# SVEET2 FINAL REPORT

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

## ESTCP Project ER-201731

**June 27, 2021**

Pacific Northwest National Laboratory

**Christian D. Johnson**
**Katherine A. Muller**
**Michael J. Truex**
**Guzel Tartakovsky**

US Army Corps of Engineers

**David J. Becker**
**Carl M. Harms**

NAVFAC Naval Facilities Engineering Command EXWC Engineering & Expeditionary Warfare Center

**Jovan Popovic**

# Contents

# Figures

# Tables

# Acknowledgments

Funding for this work was provided by the U.S. Department of Defense's Environmental Security Technology Certification Program (ESTCP) under project ER-201731.

The project team consists of the following organizations and personnel:

- Naval Facilities Engineering and Expeditionary Warfare Center (NAVFAC EXWC)
    - Jovan Popovic (Principal Investigator)
- Pacific Northwest National Laboratory (PNNL)
    - Christian Johnson
    - Katherine Muller
    - Michael Truex
- United States Army Corps of Engineers (USACE)
    - Dave Becker
    - Carl Harms

Thanks to Rob Hinchee (retired) for his involvement and guidance in the initial phases of this project.

Thanks to Guzel Tartakovsky (formerly of PNNL) for her invaluable help in running the thousands of simulations to obtain the underlying data for SVEET2. Guzel was supported by Jun Song and Ciara Varnum-Lowry, whose help with data checking and the compression algorithm is very much appreciated.

Thanks to Mart Oostrom (formerly of PNNL) for providing the foundation for the flux equivalency approach described in Appendix B and guidance in the formative phases of this project.

Thanks to Tim Appleman and Jennifer Segura for providing NAVFAC EXWC project leadership earlier in the project.

Thanks to the project personnel that shared site information and their insights on the use of the revised SVEET tool. Their participation greatly improved the SVEET update project.

McClellan – Paul Graff

Mather – Paul Graff

NASNI – Michael Pound and Vitthal Hosangadi

Hill – Elizabeth Tevault

Tooele – Nick Montgomery and Marc Sydow

CRREL – Darrell Moore

The Pacific Northwest National Laboratory is operated by Battelle Memorial Institute for the U.S. Department of Energy (DOE) under Contract DE-AC05-76RL01830.

# Acronyms and Abbreviations

| | |
|---|---|
| 3D | three dimensional |
| AFB | Air Force Base |
| BRAC | base realignment and closure |
| CRREL | Cold Regions Research and Engineering Laboratory |
| DCE | dichloroethane (1,1-DCE = 1,1-dichloroethene, cis-DCE = cis-1,2-dichloroethene) |
| DoD | U.S. Department of Defense |
| DOE | U.S. Department of Energy |
| EPA | U.S. Environmental Protection Agency |
| ER | Environmental Restoration |
| ESTCP | U.S. Department of Defense Environmental Security Technology Certification Program |
| FRTR | Federal Remediation Technologies Roundtable |
| GW | groundwater |
| IC | institutional controls |
| MC | Monte-Carlo |
| MCL | maximum contaminant level |
| NAPL | non-aqueous phase liquid |
| PCE | tetrachloroethene |
| PNNL | Pacific Northwest National Laboratory |
| q | Darcy velocity (input parameter) |
| R | recharge (input parameter) |
| RITS | Remediation Innovative Technology Seminar |
| RPM | remedial project manager |
| RSP | relative source position (input parameter) |
| SA | surface area (input parameter) |
| Sr | residual saturation (input parameter) |
| STOMP | Subsurface Transport over Multiple Phases (software name) |
| STOP | SVE termination or optimization process |
| STR | source thickness ratio (input parameter) |
| SVE | soil vapor extraction |
| SVEET | Soil Vapor Extraction Endstate Tool (software name) |
| TCE | trichloroethene |
| VI | vapor intrusion |
| VIETUS | Vapor Intrusion Estimation Tool for Unsaturated-Zone Contaminant Sources (software name) |
| VLEACH | Vadose Zone Leaching Model (EPA) |
| VOC | volatile organic compound |
| VZT | vadose zone thickness (input parameter) |

# Abstract

***Introduction and Objectives***

A volatile organic compound (VOC) contamination source in the vadose zone presents a potential threat to underlying groundwater and/or to nearby structures through vapor intrusion. Soil vapor extraction (SVE) is a commonly applied remediation technology to address VOC contamination in the unsaturated zone. SVE performance assessment guidance provides a structured approach to evaluate whether the SVE system should be terminated, optimized, supplemented, or transitioned to an alternative remedial approach. The ability to quantify impacts of the remaining source area on groundwater and soil gas are critical to a performance assessment in support of such remedial decisions.

***Technical Approach***

The Soil Vapor Extraction Endstate Tool version 2 (SVEET2) is an updated version of the SVEET spreadsheet software for estimating contaminant concentrations in groundwater and soil gas that are caused by a vadose zone contaminant source. SVEET2 has a rigorous basis from numerical model simulations for a generalized conceptual model that cover a set of parameters and contaminants that are relevant to a wider variety of sites than SVEET version 1.0. The software update includes results from over 5500 numerical simulations to provide these expanded options for site applicability. SVEET2 itself is not a numerical model; rather, it interpolates between pre-modeled scenario numerical simulation results and scales those results for parameters with linear relationship.

***Results***

SVEET2 allows for a wider range of sites to be represented (compared to SVEET v. 1.0), including more than 93% of surveyed Department of Defense (DoD) sites. A demonstration of the SVEET2 software was performed for the purpose of model verification and obtaining user feedback about software applicability. While it is challenging to find suitable sites for rigorous ground-truthing, several sites were suitable for use in the demonstration The ground-truthing had a mixture of results, with 77% of test cases with results that were on par with observed field data or were conservative (i.e., would be protective relevant to cleanup goals) estimates with respect to decision making, and the remaining 23% of test cases less than, but within a factor of 2-3, of the observed of the field data. Overall, the software was found to be user friendly and applicable for many of the tested field sites. Technology transfer activities (though constrained by the COVID pandemic) were included in the project to publicize the software capabilities and provide users with insight on software use.

### *Benefits*

The level of effort to complete a SVE system evaluation using SVEET2 is minimal, but has the potential for significant cost savings. SVEET2's rapid evaluation capabilities and ease-of-use warrant its use as a tool at the forefront of SVE system performance assessment studies.

### *Publications*

Johnson, C.D., K.A. Muller, M.J. Truex, G. Tartakovsky, D.J. Becker, C.M. Harms, and J. Popovic. "A Rapid Decision Support Tool for Estimating Impacts of a Vadose Zone Volatile Organic Compound Source on Groundwater and Soil Gas." *Groundwater Monitoring & Remediation* (early view). Available at: http://doi.org/10.1111/gwmr.12468

"Practical Management of Big Data for a Spreadsheet Software Tool." In preparation for *Computers and Geosciences (or possibly Communications of the ACM, SIAM Journal on Applied Mathematics*, or *Journal of Computational and Applied Mathematics).*

"Numerical Modelling as the Foundation for the SVEET Decision Support Software." In preparation for *Environmental Modelling and Software.*

"Using an Equivalent Flux Condition Approach for Soil Vapor Extraction Simulations." In preparation for *Vadose Zone Journal* (or similar).

# Executive Summary

### *Introduction*

Volatile organic compound (VOC) contamination in the vadose zone presents a potential threat to underlaying groundwater and/or to nearby structures through vapor intrusion. Such contamination is often addressed using soil vapor extraction (SVE), in which a vacuum is applied to the unsaturated zone to remove VOCs from the soil gas through a physical, mass transfer and extraction process. Many site-specific parameters such as soil moisture, permeability, sorption, phase partitioning, and heterogeneity (especially fine-grained units), may all affect SVE performance. Current SVE performance assessment guidance (Truex et al., 2013) provides a structured approach (Figure ES-1) for assessing remediation of volatile contaminant sources in the vadose zone. This approach involves gathering information and performing evaluations to determine whether vadose zone remediation should be terminated, optimized, supplemented, or transitioned to another technology. A major component of the SVE guidance to support remedy decisions is the quantification of the impacts of the remaining vadose zone source on groundwater and soil gas concentrations. The ability to quantify impacts of a remaining VOC source area on groundwater and soil gas are critical to evaluating existing SVE systems to support remedial decisions. The performance assessment and quantification of source zone impacts also has the potential to provide significant cost savings through optimization or termination of an existing SVE system. In 2013, The Soil Vapor Extraction Endstate Tool (SVEET) software was released as a companion to the Truex et al. (2013) SVE guidance to provide a user-friendly way to quickly determine a quantitative estimate for the impact of a vadose zone source on groundwater concentrations. SVEET was based on a generalized conceptual model, a small set of inputs, and rigorous underlying 3D numerical simulation results. Subsequently, the Vapor Intrusion Estimation Tool for Unsaturated-Zone Contaminant Sources (VIETUS) software (Johnson et al., 2016) was developed as a sister tool for estimating the impact of a vadose zone contaminant source on vapor intrusion.

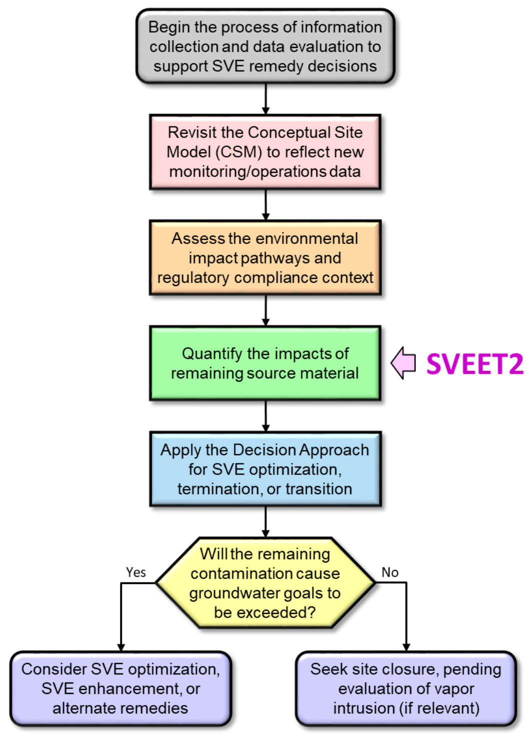


***Figure ES-1.*** *Steps in the structured approach for performance assessment to support decisions related to vadose zone volatile contaminant remediation. The SVEET2 software provides quantitative estimates of the impact of the remaining source material.*

### *Objectives*

The objective of this Environmental Security Technology Certification Program (ESTCP) project was to update SVEET version 1.0 to expand on the range of site conditions that could be represented and evaluated with the tool. Specifically, the range of site parameters needed to encompass values that are relevant for Department of Defense (DoD) sites. The SVEET software update also included a demonstration to assess applicability, performance, and usability through ground truthing and user testing with DoD sites where SVE was either used or currently being considered. Technology transfer and adoption of SVEET2 in evaluation of DoD sites to facilitate cost savings was another objective.

### *Technology Description*

The Soil Vapor Extraction Endstate Tool version 2 (SVEET2) is an updated version of the SVEET spreadsheet software for estimating contaminant concentrations in groundwater and soil gas that are caused by a vadose zone contaminant source. SVEET2 has a rigorous basis from numerical model simulations for a generalized conceptual model that cover a set of parameters and contaminants that are relevant to a wider variety of sites than SVEET version 1.0.

In SVEET2, sites are conceptualized as depicted in Figure ES-2, using commonly measured field parameters (Table ES-1). The source area is defined as a rectangular source area centered at a specific vertical location within the vadose zone, characterized by the source width ($w$), depth to the top of the source ($L1$), and source thickness ($z$). The vadose zone is characterized by inputs that include temperature ($T$), recharge ($R$), soil moisture content ($\omega$), porosity ($\theta_{total}$), bulk density ($\rho_{bulk}$), and vadose zone thickness ($VZT$). Source strength can be provided as either a gas concentration ($C_{gs}$) or mass discharge ($M_{src}$), depending on the type of field data that is available. The groundwater Darcy velocity ($q$), distance to the compliance well ($d$), and well screen length ($s$) are used when assessing effects on groundwater concentration. The longitudinal ($dx$) and transverse ($dy$) distances, as well as the depth of the basement/foundation ($dz$), are used to specify the location of interest for soil gas concentration. A total of 32 different contaminants can be selected in SVEET2 to quantitatively estimate the impacts on groundwater and/or soil gas concentrations. The permissible ranges of input parameters that are supported by SVEET2 are provided in Table ES-1.

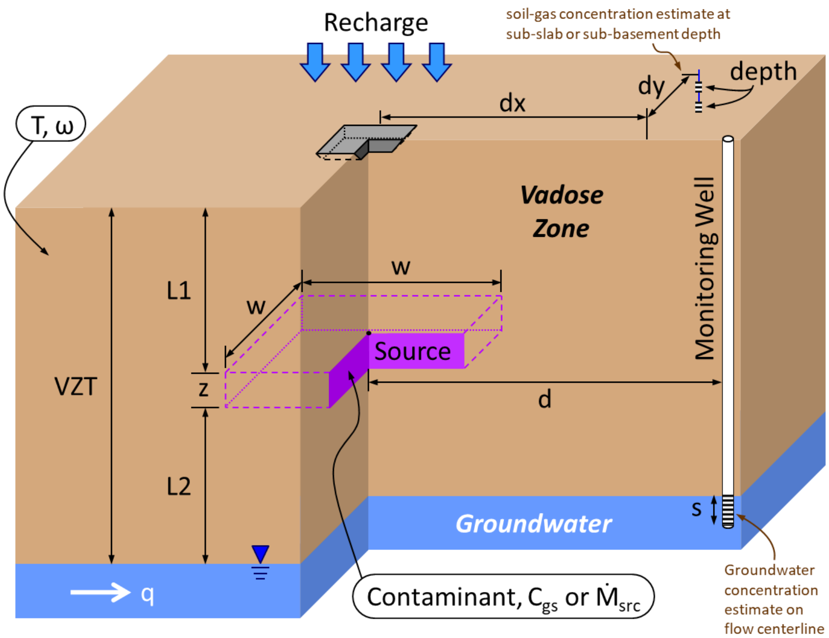


***Figure ES-2.*** *Generalized framework used by SVEET2; output is groundwater concentration at a centerline monitoring well location and/or soil gas concentration at a specified vadose zone location.*

***Table ES-1.*** *Controlling parameters and key parameter values for SVEET2. Input parameters and calculated intermediate parameters*

| Parameter Name | Parameter | Units | Permissible Range |
|---|---|---|---|
| Contaminant | *Contam.* | — | 32 options |
| Temperature | $T$ | °C | 5 – 99 |
| Avg. Recharge | $R$ | cm/yr | 0.4 – 15 |
| Avg. Soil Moisture Content | $\omega$ | wt% | varies |
| Total Porosity | $\theta_{total}$ | — | 0.1 – 0.5 |
| Dry Bulk Density | $\rho_{bulk}$ | g/mL | 1.1 – 2.0 |
| Vadose Zone Thickness | *VZT* | m | 3 – 150 |
| Depth to Top of Source | *L1* | m | 0.07 – 132 |
| Source Thickness | $z$ | m | 0.3 - 75 |
| Source Width (= Length) | $w$ | m | 10 – 100 |
| GW Darcy Velocity | $q$ | m/day | 0.005 – 1.0 |
| Compliance Well Screen Length | $s$ | m | 1 – 30 |
| Distance to GW Compliance Well | $d$ | m | 0 – 850 |
| Longitudinal Distance for Soil Gas | $dx$ | m | -850 – 850 |
| Transverse Distance for Soil Gas | $dy$ | m | 0 – 370 |
| Depth of Basement/Foundation | $dz$ | m | 1.0 or 4.0 |
| Source Gas Concentration | $C_{gs}$ | ppmv | 0.001 – 100,000 |
| Source Mass Discharge | $\dot{M}_{src}$ | g/day | 0.1 – 40,000 |

SVEET2 itself is not a numerical model, it is a spreadsheet tool that interpolates between numerical simulation results for pre-modeled scenarios and scales those results for parameters with linear relationships. The expanded permissible ranges for input parameters primarily come from expanding the underlying numerical simulations. For SVEET2, a total of 5760 pre-modeled scenarios were simulated with the Subsurface Transport over Multiple Phases (STOMP) code (White and Oostrom, 2006). STOMP is a very sophisticated, complex, and well-proven multi-phase, multi-component, three-dimensional (3D) numerical software. STOMP simulations were run to obtain steady-state concentration distributions in the gas and aqueous phases throughout the computational domain. Groundwater concentrations were then tabulated for each pre-modeled scenario for grid cell locations at and downgradient of the source center along the plume centerline (primary flow direction). Soil gas concentrations were tabulated across the domain for depths of 1 m and 4m, to represent sub-slab and sub-basement locations. Using the pre-modeled STOMP simulations results, SVEET2 estimates contaminant concentrations using lookups and interpolations for the user-specified, site-specific set of input parameters. Interpolation is applied between the collection of STOMP simulation results for parameters with nonlinear effects on results (Sr, VZT, STR, RSP, SA, and q; see Table ES-1). Parameters with a linear effect (source strength, H, s, and R; see Table ES-1) are linearly scaled from the interpolated result.

The STOMP simulations represent the equilibrium state of contaminant transport from a constant-strength vadose zone contaminant source to the groundwater and vadose zone locations under natural quiescent conditions (i.e., conditions that would be found prior to active remediation or after vadose zone remediation has been shut down). Recharge-driven processes, vapor-phase processes, and mixing into the groundwater, which have been demonstrated to be important for estimating contaminant transport (Truex et al., 2009, Oostrom et al., 2010, Brusseau et al., 2013), are all included in simulations. It is assumed that that vapor-phase diffusive transport dominates vadose zone contaminant movement, the groundwater is initially uncontaminated, the vadose zone source can be represented as a single source area, and the subsurface is homogeneous with uniform properties. The simulations do not account for attenuation mechanisms such as biodegradation or abiotic reaction, secondary sources (e.g., back diffusion from low-permeability zones outside the main source area in the vadose zone), or a groundwater monitoring well screen interval that does not start at or span the water table. SVEET2 results based on these simulations are generally conservative in that the assumptions favor higher concentration estimates, which is appropriate for predictive applications in support of remedial decision making.

### *Performance Assessment*

A demonstration of the software was completed for the purpose of model verification and getting user feedback about software ease-of-use and applicability. While it is challenging to find suitable sites for rigorous ground-truthing, several DoD sites could be used in the demonstration. The ground-truthing results demonstrated that SVEET2 can provide good estimations for field sites, though there were some discrepancies, possibly a result of the underlying SVEET2 model assumptions discussed above.

SVEET ground-truthing efforts confirmed the ability of SVEET2 to provide useable estimates of field groundwater and soil gas concentrations. SVEET2 met ground-truthing performance criteria in 46% of the test cases. The evaluation found 31% of cases with SVEET2 results that were outside the evaluation criteria and were larger than actual field concentration values. In only 23% of test cases did SVEET2 provide estimates outside the evaluation criteria that were less than field observations, although all were within a factor of 2-3 of the field data. So, 77% of test cases had results that were on par with observed field data or were conservative estimates with respect to decision making. Some of the assumptions employed for SVEET2 may only be approximately applicable for a site, thus affecting comparison of SVEET2 results to observed field values for the remaining 23% of test cases.

A site survey and qualitative user-testing were also conducted for SVEET2. Based on survey responses, SVEET2 would be applicable for decision making at 93% of DoD sites and 81% of all sites surveyed (including non-DoD sites). Overall, DoD site personnel found SVEET2 to be applicable and useful for their respective field sites. Since SVEET2 is a Microsoft Excel-based spreadsheet tool, users found it to be relatively user friendly, with straightforward inputs that were readily available from existing site data. Sites used SVEET2 for a variety of purposes including their own ground-truthing, what-if scenarios to assess the potential impacts of a source area on underlying groundwater to help determine if there was a technical justification to support SVE system shutdown, to identify the potential for vapor intrusion, and to assess parameter sensitivity. The Excel-based nature of SVEET2 allows users to perform multiple simulations nearly instantaneously, allowing for scenario testing to be completed with ease.

***Cost Assessment***

A cost analysis example was performed through evaluating the potential cost-savings associated with implementing the SVEET2 tool at a site currently operating SVE systems with diminishing contaminant recoveries. At this example site, eight locations were assessed with SVEET2 to determine the expected impacts to groundwater from the remaining source areas. Out of the eight SVE locations, SVEET2 estimates indicated that five locations could potentially be shut down. Based on current SVE operational costs, shutting down five of the eight SVE systems would result in an estimated 61.5% reduction in annual operation costs, equating to approximately $663,500 per year in cost saving. In general, the level of effort to complete an SVE system evaluation using SVEET2 is minimal, with the potential for significant cost saving.

***Implementation Issues***

Applicability and usability of the software is good, based on the range of sites that can be represented, feedback from users, and the indented use of the software. The main implementation issue surrounding SVEET2 relates to determining the appropriate input values to represent a site. While the required inputs for SVEET2 should be readily obtained from available field data, it is still necessary to define the site within the SVEET2 conceptual model framework, necessitating professional judgement.

Technology transfer activities were part of the project to publicize the SVEET2 software capabilities and provide users with insight on software use. Awareness amongst site managers, practitioners, and regulators is critical for the application of the SVEET2 software to evaluate SVE performance and opportunities for cost savings. Though constrained by the COVID-19 pandemic from early 2020, the project team has engaged in technology transfer through a journal article, conference presentation, and webinars (Johnson et al. 2019, 2021a, 2021b; Johnson and Byrnes, 2021). Three additional journal articles are in preparation. Additional interactions with Navy and Army Corps of Engineers site managers are planned through participation in workshops/meetings. A presentation/workshop is being pursued though U.S. EPA for Federal Remediation Technologies Roundtable (FRTR) members and interested personnel.

### *Conclusions*

The SVEET2 software has been demonstrated to provide useful results to support remediation decisions, though limitations/assumptions of the tool may necessitate site-specific modeling in some situations. The level of effort to complete a SVE system evaluation using SVEET2 is minimal, but has the potential for significant cost savings. SVEET2's rapid evaluation capabilities and ease-of-use warrant its use as a tool at the forefront of SVE system performance assessment studies.

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White, M.D., and M. Oostrom. 2006. *STOMP Subsurface Transport Over Multiple Phases, Version 4.0, User's Guide*. PNNL-15782, Pacific Northwest National Laboratory, Richland, Washington.

***Manuscripts in Preparation***

"Practical Management of Big Data for a Spreadsheet Software Tool." In preparation for *Computers and Geosciences* (or possibly *Communications of the ACM*, *SIAM Journal on Applied Mathematics*, or *Journal of Computational and Applied Mathematics*).

"Numerical Modelling as the Foundation for the SVEET Decision Support Software." In preparation for *Environmental Modelling and Software*.

"Using an Equivalent Flux Condition Approach for Soil Vapor Extraction Simulations." In preparation for *Vadose Zone Journal* (or similar).

# 1.0 Introduction

## 1.1 Background

Existing guidance on soil vapor extraction (SVE) performance assessment (Truex et al, 2013) provides a structured approach for assessing vadose zone volatile contaminant remediation. This approach involves gathering information and performing evaluations to determine whether the vadose zone remediation should be terminated, optimized, supplemented, or transitioned to another technology. The stepwise approach (Figure 1) goes through revisiting the conceptual site model to incorporate new information, considering/confirming the environmental impact and regulatory compliance context, quantitatively evaluating the impact of remaining vadose zone contaminant sources, and applying a decision logic approach to assess closure, optimization, augmentation, or transition options. The decision logic associated with the Truex et al. (2013) guidance is shown in Figure 2. The guidance describes specific actions and decisions to support remedy decisions, one of which is the quantification of the impacts of the remaining vadose zone source. The Soil Vapor Extraction Endstate Tool (SVEET) software was released as a companion to the Truex et al. (2013) guidance to provide a user friendly way to quickly determine a quantitative estimate for the impact to groundwater concentrations based on a generalized conceptual model, a small set of inputs, and rigorous underlying 3D numerical simulation results. Subsequently, the Vapor Intrusion Estimation Tool for Unsaturated-Zone Contaminant Sources (VIETUS) software (Johnson et al., 2016) was developed as a sister tool for estimating the impact of a vadose zone contaminant source on vapor intrusion. The work described in this report describes an update to expand the range of applicable conditions and to incorporate aspects of VIETUS in a new version titled SVEET2, thus superseding both of these previously released tools.

