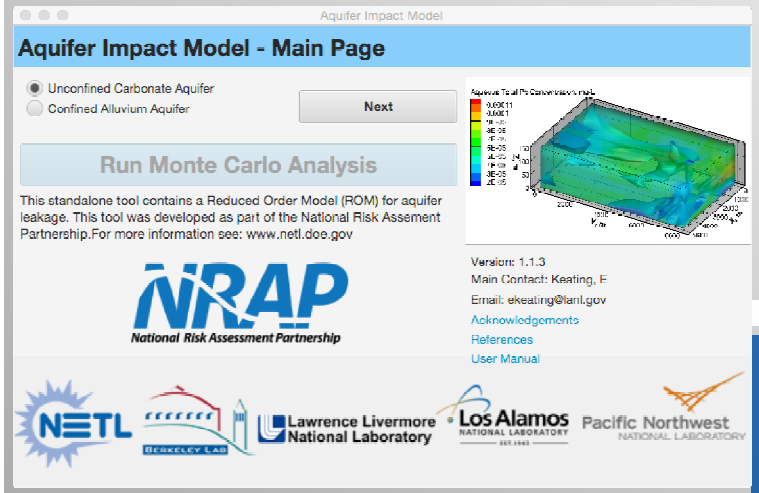


NRAP Tool Webinar Series

Webinar 5

Aquifer Impact Model: A tool for estimating risk to drinking water resources due to CO_2 and brine leaks

Monday November 9, 2015

*Presenter: *Diana Bacon[1]*
NRAP Groundwater workgroup

Contributors: Susan Carroll[2], Elizabeth Keating[3], Kayyum Mansoor[2], Liange Zheng[4]

** Presenter*
[1]Pacific Northwest National Laboratory
[2]Lawrence Livermore National Laboratory
[3]Los Alamos National Laboratory
[4]Lawrence Berkeley National Laboratory

Outline

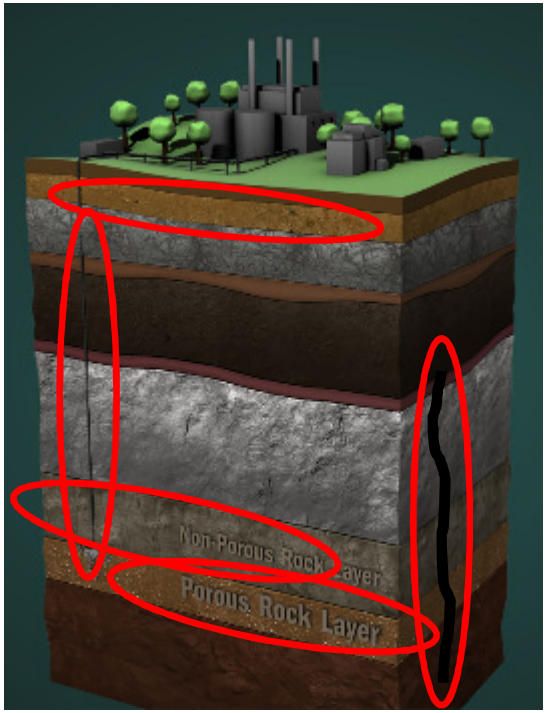
- Welcome and Overview of NRAP – Technical Approach and Tool Development
- Introduction to the NRAP Aquifer Impact Model (AIM)
- Input needed for the AIM tool
- Example use cases
- Analysis of output
- QA/QC
- Questions and Open Discussion

National Risk Assessment Partnership (NRAP)

NRAP leverages DOE's capabilities to help quantify uncertainties and risks necessary to remove barriers to full-scale CO_2 storage deployment.

Objective: Building toolset and improving the science base to address key questions about potential impacts related to release of CO_2 or brine from the storage reservoir, and potential ground-motion impacts due to injection of CO_2

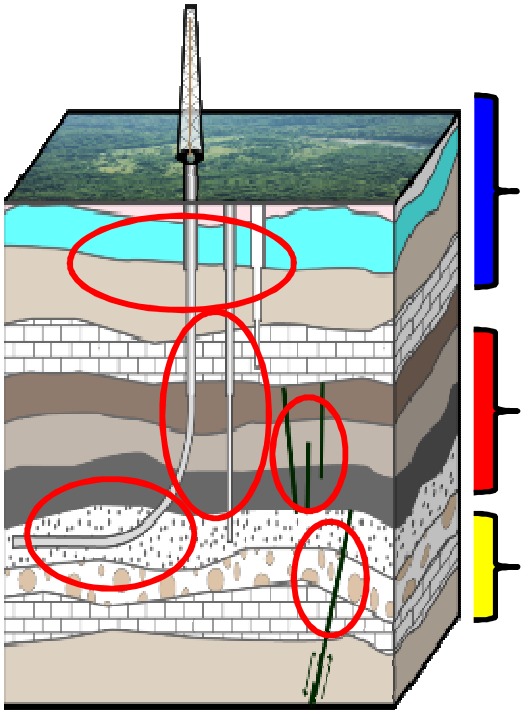
Technical Team



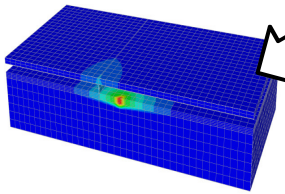
Stakeholder Group

NRAP's approach to quantifying performance relies on reduced-order models to probe uncertainty in the system.

A. Divide system into discrete components



B. Develop detailed component models that are validated against lab/field data

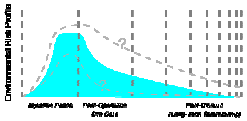


Energy Data Exchange (EDX)

