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Development of a Decision Support Tool for Vadose Zone Remediation of Volatile Contaminants

January 20, 2021

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Welcome and Introductions

Cara Patton, PMP
Noblis

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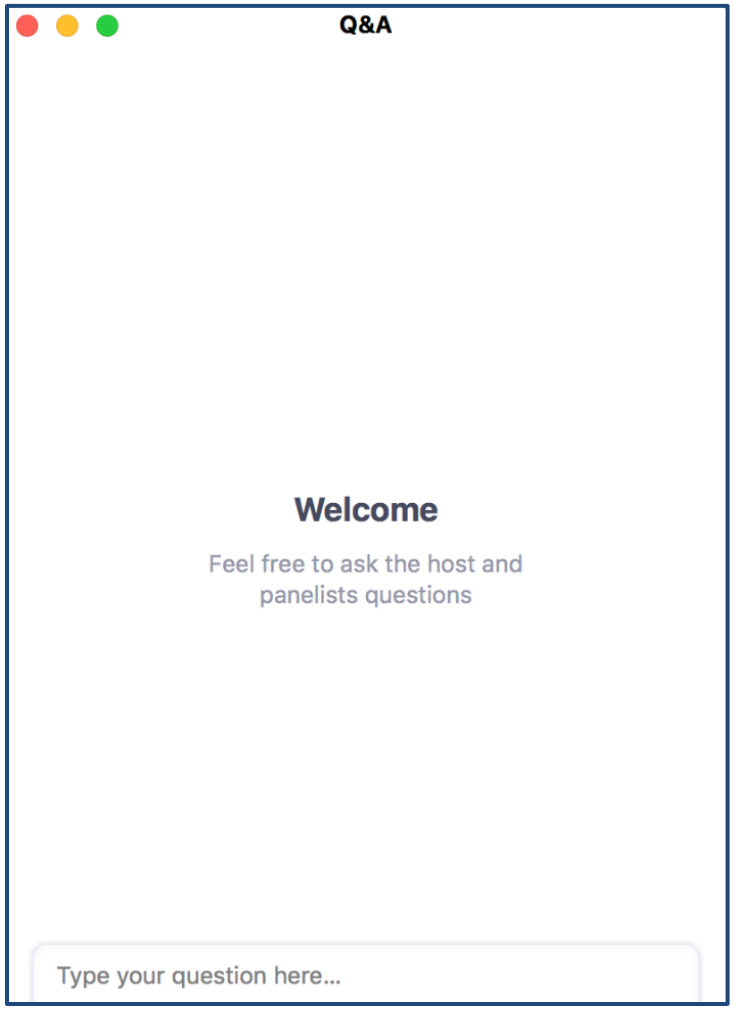

Decision Support Tool for Vadose Zone Remediation of Volatile Contaminants

Jovan Popovic
NAVFAC EXWC

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Team for ESTCP Project ER-201731

- NAVFAC EXWC
  - Jovan Popovic
- Pacific Northwest National Laboratory
  - Christian Johnson, Katherine Muller
- U.S. Army Corps of Engineers
  - David Becker, Carl Harms
- Former Team members
  - Rob Hinchee
  - Guzel Tartakovsky, Michael Truex, Mart Oostrom (PNNL)
  - Tim Appleman, Jennifer Segura (NAVFAC EXWC)

Decision Support Tool for Vadose Zone Remediation of Volatile Contaminants

Christian Johnson
Pacific Northwest National Laboratory

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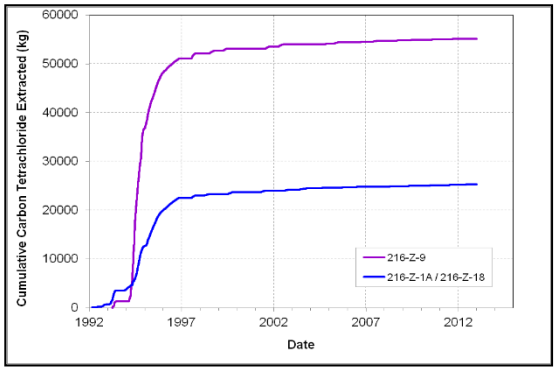
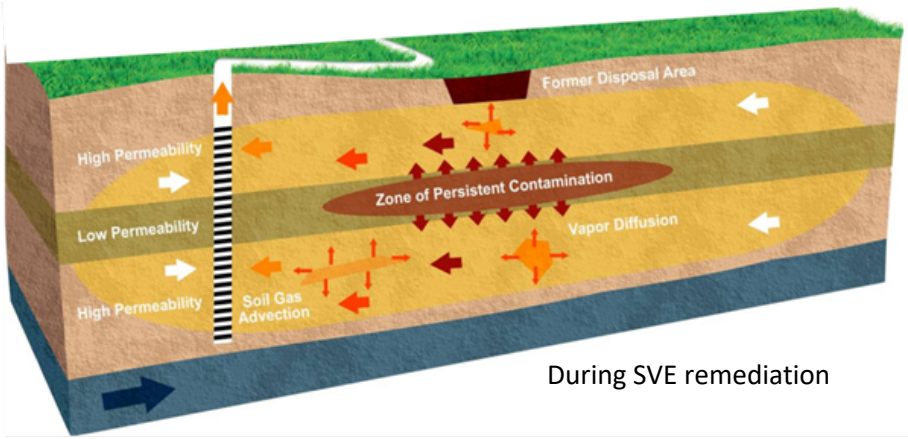
Agenda