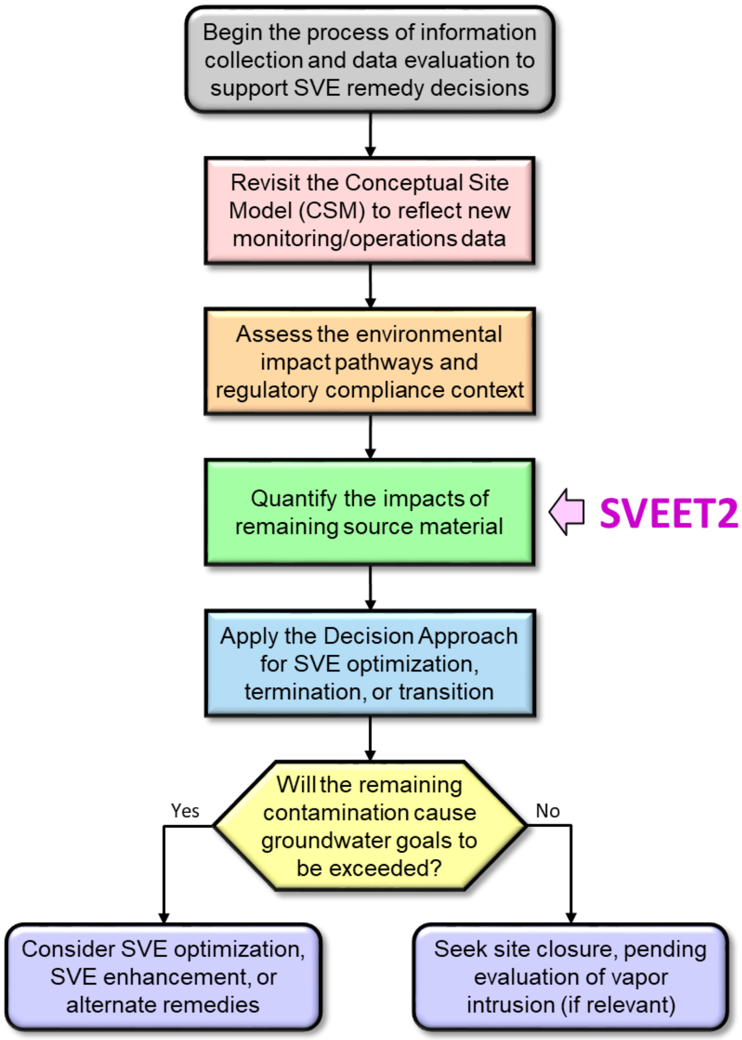
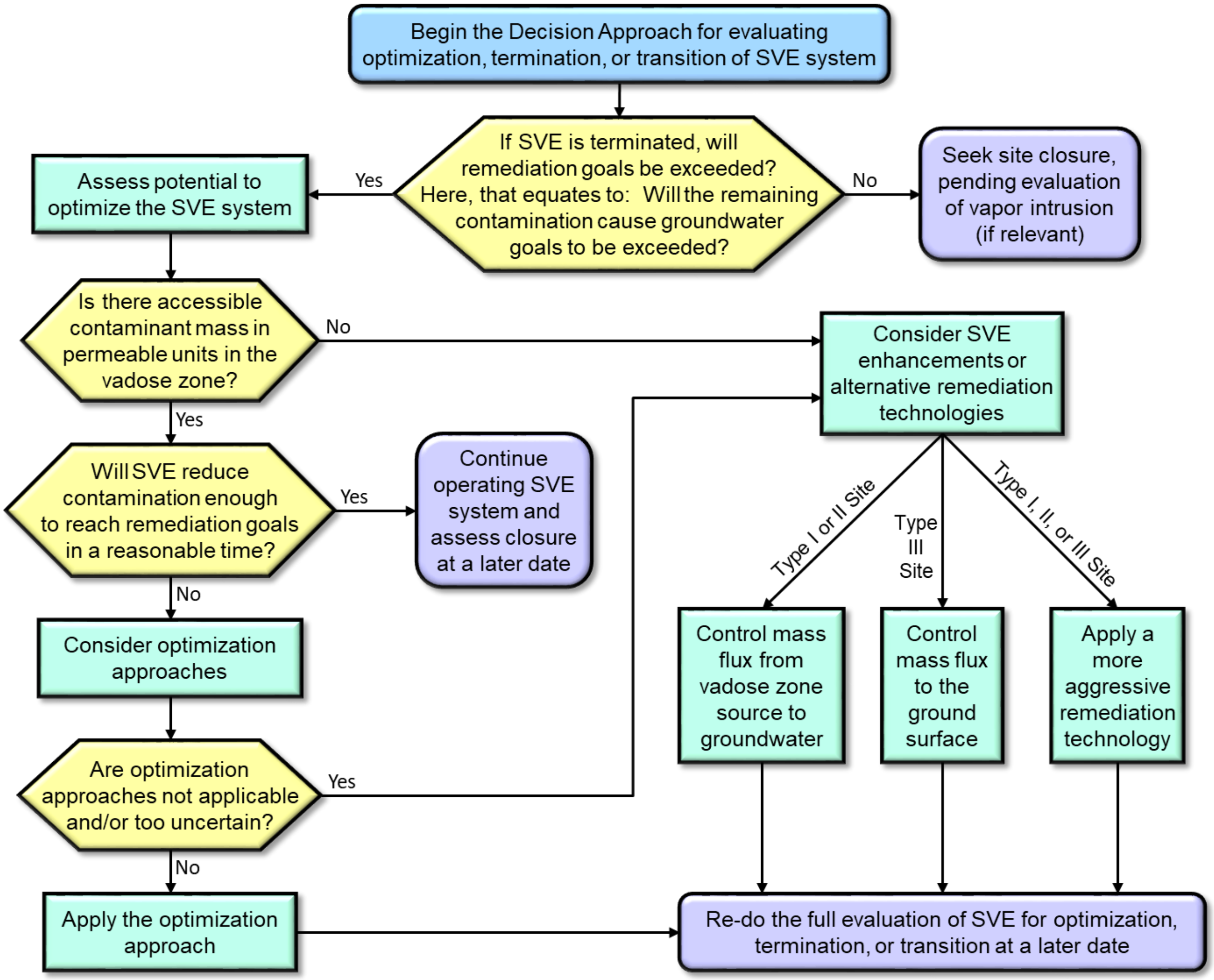



***Figure 1.*** *Steps in the structured approach for performance assessment to support decisions related to vadose zone volatile contaminant remediation. The SVEET2 software provides quantitative estimates of the impact of the remaining source material.*




Type I – Sites with contaminant source(s) in the vadose zone (e.g., a diffusion-limited low-permeability layer/lens) and only low-level dissolved phase contamination in the groundwater (near source contaminant mass transfer is from the vadose zone to the groundwater).

Type II – Sites with contaminant mass in both vadose and saturated zones (near source contaminant mass transfer may be either into our out of the groundwater and may vary locally).

Type III – Sites with the primary remaining contaminant mass located below the water table or trapped in a thick capillary fringe (contaminant mass transfer is into the vadose zone)

***Figure 2.*** *Decision logic discussed in the Truex et al. (2013) SVE guidance.*

The SVEET2 software is a spreadsheet tool that estimates contaminant concentrations in groundwater and soil gas that result from a vadose zone contaminant source at equilibrium (i.e., not influenced by active vadose zone remediation). The software provides a structured framework in the form of a generalized conceptual model (Figure 3) whereby the user can describe the site, the contamination source, and the monitoring location(s) of interest. Concentration estimates are based on the relationship between the user-specified scenario and a large suite of numerical simulations that calculate contaminant transport through the vadose zone and into the groundwater for a wide range of scenarios. SVEET2 expands on the range of scenarios that can be represented compared to the release of SVEET version 1.0 (Truex et al. 2013, Oostrom et al., 2014).

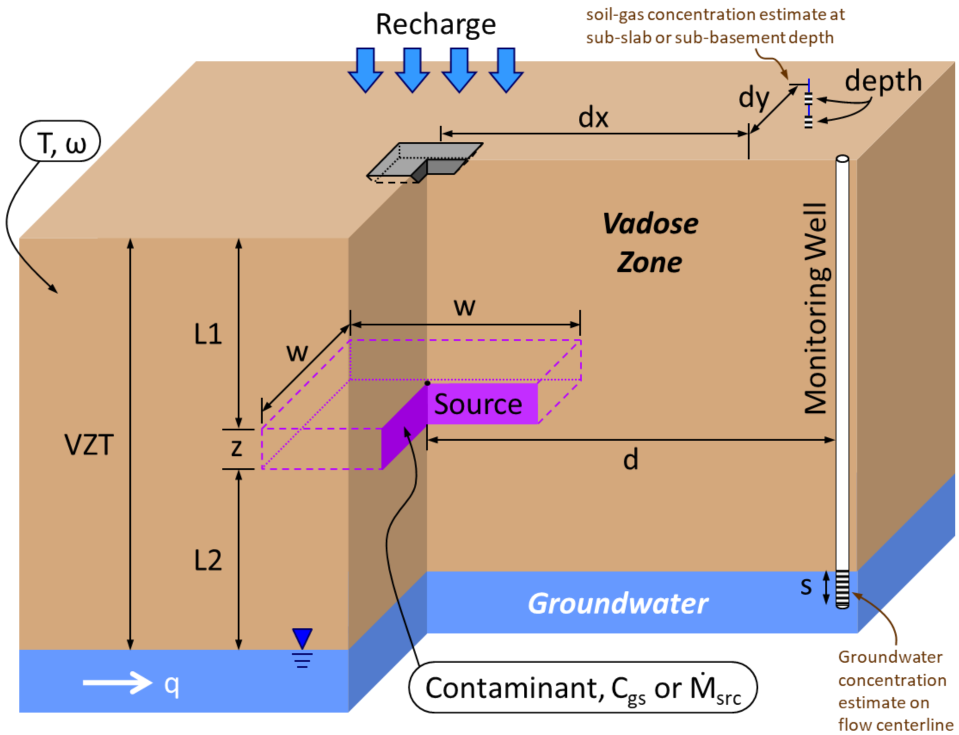



***Figure 3.*** *Generalized framework used by SVEET2; output is groundwater concentrations at a centerline monitoring well location and/or soil gas concentrations at a specified vadose zone location.*

SVEET2 input parameters and constraints, as well as results, are based on rigorous underlying numerical model simulations, which were conducted with the Subsurface Transport over Multiple Phases (STOMP) code (White and Oostrom, 2006). STOMP is a very sophisticated, complex, and well-proven multi-phase, multi-component, three-dimensional (3D) numerical software. The STOMP simulations represented contaminant transport under natural conditions (i.e., transport from a defined vadose zone contaminant source to the groundwater and vadose zone locations under quiescent conditions prior to active remediation or after vadose zone remediation has been shut down) and included recharge-driven processes, vapor-phase processes, and mixing into the groundwater, which have been demonstrated to be important for estimating contaminant transport (Truex et al., 2009, Oostrom et al., 2010, Brusseau et al., 2013). The simulations did not, however, account for attenuation mechanisms such as biodegradation or abiotic reaction. Utilizing the high-performance computing resources available to the Department of Energy (DOE) national laboratories, 5760 STOMP simulations were conducted to define the output that was used as the basis for SVEET2.

The intended use of SVEET2 is for 1) volatile organic compound (VOC) fate and transport from a vadose zone source when vapor-phase diffusive transport is a dominant transport process and 2) estimating concentrations for long-term, steady-state conditions. Under these conditions, numerical analysis showed that the groundwater concentration is controlled by a limited set of parameters (Oostrom et al., 2014; Truex et al., 2013). Evaluation of how site and contaminant parameters affect contaminant transport allowed identification of parameters having linear impacts on the groundwater contaminant concentration versus those having nonlinear impacts.

As shown in Figure 3, SVEET2 input parameters include the vadose zone thickness (*VZT*), the depth to the top of the source (*L1*), the source thickness (*z*), the source footprint area (*SA*) for a square source (of side length *w*), and the distance (*d*) to the monitoring well of interest. These dimensions also specify the relative source position (*RSP*) and the source thickness ratio (*STR*). Additional input parameters include the contaminant of interest, temperature (*T*), moisture content ($\omega$), source strength defined as either vapor concentration ($C_{gs}$) <u>or</u> mass discharge ($\dot{M}_{src}$), recharge rate (*R*), groundwater flow velocity (*q*), and monitoring well screen length (*s*). New in SVEET2, the user can also specify the lateral location (*dx*, *dy*) and depth below ground surface (*dz*) of a sub-slab (1 m) or sub-basement (4 m) location for the estimated soil gas concentration at that location. The moisture content input is converted to residual saturation (*Sr*), which is what the STOMP simulations employ. Equilibrium mass transfer between gas and aqueous phases is accounted for through a temperature-dependent, contaminant-specific Henry's Law constant (*H*). Interpolation is applied between the suite of STOMP simulation results for parameters with nonlinear effects on results (*Sr*, *VZT*, *STR*, *RSP*, *SA*, and *q*). Parameters with a linear effect (source strength, *H*, *s*, and *R*) simply scale the interpolated result. Table 1 lists the key parameters and the values used in STOMP simulations.

***Table 1.** Controlling parameters and key parameter values for SVEET2.*

| Name | Symbol | Units | Simulated Values [a] | Valid Range | Impact |
|---|---|---|---|---|---|
| Residual Water Saturation [b] | $S_r$ | — | **0.05**, 0.3, 0.55, 0.75 | 0.05 – 0.75 | Nonlinear |
| Vadose Zone Thickness | *VZT* | m | 3, 10, 30, **60**, 110, 150 | 3 – 150 | |
| Source Thickness Ratio | *STR* | — | **0.1**, 0.25, 0.5, 0.75 | 0.1 – 0.75 [c] | |
| Relative Source Position | *RSP* | — | 0.1, **1**, 10, 50 | 0.1 – 50 [c] | |
| Source Area | *SA* | m² | **100**, 400, 900, 2500, 10000 | 100 – 10,000 | |
| Groundwater Darcy Velocity | *q* | m/d | 0.005, 0.03, **0.3**, 1.0 | 0.005 – 1.0 | |
| Source Gas Concentration | $C_{gs}$ | ppmv | **159** [d] | 0.001 – 100,000 | Linear |
| Mass Discharge from Source | $\dot{M}_{src}$ | g/d | from STOMP results | 0.1 – 40,000 | |
| Henry's Law Constant | *H* | — | **0.89** | contaminant-specific | |
| Monitoring Well Screen Length | *s* | m | **5** | 1 – 30 | |
| Recharge Rate | *R* | cm/yr | **0.4** | 0.4 – 15 [e] | |

[a] STOMP base case values are shown in bold.

[b] STOMP simulations use the residual water saturation ($S_r$), which is proportional to the gravimetric moisture content (ω) requested as a user input.

[c] With limitations discussed in Section 2.0.

[d] The STOMP simulations use a source gas concentration of 1 mg/L, which was taken to be 159 ppmv for carbon tetrachloride.

[e] The user needs to consider the model assumptions about vapor-phase diffusive transport being the dominant transport process and whether the model is appropriate for higher recharge rates. See Truex et al. (2013) for further discussion.

## 1.2 Objective of the Demonstration

The objective of this Environmental Security Technology Certification Program (ESTCP) project was to update SVEET version 1.0 to expand on the range of site conditions that could be represented and evaluated with the tool. Specifically, the range of site parameters needed to encompass values that are relevant for Department of Defense (DoD) sites. The SVEET software update also included a demonstration to assess applicability, performance, and usability through ground truthing and user testing with DoD sites where SVE was either used or currently being considered. Technology transfer and adoption of SVEET2 in evaluation of DoD sites to facilitate cost savings was another objective.

## 1.3 Regulatory Drivers

Every site will have different regulatory drivers and compliance context that will be evaluated and documented with a Record of Decision or a Corrective Measures Decision. This context will provide the regulatory requirements that need to be met for a given site. For VOC contamination, regulations will likely be related to groundwater concentrations at compliance points or receptors and/or vapor intrusion into nearby buildings because these are the main routes of exposure for human and ecological receptors (Truex et al., 2013). Drinking water standards at a specific compliance location or receptor will often drive overall remedial objectives and cleanup requirements for a waste site. EPA's Subsurface Vapor Intrusion Guidance (EPA, 2015) provides details on conducting a vapor intrusion assessment, as well as providing a risk assessment framework and risk action levels.

SVE site closure and/or remedy transition hinges on assessing the potential risks from the remaining VOC contamination. Contaminant mass flux and/or groundwater concentrations may be considered when assessing groundwater impacts. SVEET2 provides quantitative estimates on the impacts of a source area on groundwater and soil gas concentrations (i.e., vapor intrusion concerns) to facilitate in the decision making progress by providing the technical justification to determine if estimated groundwater and soil gas concentrations are above or below the regulatory requirements for the site in question.

## 1.4 Report Structure

This report describes the updates to the SVEET2 software (Section 2.0), the calculations behind SVEET2 (Section 3.0), the SVEET2 installation and user guide (Section 4.0), demonstration performance objectives (Section 5.0), application and interpretation of SVEET2 results (Section 6.0), the demonstration of SVEET2 for ground truthing and use at DoD sites (Section 7.0), the potential cost savings from use of SVEET2 in a performance assessment framework (Section 8.0), and issues related to implementation (Section 9.0).

# 2.0 SVEET2 Updates

The SVEET software update process began with a survey of DoD remedial project managers (RPMs) to gather information on the nature of sites using SVE. This information was compiled and used to define the changes in parameter permissible ranges to represent site conditions in the generalized conceptual model. The survey results are summarized below, followed by a description of the updates to SVEET v. 1.0 to obtain SVEET2.

## 2.1 Soil Vapor Extraction Survey

The first step in determining the most relevant changes to parameter ranges was to conduct a survey of waste site managers (primarily DoD sites) to gather information on their site characteristics. The survey (Appendix A) was distributed to an extensive set of Army, Navy, and Air Force RPMs. Survey results were compiled (Table 2, Figure 4) and reviewed in comparison to the proposed updates to refine the relevant ranges of parameter values. Note that five additional responses are not shown because those responses were largely incomplete (either because information was not known or because of site confidentiality issues).

***Table 2.*** *Compiled survey response information.*

| Site | VZT (m) | L1 (m) | L2 (m) | z (m) | RSP | STR | SA (m$^2$) | Receptor (m) | Has Cap ? | R (cm/y) | VI Issue ? |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Camp Lejeune Site 96 | 6.1 | 0 | 0 | 6.1 | 1 | 1 | 2000 | 22.9 | N | — | Y |
| Confidential Site | 9.14 | 3.05 | 0 | 6.1 | 30.5 | 0.667 | 9300 | 168 | N | 63.5 | Y |
| Confidential European Site | 6 | 0 | 2 | 4 | 0.048 | 0.667 | 1800 | 1000 | Y | 20 | N |
| Confidential Mfgr. Facility | 2.44 | 0 | 0 | 2.44 | 1 | 1 | 3700 | 152 | N | — | Y |
| Dow Altona | 7 | 5 | 0 | 2 | 50 | 0.286 | 20000 | — | N | — | N |
| Georgetown (Burlington Env.) | 3.05 | 0.91 | 0 | 2.13 | 9.1 | 0.7 | 8000 | 30.5 | Y | 0 | Y |
| Hassayampa | 25 | 11 | 1 | 13 | 11 | 0.52 | 676 | 185 | Y | — | N |
| Hunters Point | 2.44 | 0.91 | 0.61 | 0.91 | 1.5 | 0.375 | 5 | 305 | Y | — | Y |
| Lipari | 9.14 | 0.91 | 0 | 8.23 | 9.1 | 0.9 | 24000 | 152 | Y | — | N |
| Mare Island B742 | 2.74 | 0.91 | 1.22 | 0.61 | 0.75 | 0.222 | 1 | 91 | Y | — | Y |
| McClellan/Mather | 30.5 | — | — | — | — | — | — | 152 | some | 38.1 | Y |
| North Island | 7.01 | 1.52 | 0 | 5.49 | 15.2 | 0.783 | 14000 | 610 | N | — | Y |
| Point Loma | 10 | 1.22 | 7.26 | 1.52 | 0.17 | 0.152 | 1600 | 805 | N | 2.54 | Y |
| Tooele TEAD-N Bldg 615 | 91.4 | 55 | 16.4 | 20 | 3.35 | 0.219 | 750 | 1000 | N | 1.65 | N |
| Tooele TEAD-N Bldg 620 | 95 | 60 | 15 | 20 | 4 | 0.211 | 1800 | 1000 | — | 1.65 | — |
| Tooele TEAD-N Bldg 679 | 95 | 5 | 75 | 15 | 0.067 | 0.158 | 2500 | 1000 | — | 1.65 | — |
| Tooele TEAD-N LF 006 | 95 | 10 | 65 | 20 | 0.15 | 0.211 | 2500 | 1000 | — | 1.65 | — |
| Tooele TEAD-N LF 012 | 95 | 15 | 50 | 30 | 0.3 | 0.316 | 2500 | 1000 | — | 1.65 | — |
| TPH Phoenix (Honeywell) | 24.38 | 18.9 | 0 | 5.49 | 190 | 0.225 | 194000 | 183 | Y | — | N |
| US Army CRREL | 36.6 | 6.1 | 22.9 | 7.62 | 0.27 | 0.208 | 557 | 335 | Y | 30.48 | Y |


***Figure 4.*** *Summary plots of survey data. Note that the McClellan/Mather site is not included on these plots.*

The survey data indicate several aspects that helped define the scope of the updates for SVEET2. An expanded range of VZT values is needed because multiple sites have water tables shallower or deeper (including sites at Hill Air Force Base [AFB], which are on the order of 150 m deep) than SVEET version 1.0 allowed. A number of sites, mostly with smaller VZT values, have sources that are relatively close to the water table, and thus would require a RSP value greater than 10. Sites with smaller VZT values also tend to have source contamination through a larger fraction of the vadose zone (i.e., greater STR value). Multiple sites have source areas that are greater than 2500 $m^2$, though the survey responses may be more reflective of overall contamination than the extent of a vadose zone source (e.g., residual NAPL). Receptors locations ranged from quite close to about 1000 m distant. Less is known about recharge at many sites, but ranges include dry to relatively wet. A cap (i.e., a barrier to infiltration) is relevant to a number of sites, so recharge could be expected to be lower at those sites. Vapor intrusion (VI) is a potential concern at a number of sites. All of this information was useful to help refine the nature of the SVEET2 updates.

## 2.2 Updated Aspects in SVEET2

Table 3 lists the elements that were updated in SVEET2 with this work. Ranges are expanded to the same extent or greater than identified in the project proposal, with two exceptions. The survey data indicated that few sites required an RSP less than 0.1, so an additional low-end RSP value was not added (which helps manage the total number of STOMP simulations required). Although the proposal and survey data had indicated interest in Acetone, 2,2-Dichloropropane, and total petroleum hydrocarbons as contaminants, these contaminants could not be included in SVEET2 because no temperature-dependent correlations were available for calculation of the Henry's Law Constant.

***Table 3.*** *SVEET2 update elements.*

| SVEET v. 1 | SVEET2 |
|---|---|
| *Contaminants:*<br>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 | Added these contaminants:<br>1, 2-Dichloropropane, 1, 3-Dichloropropane, 1,2,3-Trichloropropane, MIBK, MTBE, MEK, Chlorobenzene, BTEX constituents, Freons (11, 12, 113), 1,4-Dioxane<br><br>Note: biodegradation effects are not included in SVEET v. 1.0 or SVEET2. |
| *Input/Output Structure:*<br>Allows 3 concurrent scenarios | Allow 5 concurrent scenarios |
| *GW Monitoring Well Locations for Output:*<br>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:*<br>*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 – 2000 ppmv | 0.001 – 100,000 ppmv |
| *Source Mass Flux:* 0.1 – 5000 g/d | 0.1 – 40,000 g/d |
| *Recharge*<br>0.4 – 7.5 cm/yr | 0.4 – 15 cm/yr |
| *Bulk Density and Porosity:*<br>Fixed at 1.855 g/mL and 30%, respectively. | Allow user-specified bulk density and porosity values |
| *Relative Water Saturation (Moisture Content):*<br>0.05 – 0.55 (1 – 9 wt%) | 0.05 – 0.75 (% 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<br>0.75 STR is allowed for VZT ≤ 10 m |
| *Relative Source Position:* 0.1 – 10 | 0.1 – 50<br>50 RSP is allowed for VZT ≥ 30 m |
| *Source Footprint (square):* 100 – 2500 $m^2$ | 100 – 10,000 $m^2$ |
| *Groundwater Darcy Velocity:* 0.005 – 0.3 m/d | 0.005 – 1.0 m/d |

The last six elements in Table 3 required a number of new STOMP simulations to expand the permissible ranges for the Sr, VZT, STR, RSP, SA, and q parameters. Table 4 provides a depiction of the new parameter key values that provide the basis for interpolation. If this full matrix of parameter values were simulated, 7680 simulations would be required in total. As discussed in Section 2.1, the survey data indicated that extended ranges of certain parameters were mainly relevant under specific conditions. Thus, the matrix of simulations can be constrained to the conditions where STR = 0.75 and RSP = 50 are more relevant (i.e., maximum STR = 0.75 when VZT ≤ 10 and maximum RSP = 50 when VZT ≥ 30). Applying these constraints allows the number of simulations required to be refined to 5760, as shown in Table 5.

