Improving Decision Making for Vadose Zone Remediation of Volatile Contaminants

ESTCP Project ER-201731

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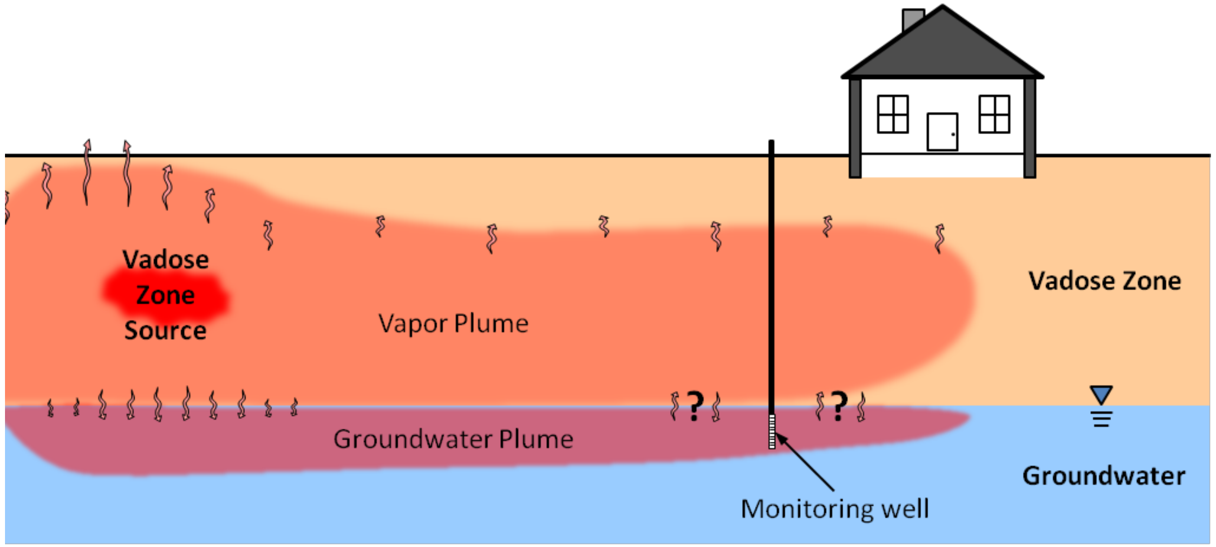
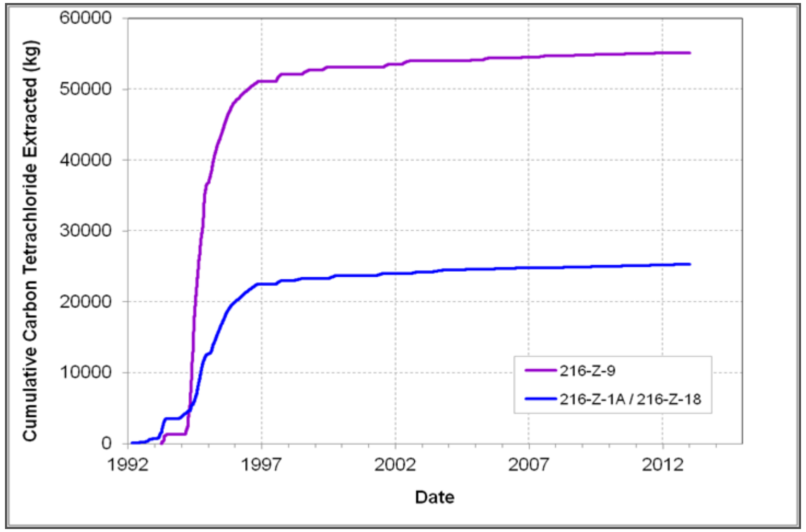
Overview

- Soil Vapor Extraction
  - Remedial Decisions
  - Guidance
- SVEET Tool to support remedial decisions
- ESTCP project: update/expand SVEET
  - Software update and prototype results
  - Planned Field Demonstration

Soil Vapor Extraction

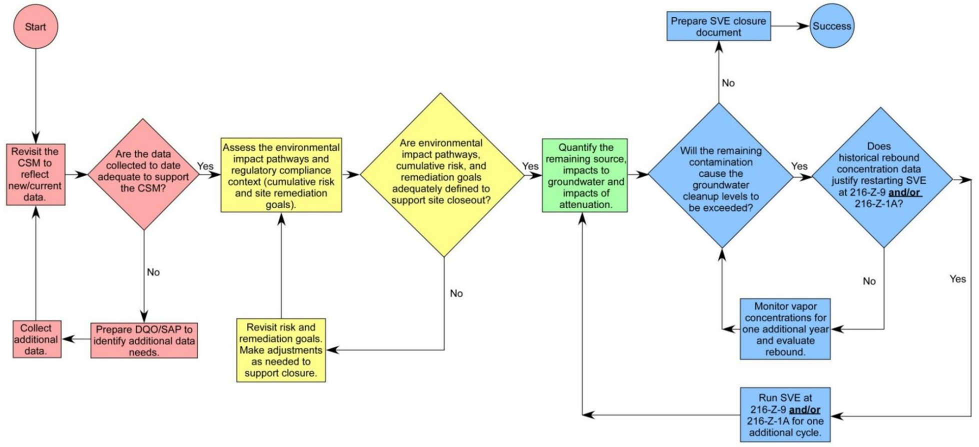
- Commonly used, effective technology
  - Volatile contaminants in vadose zone
  - But, need to determine appropriate operational duration
- Remedial Questions
  - Has a point been reached where SVE can be terminated?
    - Will the remaining mass represent a threat?
  - Can alternative technologies address the remaining mass?
    - Cost effectiveness of active SVE in question
  - Is SVE needed?
    - Is there a risk to groundwater or via vapor intrusion?
  - What are the SVE performance goals?
    - For a new or an existing system
    - What mass flux from contaminated zone or vadose soil vapor concentration is acceptable?





SVE Guidance

- *Soil Vapor Extraction System Optimization, Transition, and Closure Guidance (PNNL-21843)*
  - Process described by PNNL, USACE, & EPA
    - – Develop/update Conceptual Site Model (incorporating new data)
    - – Review environmental impact pathways and regulatory context
    - – Quantify impacts of remaining source material
    - – Apply decision approach to determine path forward
  - Applied at Hanford
    - – Closure of 200-PW-1 OU SVE system for carbon tetrachloride (DOE, 2016)
- Key component was quantifying impacts
  - Tool for this step to facilitate decision making



Success!