Data

IAM

NRAP Integrated Assessment (System) Models



Potential Receptors or Impacted Media

Release and Transport

Storage Reservoir

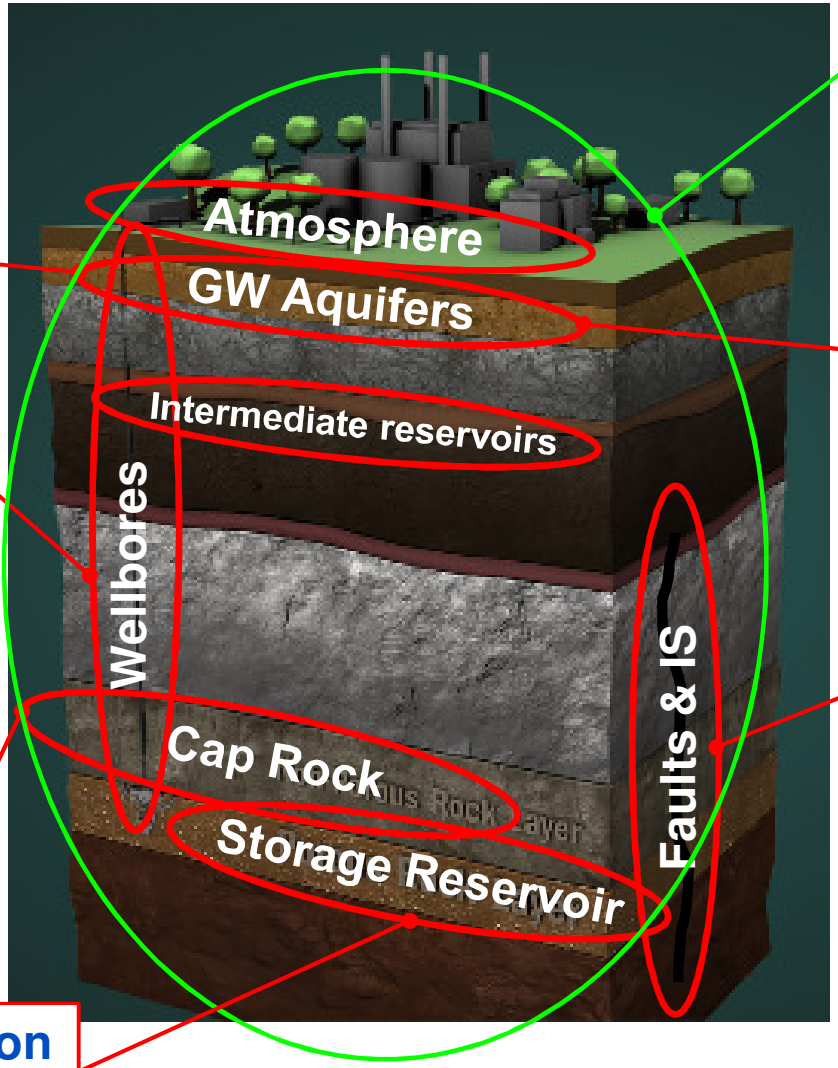
C. Develop reduced-order models (ROMs) that rapidly reproduce component model predictions

D. Link ROMs via integrated assessment models (IAMs) to predict system performance & risk; calibrate using lab/field data from NRAP and other sources

E. Develop strategic monitoring protocols that allow verification of predicted system performance

NRAP Tools

Now available for beta testing



NRAP-IAM-CS

Design for Risk Evaluation and Monitoring

Aquifer Impact Model

Wellbore Leakage Analysis Tool

Short Term Seismic Forecasting

Natural Seal ROM

Reservoir Evaluation and Visualization

www.edx.netl.doe.gov/nrap → *TOOL BETA TESTING link*

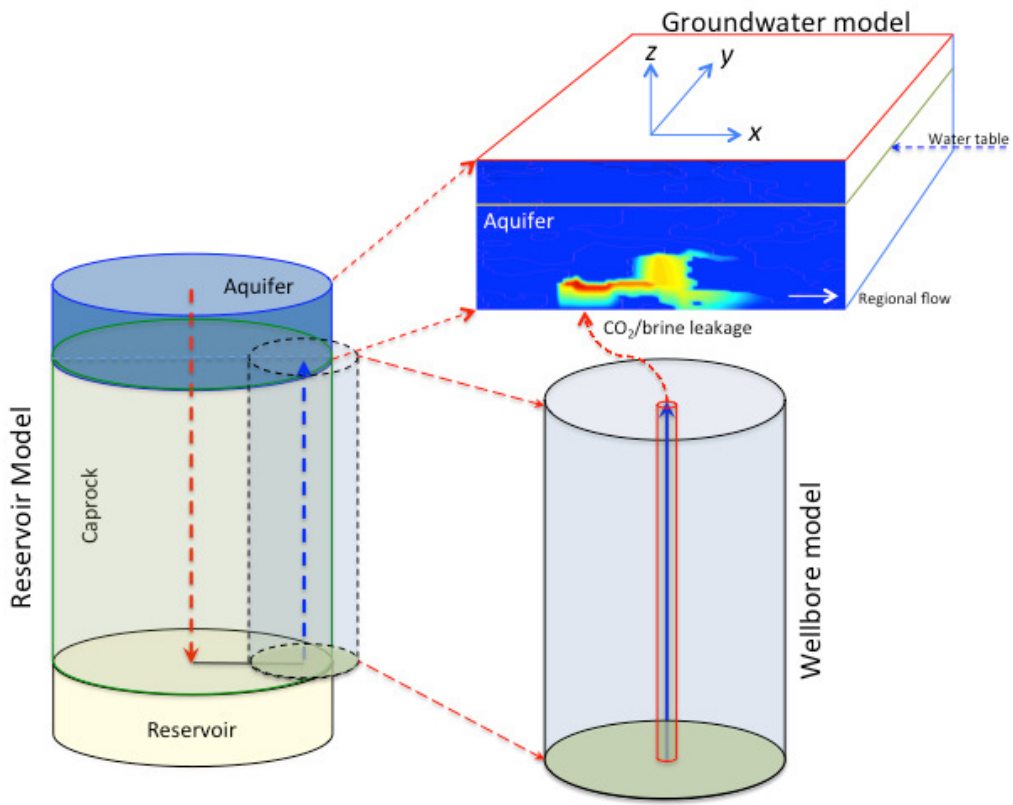
Schedule for NRAP Tool Webinar Series

Date/ Time	Tool	Presenter(s)
October 13 **Time: 1pm ET**	Integrated Assessment Model–Carbon Storage (NRAP-IAM-CS) (2.5 hours)	Rajesh Pawar
October 19 **Time: 1pm ET**	Natural Seal ROM (NSealR) (1 hour)	Nicolas Huerta, Ernest Lindner
October 26 **Time: 1pm ET**	Reservoir Evaluation and Visualization (REV) Tool (1 hour)	Seth King
November 2 **Time: 1pm ET**	Wellbore Leakage Analysis Tool (WLAT) (1.5 hour)	Nicholas Huerta
November 9 **Time: 1pm ET**	Aquifer Impact Model (AIM) (1 hour)	Diana Bacon
November 16 **Time: 1pm ET**	Design for Risk Evaluation and Monitoring (DREAM) (1 hour)	Catherine Ruprecht
November 30 **Time: 1pm ET**	Short Term Seismic Forecasting (STSF) (1 hour)	Josh White, Corinne Bachman
December 7 **Time: 1pm ET**	TBD	

Check for updates at www.edx.netl.doe.gov/nrap

Aquifer Impact Model (AIM) Development

- Used stochastic approach to incorporate uncertainties in aquifer parameters and leakage scenarios into 3D multiphase reactive transport simulations to predict the sizes and magnitudes of groundwater plumes
- Used regression analysis to develop reduced order models (ROMs)
- Coupled with ROMs for other system components to investigate various leakage scenarios



Method for ROM Development Using Geochemistry Scaling Function

Hydraulic ROM
- Simple calcite equilibrium
- Treat metals/organics as tracers
- Vary hydraulic parameters

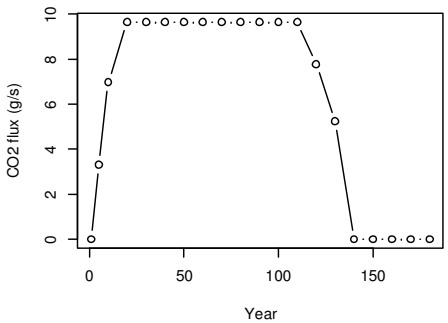
✖

Geochemistry Scaling Function
- Metal adsorption on calcite (Edwards) or clays (High Plains)
- Biodegradation/adsorption of organics
- Vary geochemical parameters
- Ratio for plume volume w/ simple and complex geochemistry