***Table 4.*** *Expansion of parameter ranges (new values are in* ***bold red****).*

| Parameter | Evaluation Points Forming the Basis for Interpolation | | | | | | # Key Values |
|---|---|---|---|---|---|---|---|
| $S_r$ | | 0.05 | 0.3 | 0.55 | **0.75** | | 4 |
| STR | | 0.1 | 0.25 | 0.5 | **0.75** | | 4 |
| VZT | **3** | 10 | 30 | 60 | **110** | **150** | 6 |
| SA | | 100 | 400 | 900 | 2500 | **10000** | 5 |
| q | | 0.005 | 0.03 | 0.3 | **1** | | 4 |
| RSP | | 0.1 | 1 | 10 | **50** | | 4 |

***Table 5.*** *Number of key values for parameters (with the actual key values in parentheses) and total number of STOMP simulations required.*

| Parameter | **SVEET 1.0** (re-run for consistency) | **Number of STOMP Simulation Key Values for SVEET2** | | |
|---|---|---|---|---|
| | | **Bulk of New Sims.** | **STR = 0.75 Sims.** | **RSP = 50 Sims.** |
| $S_r$ | 3 (0.05, 0.3, 0.55) | 4 (0.05, 0.3, 0.55, 0.75) | 4 (0.05, 0.3, 0.55, 0.75) | 4 (0.05, 0.3, 0.55, 0.75) |
| STR | 3 (0.1, 0.25, 0.5) | 3 (0.1, 0.25, 0.5) | 1 (0.75) | 3 (0.1, 0.25, 0.5) |
| VZT | 3 (10, 30, 60) | 6 (3, 10, 30, 60, 110, 150) | 2 (3, 10) | 4 (30, 60, 110, 150) |
| SA | 4 (100, 400, 900, 2500) | 5 (100, 400, 900, 2500, 10000) | 5 (100, 400, 900, 2500, 10000) | 5 (100, 400, 900, 2500, 10000) |
| q | 3 (0.005, 0.03, 0.3) | 4 (0.005, 0.03, 0.3, 1.0) | 4 (0.005, 0.03, 0.3, 1.0) | 4 (0.005, 0.03, 0.3, 1.0) |
| RSP | 3 (0.1, 1, 10) | 3 (0.1, 1, 10) | 3 (0.1, 1, 10) | 1 (50) |
| Number of Simulations | 972 | 3348 (accounting for the 972 already completed) | 480 | 960 |
| Grand Total: | **5760** | | | |

The reduced set of STOMP simulations results in minor discontinuities in possible representations of source thickness and relative source position, as depicted in Figure 5. There is no impact when both STR and RSP are at a minimum. The closest that the bottom of the source could get to the water table for the thinnest of source zones jumps from about 0.5 m at a vadose zone thickness of 30 m to a distance of about 2.4 m for a vadose zone thickness slightly less than 30 m. For the thickest of source zones, the distance from the bottom of source to the water table from has a smaller discontinuity, allowing a distance of about 0.3 m at VZT = 30 and 1.35 m for VZT just under 30. Similarly, there is a discontinuity relative to VZT for the source thickness ratio. At VZT = 10, the largest STR is 7.5 m, while at a VZT just greater than 10, the largest STR is near 5 m. Using SVEET v. 1.0 to investigate variations in groundwater concentration, it appears that such discontinuities could result in differences in groundwater concentrations that are on the order of 5 to 25 µg/L. Sites near the discontinuity bounds should evaluate the sensitivity in results to variations in the scenarios. For example, if a site actually has a 28 m vadose zone thickness, but the source is within one meter of the water table, then it is probably more appropriate to use a vadose zone thickness of 30 and appropriate RSP value to achieve a more representative distance between source and water table.

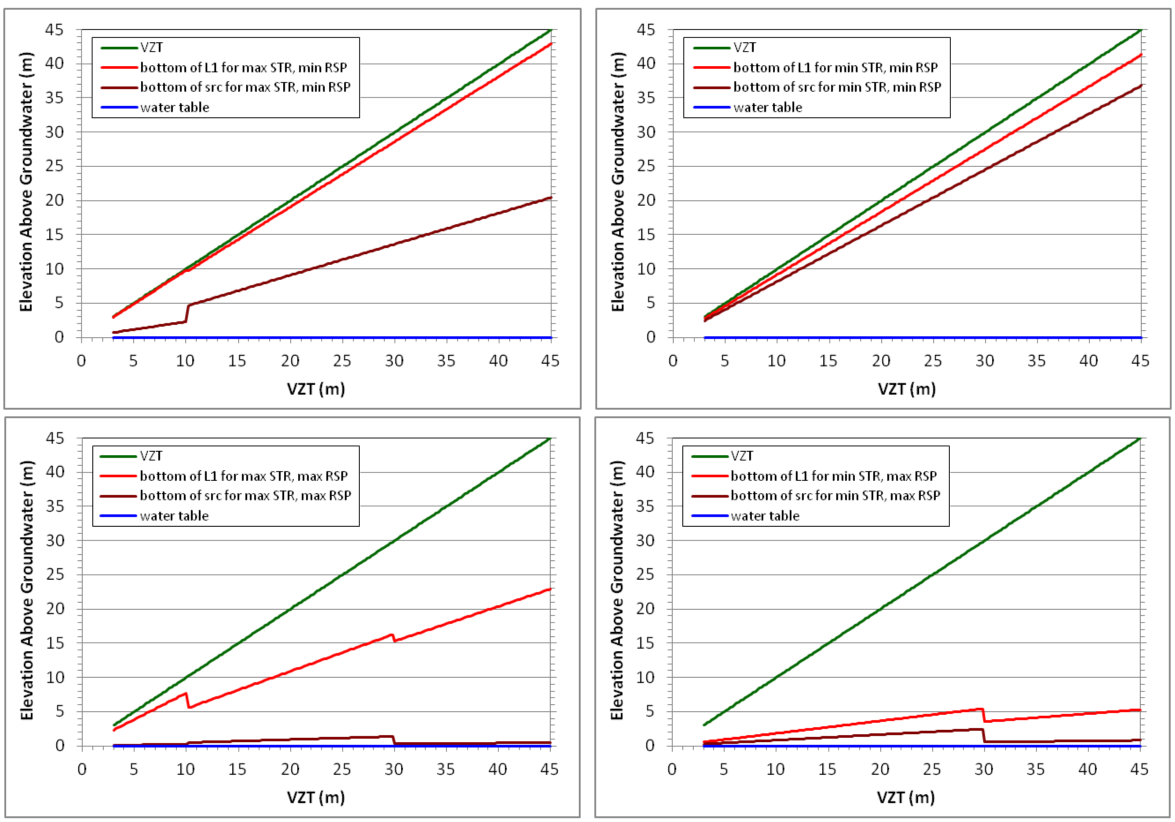



***Figure 5.*** *Options for source thickness (STR) and relative source position (RSP) as a function of vadose zone thickness for the reduced set of STOMP simulations (Table 5).*

A categorization scheme was defined for SVEET v. 1.0 to provide a structured method for managing the STOMP simulations (Table 6). Because the parameter ranges have been expanded, the categorization scheme was revised for SVEET2 to the alphabetic scheme shown in Table 7 (where a few letters have been intentionally skipped and reserved for future use).

***Table 6.*** *Categorization of pairs of VZT and STR values, as used for SVEET version 1.0.*

| **Categories** [a] | **VZT (m)** | | |
|---|---|---|---|
| **STR (–)** | 10 | 30 | 60 |
| 0.1 | Category 1 | Category 2 | Category 3 |
| 0.25 | Category 4 | Category 5 | Category 6 |
| 0.5 | Category 7 | Category 8 | Category 9 |

[a] Each category has a different vertical numerical grid discretization for RSP = 0.1, 1, and 10.

***Table 7.*** *SVEET2 categorization of pairs of VZT and STR values to assist in data organization.*

| | **VZT (m)** | | | | | |
|---|---|---|---|---|---|---|
| **STR (–)** | 3 | 10 | 30 | 60 | 110 | 150 |
| 0.1 | Category A | Category E | Category I | Category M | Category Q | Category U |
| 0.25 | Category B | Category F | Category J | Category N | Category R | Category V |
| 0.5 | Category C | Category G | Category K | Category O | Category S | Category W |
| 0.75 | Category D | Category H | L | P | T | X,Y,Z |

| Color Legend: | RSP = 0.1, 1, 10 | RSP = 0.1, 1, 10, 50 |
|---|---|---|

The SVEET2 software itself (in the form of a Microsoft Excel workbook) was modified to incorporate additional STOMP simulation results, thereby expanding the permitted input ranges, and other enhancements. The primary purpose of the new simulations is to allow expansion of permissible parameter input ranges for parameters having nonlinear effects on results. The first five elements of Table 3 describe other enhancements that were incorporated into the SVEET2 software. These other enhancements include new contaminants, allowing up to 5 concurrent scenarios, allowing more flexible options for locations where groundwater and vadose zone results can be requested, and expanding the source strength input range. The SVEET2 enhancements were incorporated in a manner designed to maintain the user-friendly nature of the software, with straightforward inputs/outputs and guidance on permissible parameter values.

## 2.3 Data Files for SVEET2

Dealing with a large amount of underlying data is important in SVEET2. In SVEET version 1.0 (Truex et al., 2013), 972 STOMP simulations formed the basis for the calculations, meaning that 972 × 5 downgradient locations = 4860 values were required, which fit well into the SVEET v. 1.0 Excel workbook. In VIETUS (Johnson et al., 2016), data from the same 972 simulations was used to provide soil gas concentration estimates for vapor intrusion analysis. However, VIETUS allowed the user to select any lateral location (on a 66 by 28 numerical grid) and one of 8 possible depths (0.5 to 4 m below ground surface in 0.5 m increments), which required storing around 13 million values. Thus, VIETUS used an external 74.63 MB text file for storing the STOMP simulation result values. SVEET2 has nearly 6 times more simulations (5760), with the groundwater including 29 more locations along the plume centerline, though the soil gas includes 2 depths instead of the 8 available in VIETUS. Thus, SVEET2 needs access to some 780,000 groundwater concentration values and 21 million soil gas concentration values. A data management approach similar to that used for VIETUS was required to accommodate this large quantity of data, while streamlining distribution and ensuring quick calculations.

Instead of storing concentration values directly, an approach was developed to store the data in a compressed format in an external file without requiring Excel to unzip the file with each calculation. The first step was to convert all results to nanograms per liter and retain the integer portion of that re-scaled value. Because of how the STOMP simulations are run with a source concentration of 1.0 mg/L, results are nominally less than that concentration, giving a maximum ng/L value of 1000000, which is a 7-character integer. The technique of numeric base conversion[1,2,3] was used to convert the 7-character integer into a 3-character base-171 value. An "alphabet" of characters was developed and the base conversion to and from base-171 was programmed into Visual Basic for Applications (VBA) procedures for incorporation into SVEET2. Base-171 allows a maximum decimal (integer) value of 5000210 to be encoded with only 3 characters. The use of 3 characters instead of 7 for all values gives a compression ratio of about 43% of the original size. Distribution of the SVEET2 software uses standard zip compression to compress the 85 MB package of files into a 19 MB compressed zip file.

[1] Weisstein, E.W. 2020. "Base." MathWorld--A Wolfram Web Resource. Available at: https://mathworld.wolfram.com/Base.html (Accessed 9/1/2020).

[2] Wikipedia. 2020. "Positional Notation." (website). Wikimedia Foundation, Inc. Available at: https://en.wikipedia.org/wiki/Positional_notation#Base_conversion (Accessed 9/1/2020).

[3] Adam Bjornson. 2016. "Number Converter." (website). Available at: http://bitfume.com/tools/number-converter/ (Accessed 9/1/2020).

# 3.0 Calculations Behind SVEET2

This section is adapted from Appendix C of Truex et al (2013) to describe the calculations implemented in the SVEET2 software.

When vapor-phase transport is an important component of the overall contaminant fate and transport from a vadose zone source, the contaminant concentration expected in groundwater and soil gas is controlled by a limited set of parameters (Oostrom et al., 2014; Truex et al., 2013), including specific site dimensions, vadose zone properties, and source characteristics. Under these circumstances, it is possible to pre-model contaminant transport for a matrix of parameter value combinations that cover a range of conditions. Results for a specific waste site can be estimated by comparing the site-specific characteristics to the characteristics of the pre-modeled scenarios. This approach consists of three steps: 1) defining site-specific inputs, 2) interpolating between pre-modeled scenario results for parameters that have nonlinear impacts on the groundwater and soil gas contaminant concentrations, and 3) scaling the interpolated results for parameters that have linear impacts on the estimated contaminant concentrations. A detailed description of the steps for this approach (summarized in Figure 6) and the required inputs is provided below. An example scenario is also used to illustrate the calculation process.

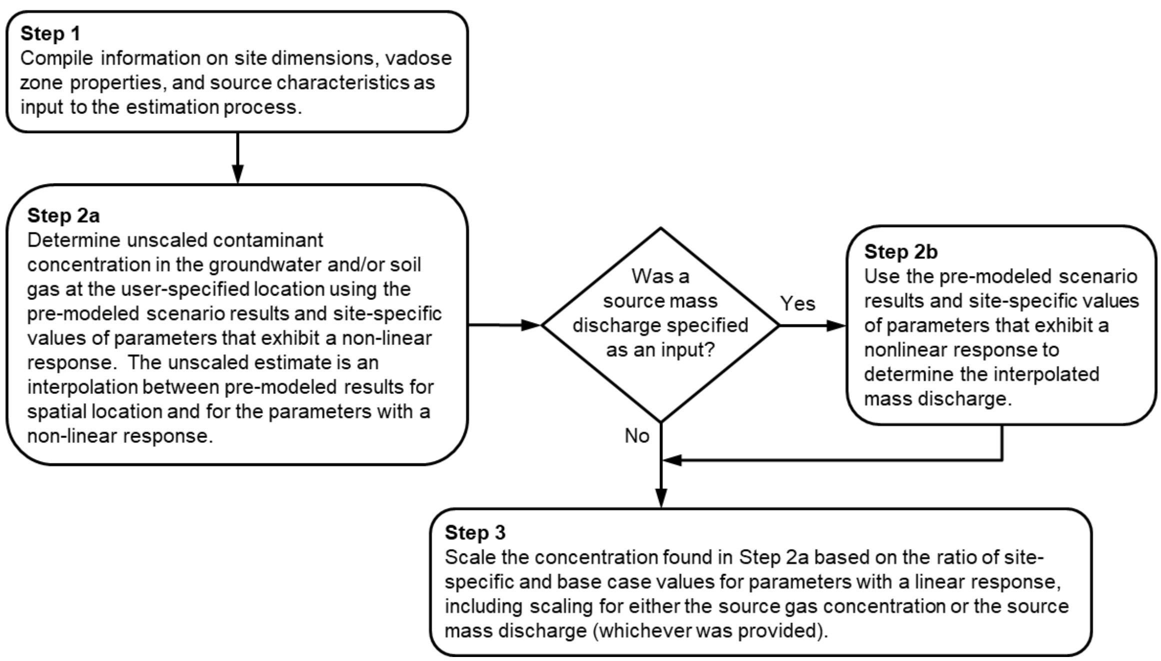



***Figure 6.*** *Flow chart of the three steps involved in the process for estimating contaminant groundwater and soil gas concentrations.*

Multiple factors may affect the estimated contaminant concentrations in the groundwater and soil gas. One category of such factors is the uncertainty of input parameter values. A sensitivity analysis can readily be conducted using SVEET2 to assess the potential impact of reasonable variation in specific input parameters on the estimated results. Other factors are outside the scope of the approach described here, but should be considered for potential site-specific impacts. Such factors include the degree of source depletion over time, adsorption, biological transformation, and other physical attenuation mechanisms. Sites will also need to consider the appropriateness of the simplifying assumptions used in the approach with respect to the site-specific conditions. For instance, the generalized conceptual model used in the approach is appropriate for sites where vapor-phase transport dominates contaminant migration.

The procedure described here is intended to estimate the contaminant concentrations for specified locations in groundwater and soil gas that result from a contaminant source located in the vadose zone. This estimation process could contribute to the design of a soil vapor extraction (SVE) system by providing information about the vadose zone remediation performance required to meet groundwater contaminant concentration goals. For existing SVE systems, this estimation process could provide input for decisions pertaining to system optimization, site closure, or transition to another remedy. Soil gas concentration estimates can be used as input to a vapor intrusion evaluation to support decisions regarding the SVE remedy or other mitigation approaches.

## 3.1 Step 1: Compilation and Conversion of Inputs

The estimation method is based on the site conceptualization depicted in Figure 7, centered on a source area present at a specified vertical location within a vadose zone of specified characteristics. Estimated concentration results are determined for a specified downgradient distance along the groundwater plume centerline or a specified lateral location at sub-slab or sub-basement vadose zone depths for a specified contaminant.

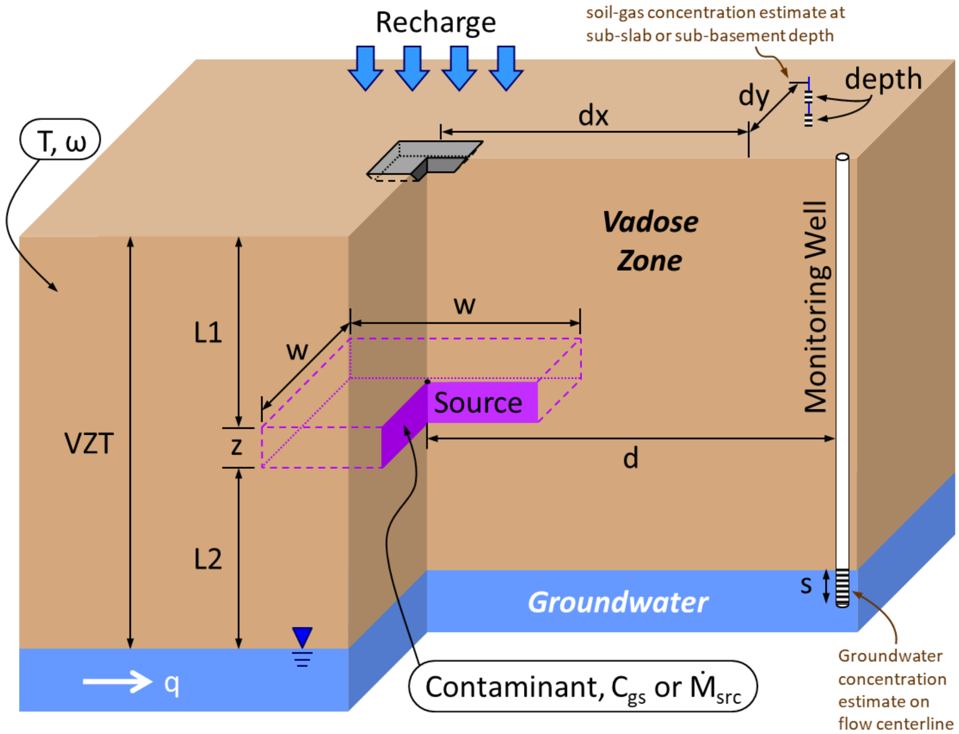



***Figure 7.*** *Conceptual framework for estimating the impact of a vadose zone contaminant source on groundwater concentration at a compliance well*

The calculational procedure for estimating the contaminant concentration in groundwater and/or soil gas at the location(s) of interest requires a set of conceptual framework inputs that describe the scenario of interest. The user is asked to provide the input parameters listed in Table 8, from which several key parameters (i.e., the parameters in the shaded rows of the table) are calculated for use in interpolation of STOMP simulation results. Truex et al. (2013) discusses approaches for determining or estimating certain information about the source area, including the lateral extent of the source area, vertical location of the source within the vadose zone, and "source strength." The source strength calculational input may be represented as either a vapor-phase contaminant concentration ($C_{gs}$) or a mass discharge of contaminant ($\dot{M}_{src}$), but not both. Because there may be uncertainty associated with input parameters, users are encouraged to conduct a sensitivity analysis, whereby multiple estimated results are determined using appropriate ranges for input parameter values. SVEET2 allows multiple (up to five) input scenarios to be evaluated as a group. The effects variations in input parameter values can be assessed to understand parameter importance and the range of potential results. Identification of parameters with the most uncertainty/largest impact can help guide where additional data collection efforts can be focused.

*Table 8. Input parameters and calculated intermediate parameters (shaded rows).*

| Parameter Name | Parameter | Units | Permissible Range | Key Values [a] and Notes |
|---|---|---|---|---|
| Contaminant | *Contam.* | — | 32 options | CT; see HLC worksheet for options |
| Temperature | $T$ | °C | 5 – 99 | 20 |
| Avg. Recharge | $R$ [b] | cm/yr | 0.4 – 15 | 0.4 |
| Avg. Soil Moisture Content | $\omega$ | wt% | varies [c] | Sr key value equivalents [c] |
| Total Porosity | $\theta_{total}$ | — | 0.1 – 0.5 [d] | 0.3 |
| Dry Bulk Density | $\rho_{bulk}$ | g/mL | 1.1 – 2.0 [d] | 1.855 |
| Vadose Zone Thickness | *VZT* | m | 3 – 150 | 3, 10, 30, 60, 110, 150 |
| Depth to Top of Source | *L1* | m | 0.07 - 132 [e] | — |
| Source Thickness | $z$ | m | 0.3 - 75 [f] | — |
| Source Width (= Length) | $w$ | m | 10 – 100 [g] | — |
| GW Darcy Velocity | $q$ | m/day | 0.005 – 1.0 [h] | 0.005, 0.03, 0.3, 1.0 |
| Compliance Well Screen Length | $s$ | m | 1 – 30 | 1, 3, 5, 9 |
| Distance to GW Compliance Well | $d$ | m | 0 – 850 | downgradient from source center |
| Longitudinal Distance for Soil Gas | $dx$ | m | -850 – 850 | dx < 0 is upgradient of source center |
| Transverse Distance for Soil Gas | $dy$ | m | 0 – 370 | transverse distance |
| Depth of Basement/Foundation | $dz$ | m | 1.0 or 4.0 | sub-slab or sub-basement |
| Source Gas Concentration | $C_{gs}$ | ppmv | 0.001 – 100,000 | 159 |
| Source Mass Discharge | $\dot{M}_{src}$ | g/day | 0.1 – 40,000 | from STOMP simulations at 3 months elapsed time |
| Residual Saturation | *Sr* | — | 0.05 - 0.75 [c] | 0.05, 0.3, 0.55, 0.75 |
| Source Thickness Ratio | *STR* | — | 0.1 - 0.75 [i] | 0.1, 0.25, 0.5, 0.75 |
| Relative Source Position | *RSP* | — | 0.1 - 50 [j] | 0.1, 1, 10, 50 |
| Areal Footprint of Source | *SA* | $m^2$ | 100 - 10,000 | 100, 400, 900, 2500, 10,000 |
| Dist. from Source Bottom to GW | *L2* | m | 0.07 – 122 [e] | — |
| Henry's Law Constant | $H$ | — | contaminant-specific [k] | 0.89 |

[a] The key values indicate either the values used in the STOMP simulations of pre-modeled scenarios (for parameters having nonlinear relationship) or the "base case" scenario values (for parameters having a linear/inverse linear or source strength relationship).

[b] For sites with recharge above 2.5 cm/yr, confirm the applicability of the estimation approach used here, as discussed in Truex et al. (2013).

[c] The STOMP simulations of pre-modeled scenarios use residual saturation (Sr), not gravimetric moisture content ($\omega$). However, weight percent gravimetric moisture content ($\omega$ = [g water / g dry soil]·100%) is requested as the input parameter for user convenience. Note that $S_r = (\omega \cdot \rho_{bulk}) / (100 \cdot \theta_{total} \cdot \rho_{water})$ Moisture content is constrained to the bounds of Sr, but the minimum and maximum permissible moisture contents will vary depending on the total porosity ($\theta_{total}$) and dry bulk density ($\rho_{bulk}$) values that are used.

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

[e] The ranges for L1 and L2 are variable because they are a function of the permissible range for RSP and the input values of z and VZT. RSP = L1 / (VZT – L1 – z) = L1 / L2

[f] The range for z is variable because it is a function of the permissible range for STR and the input value of VZT. STR = z / VZT

[g] The range for w is a function of the permissible range for SA.

[h] Darcy velocity (q) is input directly, but can be calculated from q = horizontal hydraulic conductivity)×(hydraulic gradient).

[I] STR values > 0.5 are permissible for VZT values ≤ 10 m

[j] RSP values > 10 are permissible for VZT values ≥ 30 m.

[k] The dimensionless Henry's Law Constant is calculated based on the site-specific subsurface temperature and contaminant-specific, temperature-dependent property correlations (i.e., for vapor pressure [Yaws et al. 2009] and solubility [Yaws, 2012; Horvath and Getzen, 1999; Ondo and Dohnal, 2007]).

The site characteristics listed in Table 8 can be categorized based on how the parameters are used in subsequent steps of this estimation procedure. Parameters that exhibit a nonlinear response in the contaminant concentration at the compliance well are examined in the context of the pre-modeled scenario STOMP simulation results. To avoid extrapolation outside of the pre-modeled scenarios, the input parameters are restricted to be within the permissible ranges noted in Table 8. Ranges have also been defined for parameters that exhibit a linear or inverse linear relationship to contaminant concentrations in the groundwater (including the "source strength" parameters). The range for the average recharge should be considered as described in Truex et al. (2013) because an underlying premise for the modelling is that vapor phase transport is the dominant contaminant migration method. The ranges for the source strength variables ($C_{gs}$ and $\dot{M}_{src}$) are based on reasonable extrapolation from the "base case" source strength that was used in the pre-modeled scenarios. The range for Henry's Law constant is determined by the permitted range for the subsurface temperature and the choice of the contaminant. An alternative approach (e.g., site-specific simulations) should be considered for sites with characteristics that are outside of the ranges specified here.

In SVEET2, user-specified values are allowed for porosity ($\theta_{total}$) and bulk density ($\rho_{bulk}$), whereas SVEET version 1.0 applied the fixed values that were defined for the STOMP simulations (Table 3). An equivalent flux approach, described in Appendix B, is applied in SVEET2 to calculate an effective residual saturation, *Sr*, for use in the estimation procedure. Because porosity and bulk density can be specified by the user, the minimum and maximum moisture content values are calculated as a function of those parameters and the density of water ($\rho_w$) as follows, using the base case porosity (0.3) and the *Sr* minimum (0.05) or maximum (0.75) values.