CSM

Goals/ Pathways

Quantify

Decision Logic

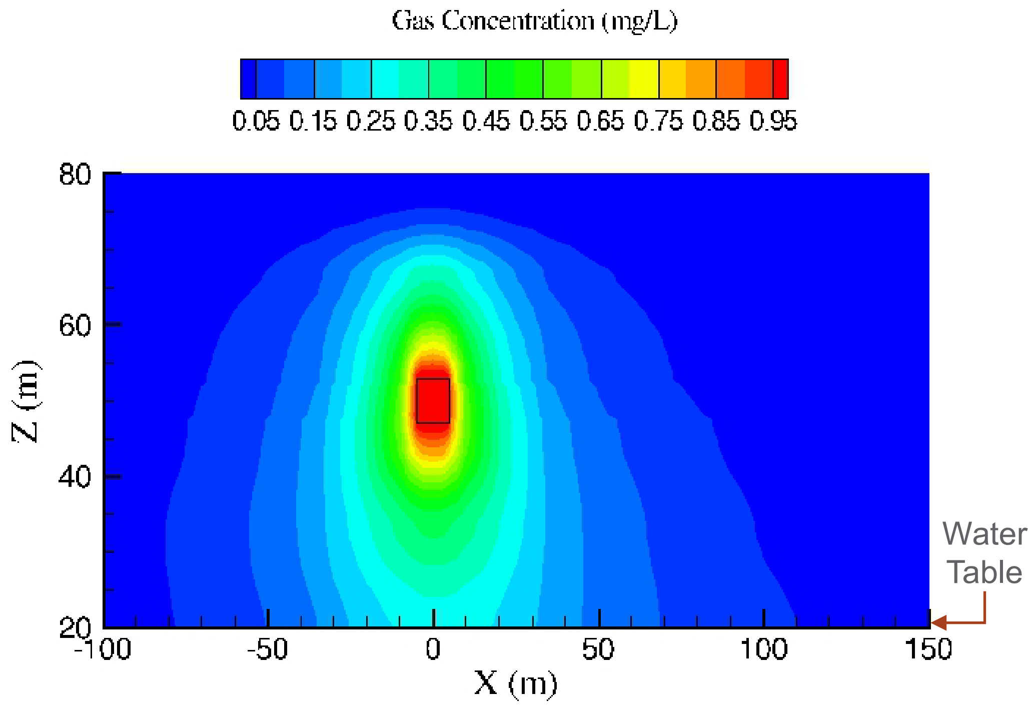
SVEET – Soil Vapor Extraction Endstate Tool

- SVEET – an existing, well-documented tool
  - Spreadsheet interface to access rigorous 3D numerical model results
    - Simple calculations using pre-modeled results (does not run simulations)
  - Estimates VOC concentrations at a distance from a defined source
  - Available at http://bioprocess.pnnl.gov/SVEET_Request.htm

- Tool use
  - Define site using structured framework
  - Tool accesses a lookup table of pre-modeled 3D simulation results
  - Tool interpolates and scales to provide site-specific results
  - Results are instantaneous
  - Easy to change the inputs for rapid sensitivity assessments

STOMP Code and Simulations

- STOMP (Subsurface Transport Over Multiple Phases)
- Fully-implicit, integrated, 3D, multi-phase, finite difference model
  - (White and Oostrom, 2006)
  - Water, organic compounds, and air
- Assumptions/configuration
  - The SVE process itself is not simulated
  - Vadose zone source is constant (no source depletion)
    - Immobile, organic, liquid-phase source
  - Transport simulations conducted until steady-state conditions reached
    - Thus, effects of sorption can be neglected (Carroll et al., 2012)
  - Vapor-phase diffusive transport dominates



SVEET – Current Interface

- User friendly spreadsheet tool
  - Rapid calculation
  - Rigorous underlying basis
- Supports remedial decisions
  - Estimates impact of vadose zone contamination on groundwater at a point of compliance
  - Improved technical basis for better decision making
- Can be applied using readily available site data

SVE Endstate Tool (SVEET) — Version 1.0.0

Described in: *Soil Vapor Extraction System Optimization, Transition, and Closure Guidance* — 2012-Sep-24

Inputs

User Input					
	Scenario Name:	—	Case A	Case B	Case C
	Contaminant:	—	CT	TCE	TCE
T	Temperature:	[°C]	19.6	20	20
ω	Avg. Moisture Content:	[wt %]	8	1	1
R	Avg. Recharge:	[cm/yr]	0.5	0.5	0.5
VZT	Vadose Zone Thickness:	[m]	60	30	30
L1	Depth to Top of Source:	[m]	40	21	21
z	Source Thickness:	[m]	10	5	5
w (= l)	Source Width (= Length):	[m]	50	15	15
q	GW Darcy Velocity:	[m/day]	0.3	0.165	0.165
d	Distance to Compliance Well:	[m]	25	50	50
s	Compl. Well Screen Length:	[m]	5	10	10
	Source Strength Input Type:	—	Gas Concentration	Gas Concentration	Mass Discharge
C_{gs}	Source Gas Concentration:	[ppmv]	159	50	
$\dot{M}_{src}$	Source Mass Discharge:	[g/day]			10
Calculated Input					
STR	Source Thickness Ratio*:	[--]	0.167	0.167	0.167
SA	Areal Footprint of Source*:	[m²]	2500	225	225
RSP	Relative Source Position*:	[--]	4.00	5.25	5.25
L2	Distance – Source to GW:	[m]	10.00	4.00	4.00
H	Henry's Law Constant**:	[--]	0.890	0.263	0.263
Result – Estimated Groundwater Contaminant Concentration at Selected Compliance Well					
C_w	Final Groundwater Conc'n:	[µg/L]	16	15	31

Calcs.

Result

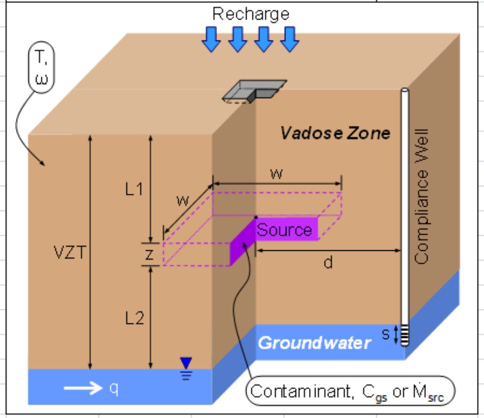
* See below for permissible ranges of intermediate calculated values.

** See the 'HLC' worksheet for details of the temperature-dependent calculation of H.

Parameter Name	Permissible Range	Key Values
T	10 - 30	20
ω	1 - 9 [a]	1, 5, 9 [a]
R	0.4 - 7.5 [b]	0.4
VZT	10 - 60	10, 30, 60
L1	varies [c]	—
z	varies [d]	—
w	10 - 50 [e]	—
q	0.005 - 0.3	0.005, 0.03, 0.3
d	10 [f], 25, 50, 75, 100	10, 25, 50, 75, 100
s	5 - 30	5
C_{gs}	1 - 2000	159
$\dot{M}_{src}$	0.1 - 5000	from STOMP simulations at 3 months elapsed time

See footnotes below.

Allow ω down to Sr = 0.05? FALSE



Parameter Name	Permissible Range	Key Values
STR	0.1 - 0.5	0.1, 0.25, 0.5
SA	100 - 2500	100, 400, 900, 2500
RSP	0.1 - 10	0.1, 1, 10
L2	0.5 - 49	—
H	contaminant-specific	0.89

[a] The pre-modeled scenarios actually use residual saturation (S_r), not gravimetric moisture content. However, for user convenience gravimetric moisture content is used as the input parameter. The key values for S_r were 0.05, 0.3, and 0.55, which correspond to moisture content values of 0.8078, 4.843, and 8.879, respectively. Again for convenience, the moisture content range is truncated at 1 wt% and extended to 9 wt%, although values at or above 8.879 wt% are treated as S_r values of 0.55.

[b] The applicability of the estimation approach used here should be confirmed for sites with recharge between 2.5 and 7.5 cm/yr. See Section 4.2.2.1 of the PNNL report entitled *Soil Vapor Extraction System Optimization, Transition, and Closure Guidance* for further discussion.

[c] The range for L1 is variable (with a maximum range of 0.5 - 49 m) because it is a function of the permissible range for RSP and the input values of z and VZT.

[d] The range for z is variable (with a maximum range of 1 - 30 m) because it is a function of the permissible range for STR and the input value of VZT.

[e] The range for w is a function of the permissible range for SA and the square footprint of the source area.

[f] The source width must be less than or equal to 20 m to use d = 10.

Notice | SVEET | HLC

Generalized Conceptual Model as a Framework for Analysis

Props.

