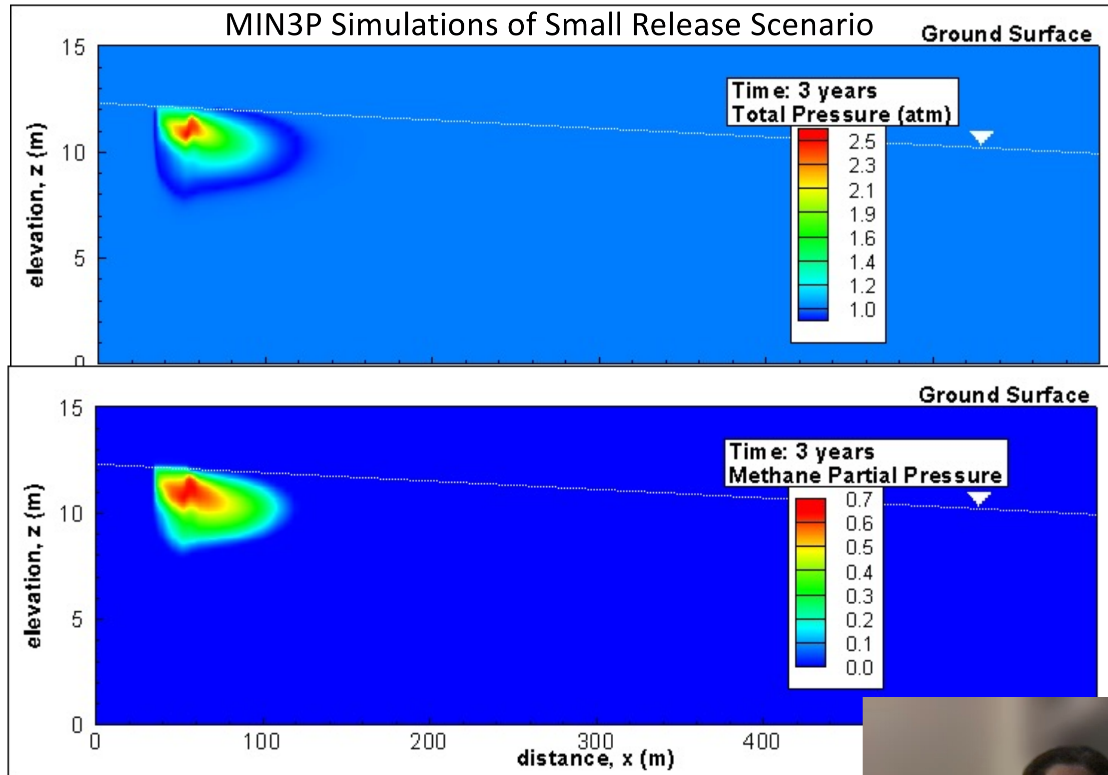


Gas Transport Across the Capillary Fringe

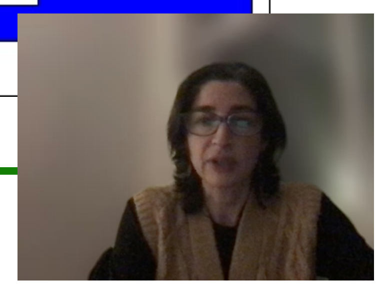
Results of baseline scenarios for both the small and large release simulations indicate significant build-up of and methane and pressure.

Also marked by decrease in N_2 and Ar concentrations

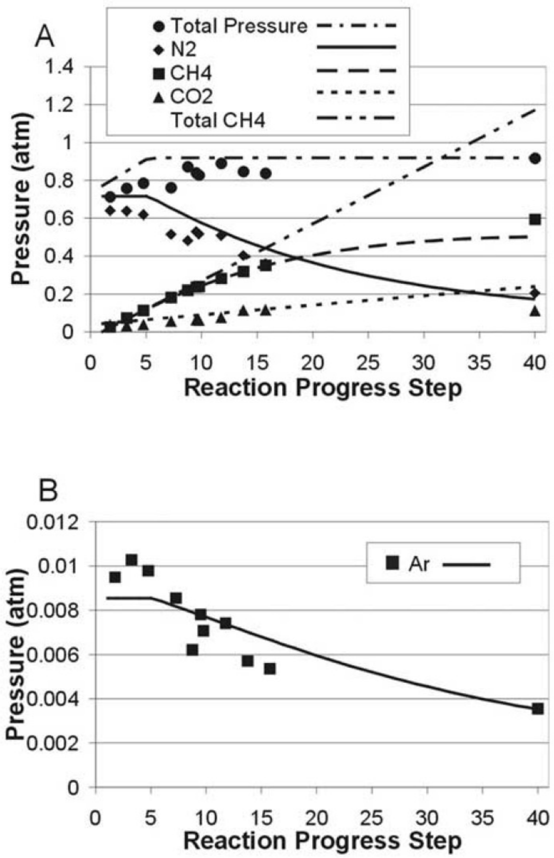
Model with degassing option needed to best represent the selected baseline scenarios.