- Soil vapor extraction performance assessment
- Project objectives
- Description of SVEET2
- SVEET2 Updates/Interface
- SVEET2 Demonstration
- Cost Savings
- Takeaways/Benefits

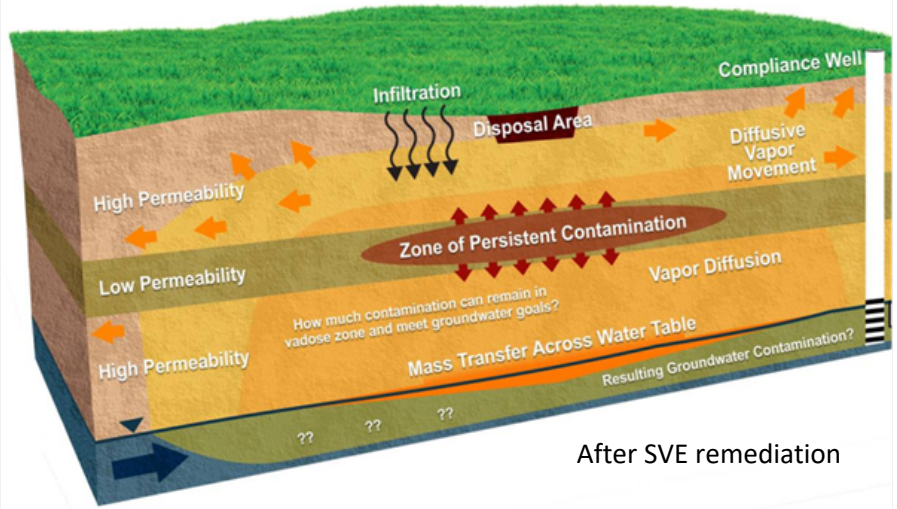
Soil Vapor Extraction (SVE)

- Effectively removes contaminant vapors
  - Typically, cannot remove all contaminant mass
    - Diminishing returns





During SVE remediation



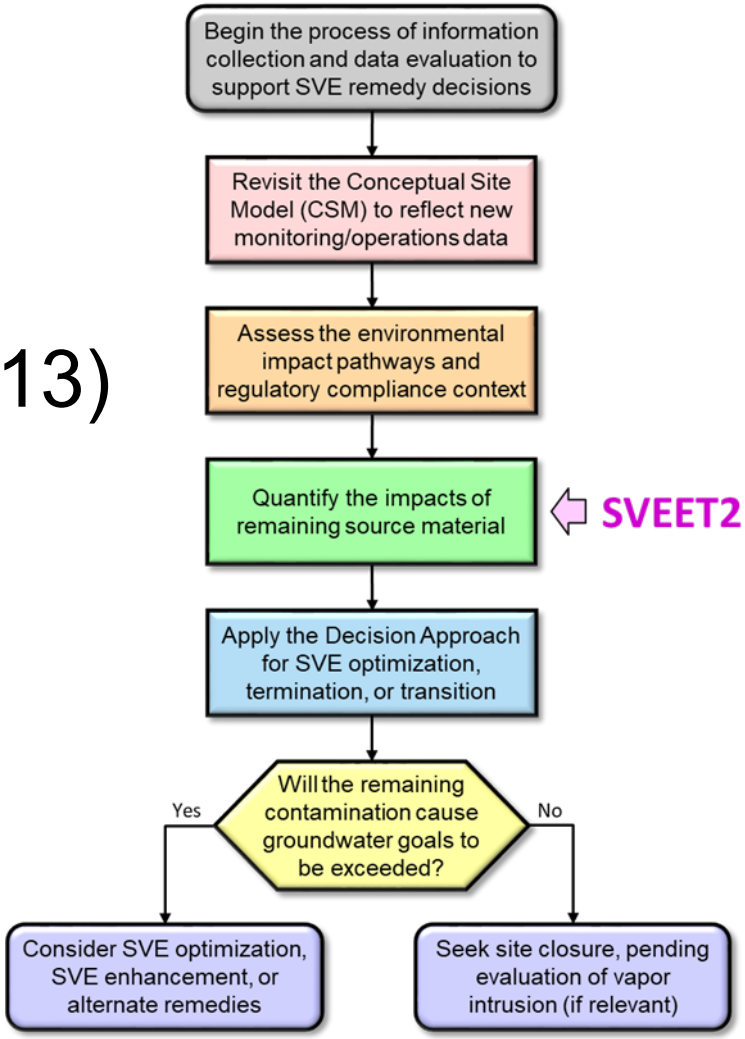
After SVE remediation

Typical Remediation Questions

- Is SVE needed?
  - Does the source pose a risk to groundwater or via vapor intrusion?
- What are the SVE performance goals?
  - For new or operating system
  - What mass flux from contaminated zone or soil vapor concentration is acceptable?
- Can SVE be terminated?
  - Will the remaining mass represent a threat?
- Can alternative technologies address the remaining mass?
  - Cost effectiveness of active SVE in question