=

Coupled Groundwater ROM

ROM Input



- *Brine and CO_2 leak rates,*
- *Concentration of salts and contaminants in brine*

Aquifer characteristics

Hydrologic

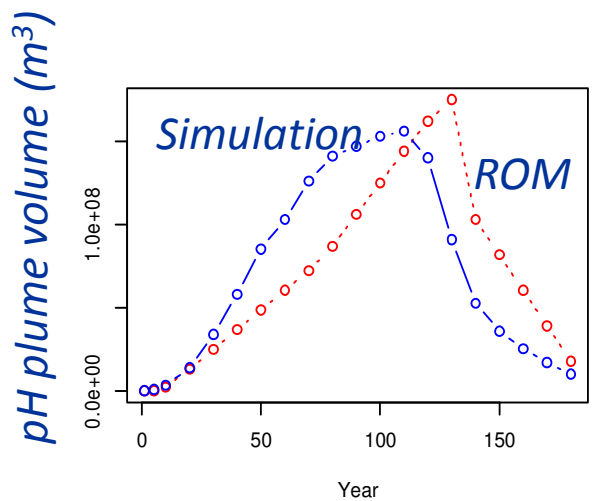
Geochemical

AIM

ROM Output

Plume volume

pH
TDS
Trace metals
Organics



Aquifer Impact Model (AIM) Features and Outputs

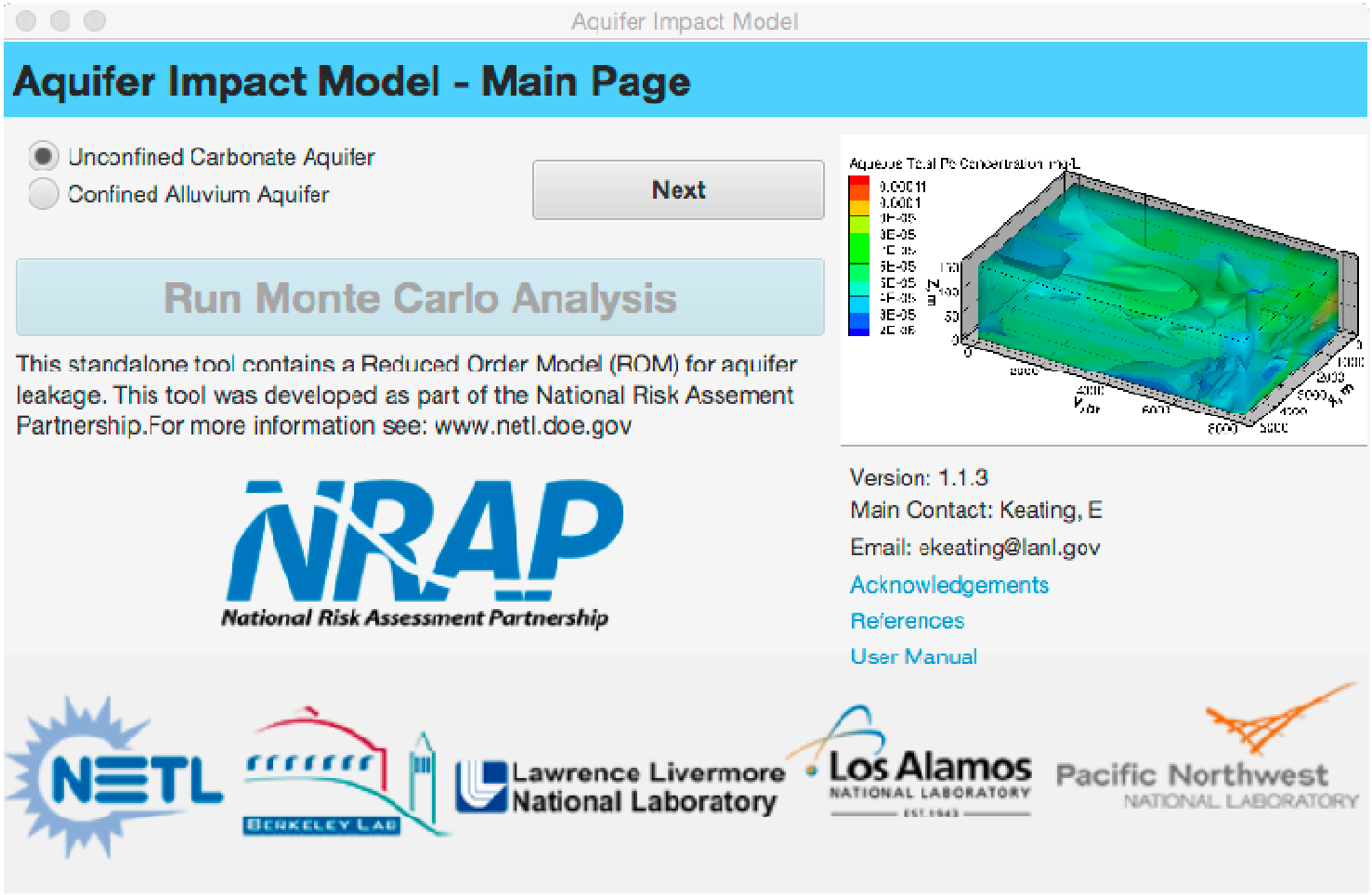
- **Can be used as a site screening tool to compare groundwater quality impacts due to CO_2 or brine leaks**
- **Two aquifer models:**
  - Unconfined carbonate aquifer
  - Confined alluvium aquifer
- **Calculates volume of aquifer beyond threshold concentrations:**
  - pH
  - TDS
  - Trace metals: arsenic, barium, cadmium, lead
  - Organics: benzene, naphthalene, phenol
- **Two threshold values for each volume calculation:**
  - MCL
  - No-impact (background 95th percentile)