## 3.2 Step 2: Pre-Modeled Scenario Result Interpolation for Nonlinear Variables

A total of 5760 pre-modeled scenarios (Table 5) were simulated with the STOMP code (White and Oostrom 2006) to assess the impact of variation in parameters that have a nonlinear relationship with concentrations in groundwater and soil gas. These variables include *Sr*, *STR*, *VZT*, *RSP*, *q*, and *SA*. Table 8 lists the key values used for each of the parameters with a nonlinear relationship to contaminant concentrations. It is the combinations of these key values that comprise the suite of pre-modeled scenarios, as described in Table 4. Scoping simulations were used to select the key values for the parameters that exhibit a nonlinear response in groundwater concentrations, with the objective that linear interpolation between bounding cases gives a reasonable estimate. Further details of the STOMP simulation basis are given in Truex et al. (2013). The pre-modeled scenarios all used "base case" values for the linear parameters, which include *H*, *R*, $C_{gs}$, and $\dot{M}_{src}$. The base case values represent a site with 0.4 cm/yr of recharge, a 159 ppmv source (equivalent to 1 $mg/L_{gas}$ for carbon tetrachloride), a Henry's Law constant of 0.89, a porosity of 0.3, and a dry bulk density of 1.855 g/mL. STOMP simulations were run to obtain steady-state concentration distributions in the gas and aqueous phases throughout the computational domain. Groundwater concentrations were then tabulated for each pre-modeled scenario for grid cell locations at and downgradient of the source center along the plume centerline (primary flow direction). Soil gas concentrations were tabulated across the domain (actually, a half domain in the transverse direction is used due to symmetry) for depths of 1 m and 4 m below ground surface, which are intended to represent depths relevant to sub-slab and sub-basement locations.

This second step in the estimation of the contaminant concentrations is based on a sequence of lookups and linear interpolations to find the unscaled groundwater concentration ($C_{wu}$) at the compliance well for the site-specific parameters. Interpolation is a two-part process. Interpolation to the specified location (longitudinal distance and screen length for groundwater concentration; longitudinal and transverse distance for soil gas concentration) is performed first. Then, interpolation between the pre-modeled scenarios is performed, unless all site-specific values correspond exactly to one of the pre-modeled scenarios. Interpolated values are calculated using Equation 1, where *P* denotes the parameter value, *C* is the simulation concentration, and the subscripts *upper* and *lower* represent the known values above and below the interpolation point of interest (*interp*). If the input for a nonlinear relationship parameter consists of a value that is equal to one of the key values in Table 8, then no interpolation is needed with respect to that parameter. Otherwise, linear interpolation will be performed using results from the bounding simulations. The lookups/interpolations are performed in the sequence of *SA*, *q*, *RSP*, *VZT*, *STR*, and *Sr* (calculated from $\omega$). Interpolation for the six nonlinear relationship parameters (*SA*, *q*, *RSP*, *VZT*, *STR*, and *Sr*) uses $2^6 = 64$ $C_{sim}$ values from the pre-modeled scenarios (interpolated to the specified location), which represent the lower and upper bounds of the range into which each of the six parameters falls.

$$C_{interp} = \left[ \frac{P_{interp} - P_{lower}}{P_{upper} - P_{lower}} \right] \cdot (C_{upper} - C_{lower}) + C_{lower} \qquad (1)$$

If the source strength input parameter provided was the $\dot{M}_{src}$ value (i.e., not the $C_{gs}$ value), then a second sequence of lookups/interpolations is performed to determine the simulated contaminant mass discharge ($\dot{M}_{sim}$) corresponding to the input site parameters. This $\dot{M}_{sim}$ value is needed in Step 3 of the procedure as a linear scaling factor. The process for obtaining the interpolated $\dot{M}_{sim}$ mass discharge value is the same as for $C_{wu}$, except that the distance interpolation does not apply.

## 3.3 Step 3: Scaling for Linear Variables

The last step in the procedure to estimate the site-specific contaminant concentrations is to scale the $C_{wu}$ value obtained in Step 2 to account for the parameters where the contaminant concentrations vary linearly or inverse linearly with the parameter value. The base case (key) values discussed above and listed in Table 8 form the basis for the scaling.

The Henry's Law constant for the site conditions (contaminant and temperature) is required as part of the scaling process. In Table 8 it was noted that the Henry's Law constant can be calculated based on the site-specific subsurface temperature and contaminant-specific, temperature-dependent chemical property correlations. The Henry's Law constant and its temperature dependence have been examined in a wide range of literature for contaminants of environmental interest (e.g., Staudinger and Roberts 2001; Warneck 2007; Chen et al. 2012). Brennan et al. (1998) suggested calculating the Henry's Law constant as the ratio of the vapor pressure to the water solubility as the preferred approach for dilute contaminant concentrations (< 0.02 mol fraction). Thus, a temperature-dependent Henry's Law constant can be found using temperature-dependent vapor pressure and water solubility values. However, the accuracy of this approach depends on the accuracy of the vapor pressure and water solubility information.

The temperature-dependent correlation for vapor pressure selected for use in this work is the Antoine correlation given in Equation 2 where $T$ is temperature in °C, $P_{vap}$ is the vapor pressure in mm Hg, and $A$, $B$, and $C$ are contaminant-specific correlation coefficients (Yaws et al. 2009).

$$Log_{10}(P_{vap}) = A - \frac{B}{T+C} \qquad \text{T is in °C} \qquad (2)$$

For most of the 32 contaminants (with 3 exceptions), the temperature-dependent water solubility correlation of Yaws (2012) is used, as shown in Equation 3. Here, $x_p$ is the mass fraction in weight percent, $T_k$ is temperature in K, and $A$, $B$, and $C$ are tabulated contaminant-specific correlation coefficients (Yaws, 2012). Correlation data were not available in Yaws (2012) for 1,3-dichloropropane or 1,2,3-trichloropropane, so solubility correlation coefficients ($A$, $B$, and $C$) from Horvath and Getzen (1999) were used instead in Equation 4. Yaws (2012) also does not have water solubility correlation information for 1,4-dioxane, so the correlation for the Henry's Law constant provided in Ondo and Dohnal (2007) was used to directly obtain $H_{px}$ (kPa) from Equation 5. Weight percent mass fraction values are converted to mole fraction, $x$, in Equation 6 by multiplying by the ratio of the molecular weight of water ($MW_w$, 18.01528 g/mol) to the molecular weight of the contaminant ($MW_i$, g/mol).

$$\mathrm{Log}_{10}(x_p) = A + B/T_k + C \cdot \mathrm{Log}_{10}(T_k) \qquad T_k \text{ is in K} \qquad (3)$$

$$x_p = A + B \cdot T_k + C \cdot T_k^2 \qquad T_k \text{ is in K} \qquad (4)$$

$$\ln(H_{px}) = A + B/T_k + C \cdot \ln(T_k) + D \cdot T_k \qquad T_k \text{ is in K} \qquad (5)$$

$$x = \frac{x_p}{100} \cdot \frac{MW_w}{MW_i} = x_f \cdot \frac{MW_w}{MW_i} \qquad x_f \text{ is mass fraction} \qquad (6)$$

The contaminants available in the software and their tabulated correlation coefficients (and molecular weights) are shown in Table 9.

***Table 9.*** *Tabulated correlation coefficients for contaminants of interest from Yaws et al. (2009), Yaws (2012), Horvath and Getzen (1999), and Ondo and Dohnal (2007)*

| | | | Correl. Coef. for Calculating Vapor Pressure | | | Correlation Coefficients for Calculating Solubility or H | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Contaminant Abbrev.** | **Contaminant** | **Molecular Weight** (g/mol) | **A** | **B** | **C** | **Eqn** | **A** | **B** | **C** | **D** |
| CT | Carbon Tetrachloride | 153.823 | 7.01144 | 1278.54 | 232.888 | 4 | -7.4600 E+1 | 3.3774 E+3 | 2.5130 E+1 | 0 |
| CF | Chloroform | 119.378 | 7.11148 | 1232.79 | 230.213 | 4 | -8.5244 E+1 | 3.9461 E+3 | 2.9057 E+1 | 0 |
| DCM | Dichloromethane | 84.933 | 7.11464 | 1152.41 | 232.442 | 4 | -1.3856 E+2 | 6.4354 E+3 | 4.7322 E+1 | 0 |
| CM | Chloromethane | 50.488 | 6.99771 | 870.17 | 235.586 | 4 | 3.0022 E+1 | -1.6520 E+2 | -1.2013 E+1 | 0 |
| PCE | Tetrachloroethene | 165.833 | 7.06892 | 1458.45 | 226.986 | 4 | -9.0823 E+1 | 3.8474 E+3 | 3.0813 E+1 | 0 |
| TCE | Trichloroethene | 131.388 | 6.87981 | 1157.83 | 202.580 | 4 | -2.4133 E+1 | 9.3612 E+2 | 8.0968 E+0 | 0 |
| 1,1-DCE | 1,1-Dichloroethene | 96.943 | 7.21678 | 1181.12 | 240.840 | 4 | -1.3500 E+2 | 6.2391 E+3 | 4.5844 E+1 | 0 |
| cDCE | cis-1,2-Dichloroethene | 96.943 | 7.21953 | 1290.28 | 236.887 | 4 | -2.1907 E+2 | 9.8827 E+3 | 7.5057 E+1 | 0 |
| tDCE | trans-1,2-Dichloroethene | 96.943 | 7.21356 | 1244.35 | 239.497 | 4 | -4.1184 E+1 | 2.0908 E+3 | 1.3671 E+1 | 0 |
| VC | Vinyl Chloride | 62.498 | 6.91423 | 911.15 | 239.800 | 4 | -1.5730 E+1 | 1.7686 E+3 | 3.7087 E+0 | 0 |
| 1,1,1,2-TeCA | 1,1,1,2-Tetrachloroethane | 167.849 | 7.03897 | 1467.16 | 222.340 | 4 | -1.0665 E+2 | 4.6697 E+3 | 3.6381 E+1 | 0 |
| 1,1,2,2-TeCA | 1,1,2,2-Tetrachloroethane | 167.849 | 6.91043 | 1378.88 | 197.086 | 4 | -9.8030 E+1 | 4.3230 E+3 | 3.3535 E+1 | 0 |
| 1,1,1-TCA | 1,1,1-Trichloroethane | 133.404 | 7.00718 | 1253.2 | 229.624 | 4 | -4.3707 E+1 | 1.8793 E+3 | 1.4757 E+1 | 0 |
| 1,1,2-TCA | 1,1,2-Trichloroethane | 133.404 | 7.14357 | 1457.65 | 228.099 | 4 | -4.0116 E+1 | 1.6121 E+3 | 1.3890 E+1 | 0 |
| 1,1-DCA | 1,1-Dichloroethane | 98.959 | 7.18316 | 1269.43 | 237.755 | 4 | -8.5877 E+1 | 3.9414 E+3 | 2.9241 E+1 | 0 |
| 1,2-DCA | 1,2-Dichloroethane | 98.959 | 7.29525 | 1407.85 | 235.480 | 4 | -9.8869 E+1 | 4.3265 E+3 | 3.4065 E+1 | 0 |
| CE | Chloroethane | 64.514 | 7.13047 | 1097.6 | 246.009 | 4 | -1.2101 E+1 | 5.4702 E+2 | 4.0491 E+0 | 0 |
| 1,2-DCP | 1,2-Dichloropropane | 112.986 | 7.17775 | 1448.2346 | 240.189 | 4 | -7.5844 E+1 | 3.2495 E+3 | 2.6026 E+1 | 0 |
| 1,3-DCP | 1,3-Dichloropropane | 112.986 | 7.15546 | 1490.3725 | 227.804 | 3 | -6.4093 E-1 | 3.0872 E-3 | 0 | 0 |
| TCP | 1,2,3-Trichloropropane | 147.431 | 7.44393 | 1680.6413 | 212.460 | 3 | -1.4676 E+1 | 9.7906 E-2 | -1.6102 E-4 | 0 |
| MEK | 2-Butanone | 72.106 | 7.19130 | 1323.0708 | 227.093 | 4 | -1.2350 E+2 | 6.2118 E+3 | 4.2058 E+1 | 0 |
| MIBK | 4-methyl-2-pentanone | 100.159 | 7.37701 | 1527.2068 | 223.816 | 4 | -6.9319 E+1 | 3.5431 E+3 | 2.3320 E+1 | 0 |
| MTBE | Methyl tert-butyl ether | 88.148 | 7.53531 | 1376.6551 | 240.719 | 4 | -1.1391 E+2 | 5.9695 E+3 | 3.8151 E+1 | 0 |
| Dioxane | 1,4-Dioxane | 88.105 | 7.30749 | 1487.9209 | 234.976 | 1 | 9.9062 E+0 | -7.2453 E+3 | 4.8084 E+0 | -3.2545 E-2 |
| B | Benzene | 78.112 | 6.81432 | 1090.4312 | 197.146 | 4 | -5.6243 E+1 | 2.2288 E+3 | 1.9403 E+1 | 0 |
| T | Toluene | 92.138 | 7.13657 | 1457.2871 | 231.827 | 4 | -1.0938 E+2 | 4.7839 E+3 | 3.7217 E+1 | 0 |
| E | Ethylbenzene | 106.165 | 7.15610 | 1559.5452 | 228.582 | 4 | -5.7526 E+1 | 2.1651 E+3 | 1.9605 E+1 | 0 |
| X | Xylenes | 106.165 | 7.21217 | 1546.919 | 217.144 | 4 | -5.4409 E+1 | 1.7266 E+3 | 1.8850 E+1 | 0 |
| CB | Chlorobenzene | 112.557 | 7.17262 | 1571.7847 | 234.229 | 4 | -1.0092 E+2 | 3.9016 E+3 | 3.4984 E+1 | 0 |
| Freon 11 | Trichlorofluoromethane | 137.368 | 6.99521 | 1081.984 | 239.265 | 4 | -1.1225 E+1 | 1.5619 E+3 | 2.0593 E+0 | 0 |
| Freon 12 | Dichlorodifluoromethane | 120.914 | 6.92200 | 865.3109 | 243.873 | 4 | -5.2398 E+1 | 3.3867 E+3 | 1.5972 E+1 | 0 |
| Freon 113 | Trichlorotrifluoroethane | 187.376 | 6.95822 | 1139.7442 | 231.677 | 4 | -1.4524 E+1 | 7.3371 E+1 | 5.0415 E+0 | 0 |

As discussed above, the dimensionless Henry's Law constant itself is calculated from the ratio of the vapor pressure ($P_{vap}$) to the mole fraction ($x$), with appropriate conversions from units of atm/mol fraction to a dimensionless value (i.e., units of concentration per concentration). See Sander (2015) for a thorough job of distinguishing between multiple representations of the units for the Henry's Law constant. Equation 7 shows the calculation for the unitless Henry's Law constant ($H$), where $\rho_w$ is the density of water (g/mL), $R_{gas}$ is the gas constant (0.08205746 $L \cdot atm \cdot K^{-1} \cdot mol^{-1}$), $T$ is the average subsurface temperature (K), and other quantities were defined above. The density of water is obtained from a fit of standard density data (HBCP, 2015a) and the gas constant is from Mohr et al. (2012). The Henry's Law constant calculated for 1,4-dioxane using Equation 5 is converted to a unitless $H$ using Equation 8.

$$H = \frac{P_{vap}}{x} \cdot \frac{MW_w}{\rho_w \cdot R_{gas} \cdot T} \cdot \frac{1\,L}{1000\,mL} \cdot \frac{1\,atm}{760\,mmHg} \qquad \text{T is in K} \qquad (7)$$

$$\mathrm{H} = (\mathrm{MW_w} / \rho_w) \cdot (\mathrm{H_{px}}/(\mathrm{R} \cdot \mathrm{T_k})) \qquad \text{T}_\text{k} \text{ is in K, H calculation for 1,4-dioxane} \qquad (8)$$

The impact of recharge on the contaminant concentration in groundwater at the compliance well is a function of both the recharge rate ($R$) and the groundwater flux ($q$). This interrelationship stems from the process of the recharge water mixing with the groundwater at the water table. For a given groundwater flux, STOMP simulations show that variation in recharge has a linear (albeit not one-to-one) impact on the contaminant groundwater concentration at a compliance well. Figure 8 shows an example of the variation in groundwater concentrations with respect to the recharge and the groundwater flux. The magnitude of the variation with recharge (i.e., the linear proportionality factor) differs to a small degree based on the distance of the compliance well from the source area. More distant locations generally show more change as recharge increases than do compliance well locations close to the source area. The proportionality factor magnitude changes more significantly as the groundwater flux changes. Figure 9 shows the average slope and average intercept of multiple concentration-versus-recharge plots (taking both parameters relative to the base case of 0.4 cm/yr recharge), from which it is clear that the recharge proportionality factor varies more when the groundwater flux is low. For the scaling process, the relationship of *q* and *R* is approximated as a linear variation within two regimes, a low groundwater flux regime and a high groundwater flux regime. Other positional/geometric parameters (*VZT*, *STR*, *RSP*, *SA*) were found to have negligible influence on the impact of recharge on groundwater contaminant concentrations.

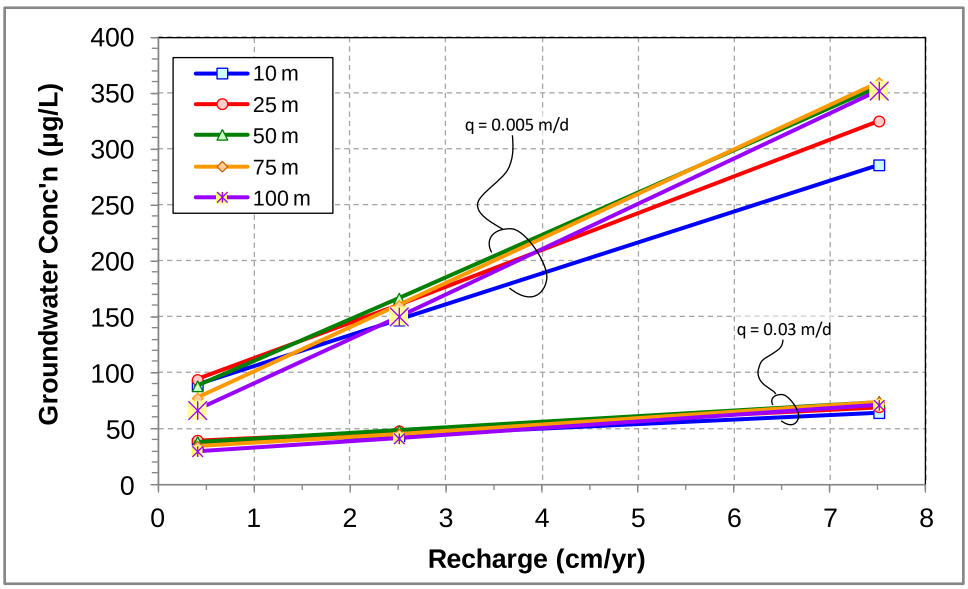



***Figure 8.*** *Example of the variation in groundwater concentration results at multiple compliance well distances (10, 25, 50, 75, and 100 m) from the source area for two groundwater flux scenarios (0.005 and 0.03 m/d). There are small differences in the slope of the linear relationships amongst the compliance well distances for a given groundwater flux, but larger differences in the nominal slope between groundwater flux scenarios.*

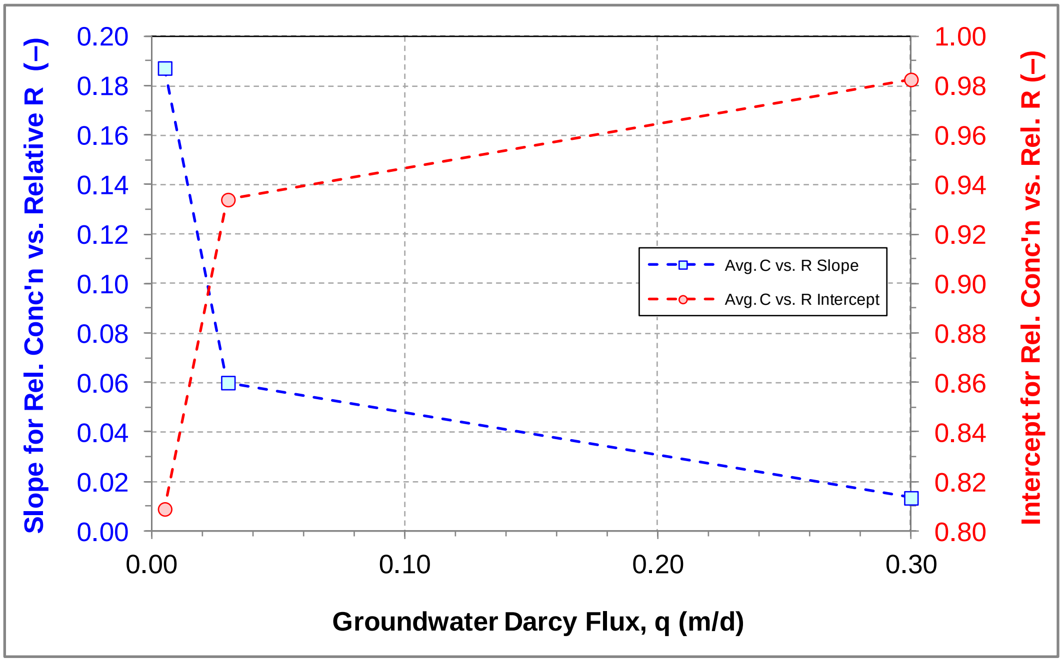



***Figure 9.*** *Variation of the average slope and intercept for concentration versus recharge plots (where the parameters are normalized relative to the 0.4 cm/yr base case).*

Equations 9 and 10 were determined from the average linear characteristics for variation of groundwater concentration as a function of recharge for a specified groundwater flux scenario. The equations are divided into a low groundwater flux regime (q < 0.03, i.e., where $q/_{0.03} < 1.0$) and a high flux regime. Equations 9 and 10 are used to determine the slope, $m_{rq}$, and intercept, $b_{rq}$, (describing the variation of groundwater concentration with recharge) for a given groundwater flux.

$$m_{rq} = \left[-2.545\cdot\left(\frac{q}{0.03}\right)+3.545\right]\cdot 0.05999 \qquad \text{for } \frac{q}{0.03} < 1.0$$

$$m_{rq} = \left[-0.0863\cdot\left(\frac{q}{0.03}\right)+1.0863\right]\cdot 0.05999 \qquad \text{for } \frac{q}{0.03} \geq 1.0 \tag{9}$$

$$b_{rq} = \left[0.161\cdot\left(\frac{q}{0.03}\right)+0.839\right]\cdot 0.934 \qquad \text{for } \frac{q}{0.03} < 1.0$$

$$b_{rq} = \left[0.00578\cdot\left(\frac{q}{0.03}\right)+0.994\right]\cdot 0.934 \qquad \text{for } \frac{q}{0.03} \geq 1.0 \tag{10}$$

After calculating the Henry's Law constant and the recharge variation slope/intercept, the unscaled concentration found in Step 2, $C_{wu}$, can be scaled to the final groundwater concentration based on the site-specific values of the Henry's Law constant ($H$), the recharge rate ($R$), the compliance well screen length ($s$), and the source strength. If the input included a value for $C_{gs}$, then Equation 11 is used to calculate the final estimated groundwater contaminant concentration, $C_w$, at the compliance well. If the input included $\dot{M}_{src}$, then Equation 12 is used to calculate $C_w$.

$$C_w = C_{wu} \cdot \frac{0.89}{H} \cdot \left[ \left( \frac{R}{0.4} \right) \cdot m_{rq} + b_{rq} \right] \cdot \frac{C_{gs}}{159.0} \tag{11}$$

$$C_w = C_{wu} \cdot \frac{0.89}{H} \cdot \left[ \left( \frac{R}{0.4} \right) \cdot m_{rq} + b_{rq} \right] \cdot \frac{\dot{M}_{src}}{\dot{M}_{sim}} \tag{12}$$

## 3.4 Example Calculation

To illustrate the procedure for estimating the contaminant concentration in groundwater at a compliance well, consider the scenarios shown in Table 10. These scenarios represent the compiled set of input data (Step 1) for two variants (Case A and Case B), which differ only in the way that the source strength is specified.