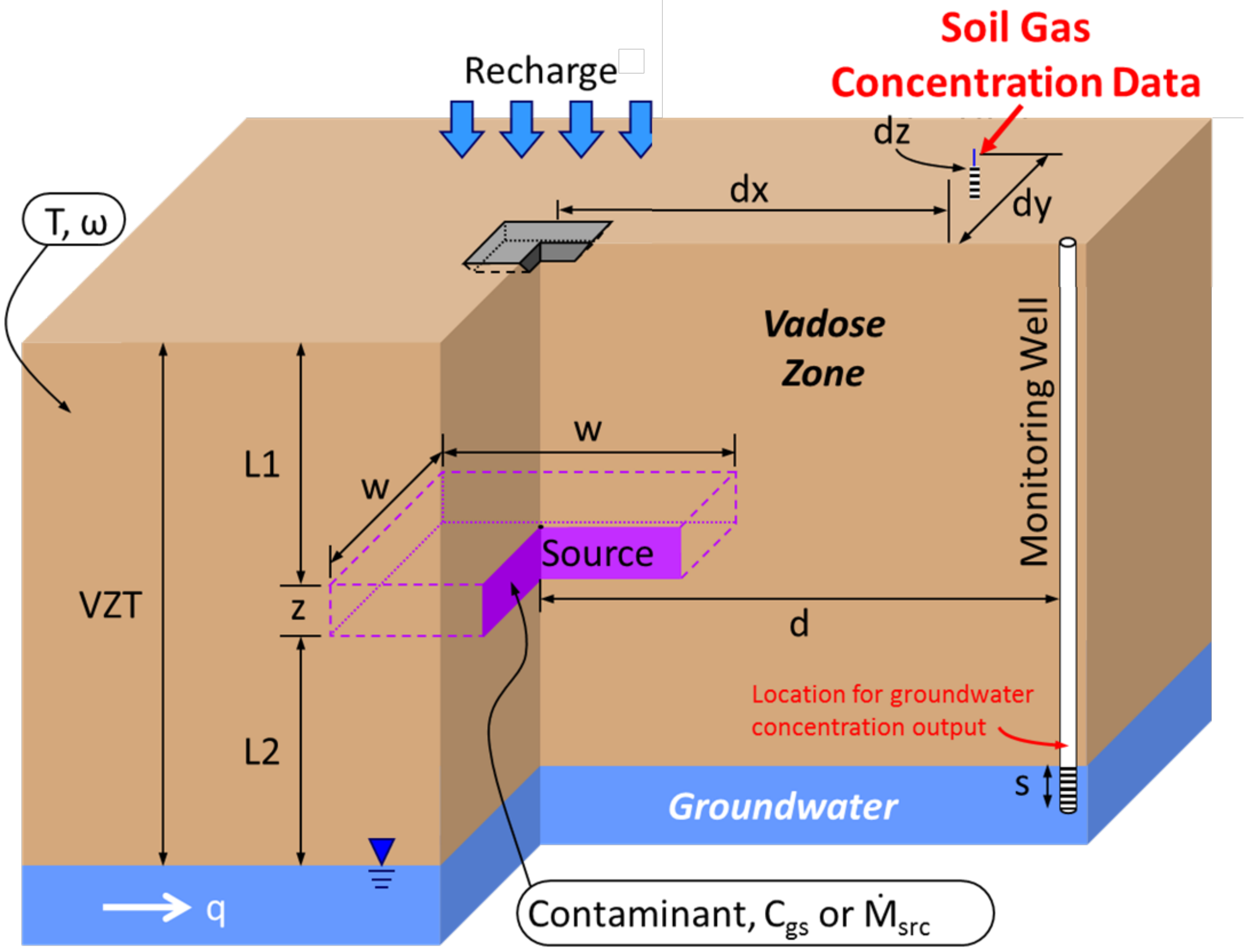
T	:	temperature
ω	:	moisture content
q	:	groundwater Darcy flux

Dimensions

VZT	:	vadose zone thickness
RSP	:	relative source position = L1 / L2
STR	:	source thickness ratio = z / VZT
SA	:	source area footprint = w × w
d	:	horizontal distance from source center to compliance well
s	:	screen length
dx, dy, dz	:	distance to soil gas location

Source Strength

C_{gs}	:	vapor concentration of the source area
$\dot{M}_{src}$	:	source vapor mass discharge



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ESTCP Project for Updating/Expanding SVEET

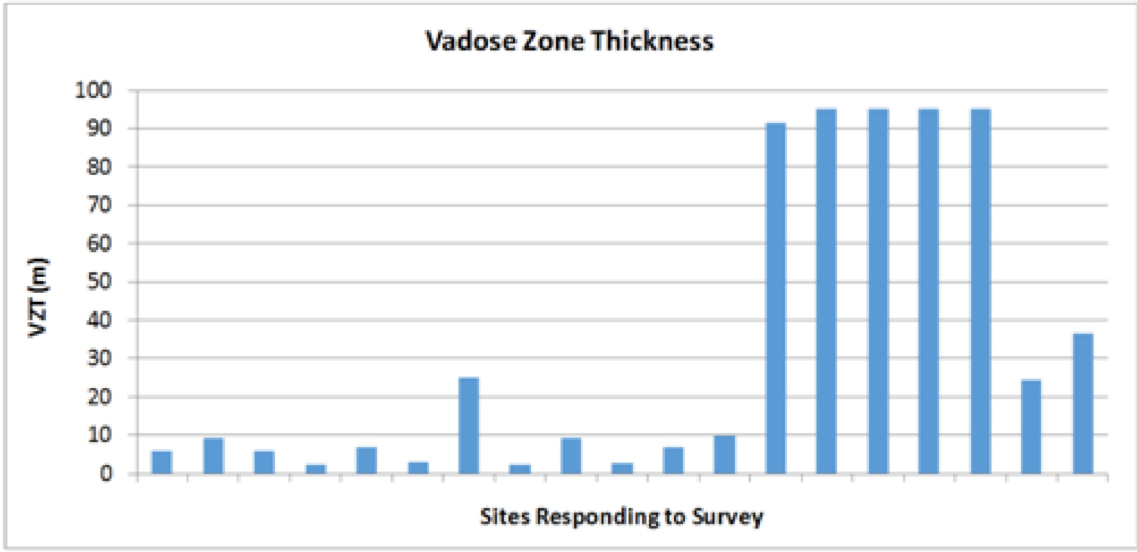
- DoD has many sites
  - wider range of characteristics than permissible SVEET inputs
- Elements of the update
  - Additional contaminants
  - Expanded parameter ranges
  - Refined input structure / user interface
    - Soil gas items, expanded ranges, etc.
  - Expanded output options
    - GW concentration at user-specified downgradient distance
    - Vadose zone gas concentration (for vapor intrusion evaluations)
- Field Demonstration
  - Ground-truthing the SVEET results
  - Assess applicability / usability