No-Impact and MCL Threshold Values

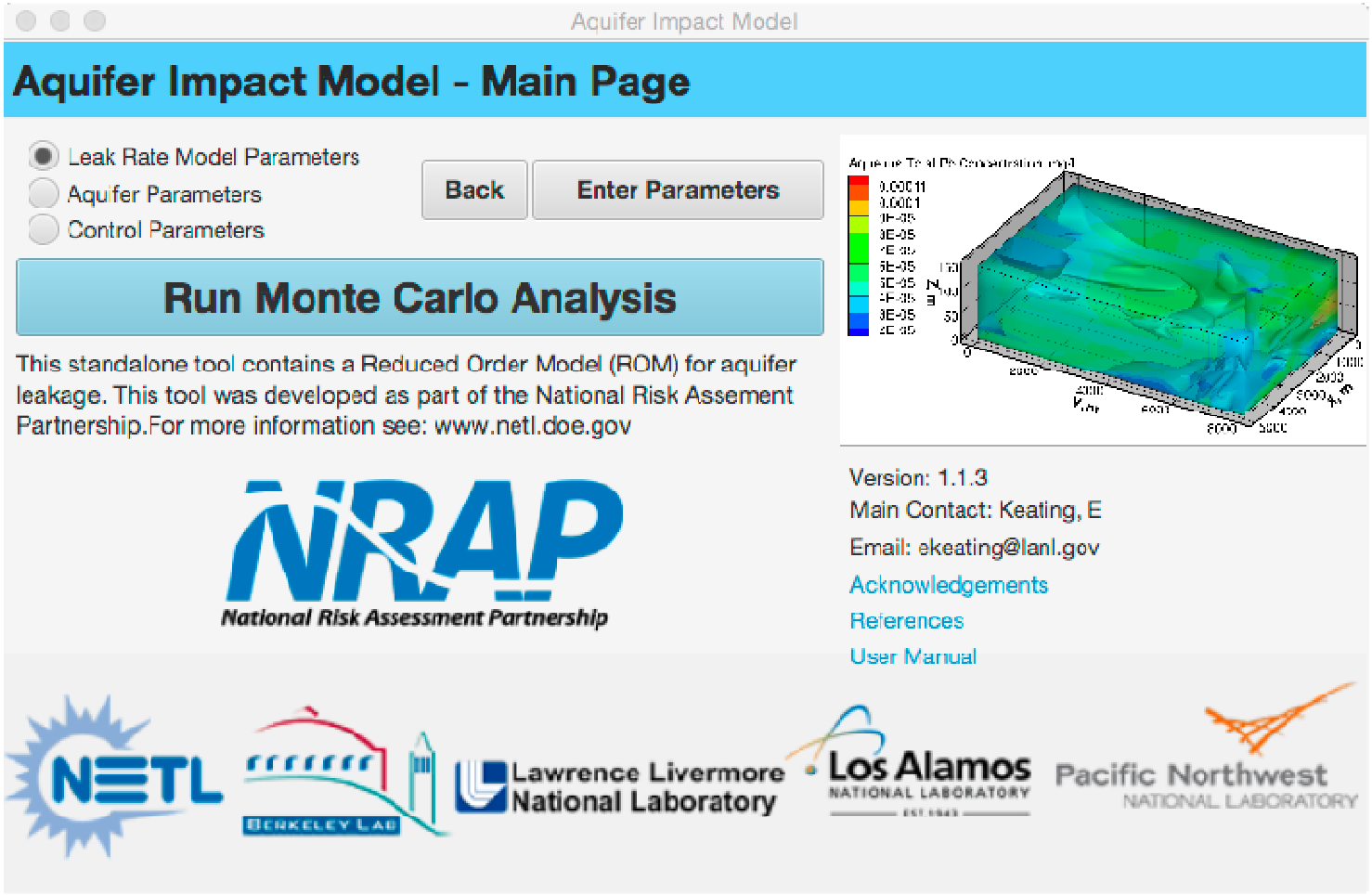
Analyte	Unconfined Carbonate Aquifer (Edwards)		Confined Unconsolidated Sands Aquifer (High Plains)		U.S. EPA Regulatory Standard
	Initial Model [a]	No-Impact Threshold [b]	Initial Model [c]	No-Impact Threshold [b]	MCL Threshold
pH	6.9	6.6	7.6	6.625 [d]	6.5
Total Dissolved Solids	330	420 mg L^{-1}	570 mg L^{-1}	1300 mg L^{-1} [e]	500 mg L^{-1}
Arsenic	0.31	0.55 µg L^{-1}	1.5 µg L^{-1}	9.3 µg L^{-1}	10 µg L^{-1}
Cadmium	0.00	0.04 µg L^{-1}	0.059 µg L^{-1}	0.25 µg L^{-1}	5 µg L^{-1}
Lead	0.06	0.15 µg L^{-1}	.086 µg L^{-1}	0.63 µg L^{-1}	15 µg L^{-1}

DRAFT

Choose aquifer type



Enter parameters



Choose leakage scenario parameters

Aquifer Impact Model

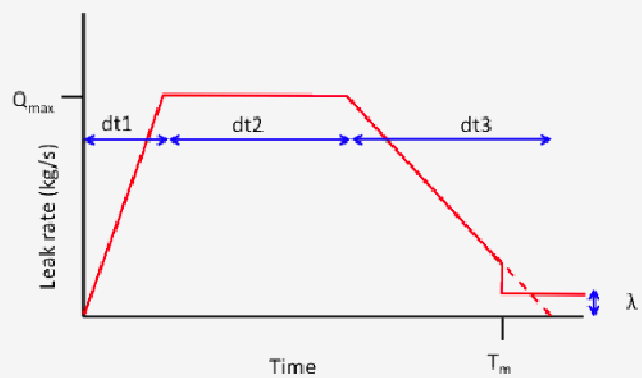
File

Leak Rate Model | Aquifer | Control

	Brine Min	Brine Max	CO2 Min	CO2 Max	Brine Lower	Brine Upper	CO2 Lower	CO2 Upper	Units
Qmax	0.005	0.075	0.001	0.5	0.005	0.075	0.001	0.5	kg/s
dt1	5.0	50.0	5.0	50.0	0	50	5	50	years
dt2	1.0	10.0	0.0	100.0	1	10	0	100	years
dt3	1.0	10.0	5.0	50.0	1	10	5	50	years
lambda	0.0		0.3		0	0.3	0	0.3	-
Tm	200.0				0.5	200	0.5	200	years
Scenarios	1000								

*Hover over a label to see its full description here.

Revert Parameters to Defaults | Cancel | Save



Choose Carbonate aquifer parameters

Aquifer Impact Model

File

Leak Rate Model | Aquifer | Control

	Min	Max	Lower Bound	Upper Bound	Units
Aquifer Type	unconfined_carbonate				
Permeability Variance	0.017	1.89	0.017	1.89	--
Correlation Length	1.0	3.95	1	3.95	km
Kx/Kz	1.1	49.1	1.1	49.1	--
Mean Permeability	-13.8	-10.3	-13.8	-10.3	log10(m^2)
Aquifer Thickness	100.0	500.0	100	500	m
Hydraulic Gradient	2.88E-4	1.89E-2	2.88E-4	1.89E-2	--
Calcite Surface Area	0.0	0.01	0	0.01	(m^2)/g
Organic C Volume Fraction	0.0	0.01	0	0.01	--
Benzene kd	1.49	1.73	1.49	1.73	log(Koc)
Benzene Decay	0.15	2.84	0.15	2.84	log(day)
Pah kd	2.78	3.18	2.78	3.18	log(Koc)
Pah Decay Constant	-0.85	2.04	-0.85	2.04	log(day)
Phenol kd	1.21	1.44	1.21	1.44	log(Koc)
Phenol Decay Constant	-1.22	2.06	-1.22	2.06	log(day)
[Cl] in leaking brine	0.1	6.0	0.1	6	mol/kg
Realizations Requested	60				