SVE Performance Assessment

- *Soil Vapor Extraction System Optimization, Transition, and Closure Guidance* (Truex et al., 2013)
  - Structured approach
    - Gather/update information
    - Quantify impacts
    - Apply decision logic
  - SVEET2 is a companion tool for quantification



ESTCP Project Objectives

- Provide DoD with a widely applicable tool to support assessment of volatile contaminant remediation in the vadose zone
  - Update to expand the permissible range of inputs
    - Enhanced functionality and acceptability for DoD applications
  - Support remediation decisions (optimization, site closure, transition to another remedy)
    - For groundwater protection and potential vapor intrusion
- Demonstrate the tool (verification and usability)
- Provide basis for potentially significant reductions in DoD's cost to complete

Brief Description of SVEET2

- Soil Vapor Extraction End-state Tool (v. 2)
- User-friendly spreadsheet tool
  - Input a small number of site parameters
  - Estimates contaminant concentrations in groundwater and soil gas
    - Result of a vadose zone contaminant source
- Rigorous underlying basis
  - 5760 STOMP numerical simulations (pre-modeled scenarios)
  - Contaminant transport under natural conditions
  - Includes vapor-phase diffusion, recharge-driven processes, and mixing into groundwater
- SVEET2 itself is not a numerical model
  - Interpolates between pre-modeled scenarios
  - Scales for parameters with linear relationship

SVEET2 for Decision Support

- Help site managers make decisions about vadose zone remediation
  - Initiate, continue, optimize, terminate, or transition to another remedy
- Provides defensible estimate of contaminant transport as a basis for supporting remedy decisions

SVEET2 Assumptions

- Vapor-phase transport dominates vadose zone contaminant movement
  - But recharge-driven transport is accounted for
- Groundwater is initially uncontaminated
- Contaminant source can be represented as a single source area
- Homogeneous subsurface with uniform properties
- Steady-state / equilibrium site conditions
- Constant strength vadose zone source
  - No source depletion
- Well screen starts at the water table

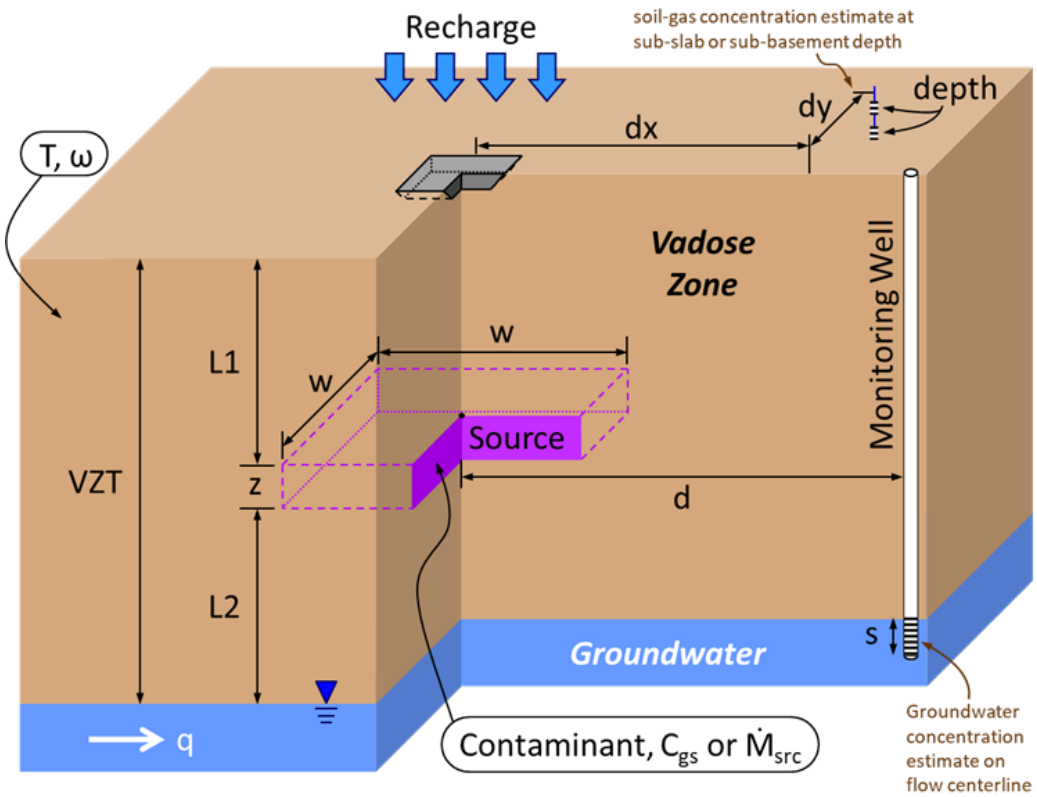
Not Included in SVEET2

- Adsorption
- Biological reactions/degradation
- Off-centerline groundwater concentration estimates