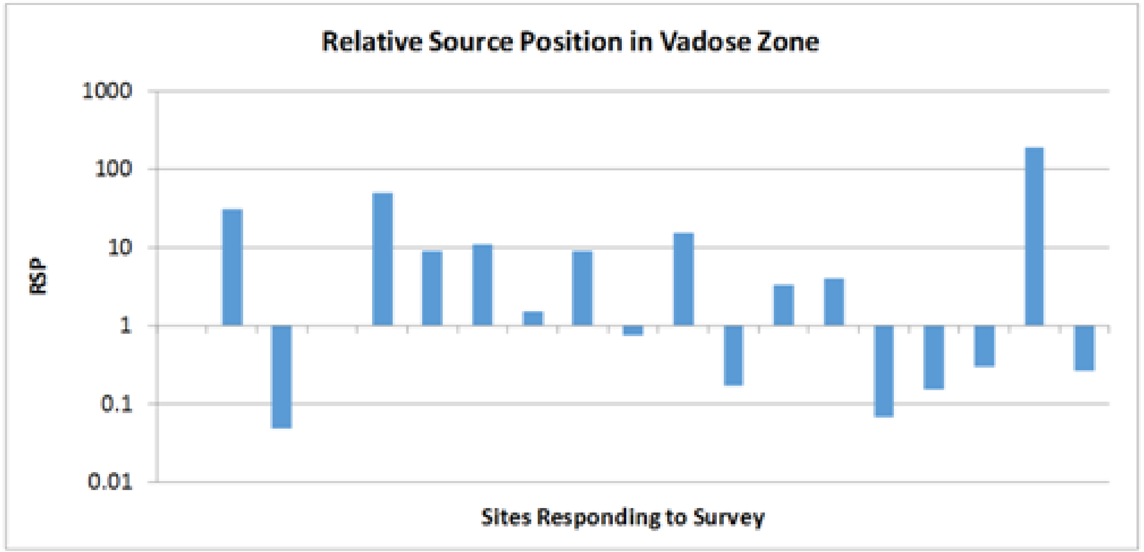
Partial List:

Current Element	Update
Contaminants: Chloroform, Dichloromethane, Chloromethane, Chloroethane, Vinyl Chloride, Tetrachloroethene, Trichloroethene, 1,1-Dichloroethene Carbon Tetrachloride, cis-1,2-Dichloroethene, trans-1,2-Dichloroethene, 1,1,1,2-Tetrachloroethane, 1,1,2,2-Tetrachloroethane, 1,1,1-Trichloroethane, 1,1,2-Trichloroethane, 1,1-Dichloroethane, 1,2-Dichloroethane	Add these contaminants: 1,2,3-Trichloropropane Dichloropropane isomers Chlorobenzene BTEX constituents/generic TPH Freons (11, 12, 113) 1,4-Dioxane Acetone, MTBE, MEK, MIBK
GW Monitoring Well Locations for Output: 10, 25, 50, 75 and 100 m downgradient along groundwater flow centerline from source area	Allow user-specified distance ≤ 950 m, along centerline
Vadose Zone Soil Gas Concentrations for Output: *Not a SVEET output (but available in VIETUS)*	Allow user-specified lateral location & depth of 1 or 4 m (for sub-slab or basement)
Relative Water Saturation (Moisture Content): 0.05 – 0.55 (1 – 9 wt%)	0.05 – 0.75 (1 – 12 wt%) Allows wetter conditions
Vadose Zone Thickness: 10 – 60 m	3 – 150 m Allows thinner/thicker vadose
Source Thickness Ratio: 0.1 – 0.5	0.1 – 0.75 Allows a thicker source zone
Relative Source Position: 0.1 – 10	0.1 – 50 Allows source closer to GW
Source Footprint (square): 100 – 2500 m²	100 – 10,000 m² Allows bigger source area

Survey of DoD RPMs

- Surveyed remedial project managers regarding their SVE sites
- Found widespread interest and need for the tool
- Identified parameters needing expanded permissible ranges
- Improvements will make SVEET a useful tool at a majority of sites





Example Survey Results

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Expansion of Permissible Parameter Ranges

- Expand ranges to address DoD site characteristics, as identified from survey
- Full matrix of permutations is 7680 simulations
  - Exclude unlikely scenarios → 5760 simulations
  - Completed using PNNL supercomputer

Parameter	Evaluation Points as the Basis for Interpolation					
Residual Moisture Saturation		0.05	0.3	0.55	**0.75**	
Source Thickness Ratio		0.1	0.25	0.5	**0.75**	
Vadose Zone Thickness	**3**	10	30	60	**110**	**150**
Source Area (m^2)		100	400	900	2,500	**10,000**
Groundwater Velocity (m/day)		0.005	0.03	0.3	**1**	
Relative Source Position		0.1	1	10	**50**	

E.g., unlikely would be a 110 m thick vadose zone with 75% of thickness as source area

Simulation Results – Groundwater Concentrations

- Examples of the variation in simulation results
- Looking at bounding cases changing a single parameter
  - Soil moisture
  - Source thickness ratio
  - Relative source position
  - Groundwater Darcy velocity

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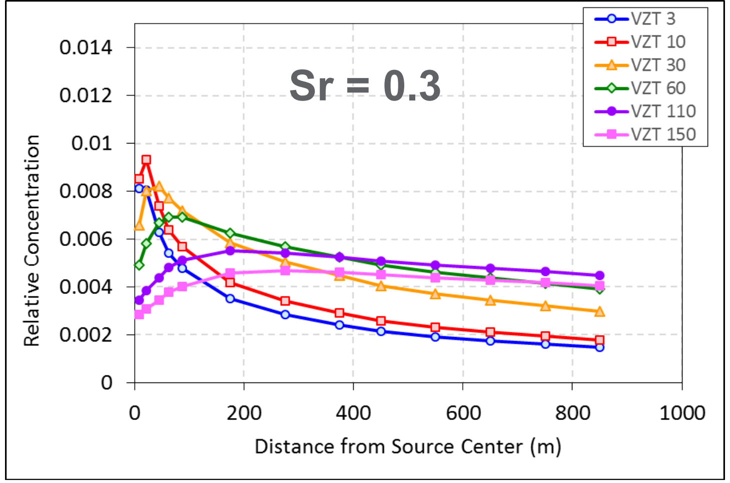
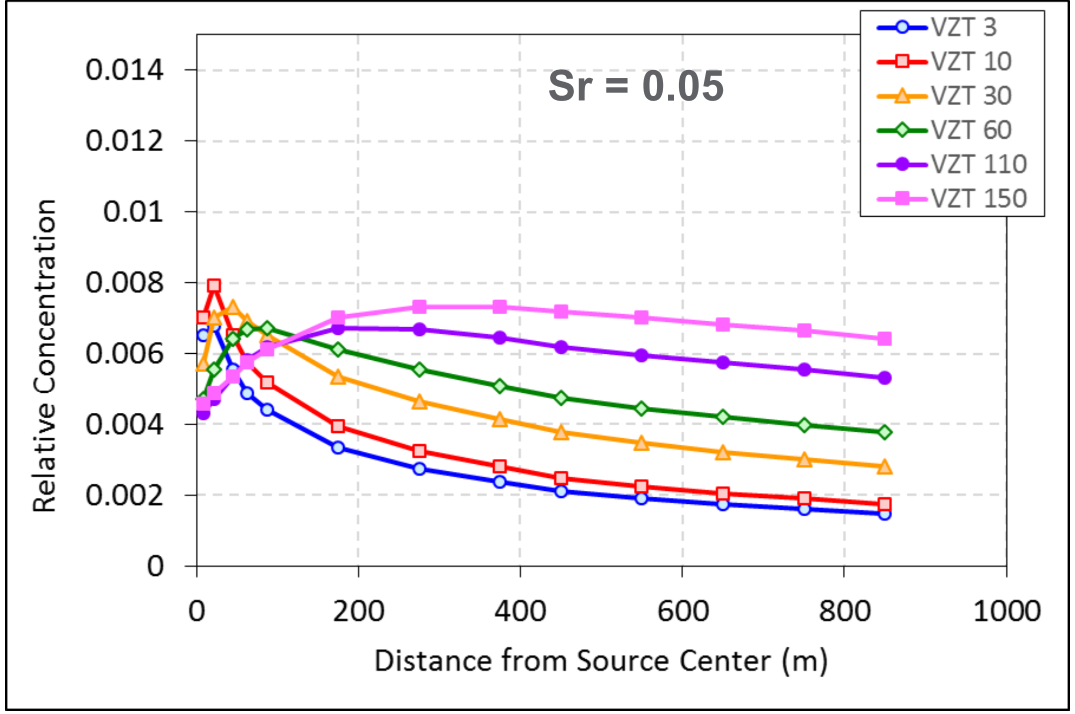