Revert Parameters to Defaults | Cancel | Save

Choose Alluvium aquifer parameters

Aquifer Impact Model

File

Leak Rate Model | Aquifer | Control

	Min	Max	Lower Bound	Upper Bound	Units
Aquifer Type	confined_alluvium				
Realizations Requested	50				
Sand Fraction	0.35	0.65	0.35	0.65	--
Correlation Length X	200.0	2500.0	200	2500	m
Correlation Length Z	0.5	25.0	0.5	25	m
Sand Permeability	-14.0	-10.0	-14	-10	log10(m^2)
Clay Permeability	-18.0	-15.0	-18	-15	log10(m^2)
Goethite	0.0	0.15	0	0.15	--
Illite	0.0	0.2	0	0.2	--
Kaolinite	0.0	0.15	0	0.15	--
Smectite	0.0	0.3	0	0.3	--
Cation Exchange Capacity	0.1	40.0	0.1	40	meq/100g
[Na] = [Cl]	-2.0	0.73	-2	0.73	log10(Molality)
[Pb]	-8.5	-5.0	-8.5	-5	log10(Molality)
[Benzene]	-8.8927	-4.8927	-8.8927	-4.8927	log10(Molality)
[As] Brine	-9.0	-5.0	-9	-5	log10(Molality)

Aquifer Impact Model

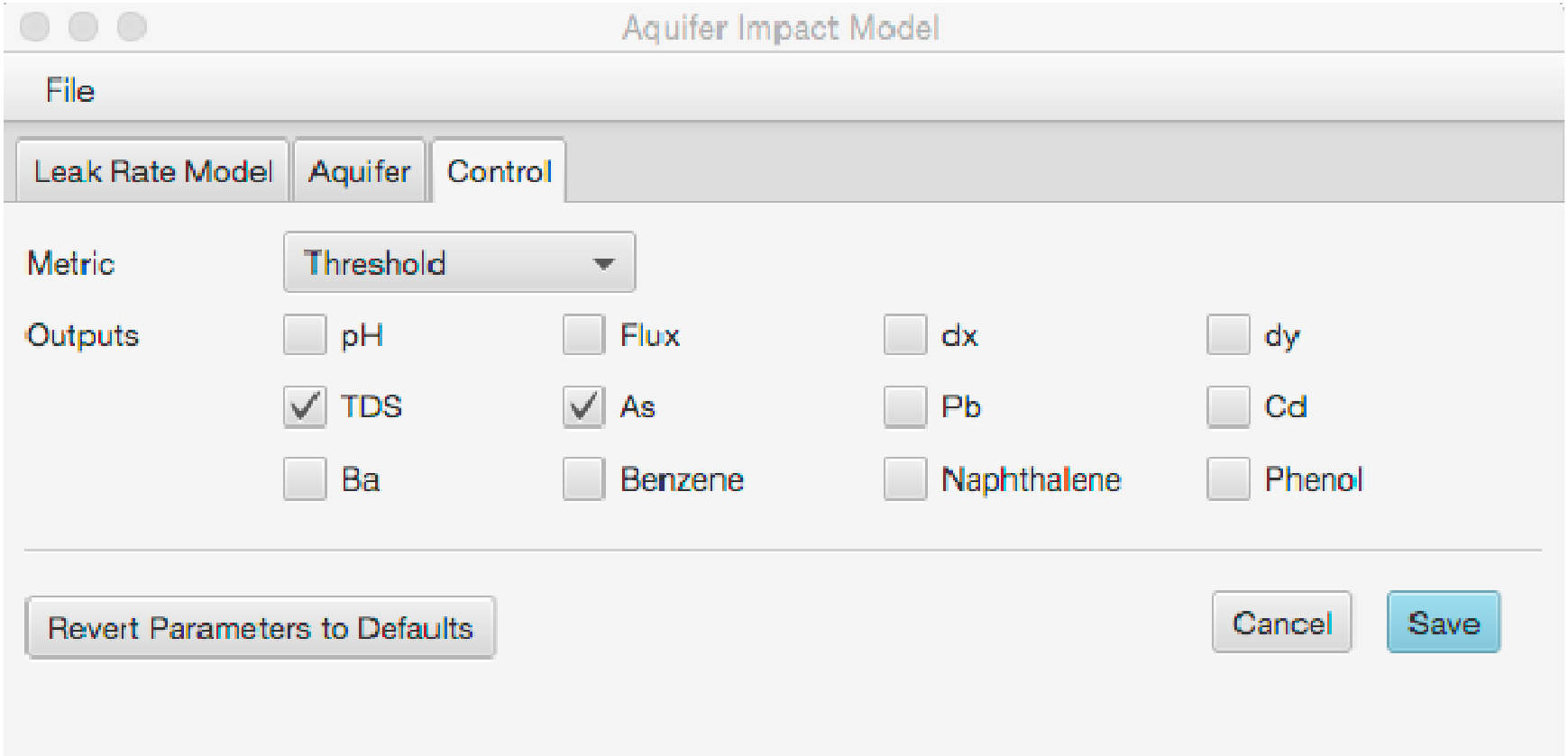
File

Leak Rate Model | Aquifer | Control

Cation Exchange Capacity	0.1	40.0	0.1	40	meq/100g
[Na] = [Cl]	-2.0	0.73	-2	0.73	log10(Molality)
[Pb]	-8.5	-5.0	-8.5	-5	log10(Molality)
[Benzene]	-8.8927	-4.8927	-8.8927	-4.8927	log10(Molality)
[As] Brine	-9.0	-5.0	-9	-5	log10(Molality)
[Ba] Brine	-5.1	-2.3	-5.1	-2.3	log10(Molality)
[Cd] Brine	-9.0	-6.0	-9	-6	log10(Molality)
Benzene Kd	-4.5	0.69	-4.5	0.69	log10 (L/kg)
Benzene Decay Constant	-10.0	-6.1	-10	-6.1	log10 (1/s)
[Pah] Brine	-10.0	-4.1	-10	-4.1	log10(Molality)
Pah Kd	-3.1	1.98	-3.1	1.98	log10 (L/kg)
Pah Decay Constant	-10.0	-6.45	-10	-6.45	log10 (1/s)
[Phenol] Brine	-10.0	-3.7	-10	-3.7	log10(Molality)
Phenol Kd	-6.0	0.15	-6	0.15	log10 (L/kg)
Phenol Decay Constant	-10.0	-5.63	-10	-5.63	log10 (1/s)