- Thus, SVEET2 is generally conservative
  - Favors higher concentration estimates
  - Appropriate for predictive applications in support of decision making

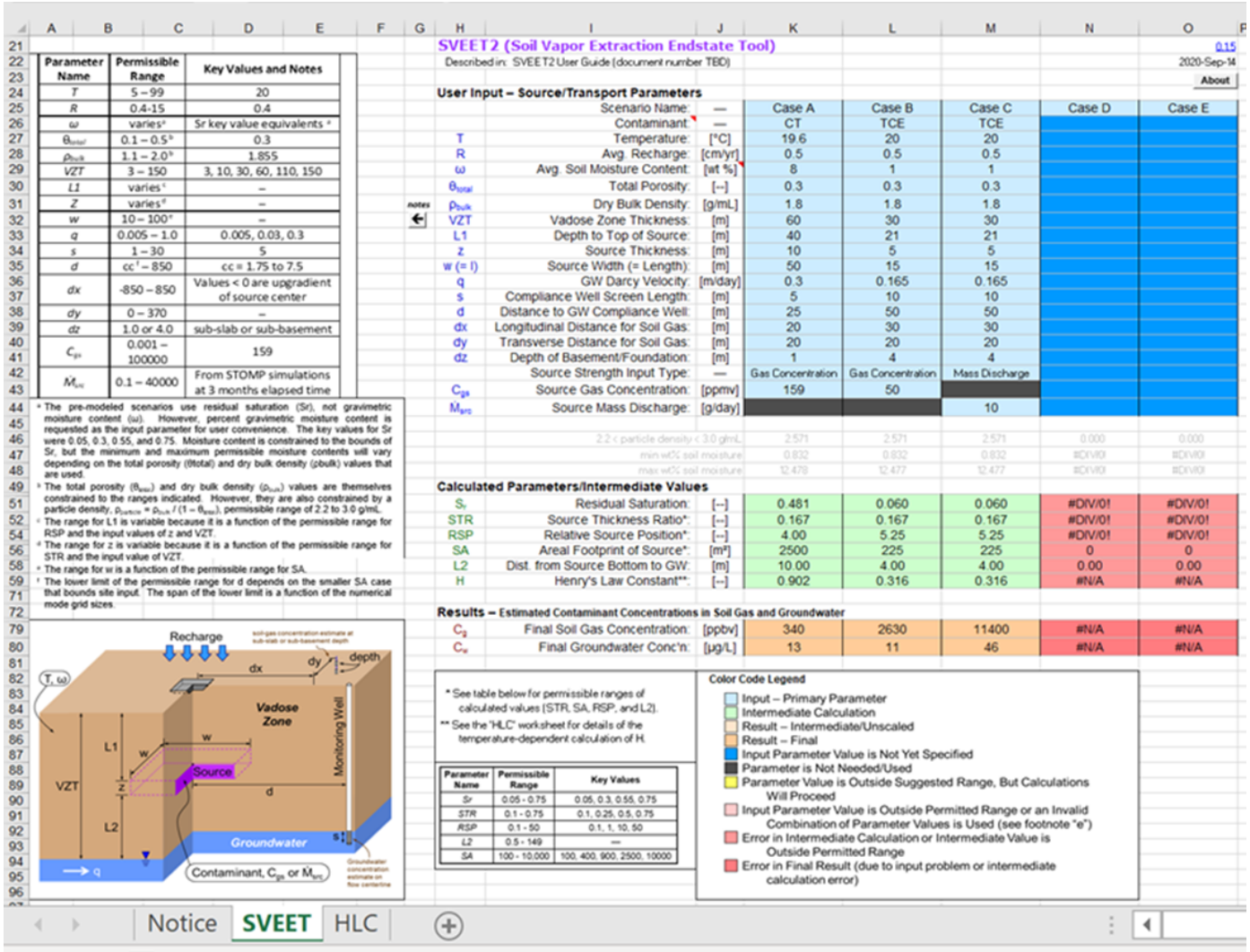
Generalized Conceptual Framework

- Conceptual framework for describing a site
- Based on prior work to determine controlling parameters



SVEET2 Interface

- Excel spreadsheet (xlsm)
- Up to 5 scenarios
- Errors and warnings flagged by cell color
- No results if inputs are invalid