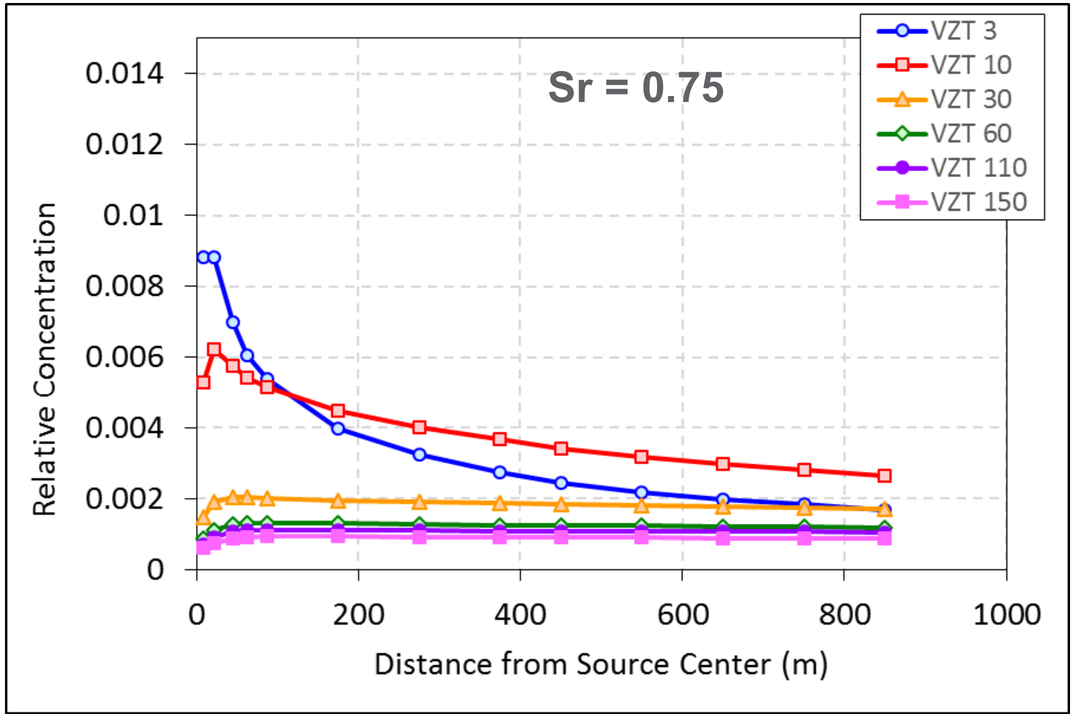
Base Case

Sr	0.3 %	q	0.3 m/d
STR	0.25	SA	900 m²
RSP	1	screen	9 m



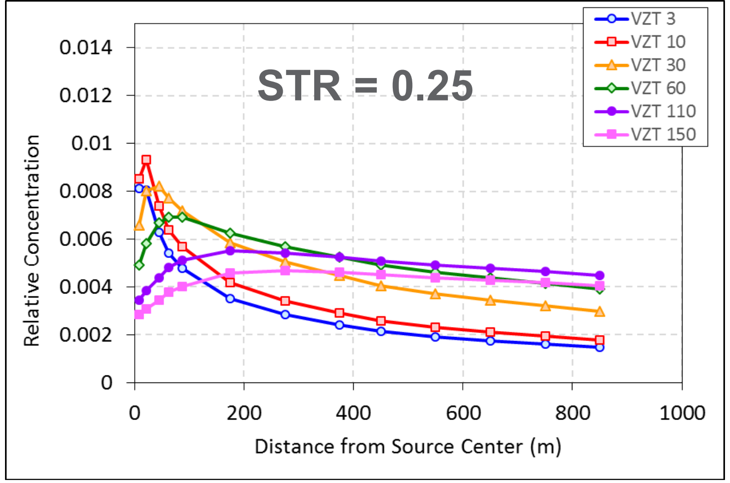
Residual Saturation (Sr)

- Increasing moisture content decreases pore space for vapor diffusion
  - Less mass transfer into groundwater



Source Thickness Ratio (STR)

- Thicker sources have more diffusion out the sides of the source
- STR has small impact on groundwater concentration for the same downgradient distance



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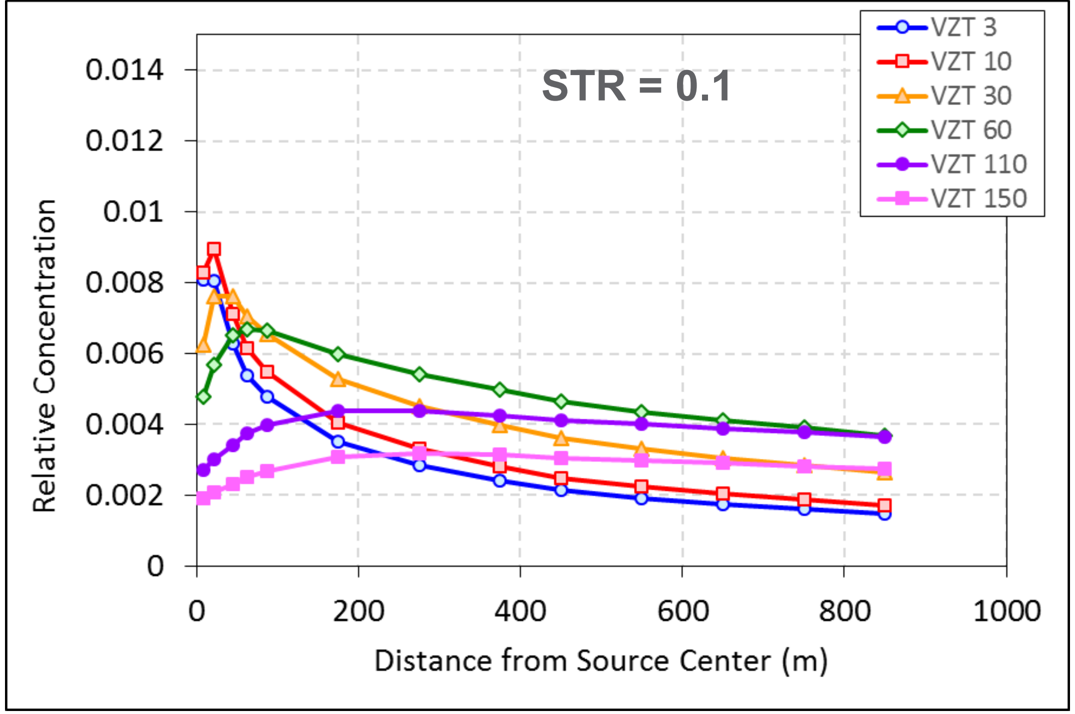