Revert Parameters to Defaults | Cancel | Save

Choose output parameters



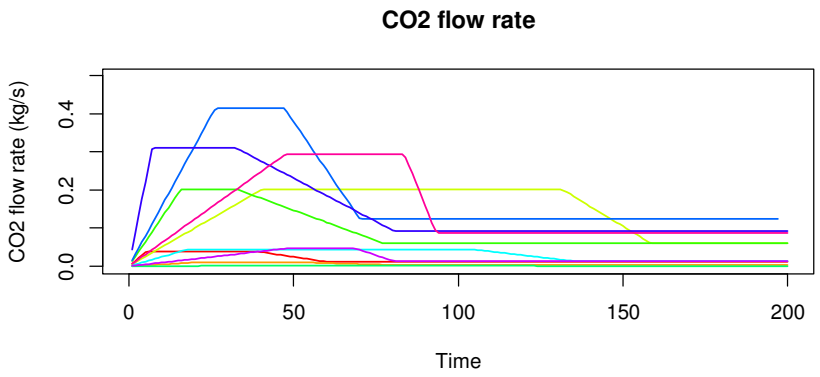
Run Monte Carlo Analysis

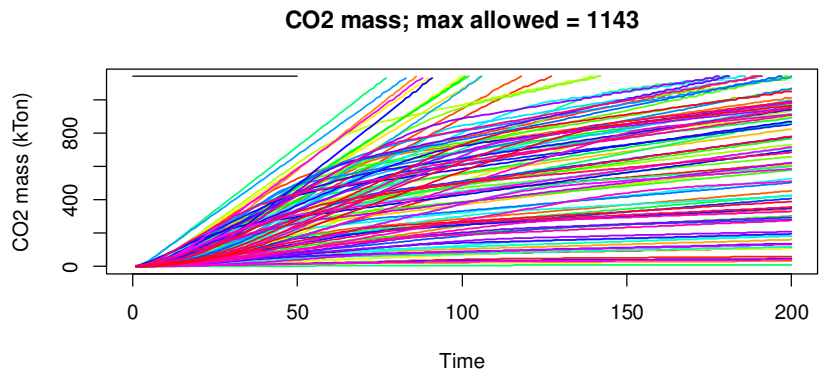
Aquifer Impact Model

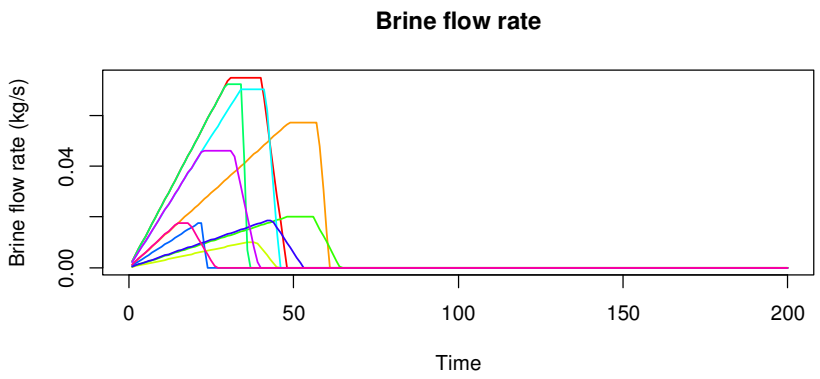
```
[INFO] Base Directory: /Users/d3a926/Desktop/nrap-aim-v1-1-3
[INFO] ROM: edwards
[INFO] bins: run-gw-rom-osx-x86_64 create-input-osx-x86_64 sa-osx-x86_64
[INFO] Creating leakage scenarios based on heuristic model values.
[INFO] Success
[INFO] Developing horsetail plots of leakage scenarios...
[INFO] Created leakage_scenarios.pdf
[INFO] Created leakage_scenarios_mass.pdf
[INFO] Running the ROM
 completed   60  aquifer parameter sets
 completed   178827 leak calculations
[INFO] Creating plots of the output...
[INFO] Created quartiles.pdf
[INFO] Created cdf.pdf
[INFO] Created sensitivities.pdf
ROM-MC.output
ROM-SA.output
create_input.output
[INFO] Script completed... Output is in the following directory:
/Users/d3a926/Desktop/nrap-aim-v1-1-3/results--2015-11-03--13-09
```