Jourabchi et al. (2018)



Methanogenesis & Bubble Formation

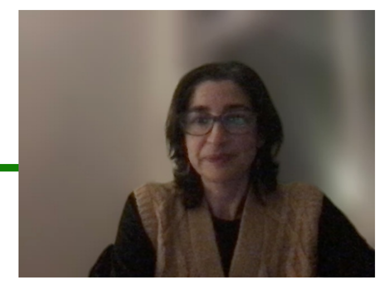


WATER RESOURCES RESEARCH, VOL. 41, W02001, doi:10.1029/2004WR003433, 2005

Use of dissolved and vapor-phase gases to investigate methanogenic degradation of petroleum hydrocarbon contamination in the subsurface

Richard T. Amos,[1] K. Ulrich Mayer,[1] Barbara A. Bekins,[2] Geoffrey N. Delin,[3] and Randi L. Williams[1]

Degassing Batch Model

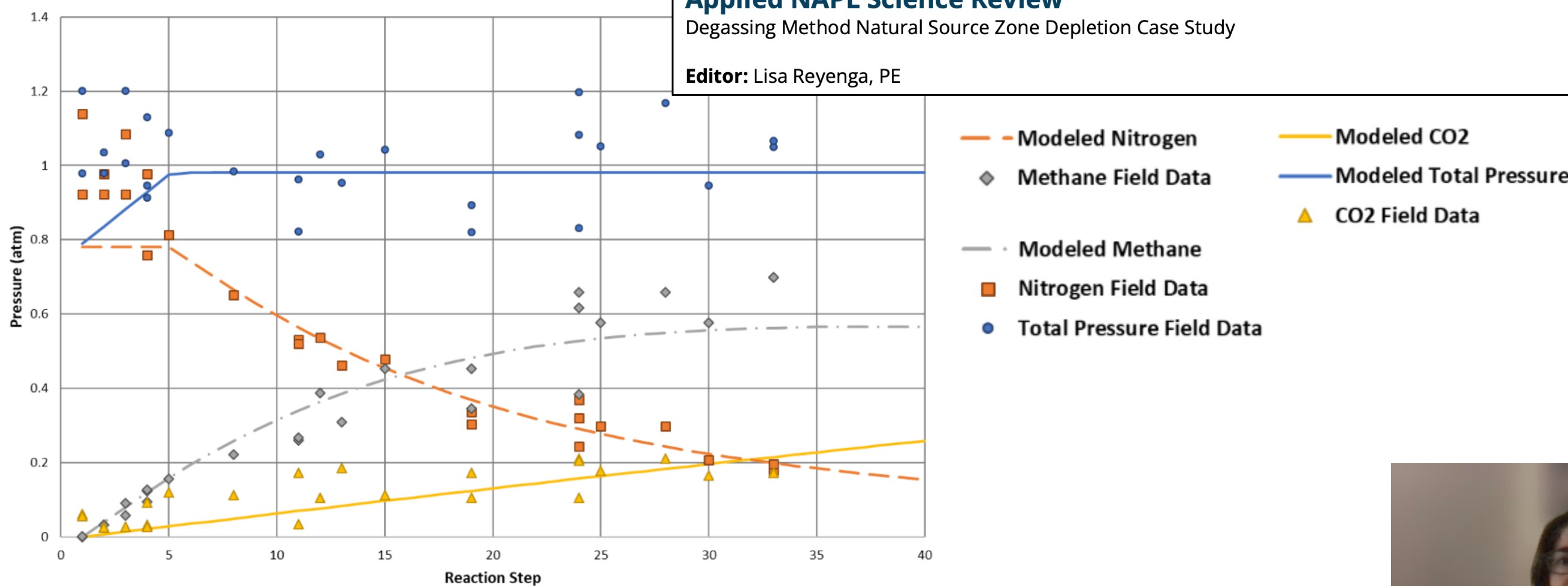


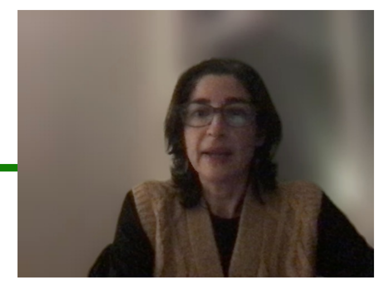
Stand-alone Implementation of Batch Model

Degassing Method Natural Source Zone Depletion Case Study
Volume 8, Issue 3 | September 2020

Applied NAPL Science Review
Degassing Method Natural Source Zone Depletion Case Study

Editor: Lisa Reyenga, PE



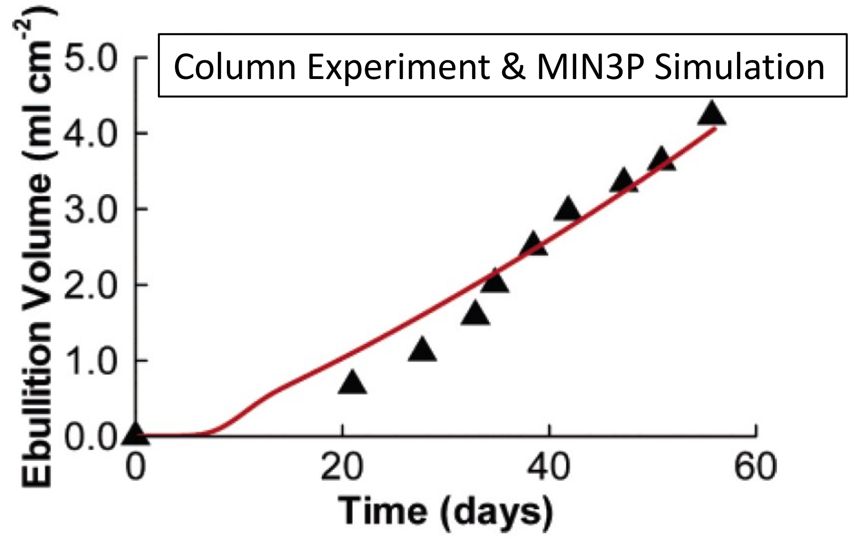


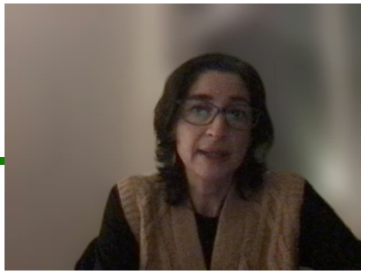
Dissolved Gas Analysis & RTM

Environ. Sci. Technol. **2006**, *40*, 5361–5367

Investigating Ebullition in a Sand Column Using Dissolved Gas Analysis and Reactive Transport Modeling

RICHARD T. AMOS* AND
K. ULRICH MAYER
Department of Earth and Ocean Sciences, University of British Columbia, Vancouver, BC, Canada





The Opportunities

Where are we? Exciting Times!

Advanced In-Situ Sensors, Artificial Intelligence, Reactive Transport Modeling (RTM), High Performance Computing RTM, Supercomputer on Digital Twin models, Python machine learning (on existing data sets, e.g. GeoTracker).

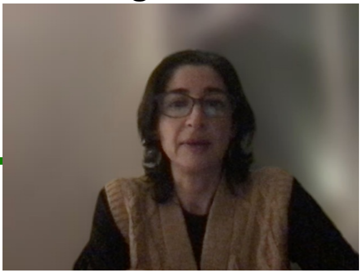
Where are we going?

Larger 'owners’ (e.g., DOE, EPA, ESTCP); are actively developing this collection of tools, akin to 'Centralized Computing' capabilities.

What does this mean for other contaminated site 'owners'?

Individual industry owners have in-house expertise & data collected on sites over time. With such an 'Innovation Playground' of tools and model capabilities, they can better predict and control costs and more easily manage their portfolio of sites, while protecting human health & the environment.

New kids in the park!



Acknowledgement:

Christof Meile (University of Georgia)

ARIS

Thank You

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