***Table 10.*** *User input for the scenario variants applied in the example calculations for the groundwater concentration estimation procedure*

| User Input – Source/Transport Parameters | | | | |
|---|---|---|---|---|
| | Scenario Name: | — | Case A | Case B |
| | Contaminant: | — | TCE | TCE |
| T | Temperature: | [°C] | 20 | 20 |
| R | Avg. Recharge: | [cm/yr] | 0.5 | 0.5 |
| ω | Avg. Soil Moisture Content: | [wt %] | 2.825 | 2.825 |
| $\theta_{total}$ | Total Porosity: | [--] | 0.3 | 0.3 |
| $\rho_{bulk}$ | Dry Bulk Density: | [g/mL] | 1.855 | 1.855 |
| VZT | Vadose Zone Thickness: | [m] | 20 | 20 |
| L1 | Depth to Top of Source: | [m] | 5.85 | 5.85 |
| z | Source Thickness: | [m] | 3.5 | 3.5 |
| w (= l) | Source Width (= Length): | [m] | 15.8 | 15.8 |
| q | GW Darcy Velocity: | [m/day] | 0.165 | 0.165 |
| s | Compliance Well Screen Length: | [m] | 3 | 3 |
| d | Distance to GW Compliance Well: | [m] | 50 | 50 |
| dx | Longitudinal Distance for Soil Gas: | [m] | 30 | 30 |
| dy | Transverse Distance for Soil Gas: | [m] | 20 | 20 |
| dz | Depth of Basement/Foundation: | [m] | 4 | 4 |
| | Source Strength Input Type: | — | Gas Concentration | Mass Discharge |
| $C_{gs}$ | Source Gas Concentration: | [ppmv] | 10 | |
| $\dot{M}_{src}$ | Source Mass Discharge: | [g/day] | | 10 |

The calculated values of *RSP*, *SA*, *STR*, and $S_r$ (i.e., the converted value of $\omega$, as indicated in Table 8), along with the user-specified values of *VZT*, and *q*, comprise the six quantities (Table 11) used in the lookup/interpolation calculations for the pre-modeled scenarios in the second step in the procedure. None of these parameter values for the example cases is equal to a corresponding key value (Table 8); thus, interpolation is required at each step.

***Table 11.*** *Parameter values for the example that are used in Step 2 for the lookup/interpolation*

| **Calculated Parameters/Intermediate Values** | | | | |
|---|---|---|---|---|
| $S_r$ | Residual Saturation: | [--] | 0.175 | 0.175 |
| STR | Source Thickness Ratio*: | [--] | 0.175 | 0.175 |
| VZT | Vadose Zone Thickness: | [m] | 20 | 20 |
| RSP | Relative Source Position*: | [--] | 0.55 | 0.55 |
| q | GW Darcy Velocity: | [m/day] | 0.165 | 0.165 |
| SA | Areal Footprint of Source*: | [m²] | 250 | 250 |
| L2 | Dist. from Source Bottom to GW: | [m] | 10.65 | 10.65 |
| H | Henry's Law Constant**: | [--] | 0.316 | 0.316 |

The step-by-step interpolation then proceeds for the six parameters (*SA*, *q*, *RSP*, *VZT*, *STR*, and *Sr*) to calculate the unscaled concentrations, $C_{wu}$ and $C_{gu}$ , for groundwater and soil gas, respectively. Interpolation of mass discharge is performed for the same six parameters to give the site-specific mass discharge, $\dot{M}_{sim}$ . Equations 11 and 12 are finally applied to obtain the scaled concentrations, $C_w$ and $C_g$ , as the final results. Table 12 lists the unscaled concentrations, site-specific mass discharge, and the final concentration results for the two example cases.

***Table 12.*** *Unscaled and final scaled results for example Cases A and B*

| **Results – Estimated Contaminant Concentrations in Soil Gas and Groundwater** | | | | |
|---|---|---|---|---|
| $C_{gu}$ | Unscaled Gas Concentration: | [ppmv] | 1.154301046 | 1.154301046 |
| $C_{wu}$ | Unscaled Aqueous Conc'n: | [µg/L] | 25.42901012 | 25.42901012 |
| $\dot{M}_{sim}$ | Unscaled Mass Discharge: | [g/day] | | 32.7 |
| $C_g$ | Final Soil Gas Concentration: | [ppbv] | 204 | 995 |
| $C_w$ | Final Groundwater Conc'n: | [µg/L] | 4.5 | 22 |

# 4.0 SVEET2 Installation and Use

The calculational procedure described in Section 3.0 for estimating the impact of vadose zone contamination on the contaminant concentration in groundwater and the soil gas is implemented in the SVEET2 spreadsheet software tool. SVEET2 allows the user to easily enter data and calculate the estimated groundwater concentration and/or soil gas concentration for one or more scenarios that conform to the generalized conceptual model. This section describes SVEET2 installation, the user interface, and user actions in the software.

## 4.1 System Requirements

The following hardware and software are recommended for use of the SVEET2 software:

- Personal computer based on Intel® IA-32 or Intel® 64 processor architectures,
- Microsoft® Windows® 10 operating system,
- Microsoft® Excel® 2016 (Office 365)

Earlier versions of Windows (back to Windows® XP) and of Excel (back to Excel® 2003) will likely work, but have not been explicitly tested. The software is not designed for use on non-Windows systems.

## 4.2 Installation

The SVEET2 software is distributed as a 19 MB zip files that contains four files, which are the SVEET2 Excel workbook and three data files:

- SVEET2_v2.0.0.xlsm
- sveet_gas_data_ng_per_L_1m.b171
- sveet_gas_data_ng_per_L_4m.b171
- sveet_gw_data_ng_per_L.b171

The *.b171 files are the data files containing base-171 values (see Section 2.3) from the STOMP simulations and are used by SVEET2 in the calculations.

Installation simply involves placing (unzipping) these files into a convenient file directory on your computer. The unzipped files will take 85 MB of disk space. The data files should be placed in a directory and not be moved or modified. The SVEET2 Excel workbook may be placed in any directory, can be moved, and can be copied. It is recommended to keep one clean/unused copy of the SVEET2 Excel workbook in the directory with the data files and copy the SVEET2 workbook to a project directory for application on a specific project.

## 4.3 Description of the SVEET2 Workbook

The SVEET2 Excel workbook has two worksheets available, only one of which will be routinely used. The content of these worksheets is described below.

The “HLC” worksheet (Figure 10) is a repository for contaminant-specific information, including molecular weight, vapor pressure correlation coefficients, and solubility correlation coefficients. The “HLC” worksheet also has data for water density as a function of temperature and values for key constants (e.g., the ideal gas constant). As an ancillary feature unrelated to the SVEET2 calculations, the rightmost part of the “HLC” worksheet has a calculation block for “Quick Calculation” of gas concentration unit conversion and the Henry’s Law Constant as a function of temperature for a specified contaminant.

| | | Molecular | Correl. Coef. for Calculating Vapor Pressure | | | Correlation Coefficients for Calculating Solubility or H | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Contaminant Abbrev. | Contaminant | Weight (g/mol) | A | B | C | Eqn | A | B | C | D | Formula | CAS RN |
| CT | Carbon Tetrachloride | 153.823 | 7.01144 | 1278.54 | 232.888 | 4 | -7.4600 E+1 | 3.3774 E+3 | 2.5130 E+1 | 0 | $CCl_4$ | "56-23-5" |
| CF | Chloroform | 119.378 | 7.11148 | 1232.79 | 230.213 | 4 | -8.5244 E+1 | 3.9461 E+3 | 2.9057 E+1 | 0 | $CHCl_3$ | "67-66-3" |
| DCM | Dichloromethane | 84.933 | 7.11464 | 1152.41 | 232.442 | 4 | -1.3856 E+2 | 6.4354 E+3 | 4.7322 E+1 | 0 | $CH_2Cl_2$ | "75-09-2" |
| CM | Chloromethane | 50.488 | 6.99771 | 870.17 | 235.586 | 4 | 3.0022 E+1 | -1.6520 E+2 | -1.2013 E+1 | 0 | $CH_3Cl$ | "74-87-3" |
| PCE | Tetrachloroethene | 165.833 | 7.06892 | 1458.45 | 226.986 | 4 | -9.0823 E+1 | 3.8474 E+3 | 3.0813 E+1 | 0 | $C_2Cl_4$ | "127-18-4" |
| TCE | Trichloroethene | 131.388 | 6.87981 | 1157.83 | 202.580 | 4 | -2.4133 E+1 | 9.3612 E+2 | 8.0968 E+0 | 0 | $C_2HCl_3$ | "79-01-6" |
| 1,1-DCE | 1,1-Dichloroethene | 96.943 | 7.21678 | 1181.12 | 240.840 | 4 | -1.3500 E+2 | 6.2391 E+3 | 4.5844 E+1 | 0 | $C_2H_2Cl_2$ | "75-35-4" |
| cDCE | cis-1,2-Dichloroethene | 96.943 | 7.21953 | 1290.28 | 236.887 | 4 | -2.1907 E+2 | 9.8827 E+3 | 7.5057 E+1 | 0 | $C_2H_2Cl_2$ | "156-59-2" |
| tDCE | trans-1,2-Dichloroethene | 96.943 | 7.21356 | 1244.35 | 239.497 | 4 | -4.1184 E+1 | 2.0908 E+3 | 1.3671 E+1 | 0 | $C_2H_2Cl_2$ | "156-60-5" |
| VC | Vinyl Chloride | 62.498 | 6.91423 | 911.15 | 239.800 | 4 | -1.5730 E+1 | 1.7686 E+3 | 3.7087 E+0 | 0 | $C_2H_3Cl$ | "75-01-4" |
| 1,1,1,2-TeCA | 1,1,1,2-Tetrachloroethane | 167.849 | 7.03897 | 1467.16 | 222.340 | 4 | -1.0665 E+2 | 4.6697 E+3 | 3.6381 E+1 | 0 | $C_2H_2Cl_4$ | "630-20-6" |
| 1,1,2,2-TeCA | 1,1,2,2-Tetrachloroethane | 167.849 | 6.91043 | 1378.88 | 197.086 | 4 | -9.8030 E+1 | 4.3230 E+3 | 3.3535 E+1 | 0 | $C_2H_2Cl_4$ | "79-34-5" |
| 1,1,1-TCA | 1,1,1-Trichloroethane | 133.404 | 7.00718 | 1253.2 | 229.624 | 4 | -4.3707 E+1 | 1.8793 E+3 | 1.4757 E+1 | 0 | $C_2H_3Cl_3$ | "71-55-6" |
| 1,1,2-TCA | 1,1,2-Trichloroethane | 133.404 | 7.14357 | 1457.65 | 228.099 | 4 | -4.0116 E+1 | 1.6121 E+3 | 1.3890 E+1 | 0 | $C_2H_3Cl_3$ | "79-00-5" |
| 1,1-DCA | 1,1-Dichloroethane | 98.959 | 7.18316 | 1269.43 | 237.755 | 4 | -8.5877 E+1 | 3.9414 E+3 | 2.9241 E+1 | 0 | $C_2H_4Cl_2$ | "75-34-3" |
| 1,2-DCA | 1,2-Dichloroethane | 98.959 | 7.29525 | 1407.85 | 235.480 | 4 | -9.8869 E+1 | 4.3265 E+3 | 3.4065 E+1 | 0 | $C_2H_4Cl_2$ | "107-06-2" |
| CE | Chloroethane | 64.514 | 7.13047 | 1097.6 | 246.009 | 4 | -1.2101 E+1 | 5.4702 E+2 | 4.0491 E+0 | 0 | $C_2H_5Cl$ | "75-00-3" |
| 1,2-DCP | 1,2-Dichloropropane | 112.986 | 7.17775 | 1448.2346 | 240.189 | 4 | -7.5844 E+1 | 3.2495 E+3 | 2.6026 E+1 | 0 | $C_3H_6Cl_2$ | "78-87-5" |
| 1,3-DCP | 1,3-Dichloropropane | 112.986 | 7.15546 | 1490.3725 | 227.804 | 3 | -6.4093 E-1 | 3.0872 E-3 | 0 | 0 | $C_3H_6Cl_2$ | "142-28-9" |
| TCP | 1,2,3-Trichloropropane | 147.431 | 7.44393 | 1680.6413 | 212.460 | 3 | -1.4676 E+1 | 9.7906 E-2 | -1.6102 E-4 | 0 | $C_3H_5Cl_3$ | "96-18-4" |
| MEK | 2-Butanone | 72.106 | 7.19130 | 1323.0708 | 227.093 | 4 | -1.2350 E+2 | 6.2118 E+3 | 4.2058 E+1 | 0 | $C_4H_8O$ | "78-93-3" |
| MIBK | 4-methyl-2-pentanone | 100.159 | 7.37701 | 1527.2068 | 223.816 | 4 | -6.9319 E+1 | 3.5431 E+3 | 2.3320 E+1 | 0 | $C_6H_{12}O$ | "108-10-1" |
| MTBE | Methyl tert-butyl ether | 88.148 | 7.53531 | 1376.6551 | 240.719 | 4 | -1.1391 E+2 | 5.9695 E+3 | 3.8151 E+1 | 0 | $C_5H_{12}O$ | "1634-04-4" |
| Dioxane | 1,4-Dioxane | 88.105 | 7.30749 | 1487.9209 | 234.976 | 1 | 9.9062 E+0 | -7.2453 E+3 | 4.8084 E+0 | -3.2545 E-2 | $C_4H_8O_2$ | "123-91-1" |
| B | Benzene | 78.112 | 6.81432 | 1090.4312 | 197.146 | 4 | -5.6243 E+1 | 2.2288 E+3 | 1.9403 E+1 | 0 | $C_6H_6$ | "71-43-2" |
| T | Toluene | 92.138 | 7.13657 | 1457.2871 | 231.827 | 4 | -1.0938 E+2 | 4.7839 E+3 | 3.7217 E+1 | 0 | $C_7H_8$ | "108-88-3" |
| E | Ethylbenzene | 106.165 | 7.15610 | 1559.5452 | 228.582 | 4 | -5.7526 E+1 | 2.1651 E+3 | 1.9605 E+1 | 0 | $C_8H_{10}$ | "100-41-4" |
| X | Xylenes | 106.165 | 7.21217 | 1546.919 | 217.144 | 4 | -5.4409 E+1 | 1.7266 E+3 | 1.8850 E+1 | 0 | $C_8H_{10}$ | "1330-20-7" |
| CB | Chlorobenzene | 112.557 | 7.17262 | 1571.7847 | 234.229 | 4 | -1.0092 E+2 | 3.9016 E+3 | 3.4984 E+1 | 0 | $C_6H_5Cl$ | "108-90-7" |
| Freon 11 | Trichlorofluoromethane | 137.368 | 6.99521 | 1081.984 | 239.265 | 4 | -1.1225 E+1 | 1.5619 E+3 | 2.0593 E+0 | 0 | $CCl_3F$ | "75-69-4" |
| Freon 12 | Dichlorodifluoromethane | 120.914 | 6.92200 | 865.3109 | 243.873 | 4 | -5.2398 E+1 | 3.3867 E+3 | 1.5972 E+1 | 0 | $CCl_2F_2$ | "75-71-8" |
| Freon 113 | Trichlorotrifluoroethane | 187.376 | 6.95822 | 1139.7442 | 231.677 | 4 | -1.4524 E+1 | 7.3371 E+1 | 5.0415 E+0 | 0 | $C_2Cl_3F_3$ | "76-13-1" |

$x = (xp / 100) \cdot (MW_w / MW_i) = xf \cdot (MW_w / MW_i)$
$H = [ (P / 760) / x ] \cdot [ MW_w / (\rho_w \cdot R_{gas} \cdot Tk) ]$

$Log(P_{vap}) = A - B/(Tc + C)$ Yaws et al., 2009
$P_{vap}$ = Vapor Pressure (mm Hg)

1: $ln(Hpx) = A + B/Tk + C \cdot ln(Tk) + D \cdot Tk$ Ondo and Dohnal, 2007
2: $log(Hpx) = A + B/Tk + C \cdot log(Tk) + D \cdot Tk$ Not used
3: $xp = A + B \cdot Tk + C \cdot Tk^2$ Horvath & Getzen, 1999
4: $Log(xp) = A + B/Tk + C \cdot Log(Tk)$ Yaws, 2012
xp = mass fraction × 100% xf = mass fraction Hpx = Henry's Law Const. (kPa)

MW from Wieser & Berglund, 2009 Tc = Temp. in °C Tk = Temp. in K

***Figure 10.*** *View of the primary data (molecular weights and correlation coefficients) on the “HLC” worksheet of the SVEET2 workbook (information for constants and the water density correlation are not shown)*

The primary worksheet for user interaction, the “SVEET” worksheet (Figure 11) is divided into areas for data input (blue shading), intermediate calculated values (green shading), and the final estimate for groundwater concentration (tan shading). Additional information is presented on the left side of the worksheet, showing the generalized conceptual model figure to clarify the meaning of parameters and a table of the parameter value permissible ranges and key values. By default, the “SVEET” worksheet has space for up to five independent scenarios (columns K through O).

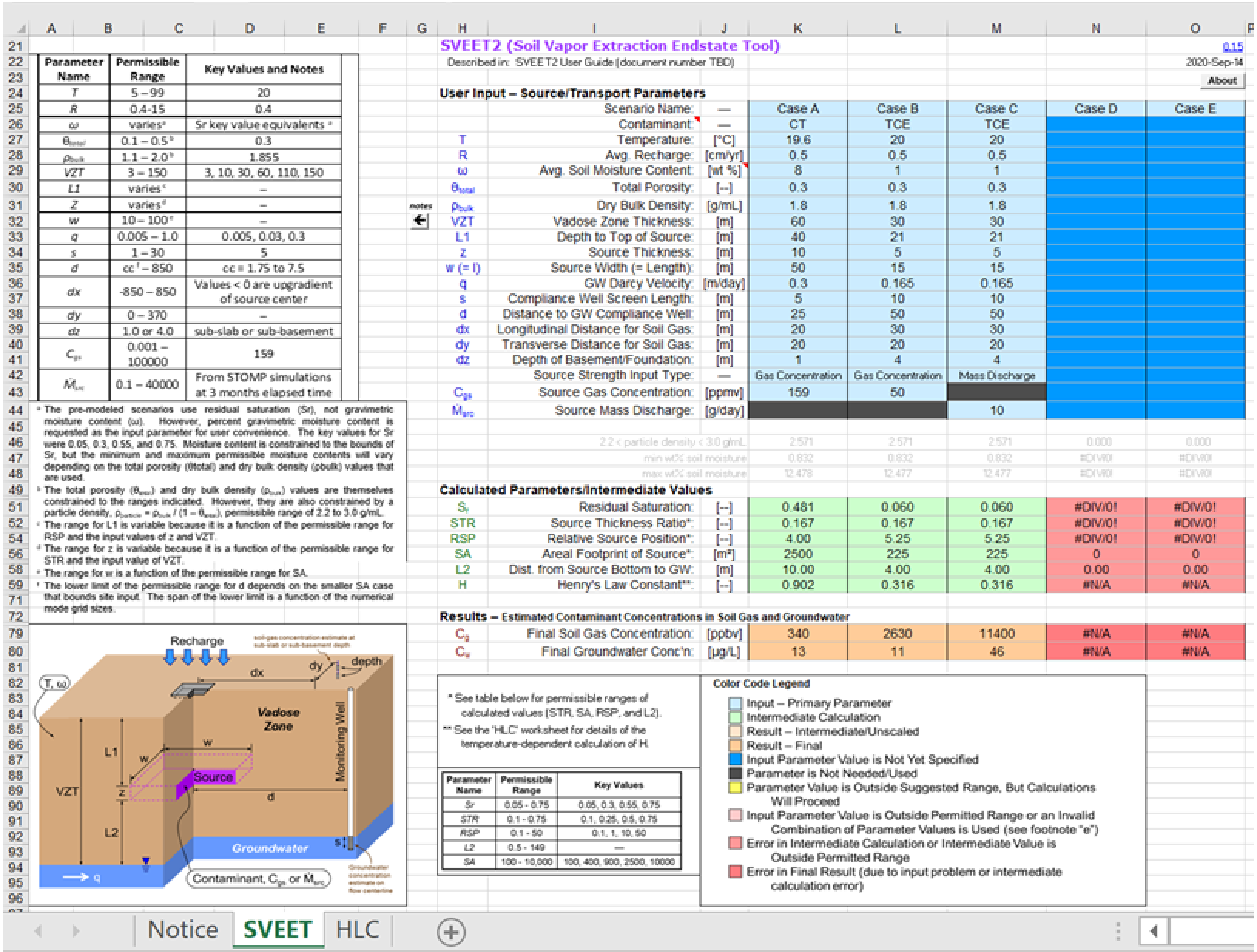



***Figure 11.*** *View of the “SVEET” worksheet, showing inputs, intermediate calculations, results, and reference/help information.*

## 4.4 Using the Software

### 4.4.1 Getting Started

On opening the SVEET2 Excel workbook, the user will have an option to enable macros or not. Macros must be enabled for the SVEET2 software to function. The SVEET2 workbook uses a user-defined function (macro) to retrieve data and perform the interpolations. If not presented with an option to enable macros, the user can try closing and re-opening the file or altering the macro security settings of Excel. Depending on the settings in Excel and the directory location of the

SVEET2 workbook file, the user may not be prompted to enable macros when opened a second or subsequent time because the file is considered a trusted document. Recent versions of Excel have security options found under the name of "Macro Security" or "Trust Center" (depending on the version of Excel) where a macro security option can be selected to prompt/notify the user to confirm, on an individual workbook basis, whether macros should be enabled or not and where trusted document settings can be viewed or modified.

After macros are enabled, the first use of a SVEET2 workbook will prompt the user for the location of the data files. This data file directory location is stored in the Windows registry and will not be requested again unless the data files are moved or deleted from the specified directory.

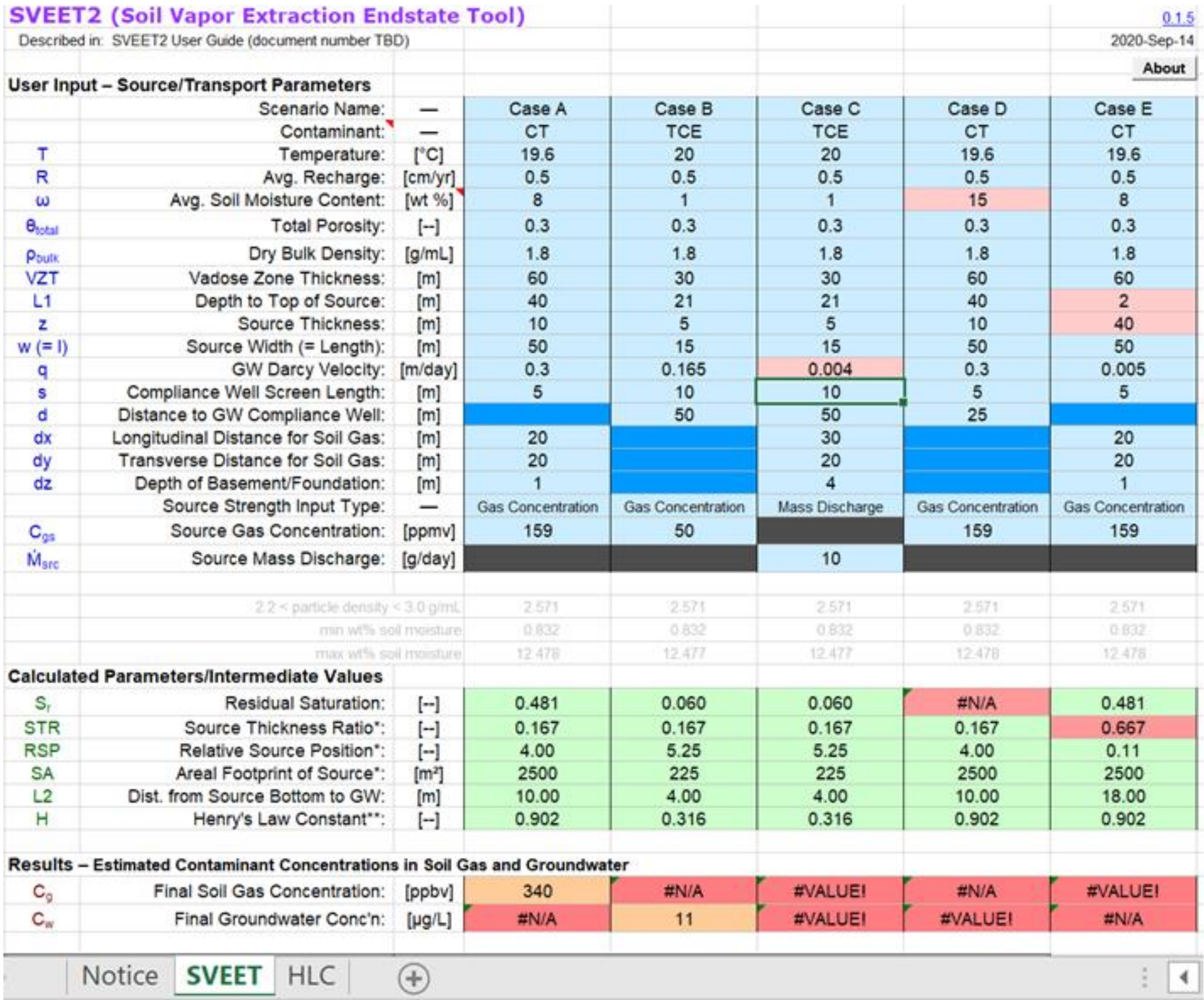
With these initial steps completed, the user can proceed to enter input values and use the software.

### 4.4.2 Performing Calculations

Performing calculations with the SVEET2 software is as simple as entering the required input data (based on the site conceptual model, data collection, and procedures discussed in Truex et al. [2013]). On input of valid data, results are available immediately. Data entry for most items consists of entering numeric values for parameters in the blue shaded cells for a particular scenario. Three of the inputs (contaminant name, depth of basement/foundation, and source strength input type) use a selection list to ensure that valid data are input. The selection list is activated by selecting the input cell on the spreadsheet, then clicking on the arrow button that appears. The selection of the source strength input type modifies the requested input data to be either source gas concentration or source mass discharge, while graying out the unused parameter.