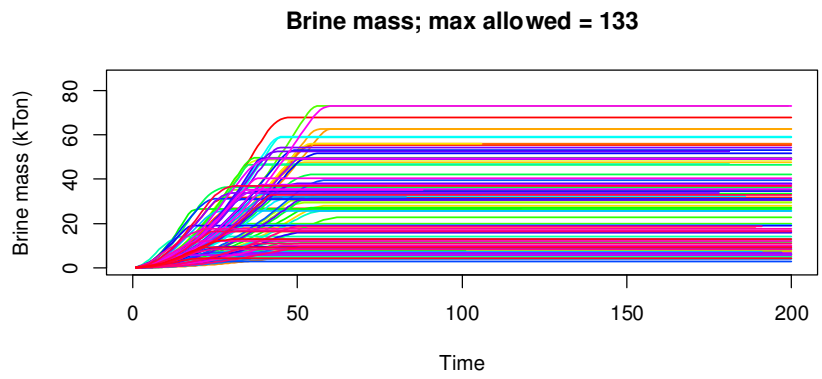
Return To Main Screen

Leakage Scenarios



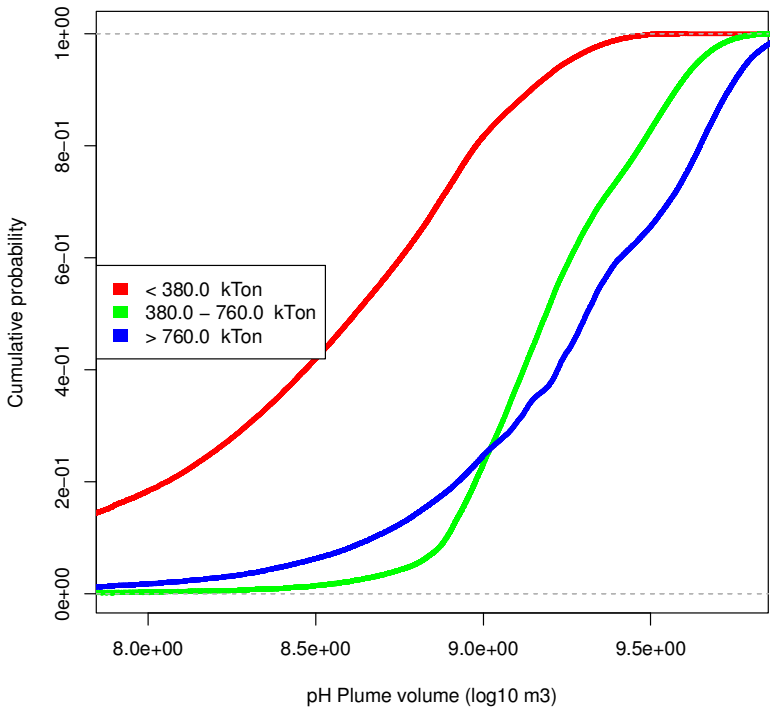




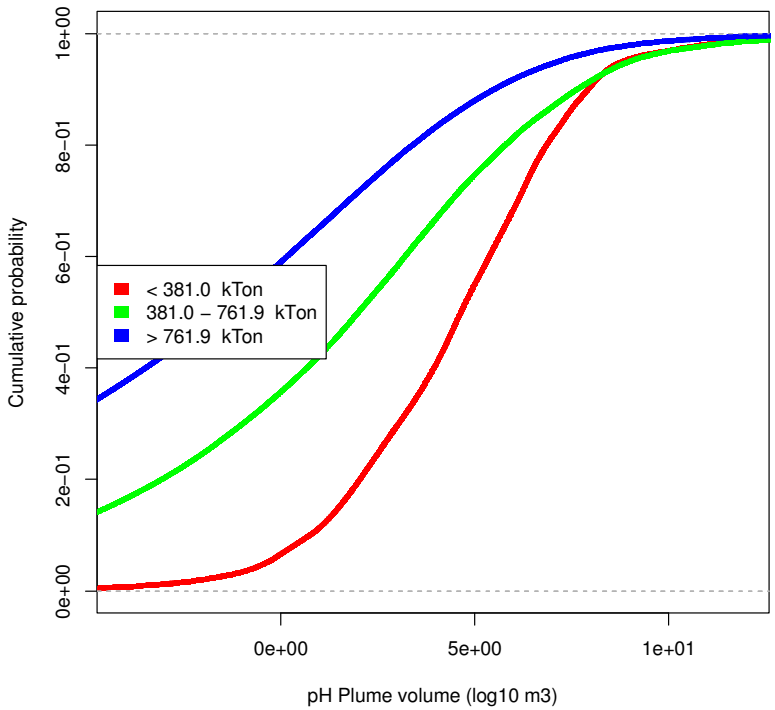


Application: Site Screening

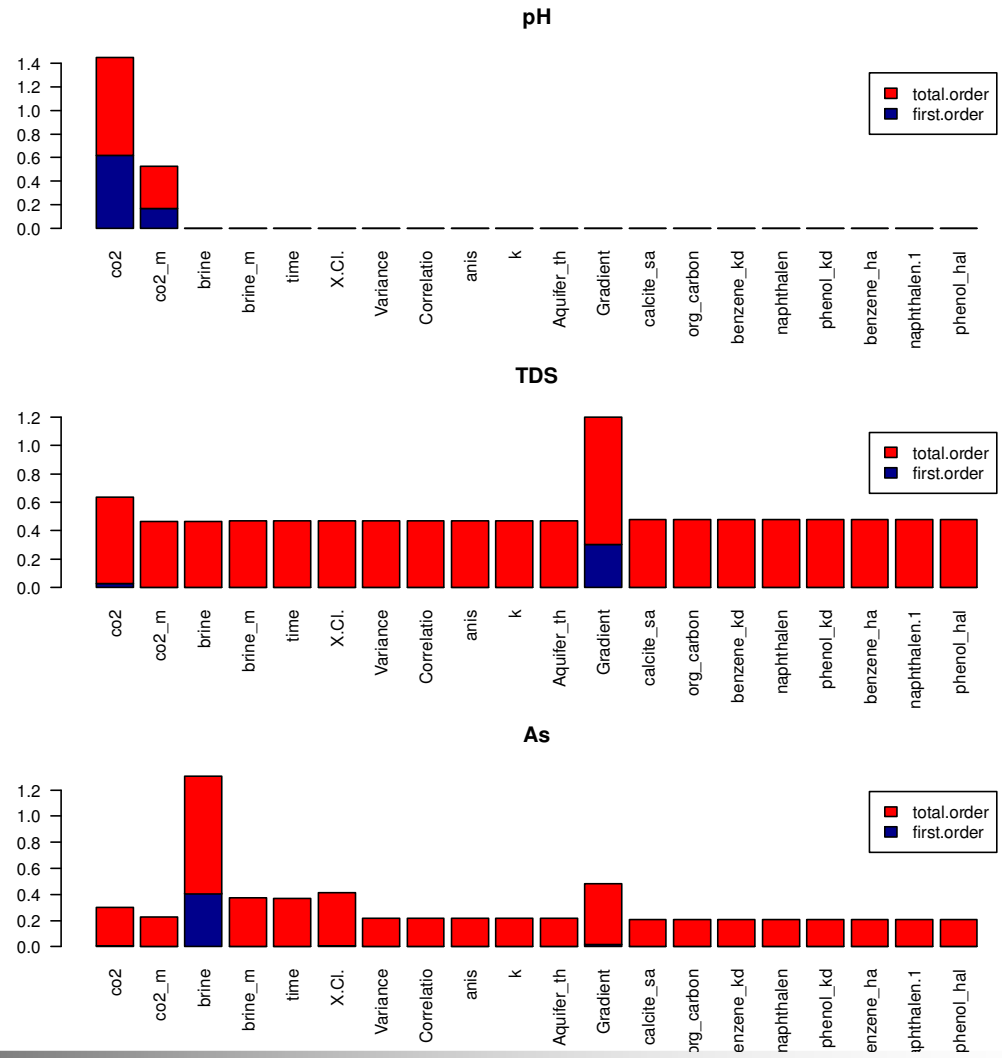
Carbonate Aquifer



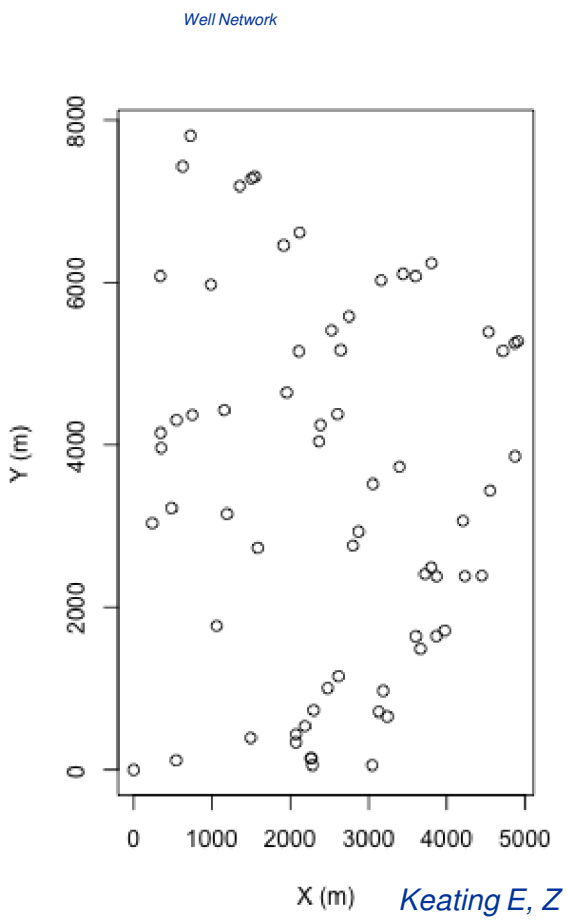
Sand and Gravel Aquifer

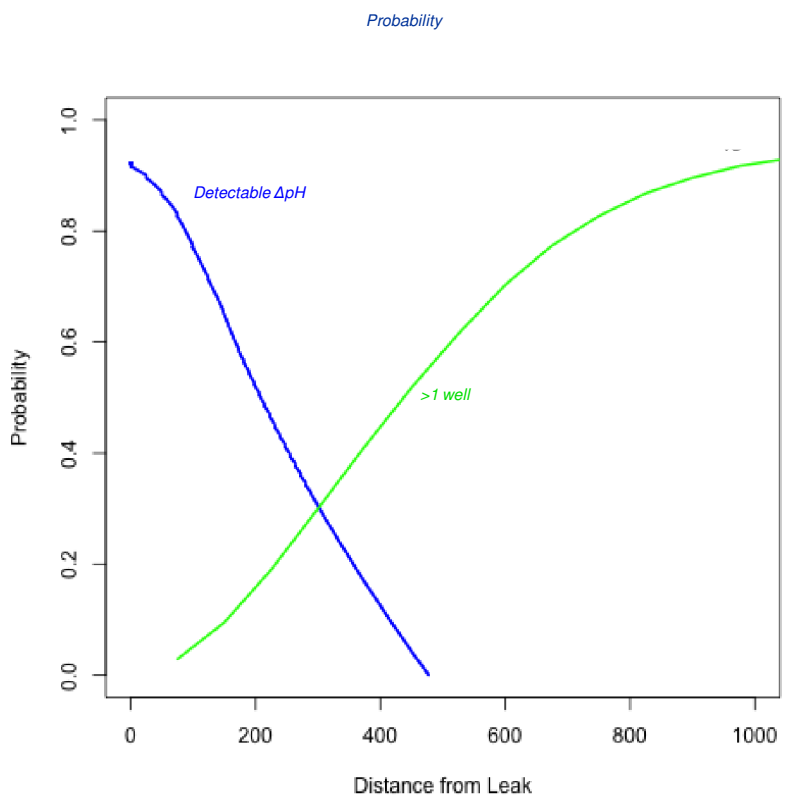


Application: Prioritizing Site Characterization Studies



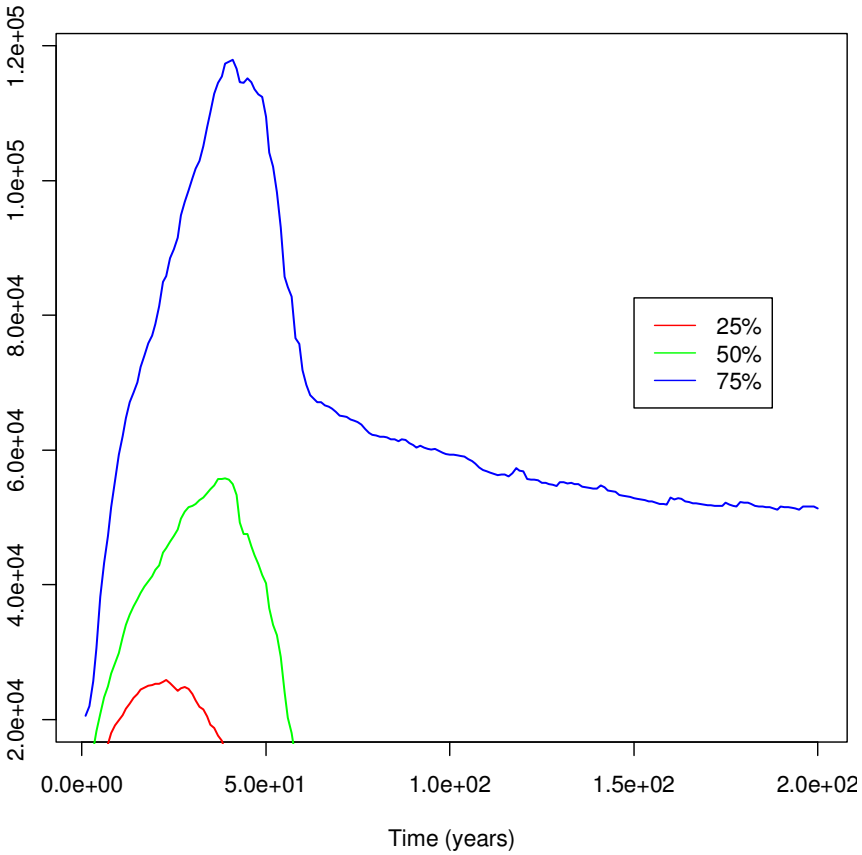
Application: Evaluation/design of a monitoring network for plume detection





Keating E, Z Dai, D Dempsey, and R Pawar. 2014. "Effective detection of CO_2 leakage: a comparison of groundwater sampling and pressure monitoring." Energy Procedia 63:4163-4171

Application: Evaluating Potential for Health Impacts from Arsenic



- **Carbonate Aquifer**
- **U.S. EPA Maximum Contaminant Level (MCL) threshold for plume size**
- **Plume size decreases with time due to dispersion**

Criteria for Application of AIM to a New Site

1. ***Do the physical and chemical characteristics of the aquifer at the new site fall within the uncertainty range of existing ROM input parameters?***

YES

NO

Are ROMs sensitive to these parameters?

NO

YES

Existing ROM may be useful

Existing ROM should not be used

2. Do the potential leakage scenarios at the site fall within the range considered by our ROMs? (leak rates, brine composition)

Quality Assurance

- **Each AIM aquifer model is based on two multiphase flow and reactive transport models**
  - One with simple geochemistry where the hydraulic parameters have been varied
  - The other with complex geochemistry where the geochemical parameters have been varied
- **The component ROMs have been compared to their associated reactive transport model's output**
  - Bacon DH, Z Dai, and L Zheng. 2014. "Geochemical Impacts of Carbon Dioxide, Brine, Trace Metal and Organic Leakage into an Unconfined, Oxidizing Limestone Aquifer." *Energy Procedia* 63:4684-4707. 10.1016/j.egypro.2014.11.502.