Parameter Name	Permissible Range	Key Values and Notes
T	5 – 99	20
R	0.4-15	0.4
ω	varies[a]	Sr key value equivalents [a]
θ_{total}	0.1 – 0.5[b]	0.3
ρ_{bulk}	1.1 – 2.0[b]	1.855
VZT	3 – 150	3, 10, 30, 60, 110, 150
L1	varies[c]	--
Z	varies[d]	--
w	10 – 100[e]	--
q	0.005 – 1.0	0.005, 0.03, 0.3
s	1 – 30	5
d	cc[f] – 850	cc = 1.75 to 7.5
dx	-850 – 850	Values < 0 are upgradient of source center
dy	0 – 370	--
dz	1.0 or 4.0	sub-slab or sub-basement
C_{gs}	0.001 – 100000	159
$\dot{M}_{src}$	0.1 – 40000	From STOMP simulations at 3 months elapsed time

[a] The pre-modeled scenarios use residual saturation (Sr), not gravimetric moisture content (ω). However, percent gravimetric moisture content is requested as the input parameter for user convenience. The key values for Sr were 0.05, 0.3, 0.55, and 0.75. Moisture content is constrained to the bounds of Sr, but the minimum and maximum permissible moisture contents will vary depending on the total porosity (θtotal) and dry bulk density (ρbulk) values that are used.

[b] The total porosity (θ_{total}) and dry bulk density (ρ_{bulk}) values are themselves constrained to the ranges indicated. However, they are also constrained by a particle density, $\rho_{particle} = \rho_{bulk} / (1 - \theta_{total})$, permissible range of 2.2 to 3.0 g/mL.

[c] The range for L1 is variable 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 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.

[f] The lower limit of the permissible range for d depends on the smaller SA case that bounds site input. The span of the lower limit is a function of the numerical mode grid sizes.

SVEET2 (Soil Vapor Extraction Endstate Tool)

Described in: SVEET2 User Guide (document number TBD)

0.15

2020-Sep-14

About

User Input – Source/Transport Parameters

			Case A	Case B	Case C	Case D	Case E
	Scenario Name:	—	Case A	Case B	Case C	Case D	Case E
	Contaminant:	—	CT	TCE	TCE		
T	Temperature:	[°C]	19.6	20	20		
R	Avg. Recharge:	[cm/yr]	0.5	0.5	0.5		
ω	Avg. Soil Moisture Content:	[wt %]	8	1	1		
θ_{total}	Total Porosity:	[--]	0.3	0.3	0.3		
ρ_{bulk}	Dry Bulk Density:	[g/mL]	1.8	1.8	1.8		
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		
s	Compliance Well Screen Length:	[m]	5	10	10		
d	Distance to GW Compliance Well:	[m]	25	50	50		
dx	Longitudinal Distance for Soil Gas:	[m]	20	30	30		
dy	Transverse Distance for Soil Gas:	[m]	20	20	20		
dz	Depth of Basement/Foundation:	[m]	1	4	4		
	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		
	2.2 < particle density < 3.0 g/mL		2.571	2.571	2.571	0.000	0.000
	min wt% soil moisture		0.832	0.832	0.832	#DIV/0!	#DIV/0!
	max wt% soil moisture		12.479	12.477	12.477	#DIV/0!	#DIV/0!

Calculated Parameters/Intermediate Values

S_r	Residual Saturation:	[--]	0.481	0.060	0.060	#DIV/0!	#DIV/0!
STR	Source Thickness Ratio*:	[--]	0.167	0.167	0.167	#DIV/0!	#DIV/0!
RSP	Relative Source Position*:	[--]	4.00	5.25	5.25	#DIV/0!	#DIV/0!
SA	Areal Footprint of Source*:	[m²]	2500	225	225	0	0
L2	Dist. from Source Bottom to GW:	[m]	10.00	4.00	4.00	0.00	0.00
H	Henry's Law Constant**:	[--]	0.902	0.316	0.316	#N/A	#N/A

Results – Estimated Contaminant Concentrations in Soil Gas and Groundwater

C_g	Final Soil Gas Concentration:	[ppbv]	340	2630	11400	#N/A	#N/A
C_w	Final Groundwater Conc'n:	[µg/L]	13	11	46	#N/A	#N/A

* See table below for permissible ranges of calculated values (STR, SA, RSP, and L2).

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

Parameter Name	Permissible Range	Key Values
Sr	0.05 - 0.75	0.05, 0.3, 0.55, 0.75
STR	0.1 - 0.75	0.1, 0.25, 0.5, 0.75
RSP	0.1 - 50	0.1, 1, 10, 50
L2	0.5 - 149	---
SA	100 - 10,000	100, 400, 900, 2500, 10000

Color Code Legend

- Input – Primary Parameter
- Intermediate Calculation
- Result – Intermediate/Unscaled
- Result – Final
- Input Parameter Value is Not Yet Specified
- Parameter is Not Needed/Used
- Parameter Value is Outside Suggested Range, But Calculations Will Proceed
- Input Parameter Value is Outside Permitted Range or an Invalid Combination of Parameter Values is Used (see footnote "e")
- Error in Intermediate Calculation or Intermediate Value is Outside Permitted Range
- Error in Final Result (due to input problem or intermediate calculation error)