If invalid input values (or combinations of values) are entered, affected cells are highlighted in a light red shading. The warnings may be visible in either the user inputs or intermediate calculated values. The primary cause for errors is likely to be data values outside the permissible ranges or values that are inconsistent with each other (e.g., a 40 ft source thickness for a 30 ft thick vadose zone). A table of permissible ranges and a diagram of the generalized conceptual model is included directly on the worksheet to help the user identify issues with improper input values. Figure 12 shows three examples of invalid input data. In Case C of the figure, the groundwater Darcy velocity is too low, outside the permissible range. In Case D of the figure, the soil moisture content is too high, meaning that the residual saturation is outside the permissible range bounds. In Case E of the figure, the source thickness is too large for the scenario making the STR out of range, and the depth to source is too small, which will impact the RSP (once the source thickness is addressed). Figure 12 also shows that the user can ask for results for either groundwater concentrations, soil gas concentration, or both.

The SVEET2 workbook includes two features to help maintain the integrity of the calculations. The associated macro code (for doing the interpolations) is locked for viewing or editing. Also, the worksheets are protected and data entry is only allowed in appropriate data input cells.



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **SVEET2 (Soil Vapor Extraction Endstate Tool)** | | | | | | | 0.1.5 |
| Described in: SVEET2 User Guide (document number TBD) | | | | | | | 2020-Sep-14 |
| | | | | | | | About |
| **User Input – Source/Transport Parameters** | | | | | | | |
| | Scenario Name: | — | Case A | Case B | Case C | Case D | Case E |
| | Contaminant: | — | CT | TCE | TCE | CT | CT |
| T | Temperature: | [°C] | 19.6 | 20 | 20 | 19.6 | 19.6 |
| R | Avg. Recharge: | [cm/yr] | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| ω | Avg. Soil Moisture Content: | [wt %] | 8 | 1 | 1 | 15 | 8 |
| $\theta_{total}$ | Total Porosity: | [--] | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 |
| $\rho_{bulk}$ | Dry Bulk Density: | [g/mL] | 1.8 | 1.8 | 1.8 | 1.8 | 1.8 |
| VZT | Vadose Zone Thickness: | [m] | 60 | 30 | 30 | 60 | 60 |
| L1 | Depth to Top of Source: | [m] | 40 | 21 | 21 | 40 | 2 |
| z | Source Thickness: | [m] | 10 | 5 | 5 | 10 | 40 |
| w (= l) | Source Width (= Length): | [m] | 50 | 15 | 15 | 50 | 50 |
| q | GW Darcy Velocity: | [m/day] | 0.3 | 0.165 | 0.004 | 0.3 | 0.005 |
| s | Compliance Well Screen Length: | [m] | 5 | 10 | 10 | 5 | 5 |
| d | Distance to GW Compliance Well: | [m] | | 50 | 50 | 25 | |
| dx | Longitudinal Distance for Soil Gas: | [m] | 20 | | 30 | | 20 |
| dy | Transverse Distance for Soil Gas: | [m] | 20 | | 20 | | 20 |
| dz | Depth of Basement/Foundation: | [m] | 1 | | 4 | | 1 |
| | Source Strength Input Type: | — | Gas Concentration | Gas Concentration | Mass Discharge | Gas Concentration | Gas Concentration |
| $C_{gs}$ | Source Gas Concentration: | [ppmv] | 159 | 50 | | 159 | 159 |
| $\dot{M}_{src}$ | Source Mass Discharge: | [g/day] | | | 10 | | |
| | 2.2 < particle density < 3.0 g/mL | | 2.571 | 2.571 | 2.571 | 2.571 | 2.571 |
| | min wt% soil moisture | | 0.832 | 0.832 | 0.832 | 0.832 | 0.832 |
| | max wt% soil moisture | | 12.478 | 12.477 | 12.477 | 12.478 | 12.478 |
| **Calculated Parameters/Intermediate Values** | | | | | | | |
| $S_r$ | Residual Saturation: | [--] | 0.481 | 0.060 | 0.060 | #N/A | 0.481 |
| STR | Source Thickness Ratio*: | [--] | 0.167 | 0.167 | 0.167 | 0.167 | 0.667 |
| RSP | Relative Source Position*: | [--] | 4.00 | 5.25 | 5.25 | 4.00 | 0.11 |
| SA | Areal Footprint of Source*: | [m²] | 2500 | 225 | 225 | 2500 | 2500 |
| L2 | Dist. from Source Bottom to GW: | [m] | 10.00 | 4.00 | 4.00 | 10.00 | 18.00 |
| H | Henry's Law Constant**: | [--] | 0.902 | 0.316 | 0.316 | 0.902 | 0.902 |
| **Results – Estimated Contaminant Concentrations in Soil Gas and Groundwater** | | | | | | | |
| $C_g$ | Final Soil Gas Concentration: | [ppbv] | 340 | #N/A | #VALUE! | #N/A | #VALUE! |
| $C_w$ | Final Groundwater Conc'n: | [μg/L] | #N/A | 11 | #VALUE! | #VALUE! | #N/A |

Notice | SVEET | HLC

***Figure 12.*** *Example of invalid (red shading) and missing (darker blue shading) data on the "SVEET" worksheet*

Based on user testing for this project, personnel who are unfamiliar with the SVEET2 software functionality could expect to spend roughly 16 hours of labor to run site-specific scenarios . See Section 8.2 for additional discussion of time spent and the associated cost impacts.

# 5.0 Performance Objectives

Performance objectives for the demonstration are described in Table 13. Performance objectives are identified for both the ground-truthing (Type 1) demonstration sites and the ease-of-use/applicability (Type 2) sites.

***Table 13.*** *Performance objectives for demonstration elements.*

<table>
<tr><th>Performance Objective</th><th>Data Requirements</th><th>Success Criteria</th></tr>
<tr><td colspan="3">Type 1 - Quantitative Performance Objectives</td></tr>
<tr><td>Test SVEET Tool<br><br>Ground-Truthing</td><td>Current and/or historical groundwater and soil vapor contaminant concentrations</td><td>At a minimum of 2 sites data will be input to the SVEET tool. A sensitivity analysis will be conducted using a reasonable range of input parameters. Success will be determined based on:<br>• Observed site values falling within 3 standard deviations of the mean calculated from sensitivity results for SVEET estimations for the site.<br>• The range predicted from the sensitivity analysis being useful to the DoD staff working on the project.</td></tr>
<tr><td colspan="3">Type 2 – Qualitative and Quantitative Performance Objectives</td></tr>
<tr><td>Ease of use and applicability<br><br>User Testing</td><td>Input from DoD user community and readily available data on DoD site characteristics</td><td>At a minimum of 2 sites available data will be input into the tool, as above a sensitivity analysis will be conducted using a reasonable range of input parameters. Success will be determined based on:<br>• Providing output that is used by the DoD entity in setting remedial strategies.<br>• Updated SVEET is applicable to 80% of DoD sites investigated.<br>• Obtaining feedback from the DoD user that informs update of SVEET.</td></tr>
<tr><td colspan="3">For clarity, ground-truthing sites are referred to as Type 1 sites. Sites for assessing ease of use and applicability are referred to as Type 2 sites. It is possible that a single site may serve as both a Type 1 and Type 2 site.</td></tr>
</table>

## 5.1 Type 1 – Quantitative Performance Objective

The quantitative performance objective was to test the SVEET2 software and evaluate the results of predicted soil gas and groundwater concentrations at actual field sites. The objective was to show that the field-measured concentrations are within the range predicted by SVEET2. The range of SVEET2 estimates was generated through a sensitivity analysis based on a range of input parameters suitable for the site.

Recognizing that uncertainty is intrinsic to the nature of the input values (e.g., extent and location of contamination, site properties, etc.), SVEET results were compared to site data by assessing whether observed site values are within the bounds of the "most likely" scenario result plus/minus three standard deviations calculated from the sensitivity results for the site. To assess this performance metric, first a single SVEET2 scenario was conducted using input values that were most likely representative of the site parameters for each site (designated as "most likely" SVEET2 estimations). To include the variability and uncertainty in site inputs, ground-truthing SVEET2 scenarios were also completed using a Monte-Carlo (MC) analysis ($n$ =2,500) where input parameters were randomly selected between defined minimum and maximum input values of each parameter. A standard deviation was calculated from the MC analysis results. The results of the ground-truthing evaluation are summarized in Table 14, with full results presented in Section 7.1 (model verification).

***Table 14.*** *Summary of performance criteria and ground-truthing outcomes.*

| **Groundwater** | | | | | |
|---|---|---|---|---|---|
| **Installation** | **Monitoring Well** | **Contaminant [a]** | **SVEET prediction range [b] [μg/L]** | **Field Concentration [μg/L]** | **Yes/No Meets Performance Criteria? [c]** |
| McClellan IC 1 | MW-235 | PCE | 0 – 47 | 4 | Y |
| | MW-364 | | 0 – 39 | 3 | Y |
| | ME-366 | | 0 – 26 | 11 | Y |
| McClellan IC 19 | MW-354 | PCE | 0 – 34 | 96 | N (low) |
| | EW-379 | PCE | 0.4 – 1.0 | 1.8 | N (low) |
| | | TCE | 208 – 527 | 1.6 | N (high) |
| | | 1,1-DCE | 19 – 40 | 0.7 | N (high) |
| | MW-355 | PCE | 0.2 – 1.4 | <0.2 | Y |
| | | TCE | 214 – 826 | 1.2 | N (high) |
| | | 1,1-DCE | 20 – 62 | 1.3 | N (high) |
| CRREL | MW 14-107 | TCE | 0 – 15,252 | 22,961 | N (low) |
| Mather | MAFB-341 | PCE | 0 – 58 | 0.2 | Y |
| **Soil Gas** | | | | | |
| **Installation** | **Monitoring Location** | **Contaminant [a]** | **SVEET prediction range [b] [ppbv]** | **Field Concentration [ppbv]** | **Meets Performance Criteria?** |
| CRREL | Multipurpose Room | TCE | 0– 710,590 | 20,127 | Y |

[a] PCE = tetrachloroethene, TCE = trichloroethene, and 1,1-DCE = 1,1-dichloroethene
[b] The SVEET prediction range is computed as "most likely" ± 3×standard deviation. The standard deviation is calculated from the MC analysis results.
[c] Where the performance criteria was not met, the notation in parentheses indicates whether the SVEET2 estimate was higher or lower than the observed value. SVEET2 estimates higher than the observed value are conservative with respect to remedial decision-making. Note that estimates that are lower than the observed values are within a factor of 2-3 of the observed values.

Overall, SVEET2 provided reasonable groundwater concentration and soil gas estimates for the Type 1 field sites evaluated. Six of the tested cases met the ground-truthing performance criteria and matched observed data. Four test cases resulted in estimates larger than field data. In three instances, the SVEET2 estimated concentrations that were less than observed data, but all were still within a factor of about 2-3 of the observed values.

It should be noted that SVEET2 is not intended to be used for ground-truthing efforts, but rather to aid remedial decision making. SVEET2 groundwater concentration estimates are appropriate for predictive applications because the downgradient plume centerline concentrations are maximum values and therefore are conservative estimates. For ground-truthing with existing wells, however, downgradient groundwater wells may not be directly downgradient from the source area and along the plume centerline. This was the case with several of the Type-1 sites used for ground-truthing. To provide a comparison with existing groundwater wells on site, an internal version of SVEET2 had to be adapted to estimate concentrations for monitoring wells located laterally off the downgradient groundwater plume centerline. Overall, the ground-truthing results highlight the ability of SVEET2 to provide reasonable estimations for both groundwater concentrations and soil gas.

## 5.2 Type 2 – Qualitative and Quantitative Performance Objectives

SVEET2 was also assessed for applicability to DoD sites. Success on this front was defined through the associated performance metric that the SVEET2 be applicable to 80% of DoD sites investigated. Data from the initial survey (Section 2.1, Appendix F) was used to assess this performance metric. The survey asked site managers to estimate SVEET2 parameters for their site and both DoD and non-DoD sites were included. Based on the responses, SVEET2 would be applicable for decision making at 93% of DoD sites and 81% of all sites surveyed. A subsect of these sites was identified as potentially requiring further characterization to assess whether the tool can capture the site conditions or if site-specific modeling may be useful. The source area (footprint) was the main parameter that disqualified field sites for use in SVEET2. Field sites with a source area that is either too small (less than 100 $m^2$) or too large (greater than 1000 $m^2$) cannot be simulated using SVEET2. Sites that list a very large source areas may still be applicable to SVEET2, if more detailed site characterization can better define the source area size, allowing it to be described with a smaller footprint. Overall, results indicate that the expanded input parameter ranges employed in the SVEET2 update allow the tool to be applicable to the majority of surveyed DoD sites.

An additional qualitative objective was to demonstrate the ease-of-use of the SVEET2 by DoD end users. This was judged by actual use of the tool by DoD users involved with the demonstration sites. User feedback was obtained from site teams, in the form of both verbal discussions and through written responses to a user feedback survey. Further details on user feedback are provided in Section 7.2. Overall, the response from users was very positive; users found SVEET2 to be applicable and helpful at their respective field sites. The spreadsheet nature of SVEET2 was found to be relatively user friendly, with straightforward input requirements that were readily obtained based on available site data.

# 6.0 Application and Interpretation of SVEET2

Like any other model, the approach to configuring scenarios and interpreting results is important for use of the SVEET2 tool in support of making remedy decisions. As recommended in the Soil Vapor Extraction System Optimization, Transition, and Closure Guidance (Truex et al., 2013), scenarios should be configured using estimates of the site properties required for the SVEET2 model. For each of the inputs, users should consider configuring scenarios for a range of parameter values, depending on the certainty of the parameter value. With this approach, the scenario results will be a range of estimated contaminant concentrations at the selected location for comparison to a remediation objective (e.g., groundwater standard), to an associated metric (e.g., active remediation target), or for "ground-truthing" of the results. Thus, for evaluating the SVEET2 results as part of the field demonstration, a range of input parameters were applied to obtain a corresponding range of results. However, interpretation of results also requires additional considerations beyond the direct comparison of scenario results to measured concentration values at a defined location.

Interpretation of SVEET2 scenario results and comparison to measured concentration values or to remediation target concentrations at a defined location should consider how the comparison will be used to support the decision to be made. For instance, in some cases, SVEET2 results will be generated to compare to a remediation objective such as a groundwater drinking-water standard. The decision from the SVEET2 result in this case is whether it is acceptable to stop active treatment of a source zone (or potentially to not start active treatment) because the source will no longer cause a groundwater plume of concern. For this decision, consideration of the SVEET2 results as a predictive estimate is needed to determine if there is confidence by the decision-makers that the results represent a reasonable likelihood that the groundwater objective will be met (or maintained) in the future or not. In some cases, the range of SVEET2-estimated results may not be below the objective. The decision-makers will need to determine whether it is reasonable to anticipate that future site conditions will be acceptable if, for instance, the range of SVEET2-estimated concentration values is the same order of magnitude as the groundwater objective. In this case, the site decision makers would consider the uncertainty in the SVEET2 estimate and site conditions as part of evaluating termination of source treatment. That is, if the objective is 5 ppb and the range of SVEET2 values is 3-10 ppb, the site could determine that within the accuracy of site knowledge the values are comparable and support the source termination decision, potentially with caveats related to ongoing verification monitoring. This decision may be due, in part, to the generally conservative approach (e.g., biased toward higher concentrations) of the SVEET2 tool (e.g., because SVEET2 does not include attenuation processes).

In the case of the field demonstration, SVEET2 estimated-concentration result ranges are compared to a single measured value at the designated comparison well or vapor sampling location. Interpretation of the comparability between these should also consider the concentration magnitude and how the information would be used to support a remediation decision. If both the

SVEET2 estimates and the measured values are very low and below the decision threshold, even though the concentrations may differ, they functionally both support the decision related to being below the threshold (e.g., to terminate an SVE system). Similarly, if both concentrations are much higher than a decision threshold and they also differ in magnitude, they both support the same decision (e.g., to continue SVE). In either of these cases, differences by a factor of 2-5 may have little impact on a decision. As described in the preceding paragraph, decision makers will need to carefully consider values close to a decision threshold. In this case, it is worthwhile to note that the SVEET2 estimates are generally conservative (e.g., because SVEET2 does not include attenuation processes). Thus, in the ground-truthing comparison portion of the field demonstration, discussion is included to evaluate whether observed differences between SVEET2-estimated values and measure site values are relevant with respect to the type of decision that would be supported by the SVEET2 results.

In addition, with respect to comparing SVEET2 results to a measured value (e.g., for "ground-truth" evaluations), the interpretation should consider that there are factors beyond those included in the SVEET2 tool estimates that can increase the magnitude of the difference. For instance, if the monitoring location is not directly along the groundwater flow centerline from the source centerline, the monitoring location concentration may be lower than the SVEET2 estimate depending on the plume transverse dispersion. SVEET2 does not include attenuation processes other than physical dispersion and assumes both a constant source and that the site conditions have reached a long-term equilibrium with the source area, both of which may only be approximately applicable to the site condition with respect to the measured value for ground-truth comparisons. SVEET2 also does not include any secondary sources (e.g., back diffusion from low-permeability zones outside the main source area in the vadose zone). Thus, these site-specific factors are important to consider for interpretation of the differences between SVEET2 estimates and measured concentrations. Note that these caveats apply to any type of predictive model because all models are an abstraction of actual conditions to some degree.

# 7.0 Demonstration of SVEET2

SVEET2 demonstration testing was conducted for five installations: McClellan Air Force Base, U.S. Army Cold Regions Research and Engineering Laboratory (CRREL), Mather Air Force Base, Tooele Army Depot, and Hill Air Force Base. Waste sites at these installations encompass both Type 1 (ground-truthing/model verification) and Type 2 (ease of use/applicability testing) sites.

## 7.1 Model Verification

In addition to installation personnel working with SVEET2 on their own and in consultation with the SVEET project team, documents obtained by the project team (e.g., from the administrative record) were used to create SVEET2 inputs for ground-truthing (verification) of SVEET2. Data for groundwater and/or soil vapor was compiled for four source areas at three installations for multiple contaminants, for a total of 13 ground-truthing assessments. A summary of the field demonstration ground-truthing efforts are detailed in Table 15. The SVEET2 ground-truthing analysis complied from existing site documents was augmented with any site-specific input collected during interactions with the sites. First, a single SVEET2 scenario was conducted using input values that were most likely representative of the site parameters. These scenarios are designated as "most likely" SVEET2 estimations. To include the variability and uncertainty in site inputs, ground-truthing SVEET2 scenarios were also completed using a Monte-Carlo (MC) analysis ($n$ =2,500) where input parameters were randomly selected between defined minimum and maximum input values of each parameter. The required MC sample size ($n$) to be representative was determined through a sample size analysis (Appendix C). Sample size analysis showed that at least 2,200 realizations were required to produce a stable result. Here, 2,500 MC realizations were used to produce the range in SVEET2 estimations for each ground-truthing comparison. Ground-truthing comparisons for individual sites and relevant monitoring locations are compiled in the sections below.

***Table 15.** Ground-Truthing (Type 1) SVEET2 Demonstrations*

| Site | Source Area | Contaminant [a] | Groundwater / Soil Gas [b] | Monitoring Location |
|---|---|---|---|---|
| McClellan | IC 1 | PCE | GW | MW-235 |
| McClellan | IC 1 | PCE | GW | MW-364 |
| McClellan | IC 1 | PCE | GW | MW-366 |
| McClellan | IC 19 | PCE | GW | MW-354 |
| McClellan | IC 19 | PCE | GW | EW-379 |
| McClellan | IC 19 | TCE | GW | EW-379 |
| McClellan | IC 19 | 1,1-DCE | GW | EW-379 |
| McClellan | IC 19 | PCE | GW | MW-355 |
| McClellan | IC 19 | TCE | GW | MW-355 |
| McClellan | IC 19 | 1,1-DCE | GW | MW-355 |
| CRREL | AOC 2 | TCE | SG | Multipurpose Room |
| CRREL | AOC 2 | TCE | GW | MW 14-107 |
| Mather | 23 C | PCE | GW | MAFB-341 |

[a] PCE = tetrachloroethene, TCE = trichloroethene, and 1,1-DCE = 1,1-dichloroethene
[b] GW = groundwater, SG = soil gas

### 7.1.1 McClellan IC 1

Based on existing site documents for McClellan IC 1, in July 2017, SVE was terminated because the remaining residual vadose zone soil gas volatile organic compounds was found to not extend the time or cost of groundwater remediation, and thus continued SVE was deem unnecessary. The McClellan IC 1 STOP evaluation was completed using groundwater fate and transport modeling, including various VLEACH (EPA, 1997) calculations, to estimate the impact of the residual source area on groundwater.

SVEET2 was used to estimate the potential impact of the source areas on groundwater and compare results to field measured concentrations. SVEET2 input values for the McClellan IC 1 installation were collected from available site documentation, including the final STOP evaluation documentation, on general site conditions, source area characterization, and groundwater monitoring values for the contaminants of interest. Input values for the various McClellan ground-truthing runs are presented in Appendix D.

It should be noted that, while McClellan IC 1 has historically measured various contaminants in the soil gas (e.g., tetrachloroethene [PCE], trichloroethene [TCE], cis-1,2-dichloroethene [cis-DCE]) and both PCE and TCE in groundwater, the source area is presumed to be comprised solely of PCE. Elevated levels of daughter products, such as TCE and cis-DCE are likely due to PCE degradation. Contamination due to degradation and transformation processes are not estimated with SVEET2, and are not considered herein.

SVEET2 estimations for McClellan IC 1 slightly overpredicted the field measured PCE concentrations for the two of the three groundwater wells used for comparison (Table 16; Figure 13). Based on site information, the groundwater wells were assumed to be directly along the groundwater flow centerline. The "most likely" SVEET2 scenarios were able to successfully estimate field measured groundwater concentrations, while the MC output provided a reasonable range expected PCE concentrations for the various groundwater monitoring wells. Using the most likely input parameters to describe the field conditions, SVEET2 estimated concentrations between 6.0 and 6.7 µg/L, providing very good estimations for the measured concentrations that ranged from 3 to 11 µg/L. When parameter uncertainties were applied, the MC SVEET2 estimations tended to overestimate the impact of the source area on groundwater, thus overall providing a conservative estimation.

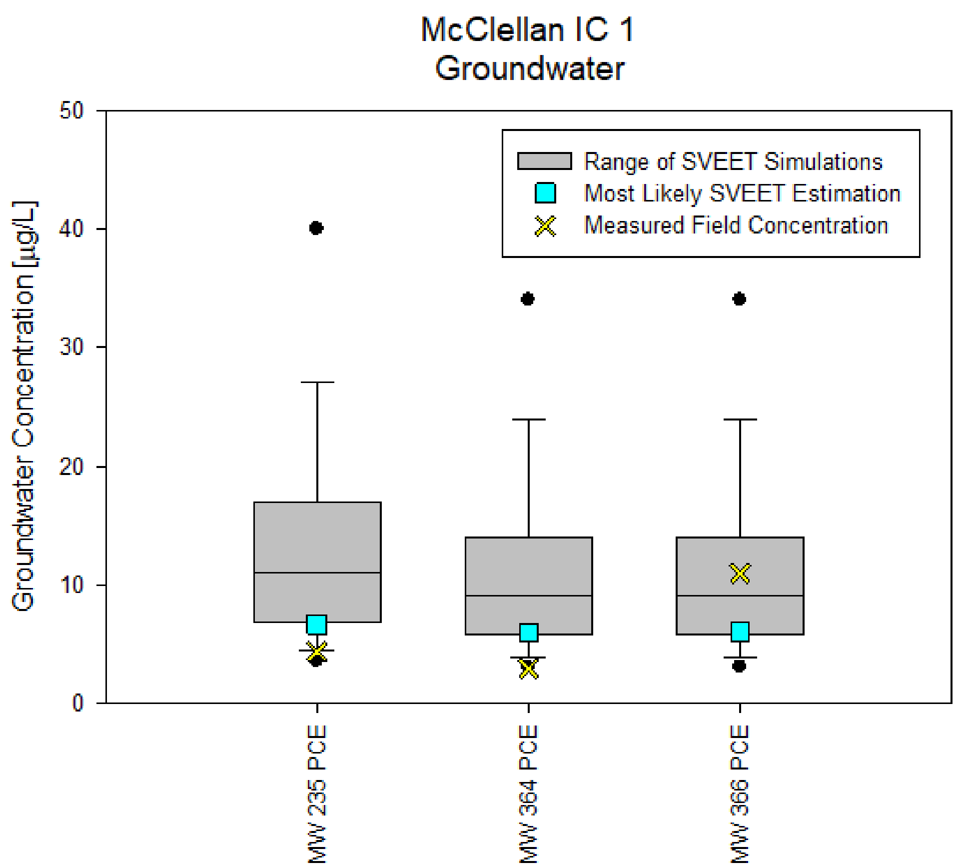



***Figure 13.*** *Comparison of field measured PCE groundwater concentration with SVEET2 scenario values at McClellan IC 1 for monitoring well MW-235, MW-364, and MW-366 located 45, 67, and 61 m from the source area, respectively. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field groundwater concentration is shown with a yellow X.*

**Table 16.** *McClellan IC 1 Groundwater Comparisons*

| | McClellan IC 1 Groundwater Monitoring | | |
|---|---|---|---|
| Well | MW-235 | MW-364 | ME-366 |
| Contaminant | PCE | PCE | PCE |
| **SVEET2 Estimations** | | | |
| Most Likely [µg/L] [a] | 6.7 | 6.0 | 6.1 |
| Mean [µg/L] | 14.5 | 12.3 | 7.1 |
| Median [µg/L] | 11.0 | 9.1 | 5.20 |
| Maximum [µg/L] | 146 | 112 | 61 |
| Minimum [µg/L] | 0.97 | 1.1 | 0.53 |
| Standard Deviation [µg/L] | 13.3 | 11.0 | 6.6 |
| Relative Standard Deviation [µg/L] | 92% | 89% | 94% |
| **Field Data** | | | |
| Well distance (downgradient) [m] [b] | 45.7 | 67.1 | 61.0 |
| PCE Concentration [µg/L] | 4.4 | 3.0 | 11.0 |

[a] SVEET2 estimation for most likely input values
[b] 15% uncertainty was applied to well distance

### 7.1.2 McClellan IC 19

The IC 19 site at McClellan is about 20 acres in the north-central part of Operable Unit C. Previous site investigations identified five disposal pits where industrial waste and ash residues were disposed of. Due to the proximity of these disposal pits, they have been grouped together as a single source area. Historically, PCE, TCE, and 1,1-dichloroethene (1,1-DCE) were the main VOCs detected in the soil gas and groundwater at the site and have been identified in the soil gas of the source area. Other compounds, including vinyl chloride, cis-DCE, 1,1-dichloroethane, 1,2-dichloroethane, and carbon tetrachloride have been measured above the State of California drinking water maximum contaminant levels (MCLs), but are not the primary drivers for remediation.