Related Articles in IJGGC Special Issue on NRAP

- Hou, Z., Bacon, D.H., Engel, D.W., Lin, G., Fang, Y., Ren, H., Fang, Z., 2014. Uncertainty analyses of CO_2 plume expansion subsequent to wellbore CO_2 leakage into aquifers. International Journal of Greenhouse Gas Control 27, 69-80, doi:10.1016/j.ijggc.2014.05.004.
- Carroll, SA, E Keating, K Mansoor, Z Dai, Y Sun, W Trainor-Guitton, CR Brown, DH Bacon, 2014, “Key Factors for Determining Groundwater Impacts Due to Leakage from Geologic Carbon Sequestration Reservoirs”, doi:10.1016/j.ijggc.2014.07.007.
- G Wang, NP Qafoku, AR Lawter, M Bowden, O Harvey, CS Sullivan and CF Brown, “Geochemical Impacts of Leaking CO_2 from Subsurface Storage Reservoirs to an Unconfined Aquifer”, doi:10.1016/j.ijggc.2015.07.002.
- Bacon, DH, NP Qafoku, Z Dai, E Keating, CF Brown, “Modeling the Impact of Carbon Dioxide Leakage into an Unconfined, Oxidizing Carbonate Aquifer”, doi:10.1016/j.ijggc.2015.04.008.
- Lawter AR, N Qafoku, G Wang, H Shao, and CF Brown. 2015. "Evaluating Impacts of CO2 Intrusion into an Unconsolidated Aquifer: I. Experimental Data." International Journal of Greenhouse Gas Control. doi:10.1016/j.ijggc.2015.07.009.
- Zheng, L., N. P. Qafoku, A. Lawter, G. Wang, H. Shao and C. F. Brown Evaluating impacts of CO2 intrusion into an unconsolidated aquifer: II. Modeling results. International Journal of Greenhouse Gas Control. doi:10.1016/j.ijggc.2015.07.001.
- Keating, E.H., Harp, DH, Dai, Z., Pawar RJ. 2015. Reduced Order Models for Assessing CO_2 Impacts in Shallow Unconfined Aquifers. International Journal of Greenhouse Gas Control, in review.
- Keating, E, DH Bacon, SA Carroll, K Mansoor, L Zheng, “Applicability of Reduced Order Models of Groundwater Impact”, submitted.
- Last, G.V., C. J. Murray, and Y. Bott. Derivation of Groundwater Threshold Values for Analysis of Impacts Predicted at Potential Carbon Sequestration Sites. International Journal of Greenhouse Gas Control, submitted.