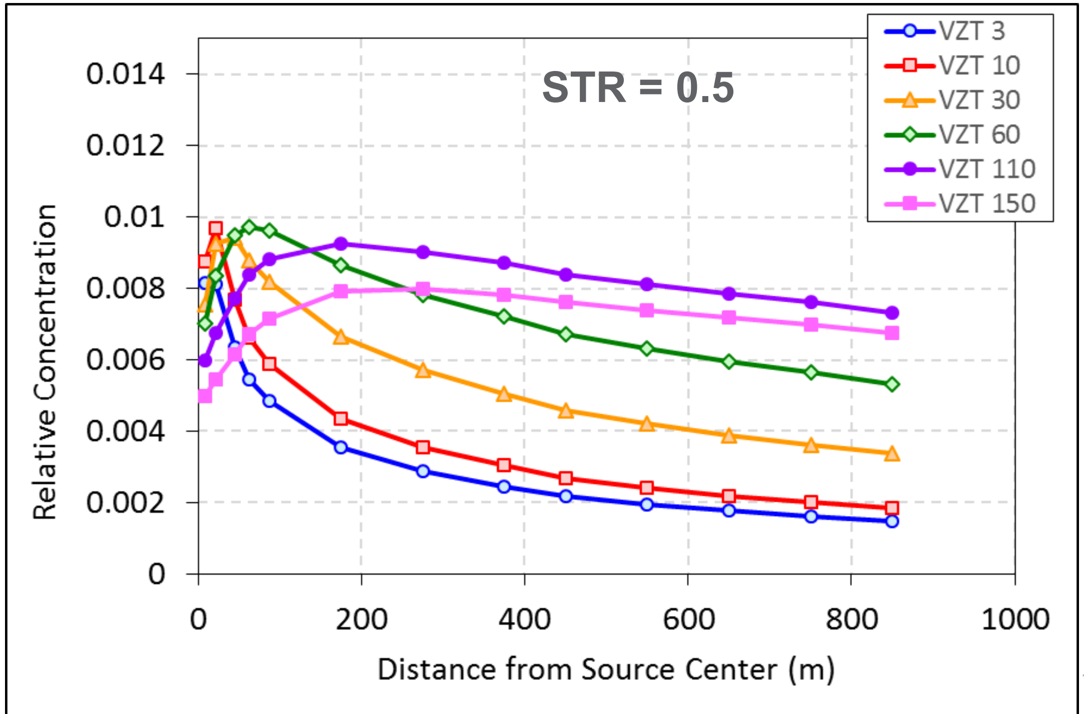

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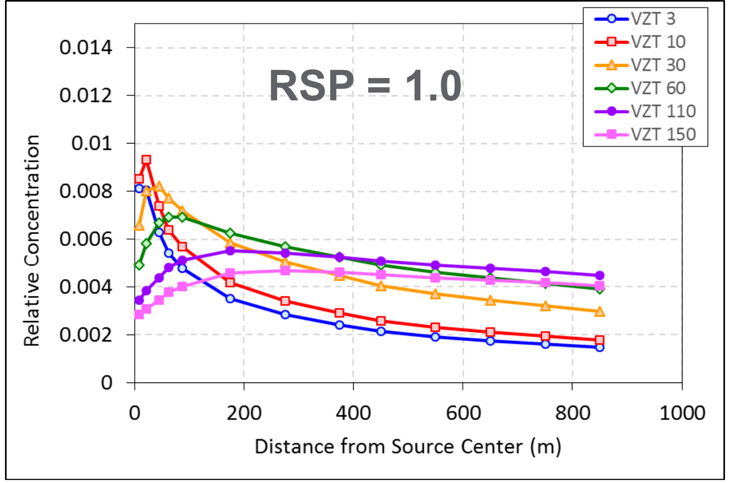

Base Case

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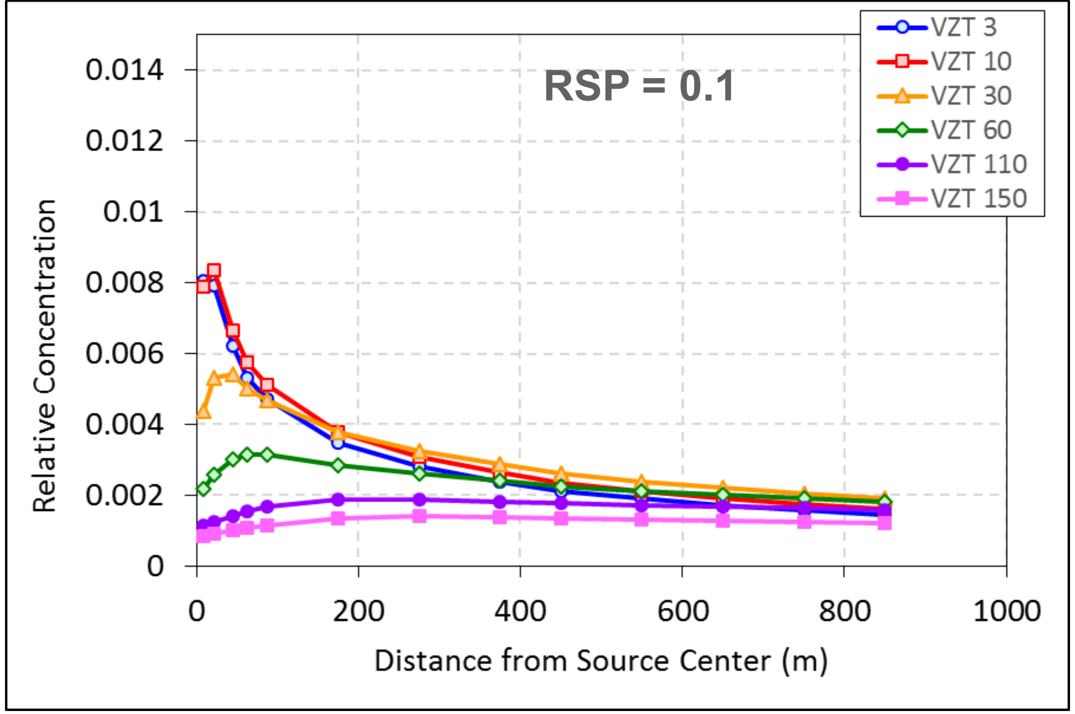
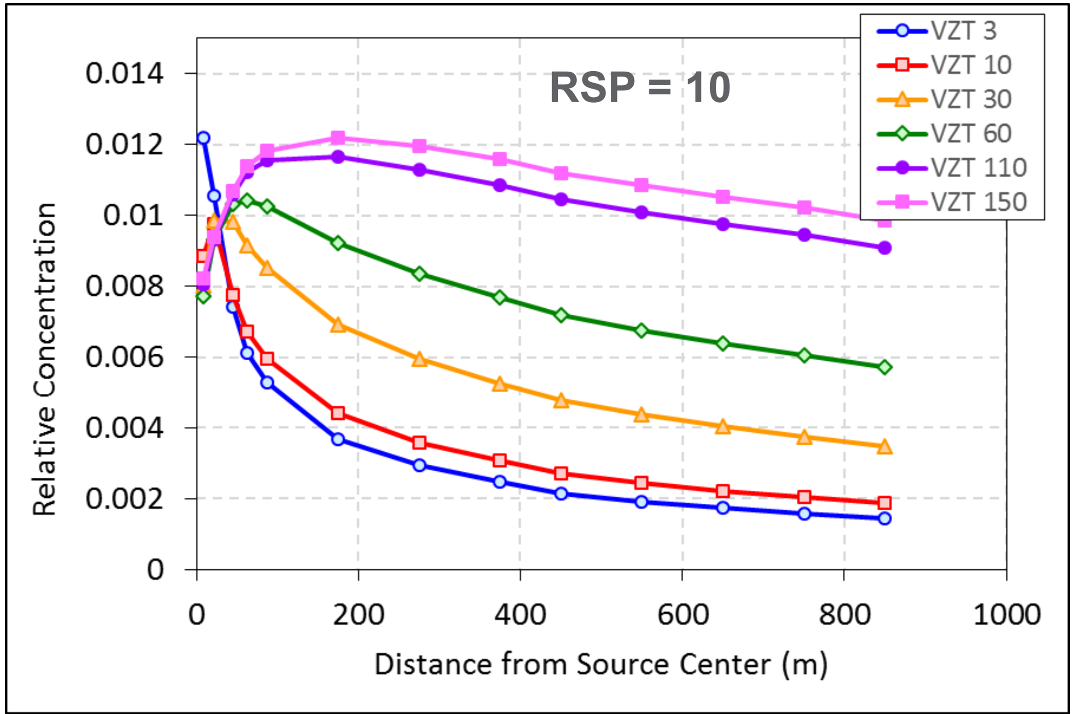
STR	0.25	SA	900 m²
RSP	1	screen	9 m