Briefly, SVE operations started at McClellan IC 19 in June 1997 and ran through March 2016 with brief shutdown periods for system repairs. Shutdown periods included from May 12, 1999 to August 12, 1999; and from August 17, 2001 to January 21, 2002. The SVE system was shut down for a rebound study on March 08, 2016. Estimates approximated there was between 10,342 and 16,200 pounds of VOC mass initial contained in the source area. After the 19 years of SVE operations, approximately 23,760 pounds of total VOC was removed, nearly double the contaminant original mass estimate. Site documents delineate two contaminant source areas, where Area A contains a PCE source area, and Area B contains both TCE and 1,1-DCE source areas.

In December 2017, an external STOP evaluation was completed for McClellan IC 19. The STOP evaluation utilized groundwater fate and transport modeling, including various VLEACH (EPA, 1997) calculations, to estimate the impact of the residual source area on groundwater. PCE, TCE, and 1,1-DCE were all presumed to be vadose zone sources. The STOP evaluation at McClellan IC 19 found that the remaining residual vadose zone soil gas volatile organic compounds would not extend the time or cost of groundwater remediation, and thus continued SVE was deemed unnecessary.

Here, SVEET2 was used to estimate the impact of the source area on groundwater. SVEET2 estimations were then compared to field values as a means of ground-truthing. SVEET2 input values for the McClellan IC 19 installation were collected from available site documentation, including the STOP evaluation documentation, on general site conditions, source area characterization, and groundwater monitoring values for the contaminants of interest. Input values for the various McClellan 19 ground-truthing runs are presented in Appendix D. Ground-truthing comparisons were completed for post SVE shutdown conditions using field data collected in 2017 for the rebound analysis. By January and September 2017, the SVE system had been shut down for approximately one year with site date indicating the rebounding concentrations had stabilized by this point.

At McClellan IC 19, some of the field groundwater monitoring wells were not located directly on the groundwater flow centerline. The original SVEET2 model assumes monitoring locations are directly downgradient from the source area, and thus the estimations were systematically over predicting field concentrations.

For the intended use of SVEET2 (i.e., predictive modeling aimed to inform regulatory decisions) providing an estimate of the maximum concentration is desired. However, for ground-truthing efforts where a monitoring location is situated off the groundwater flow centerline, such an assumption overpredicts concentrations. A version of SVEET2 was developed for internal testing purposes to provide estimates of contaminant concentrations laterally away from the plume centerline. Transverse SVEET2 was used to further refine estimates for MW-354 and MW-355 at McClellan IC 19. An example of how contaminant concentrations change as a function of distance away from the plume center is shown in Figure 14.

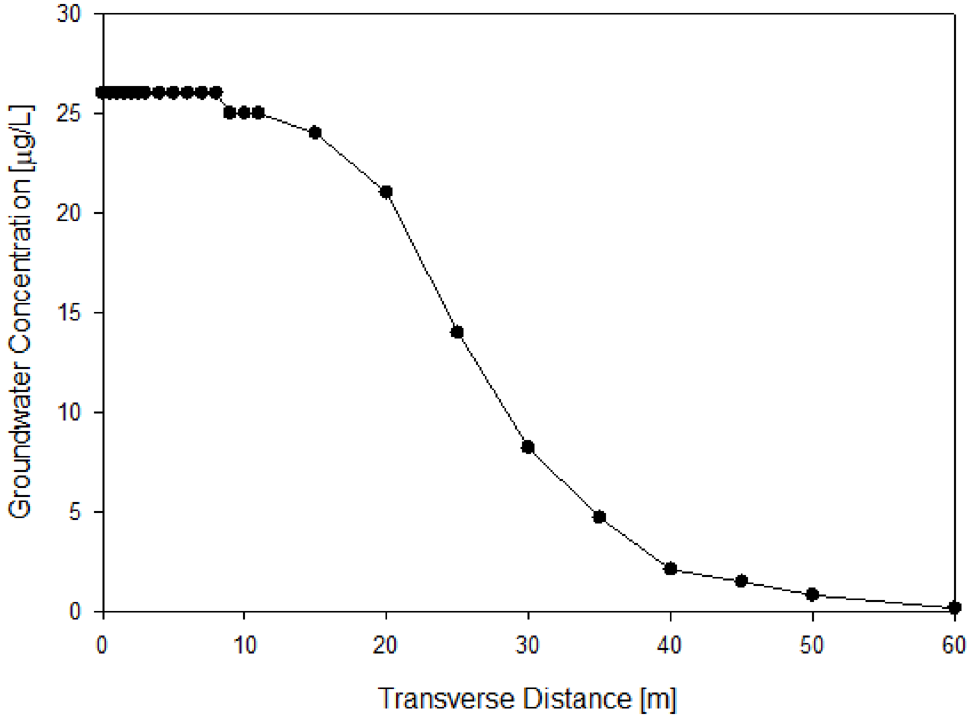



***Figure 14.*** *Spatial plume concentrations for McClellan IC 19 PCE source area as a function of transverse distance away from the plume centerline at a distance of 65 m downgradient.*

Ground-truthing results for McClellan IC 19 are listed for each of the monitoring wells, contaminants, and contaminant source area. Transverse SVEET2 was used for groundwater monitoring well MW-354 comparisons, because this well represents down-cross gradient contaminant conditions being located 30.5 m downgradient and 23 m laterally from Source Area A (Figure 15). Two groundwater monitoring wells represent the plume resulting from Source Area B. Monitoring well EW-379 is located 101 m directly downgradient, whereas MW-355 is located 53 m downgradient and 21.3 m laterally from Source Area B. Ground-truthing results are shown in Figure 16, Figure 17 and Figure 18 for PCE, TCE and 1,1 DCE, respectively.

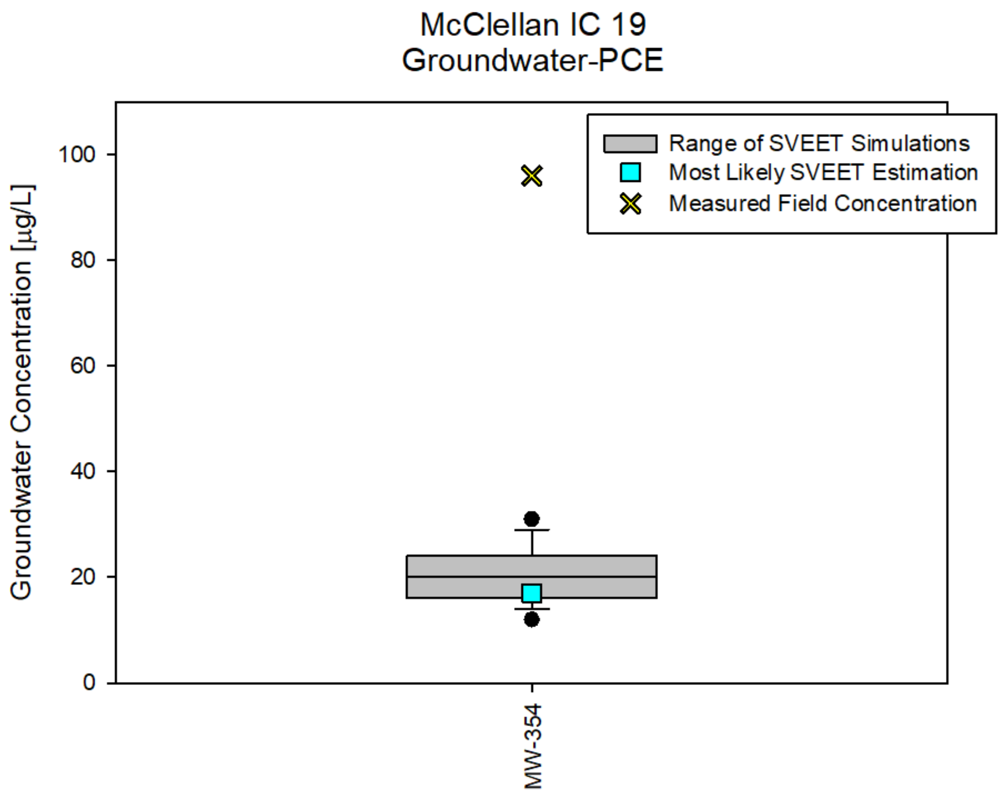



***Figure 15.*** *Comparison of field measured PCE groundwater concentration with SVEET2 scenario values at McClellan IC 19 for monitoring well MW-354, located 30.5 m downgradient, and 23 m laterally, from the Source Area A. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field groundwater concentration is shown with a yellow X.*

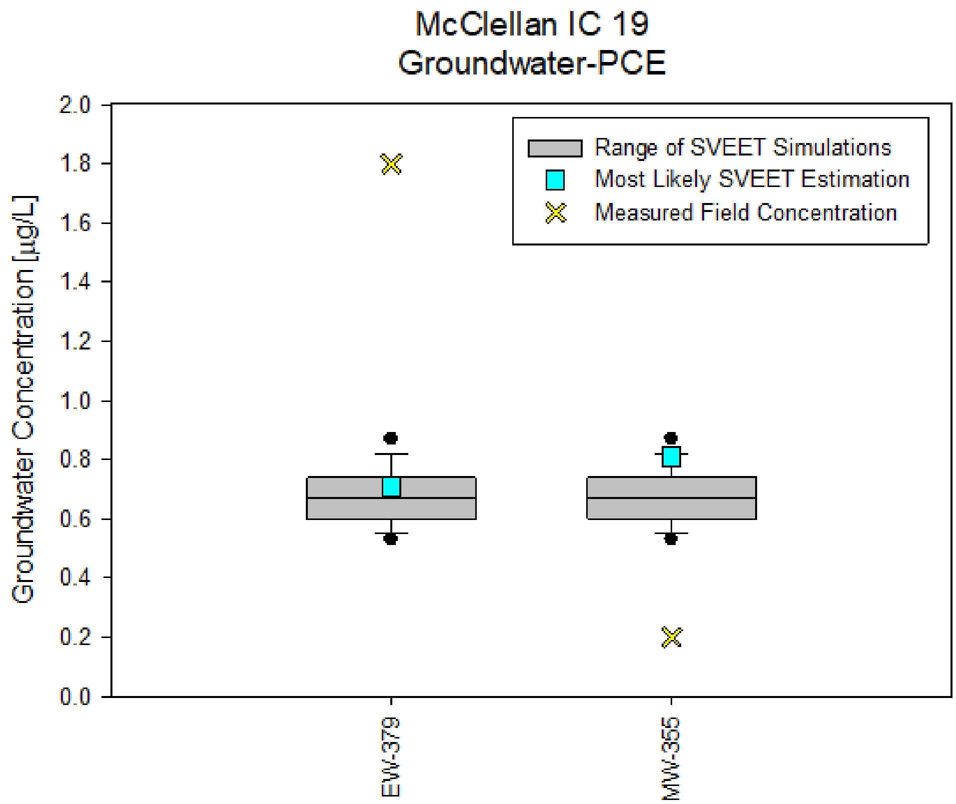



***Figure 16.*** *Comparison of field measured PCE groundwater concentration with SVEET2 scenario values at McClellan IC 19 for monitoring well EW-379 and MW-355, located 101m downgradient and 0 m laterally, and 53 m downgradient and 21.3 m laterally, from Source Area B, respectively. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field groundwater concentration is shown with a yellow X.*

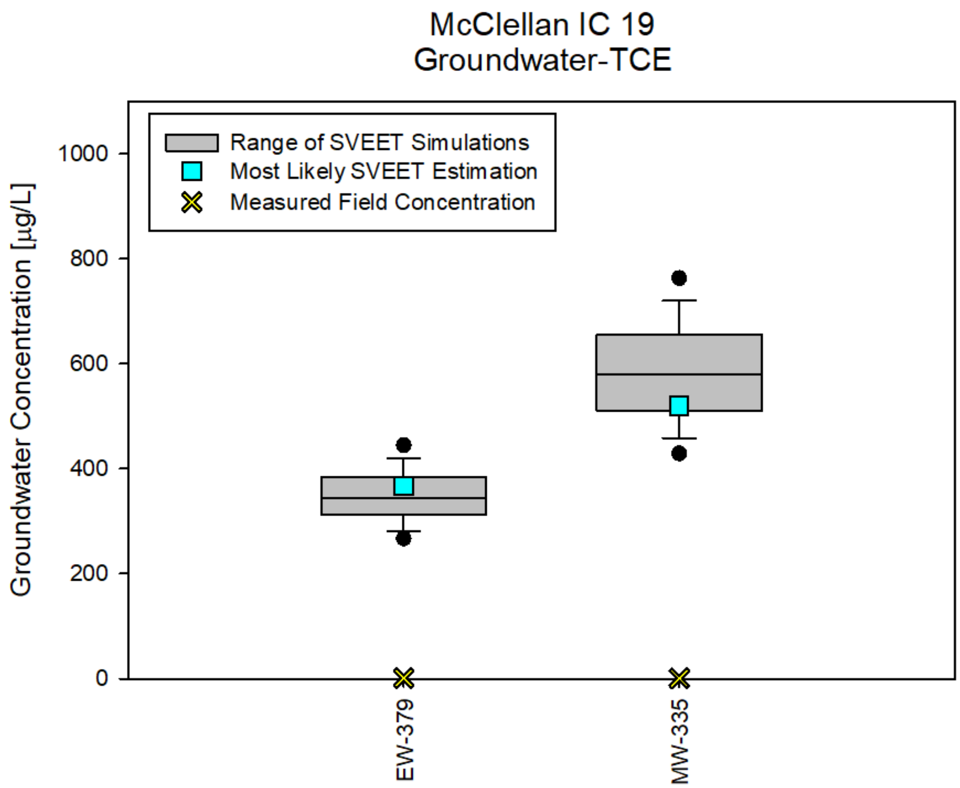



***Figure 17.*** *Comparison of field measured TCE groundwater concentration with SVEET2 scenario values at McClellan IC 19 for monitoring well EW-379 and MW-355, located 91 directly downgradient, and 53 m downgradient and 21 m laterally from Source Area B, respectively. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field groundwater concentration is shown with a yellow X.*

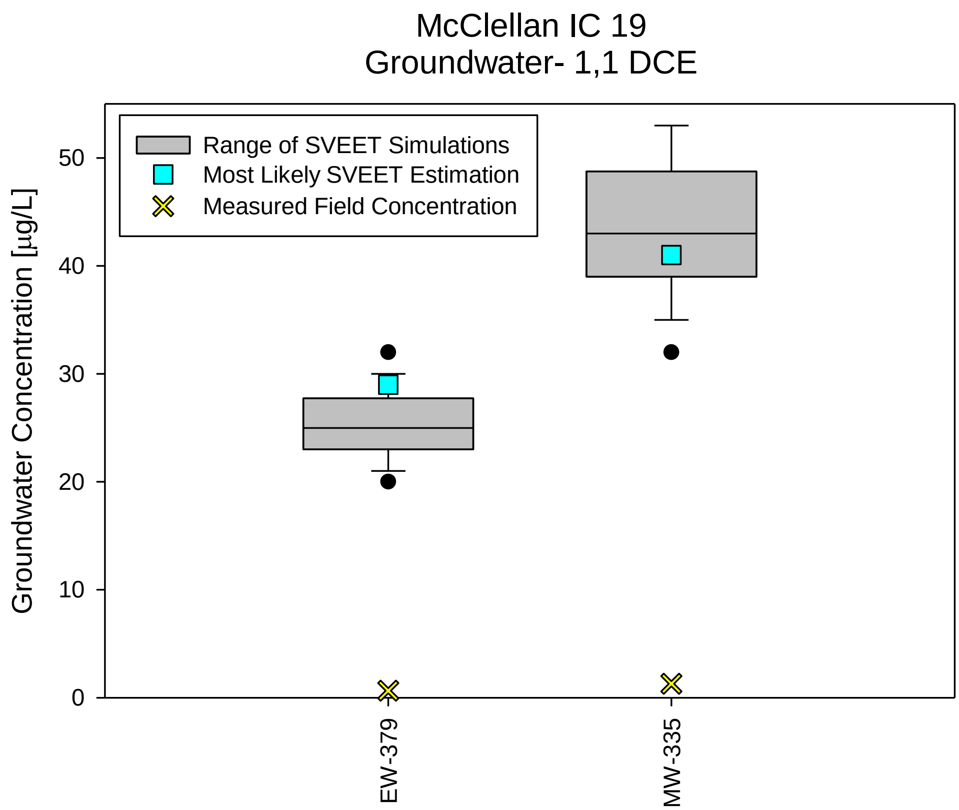



***Figure 18.*** *Comparison of field measured 1,1-DCE groundwater concentration with SVEET2 scenario values at McClellan IC 19 for monitoring well EW-379 and MW-355, located 101, and 53 m from the Source Area B, respectively. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field groundwater concentration is shown with a yellow X.*

*Table 17. McClellan IC 19 Groundwater Comparisons*

| McClellan IC 19 Groundwater Monitoring Well | MW-354 | EW-379 | | | MW-355 | | |
|---|---|---|---|---|---|---|---|
| Contaminant | PCE | PCE | TCE | 1,1-DCE | PCE | TCE | 1,1-DCE |
| **SVEET2 Estimations** | | | | | | | |
| Most Likely [µg/L] [a] | 17 | 0.71 | 367 | 29 | 0.81 | 520 | 41 |
| Mean [µg/L] | 21 | 0.7 | 349 | 25 | 1.1 | 585 | 44 |
| Median [µg/L] | 20 | 0.67 | 345 | 25 | 1.1 | 579 | 43 |
| Maximum [µg/L] | 46 | 1.1 | 526 | 39 | 1.9 | 1030 | 68 |
| Minimum [µg/L] | 7.2 | 0.43 | 219 | 16 | 0.6 | 319 | 25 |
| Standard Deviation [µg/L] | 5.8 | 0.1 | 53.1 | 3.5 | 0.2 | 102 | 7.0 |
| Relative Standard Deviation [%] | 28% | 15% | 15% | 14% | 19% | 18% | 16% |
| **Field Data** | | | | | | | |
| Well distance (downgradient) [m] [b] | 30.5 | 101 | | | 53 | | |
| Well distance (laterally from flow centerline) [m] [b] | 23 | 0 | | | 21 | | |
| Concentration [µg/L] | 96 | 1.8 | 1.6 | 0.66 | < 0.2 | 1.2 | 1.3 |

[a] SVEET2 estimation for most likely input values
[b] 15% uncertainty was applied to well distance

### 7.1.3 CRREL

Area of concern 2 (AOC 2) at the CRREL facility is associated with a release of TCE from an underground storage tank and distribution system. The TCE was used as a refrigerant for operations in the adjacent laboratory building. Contamination was identified in the early 1990s and subsequent investigations have defined the extent of the groundwater and soil vapor contamination associated with the release. The release has impacted unconsolidated glacially derived fine sands, silts, and clays. The water table is approximately 115 feet below the surface. Permeability of the soils tends to increase with depth, and the materials above 50 feet are fine-grained. Underlying metamorphic bedrock is encountered at depths of approximately 170 feet and has not been significantly impacted. The releases at AOC 2 and another significant TCE release at AOC 9 to the southwest of AOC 2 have resulted in vapor intrusion concerns in the laboratory building.

Past remedial activities at AOC 2 included a pilot test of air sparging in 1995, the removal of soil and the underground TCE tank around 2001, and a pilot test of permanganate injection into the vadose zone soils in 2003.

Site data was collected for, specifically for Area of Concern 2 (AOC 2) for SVEET2 ground-truthing efforts for both groundwater and soil gas concentrations within existing buildings. In 2014, a SVE pilot test was conducted at CRREL AOC 2 to identify locations of continual source contamination and collect necessary data to aid in a full-scale design of an SVE system. Rebound testing at the site was conducted between December 2015 and January 2016. Groundwater and vapor concentrations in the vicinity of AOC 2 declined substantially coincident with the SVE pilot test. SVEET2 ground-truthing efforts were completed using pre-SVE pilot data collected in 2014.

Installation of a sub-slab depressurization system was initiated at the laboratory building in 2012 and completed in 2014. The operations of the system affected soil gas concentrations under and inside the building following that timeframe.

The information from the site was used to verify the SVEET2 modeling under this project. SVEET2 estimations were compared to field values as a means of ground-truthing. SVEET2 input values for the CRREL AOC 2 site were collected from available site documentation. Input values for the various CRREL AOC 2 ground-truthing runs are presented in Appendix D. In addition, the project team used the original SVEET2 tool during the Feasibility Study to assess cleanup levels and conducted testing of the new SVEET2 tool under this study. The feedback from this testing is provided in Section 7.2.

For both groundwater and soil gas concentrations at CRREL, SVEET2 provided reasonable comparisons to field data. Field-measured TCE groundwater concentrations fell within the range of SVEET2 estimations (Figure 19). SVEET2 generally overpredicted the soil gas concentrations within the Multipurpose room (Figure 20), which may be related to the sub-slab depressurization system. However, the SVEET2 estimate of soil gas was within the performance criteria (Section 5.1) and is a conservative results with respect to evaluating potential vapor intrusion effects.