Notice | SVEET | HLC

Updates for SVEET2

- Range of updates to improve usability and applicability
  - New contaminants
  - More scenarios
  - Flexible groundwater well locations
  - Soil gas output
  - Increased permissible ranges
    - Source concentration
    - Recharge
    - Sr
    - VZT
    - RSP
    - SA
    - q
  - Can specify porosity and bulk density

SVEET v. 1.-	SVEET2
Contaminants: Chloroform, Carbon Tetrachloride Dichloromethane, cis-1,2-Dichloroethene Chloromethane, trans-1,2-Dichloroethene Chloroethane, 1,1,1,2-Tetrachloroethane Vinyl Chloride, 1,1,2,2-Tetrachloroethane Tetrachloroethene, 1,1,1-Trichloroethane Trichloroethene, 1,1,2-Trichloroethane 1,1-Dichloroethene, 1,1-Dichloroethane 1,2-Dichloroethane	Added these contaminants: 1, 2-Dichloropropane, 1, 3-Dichloropropane 1,2,3-Trichloropropane, MIBK MTBE, MEK Chlorobenzene, BTEX constituents Freons (11, 12, 113), 1,4-Dioxane Note: biodegradation effects are not included in SVEET v. 1.0 or SVEET2.
Input/Output Structure: 3 concurrent scenarios are allowed	Allow 5 concurrent scenarios
GW Monitoring Well Locations for Output: 10, 25, 50, 75 and 100 m downgradient along groundwater flow centerline from source area	Allow any user-specified distance ≤ 850 m, along centerline
Vadose Zone Soil Gas Concentrations for Output: Not a SVEET output (but available in VIETUS)	Allow user-specified lateral location (-850 to 850 m in x direction, 0 to 370 m in y direction) and depth of 1 or 4 m (for sub-slab or basement)
Source Gas Concentration: 1 – 2,000 ppmv	0.001- 100,000 ppmv
Source Mass Flux: 0.1 – 5,000 g/d	0.1 – 40,000 g/d
Recharge: 0.4 – 7.5 cm/yr	0.4 – 15 cm/yr
Bulk Density and Porosity: Fixed at 1.855 g/mL and 30%, respectively.	Allow user-specified bulk density and porosity values
Relative Water Saturation (Moisture Content): 0.05 – 0.55 (1 – 9 wt%)	0.05 – 0.75 Allowable moisture content depends on bulk density and porosity
Vadose Zone Thickness: 10 – 60 m	3 – 150 m
Source Thickness Ratio: 0.1 – 0.5	0.1 – 0.75 0.75 STR is allowed for VZT ≤ 10 m
Relative Source Position: 0.1 – 10	0.1 – 50 50 RSP is allowed for VZT ≥ 30 m
Source Footprint (square): 100 – 2,500 m²	100 – 10,000 m²
Groundwater Darcy Velocity: 0.005 – 0.3 m/d	0.005 – 1.0 m/d