Relative Source Position (RSP)

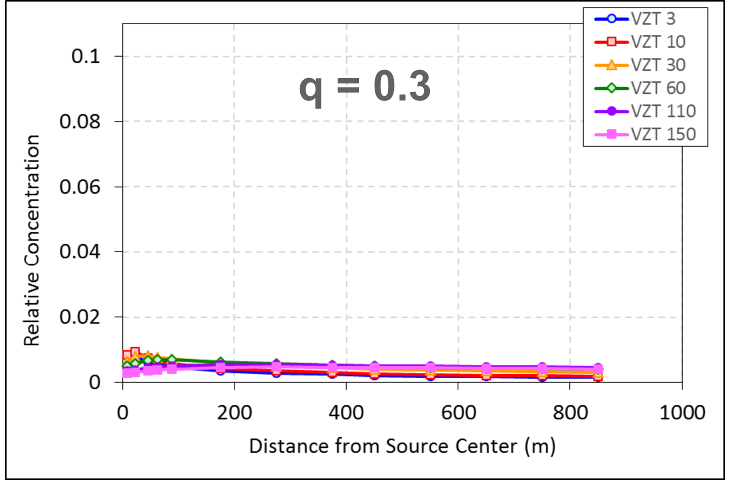
- Near-surface sources lose more mass to atmosphere
- Near-groundwater sources transfer more mass into the groundwater





Groundwater Darcy Velocity (q)

- Groundwater flow has a significant effect on amount of diffusional mass transfer
  - High flow has much less mass transfer
  - Low flow rate has much more mass transfer



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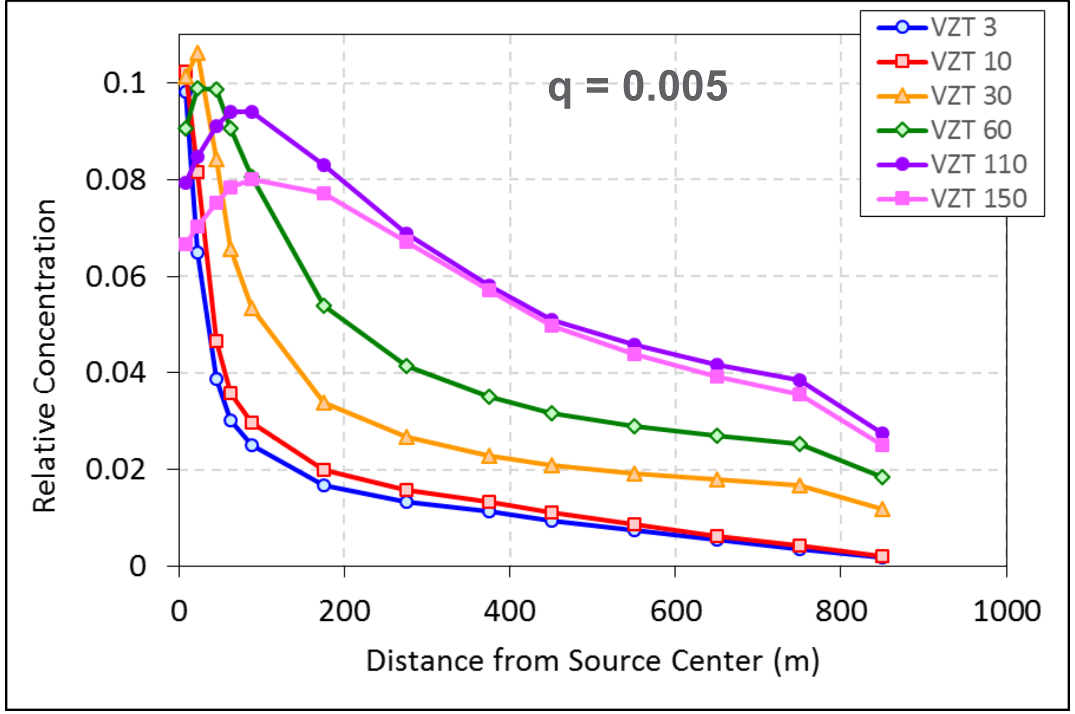
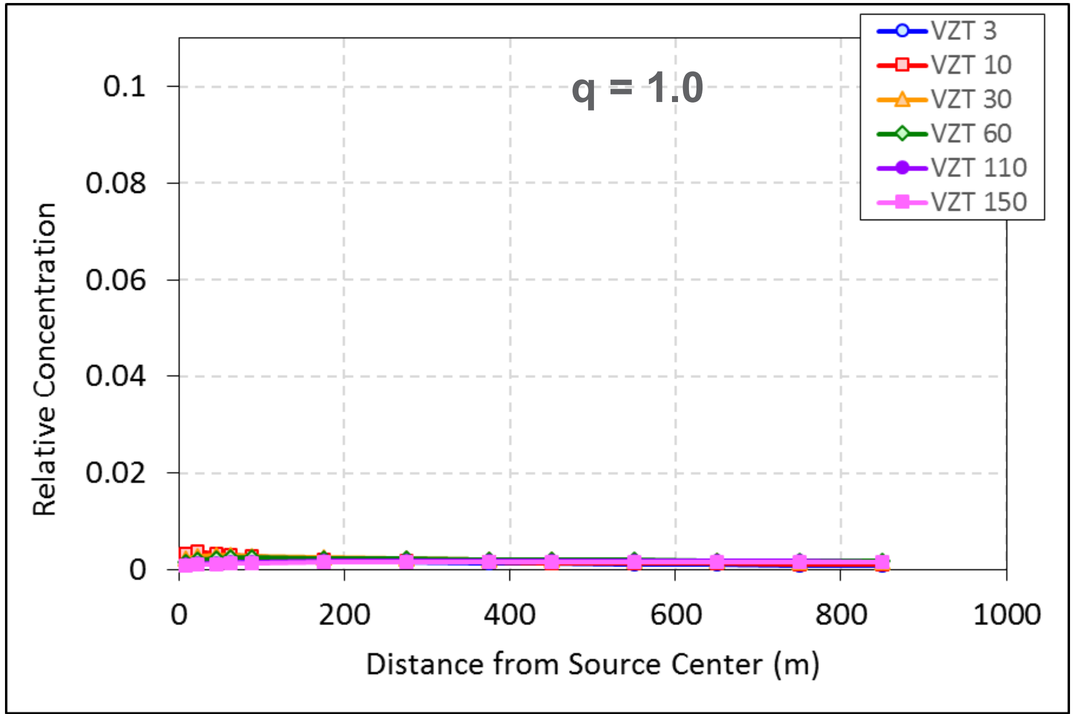
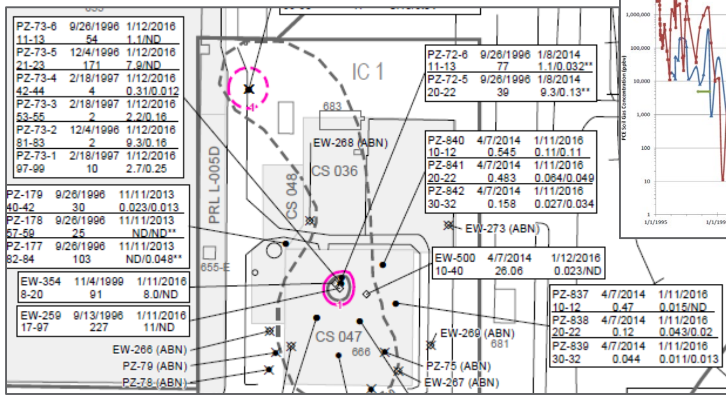
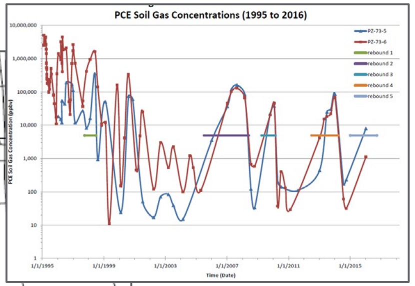