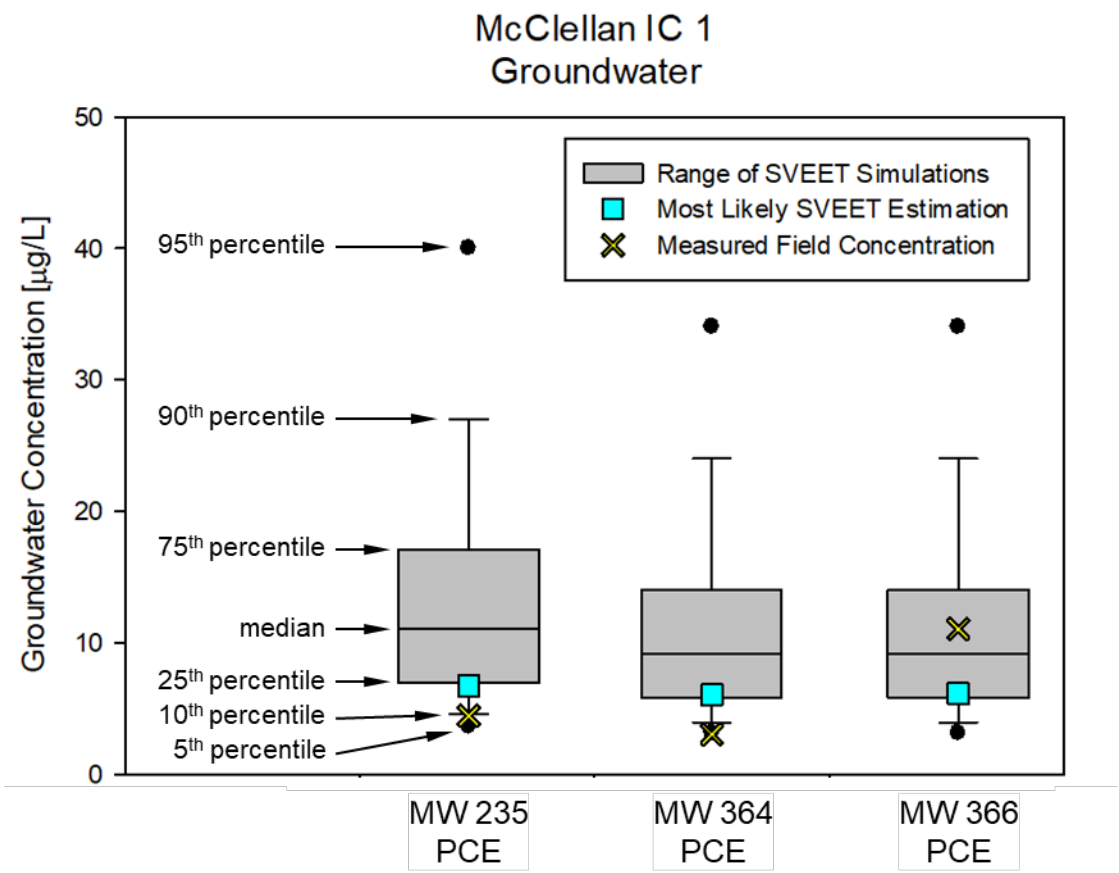
Demonstration Elements

- Type 1 – SVEET2 Ground-Truthing (2+ sites)
  - The site must have reached equilibrium conditions
    - Ideally, demonstrated by long term data
  - Soil gas and/or groundwater data required for comparison to SVEET2 results
  - Performance metric: observed values are within 3 standard deviations of SVEET2 sensitivity results

- Type 2 – SVEET2 Tool User Testing (2+ sites)
  - Ideally, had SVE operations approaching asymptotic removal and shutdown is being considered
  - Soil gas and/or groundwater data required
  - Qualitative feedback on usability and applicability
  - Performance metric: Applicable to ≥ 80% of sites investigated

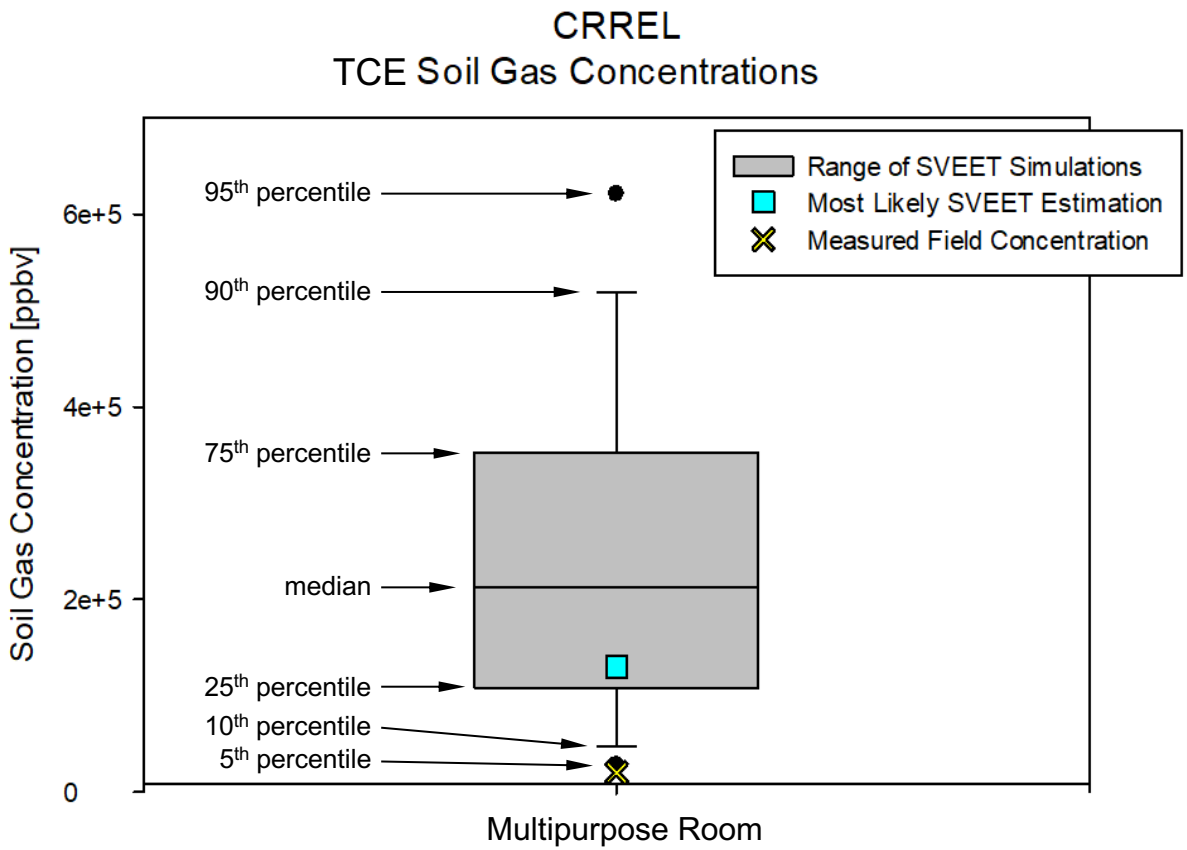
SVEET2 Demo – McClellan IC-1

- Tetrachloroethene (PCE) source impact on groundwater at McClellan AFB IC-1
  - SVE was recently terminated
  - Comparison for three monitoring wells
- SVEET2 estimates met performance objectives, matching observed data



SVEET2 Demo – CRREL AOC 2

- Trichloroethene (TCE) source impact on soil gas for CRREL AOC 2 to assess vapor intrusion
- SVEET2 estimate met performance objectives, matching observed data



Ground-Truthing Demo Summary

- Overall, SVEET2 provided reasonable concentration estimates
  - Six cases matched observed data, meeting the performance metric
  - Three cases had estimates less than observed data
    - Estimates for all were within a factor of 2-3 of observed data
  - Four cases had estimates larger than observed data
    - Conservative
- Challenging to find a site meeting all SVEET2 assumptions
  - Need to distinguish between ground-truthing and application to support remedial decisions

Demo – Usability and Applicability

- Applicable to 93% of DoD sites surveyed (n = 14)
  - 29% of sites may need additional characterization
  - Issues: recharge (too great) or site size (too small/thin or too large)
- Feedback: SVEET2 was appliable and helpful
  - User friendly and straightforward input requirements
    - Inputs readily available from existing site data
- Easy to vary inputs and quickly run multiple scenarios or what-if analyses
  - Rapid assessment results
  - Major benefit vs. traditional approaches
    - Less labor effort, less data intensive
    - Lower cost to obtain estimated impacts
    - Similar level of professional judgement and assumptions
  - Helpful when inputs have high degree of uncertainty
    - Provided insight at one field site regarding controlling processes
  - Provides useful information for decision making

Demo – User Applications

- Multiple applications were tried or considered by DoD site users
  - Ground-truthing for groundwater and soil gas
  - Source impacts on groundwater for SVE endpoint evaluation
  - Identification of potential vapor intrusion concerns
  - Assess parameter sensitivity and resulting estimated impacts
  - Help define institutional control needs/boundaries
  - Feasibility study use to determine suitable performance objectives to meet cleanup goals
- User-conducted ground-truthing efforts found reasonable estimates from SVEET2
- Soil gas concentration estimates were useful
  - When SVE closure is proposed, regulatory agencies often bring up the potential for vapor intrusion

Cost Savings for DoD Site Example

- Application of SVEET2 to assess SVE endpoints
  - Usability / applicability demonstration
  - Eight systems/locations assessed
- Outcome
  - Five locations could terminate SVE system operations ("Shutdown")
  - Three locations should continue SVE operations (“Run”)
- Cost savings estimated from current SVE operational costs
  - Cost savings of roughly $663,500 per year
  - 61.5% decrease in annual operational costs

System	Run/Shutdown	Operating Cost ($/y)
1	Run	$ 142,025
2	Shutdown	$ 128,400
3	Run	$ 122,700
4	Shutdown	$ 118,650
5	Shutdown	$ 46,675
6	Shutdown	$ 161,325
7	Run	$ 151,075
8	Shutdown	$ 208,450
Estimated Potential Cost Savings for Shutdown Systems		**$663,500**

Cost Savings

- Annual SVE system operation may cost upwards of $200K (NFESC, 2005; EPA, 2007)
  - Above example was $50-200K a year
- Using SVEET2 for endpoint evaluation at a small percentage of DoD sites with SVE systems
  - Potential annual cost savings could reach millions of dollars based on operational costs alone
- Personnel unfamiliar with the SVEET2 software
  - Expect roughly 16 hours of labor to run site-specific scenarios
    - Including time for downloads/installation, learning SVEET2, gathering site data, and performing data analysis and interpretation
  - Most time will be spent in gathering site data and assessing scenario variations to support remedy decisions
- Labor estimates (new user, site-specific analyses)
  - Assuming billable rates of $80-150 per hour
  - $1280-2400 per DoD installation

Key Takeaways

- SVEET2 is an easy-to-use tool
  - Makes use of readily available data
- SVEET2 is broadly applicable to DoD sites
  - Able to represent real field conditions found at DoD sites
- Spreadsheet-fast estimates of vadose zone source impacts on groundwater and soil gas concentrations
  - Allows users to quickly perform what-if/sensitivity analyses
  - Supports a range of remedial evaluations/decisions
    - Endpoint analysis
    - Remedial performance goals
    - Assess potential vapor intrusion concerns
- Potential to save millions of dollars
  - Turn off SVE systems where continuation is not needed

Conclusions & Benefits

- SVEET2's rapid evaluation capabilities and ease-of-use warrants its use as a key tool in SVE performance assessment/optimization studies

- Primary benefit is potential cost savings
  - Rapid evaluation to obtain a defensible analysis for decision making

References

- Project Final Report will be published in February 2021
  - https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Persistent-Contamination/ER-201731
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https://www.pnnl.gov/projects/remediation-performance-assessment/soil-vapor-extraction

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Q&A Session

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