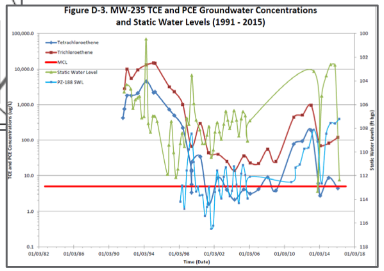


Ongoing Work: Field Demonstration for Ground Truthing Examples

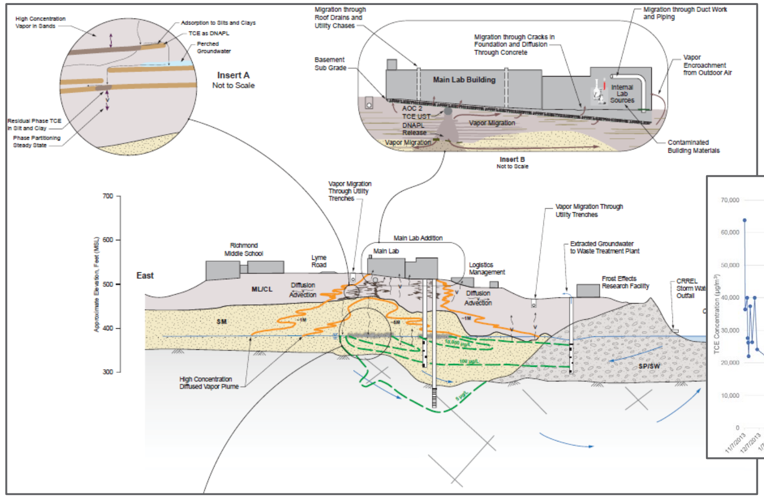
- McClellan IC1
  - ~25 years of data
  - 20 years of SVE with 6 significant rebound tests
  - Site closed VLEACH and MT3D used for support

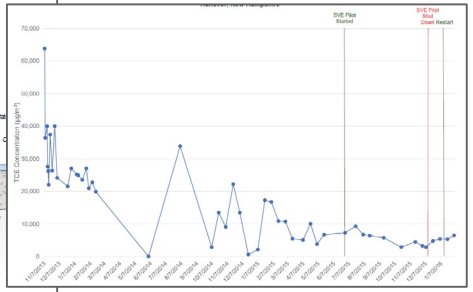






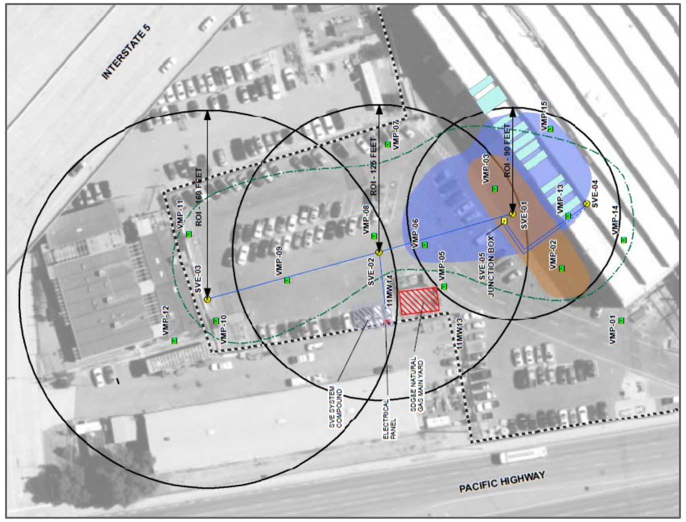
- Cold Regions Lab (CREEL)
  - Very well characterized
  - SVE ~2 years
  - Pre-SVE data available
  - No DNAPL in groundwater
  - Vapor Intrusion Issues

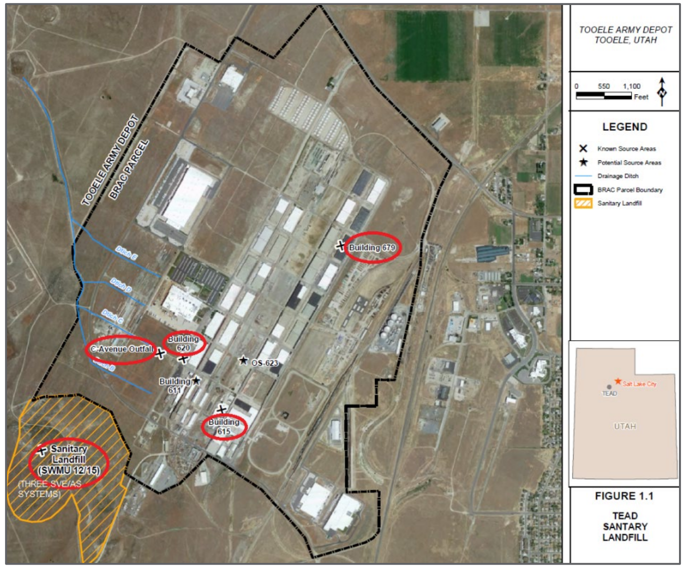




Ongoing Work: Field Demonstration for Applicability / Implementation

- SPAWAR, IR Site 11
  - 3 years of SVE operation
    - Extensive data, soil vapor, & groundwater
  - Site conducting additional characterization and assessment
  - Interested in SVEET with VI component
- Tooele (TEAD) Landfill Site
  - Depth to water 285 feet (87 m)
  - SVE to continue until no impact to groundwater (RCRA site)
  - SVE operated beginning in early 2013
    - Removal has greatly reduced contamination
    - Costs to operate ~400K/yr
  - Tooele has 4 other nearby candidate sites
    - Costs to operate ~270K/yr





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Conclusions

- SVEET is a useful tool
  - Estimate long-term impacts of a vadose zone source
    - On groundwater and soil gas concentrations
- Concentration estimates support decisions
  - Input for decisions about SVE termination, optimization, or transition
  - Provides transport estimates needed to support remedial decisions
  - Cost savings over continued operations that provide little benefit
- Current work expands range of permissible parameter values
  - Applicable to more sites
- Uncertainty in site parameters…
  - Testing parameter significance is quick and easy
  - Can determine where additional data would be most useful

References

SVEET Website: http://bioprocess.pnnl.gov/SVEET_Request.htm
(has v. 1.0 currently; v. 2.0 is targeted for October, 2019)

- Truex, M.J., D.J. Becker, M.A. Simon, M. Oostrom, A.K. Rice, and C.D. Johnson. 2013. *Soil Vapor Extraction System Optimization, Transition, and Closure Guidance*. PNNL-21843, Pacific Northwest National Laboratory, Richland, Washington. (Avalable at the website above.)
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