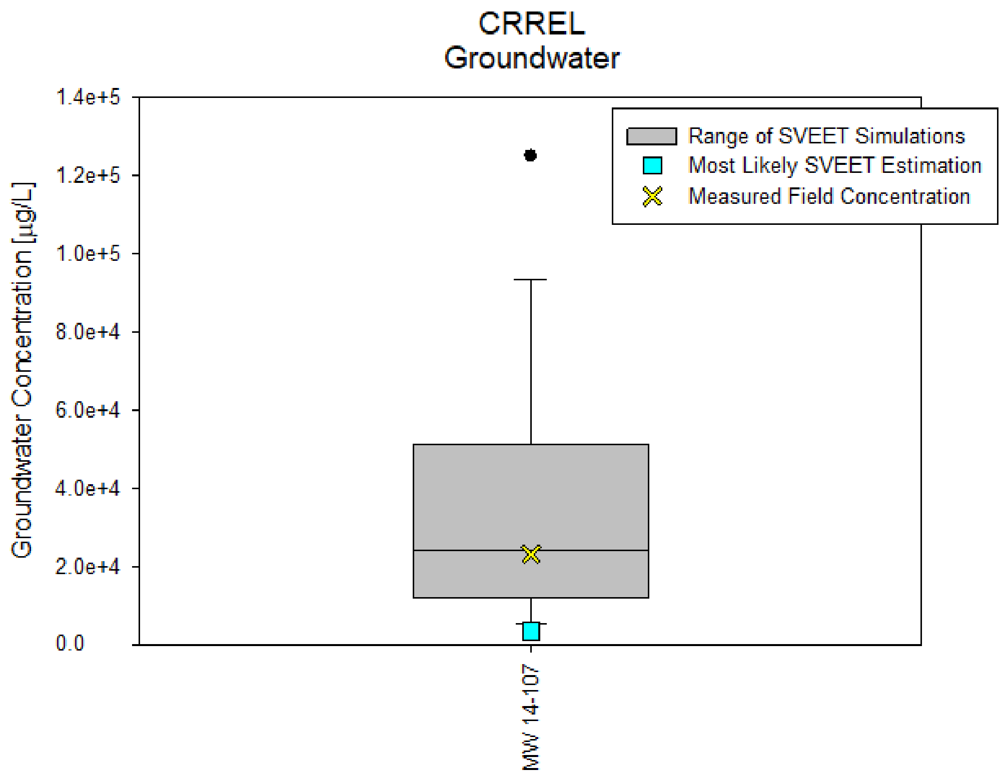



***Figure 19.*** *Comparison of field measured TCE groundwater concentration with SVEET2 scenario values at CRREL AOC 2 for monitoring well MW 14-107 located 24.4 m from the source area. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field groundwater concentration is shown with a yellow X.*

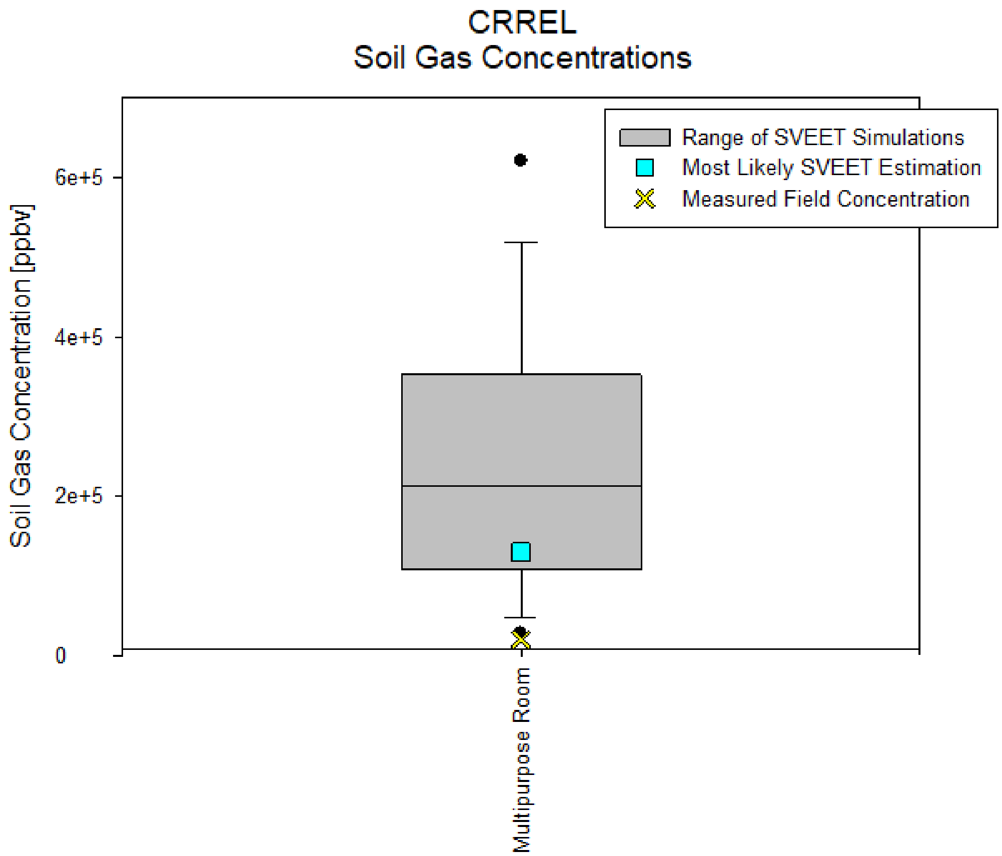



***Figure 20.*** *Comparison of field measured TCE soil gas concentrations with SVEET2 scenario values at CRREL AOC 2 for the Multipurpose Room. Soil gas sampling in the Multipurpose room was located 6 m, 23 m, 4 m (dx, dy, dz) from the source area. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field soil gas concentrations are shown with a yellow X.*

***Table 18.** CRREL Groundwater Comparison*

| | CRREL Groundwater Monitoring Well |
|---|---|
| Well | MW 14-107 |
| Contaminant | TCE |
| **SVEET2 Estimations** | |
| Most Likely [µg/L] [a] | 3,300 |
| Mean [µg/L] | 38,486 |
| Median [µg/L] | 24,200 |
| Maximum [µg/L] | 294,000 |
| Minimum [µg/L] | 231 |
| Standard Deviation [µg/L] | 3984 |
| Relative Standard Deviation [µg/L] | 103% |
| **Field Data** | |
| Well distance (downgradient) [m] [b] | 24.4 |
| TCE Concentration [µg/L] | 22,961 |

[a] SVEET2 estimation for most likely input values
[b] 15% uncertainty was applied to well distance

***Table 19.** CRREL Soil Gas Comparison*

| | CRREL |
|---|---|
| Location | Multipurpose Room |
| Contaminant | TCE |
| **SVEET2 Estimations** | |
| Most Likely [ppbv] [a] | 130000 |
| Mean [ppbv] | 254737 |
| Median [ppbv] | 212500 |
| Maximum [ppbv] | 1440000 |
| Minimum [ppbv] | 27580 |
| Standard Deviation [ppbv] | 193530 |
| Relative Standard Deviation [ppbv] | 76% |
| **Field Data** | |
| Longitudinal Distance (dy) [m] | 6.3 |
| Transverse Distance (dx) [m] | 23 |
| Depth of Basement/Foundation (dz) [m] | 4 |
| TCE Concentration [ppbv] | 20,127 |

[a] SVEET2 estimation for most likely input values

### 7.1.4 Mather

Site values were collected for Mather Air Force Base specifically for Site 23C Former Laundry and Cleaning Plan for SVEET2 ground-truthing efforts for groundwater concentrations. The 2016 SVE completion report of the soil remedial action at Site 23 C at the former Mather Air Force Base recommended SVE termination and site closure with restrictions.

A historical soil gas survey measured elevated VOC concentrations, primarily PCE, near the former laundry and cleaning plant at Bldg. 2587 at Site 23C. Using site data obtained in a 1998-1999 investigation, an SVE system was designed and constructed in 2000. A pilot SVE test was conducted from April 2000 through August 2000. The SVE system was operational from April 12, 2000 through April 30, 2015. The SVE system comprised of shallow to intermediate depth vapor extraction wells. In April 2015, the SVE system was shutdown to assess rebound and conduct a STOP evaluation. Over the 15 years of SVE operations, 6,442 pounds of VOC was removed from the site, including 4,573 pounds of PCE.

Using the site data and some of the VLEACH (EPA, 1997) parameters contained within the SVE completion report, SVEET2 ground-truthing analysis was completed using 2016 field data. One groundwater monitoring well, MAFB-341, was used for comparison (Figure 21).

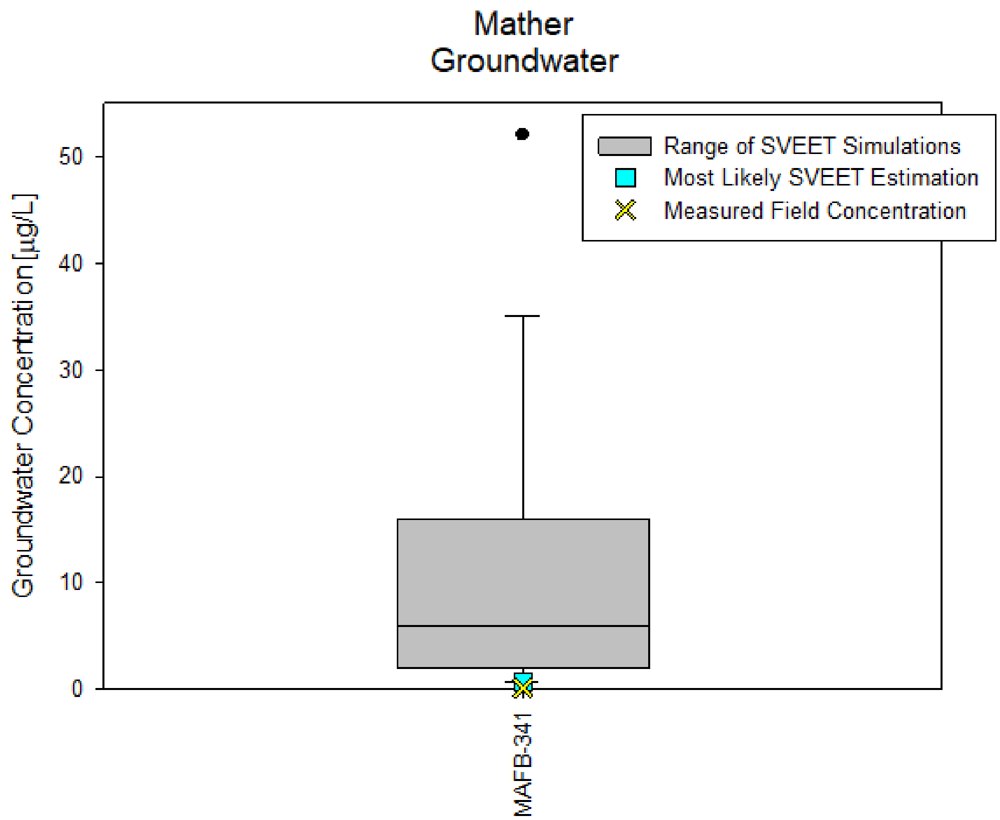



***Figure 21.*** *Comparison of field-measured PCE groundwater concentration with SVEET2 scenario values at Mather for monitoring well MAFB-341 located 91.4 m downgradient and 53.3 m laterally and from the source area. Boxes indicate the 25th and 75th percentiles, whiskers the 10th and 90th percentiles, dots the 5th and 95th percentiles, and the line is the median value of the dataset. The SVEET2 estimation using the most likely input parameter values is indicated with a blue square. The corresponding measured field groundwater concentration is shown with a yellow X.*

***Table 20.** Mather Groundwater Comparison*

| | Mather Groundwater Monitoring Well |
|---|---|
| Well | MAFB-341 |
| Contaminant | PCE |
| **SVEET2 Estimations** | |
| Most Likely [µg/L] [a] | 0.72 |
| Mean [µg/L] | 13.2 |
| Median [µg/L] | 6 |
| Maximum [µg/L] | 188 |
| Minimum [µg/L] | 0.04 |
| Standard Deviation [µg/L] | 19 |
| Relative Standard Deviation [µg/L] | 144% |
| **Field Data** | |
| Well distance (downgradient) [m] [b] | 91.4 |
| Well distance (laterally from flow centerline) [m] [b] | 53.3 |
| PCE Concentration [µg/L] | 0.16 |

[a] SVEET2 estimation for most likely input values
[b] 15% uncertainty was applied to well distance

### 7.1.5 Ground-Truthing Summary and Limitations

The SVEET2 software demonstration showed that that the software can provide useful results to support remediation decisions, though limitations/assumptions of the tool may necessitate site-specific modeling in some situations. SVEET2 is not intended for extrapolation beyond the range of underlying STOMP simulation results. Thus, application is limited to situations where site characteristics can be represented within the bounds placed on the input parameters. For sites where input parameters are outside those bounds (e.g., high recharge), site-specific modelling should be applied. SVEET2 assumes that vapor-phase diffusive transport dominates vadose zone contaminant movement (though migration via recharge is accounted for), the vadose zone source can be represented as a single source area (which could be one source or a composite of multiple nearby sources), the source has a constant strength (i.e., no source depletion over time), the groundwater is initially uncontaminated (no groundwater contaminant sources), and the subsurface is homogeneous with uniform properties. For groundwater results, SVEET2 reports concentrations along the plume centerline from the source in the direction of downgradient flow, which is assumed to be the path of most interest with respect to remediation decisions. SVEET2 does not explicitly account for contaminant adsorption, contaminant transformations (biological or abiotic degradation), any secondary sources (e.g., back diffusion from low-permeability zones outside the main source area in the vadose zone), or a groundwater monitoring well screen interval that does not start/span the water table. Because SVEET2 results represents equilibrium conditions (either undisturbed pre-remedial action or post-remediation re-equilibration), transient effects such as adsorption or migration through different geological layers do not play a role in the results and these aspects can be neglected (no adsorption, homogeneous subsurface). If transient changes are important for a site, then site-specific modeling that accounts for aspects (such as heterogeneity and adsorption) would be required.

SVEET2 results are generally conservative in that the assumptions favor higher concentration estimates, which is appropriate for predictive applications in support of remedial decision making. Given a site scenario within the constraints of the defined input parameter bounds, having a single source area, no secondary sources, and no sources in groundwater, five of the assumptions are important in leading to conservatively high concentration estimates. For the long-term state of a site post-remedial activity, the assumptions of a system at equilibrium and a constant-strength vadose zone source will provide higher concentration estimates. For short time frames, a system could be expected to not yet have reached equilibrium and would thus have lower concentrations at distance from the source. As equilibrium is reached over time, the maximum concentration impacts are attained. It depends on the contaminant mass and configuration of the vadose zone source in the subsurface, but generally a source would be expected to deplete and decrease in strength over time (e.g., Truex et al., 2012; Carroll et al., 2012). Thus, a constant-strength source would result in conservatively high concentration estimates over time, though the concentration estimates relative to a short time frame would merely be representative. Conservatively higher concentration estimates in both soil gas and groundwater also arise from not including biological or abiotic contaminant degradation/transformation. The degree of contaminant degradation at a site depends on the contaminant and subsurface environment, but it is not uncommon to see attenuation of contamination through such mechanisms. Finally, for the estimated groundwater concentration in SVEET2, it is assumed both that the monitoring location of interest is along the plume centerline downgradient from the source location and that the monitoring well screen starts at the water table where the highest mass transfer/mixing from the vadose zone would occur. The plume centerline will be the highest concentration in the groundwater; transverse/off-centerline locations could be expected to have a lower concentration, depending on the size of the plume. If a monitoring well screen interval starts at some distance below the groundwater table, then the concentrations that would be measured in that well could be expected to be lower than the SVEET2 estimates because it is sampling a lower-concentration portion of the aquifer. Taken together, the user will find that these assumptions help safeguard against potentially underestimating groundwater and soil gas impacts from a vadose zone source for many situations.

## 7.2 Site Feedback

Both quantitative (ground-truthing) and qualitative (user-testing) feedback on SVEET2 was collected from various site personnel. Introductory phone calls with site personnel for each installation were first completed. During these initial meetings, the SVEET2 project team provided an overview of the updated SVEET2 software and details on how the site can contribute to the field demonstration effort. Installation personnel were provided with the following documentation: (a) an introduction to SVEET2, (b) the updated beta version of the SVEET2 software (SVEET2_0.1.4_beta), (c) a SVEET2 user guide, (d) an example site parameter input file, and (e) a user feedback form. Follow-up phone calls were then conducted with each of the installations to collect feedback, input files compiled by their personnel, the user feedback form, and any other related feedback on the beta version of SVEET2. Feedback on SVEET2 was received from CRREL, McClellan, Mather, Hill, and Tooele.

User feedback was obtained from the site team in the form of both verbal discussions between the SVEET2 team and the site and through written responses to the provided user feedback survey questions. A summary of how each site used SVEET2 is completed in Table 21. A more extensive summary of the written feedback is provided in Appendix E. The collected feedback pointed to a few areas where SVEET2 had the potential be improved, with test users commenting on the importance of documentation to guide users with respect to inputs and considerations.

***Table 21.*** *Summary of SVEET2 user testing.*

| Site | Scenario type? | Scenarios Run | Sensitivity Analysis Conducted? | Source Strength (soil gas conc. vs. mass discharge?) | Site parameters outside of SVEET2 range? |
|---|---|---|---|---|---|
| McClellan IC 1 | Ground-truthing | GW | No | Soil gas | Yes, recharge |
| CRREL | Ground-truthing | GW, VI | Yes | Soil gas | Yes, recharge [a] |
| Mather | Ground Truthing | GW | No | Soil gas | No |
| Hill- Landfill 5 | Ground Truthing and assessment of stopping point for active SVE or other source treatment operations | GW | Yes | Soil gas | Yes, recharge, source thickness, groundwater velocity, porosity, bulk density, soil moisture, groundwater velocity |
| Tooele | Stopping point for active SVE or other source treatment operations | GW | Yes | Soil gas | No |

[a] The CRREL site team estimated a range potential of recharge values, with only some of those values falling outside the acceptable range of SVEET2 inputs.

Overall, the feedback collected indicated that users found SVEET2 to be applicable and helpful at their respective sites. The spreadsheet based SVEET2 was found to be relatively user friendly with straightforward input requirements that were readily available based on current site data. Sites used SVEET2 for a variety of purposes including in their own ground-truthing efforts where SVEET2 estimates were compared to nearby groundwater wells and soil gas concentrations were compared to sub-slab measured values. What-if scenarios were also completed to assess potential impacts of a source area on groundwater to support SVE system final shutdown and soil gas concentrations to help identify potential vapor intrusion concerns. Furthermore, SVEET2 was used to help assess parameter sensitivity, and the resulting potential impacts, by various scenarios.

Since SVEET2 is a spreadsheet tool, it can provide nearly instantaneous results, allowing users to quickly vary input conditions and running multiple scenarios readily. This ability can be especially important when site inputs have a high degree of uncertainty or are relatively unknown. For example, through conducting various scenarios quickly in SVEET2, one field site was able to obtain insight into the processes likely controlling groundwater concentrations. In this case, users did not have a measured value for recharge at their site; however, by testing various recharge inputs, the impact of recharge, and recharge rate, on groundwater conditions was it was clear that recharge was a dominant process.

A site also noted the potential to use SVEET2 in a current feasibility study to help determine the required remedial clean up objective to meet regulatory requirements for both groundwater and vapor intrusion. The ability to quickly conduct such what-if analysis in SVEET2 is a major benefit over other modeling approaches. This ability was recognized by the site personnel, particularly to support the decision-making process during feasibility analysis. Another site noted that, previously, a fairly intensive process has been required to demonstrate that SVE is either not required or is no longer necessary because the predicted VOC impact on groundwater either will not cause underlaying groundwater concentrations to exceed the clean-up level (MCL) or will not significantly lengthen the time and/or cost of the current groundwater remediation activities. In this more intensive approach, the site staff would typically use soil gas data and the VLEACH (EPA, 1997) vadose zone fate and transport model to estimate contaminant mass loading to groundwater, followed by groundwater modeling to assess the remaining potential impacts. While such a methodology has been successful, it is seen as having considerable data demands, being labor intensive, while still requiring many assumptions and professional judgment. Such assumptions and judgements are often called into question by the regulatory agencies. Site staff noted that SVEET2 does still have some of these same limitations; however, it is much quicker and easier to use. It was further noted that, in some instances, SVEET2 may be able to confirm or replace some of more traditional methodology to better assess whether a SVE system can be shut down.

Further, the ability to estimate soil gas concentrations for use in vapor intrusion assessments was particularly interesting to many of the sites. At some of the sites, SVE was previously installed and operated solely as part of groundwater remedy without consideration for vapor intrusion. While SVE is not typically applied as a shallow soil gas VOC vapor instruction remedy, regulatory agencies would, in fact, consider an active shallow soil remediation approach, like SVE. Site contractors are finding that regulatory agencies often bring up the potential for VI when an SVE system is proposed for closure based on groundwater standards. So, the ability to estimate the remaining potential VI impacts, in addition to groundwater, would be desired. Furthermore, it was noted that SVEET2 could potentially be used to help establish institutional control (IC) boundaries for a site, or assess if ICs are needed. While such scenarios were not directly tested here, such discussions with site individuals point to the wide potential application of SVEET2 to aid in decision-making processes.

Overall, the feedback from the sites was very positive.  Ground-truthing efforts conducted by the sites found that SVEET2 did fact provided reasonable estimates of the field concentrations, highlighting two important findings.  First, this confirms that the implicit assumptions of SVEET2 were able to represent real field conditions encountered at DoD sites, and secondly that individuals with knowledge of a specific site were able to distill down field data into the required input parameters for the SVEET2 scenarios.  Further, while some of the sites did not have the field conditions and/or the data to support ground-truthing, there was still interest in how SVEET2 could potentially be applied to their sites in the futures, particularly for vapor intrusion estimations.  Sites also expressed that SVEET2 may be able to act as a lower cost estimation of potential groundwater impacts, as compared to more typical VLEACH (EPA, 1997) modeling efforts.

# 8.0 Cost Assessment

An installation-specific cost analysis was performed to elucidate potential benefits and cost-savings associated with implementing the SVEET2 tool at sites currently utilizing SVE systems with diminishing recoveries. Information on SVE operational costs and the application of SVEET2 for the evaluated site are described below, followed by an assessment of the cost savings/cost avoidance.

## 8.1 SVE Operational Costs and SVEET2 Assessment

Site-specific parameters for eight SVE systems (both base realignment and closure [BRAC] and landfill sites) located at Tooele Army Depot were used to run multiple scenarios with the SVEET2 software to determine the necessity for VOC remediation using SVE systems currently in operation at the facility. Several scenarios were evaluated to assess uncertainties with respect to source zone geometry and the soil gas concentrations that were used to define source strength parameters. The SVEET2 results for the impact to groundwater were compared to the site cleanup criteria. The evaluation found that the impact to groundwater was small enough for five of the eight locations to potentially power down their existing SVE systems, while it was determined that the other three sites should continue SVE operation.

Annual operational costs (2019 values) for each SVE system were derived from installation-specific annual performance evaluation reports, with the approximate costs listed in Table 22. Data derived from these reports are inclusive of operational costs of SVE coupled to air sparging systems. Landfill SVE system costs were estimated based on total cost to operate all systems and proportion of total energy use for each system. In Table 22, the five SVE systems that could potentially be terminated are labeled “Shutdown,” and the three systems where SVE operation should continue are labeled “Run”.

***Table 22.*** *Annual operational cost comparisons between SVE systems at Tooele Army Depot.*

| System | Run/Shutdown | Operating Cost |
|---|---|---|
| **BRAC Systems** | | |
| Building 615 | Run | $ 142,000 |
| Building 620 | Shutdown | $ 128,400 |
| Building 679 | Run | $ 122,700 |
| Avenue C | Shutdown | $ 118,600 |
| **Landfill Systems** | | |
| SVE-006 | Shutdown | $ 46,700 |
| SVE-009 | Shutdown | $ 161,300 |
| SVE-012 | Run | $ 151,100 |
| SVE-023 | Shutdown | $ 208,500 |
| ***Estimated Cost Savings for Shutdown Systems*** | | **$ 663,500** |

## 8.2 Cost Savings/Avoidance

This assessment of SVE systems for the Tooele Army Depot provided an example for potential cost savings. Based on application of the SVEET2 tool and these current annual SVE operational costs, it is estimated that powering down the five SVE systems would equate to a cost savings of roughly $663,500 per year, which is about a 61.5% decrease in annual operational costs associated with these systems (Table 22).

While the data presented here are inclusive of a single case study (with multiple SVE systems), the SVEET2 tool is broadly applicable to a wide range of sites owned or managed by the DoD. SVE operational costs in this study ranged between approximately $50-210K a year (Table 22). Other reports suggest that annual SVE system operation may cost upwards of $200K (NFESC, 2005; EPA, 2007). Should only a small percentage of DoD sites that actively utilize SVE systems incorporate SVEET2 as a part of their performance monitoring process, potential annual cost savings for the DoD could reach millions of dollars just on system operational costs alone.

For personnel who are unfamiliar with the SVEET2 software functionality, roughly 16 hours of labor will be required to run site-specific scenarios. This level of effort is inclusive of time dedicated to file downloads, software installation, navigating software functionality, gathering relevant site information, configuring scenarios for calculation, and performing data analysis and interpretation. Most of that time will be spent in gathering site data and assessing scenario variations to support remedy decisions. Assuming billable rates are in the range of $80-150 per hour, labor estimates for a new user to run site-specific analyses with SVEET2 can range from $1280-2400 per DoD installation, depending on the number of SVE sites being vetted.

With all of these considerations, SVEET2's rapid evaluation capabilities and ease-of-use warrants its utilization as a tool to be used at the forefront of performance optimization studies surrounding SVE systems.

# 9.0 Implementation Issues

The main implementation issue surrounding SVEET2 relates to determining the appropriate input values to represent a site. While the required inputs for SVEET2 should be readily available from field data, it is still necessary to define the site within the SVEET2 conceptual model framework. As with any modeling effort, assumptions and professional judgement are needed to fit a complex site within a conceptualized model framework. With SVEET2, for instance, a user needs to define a square source area with a single representative soil gas concentration from existing field measurements, requiring an understanding of the site, available data, and professional judgement.

Many field sites and source areas can be represented with the SVEET2 conceptual model. However, if the level of complexity at a site is too great, then it may be necessary to perform site-specific modeling. For instance, if the site has NAPL present, multiple source areas that cannot be represented as a single source area, or if the site conditions fall significantly outside the permissible range of input parameters, then the SVEET2 generalized conceptual model may not provide an adequate representation of the site. For example, very high recharge rates at a site would be outside the boundaries/assumptions of the underlying STOMP simulations (with respect to vapor diffusion dominated transport versus recharge dominated contaminant transport).

## 9.1 Example Use of SVEET2

To illustrate how site data can be applied towards the SVEET2 inputs, a Type 1 DoD site used for ground-truthing (Section 7.1) will be used as an example. Data obtained for the example site included several reports that detailed site characterization information, including soil properties, historic SVE operations, site maps, source zone characterization efforts, and groundwater monitoring data. The general site characterization information provided estimates for many of the subsurface and porous media input parameters, including temperature, moisture content, porosity, dry bulk density, and recharge. Groundwater flow direction and velocity were used to calculate the groundwater Darcy velocity and to determine groundwater location/wells potentially impacted by the VOC source zone. To define the source area terms, source zone maps and corresponding soil gas sampling data was used. Vadose zone thickness (VZT) was estimated from a cross-section through the source area, using the water table evaluation in comparison to the ground surface. In this example, site sampling identified three subsurface areas that had elevated VOC soil gas concentrations. Soil gas concentration data with depth further suggested that only one of the elevated areas was likely a main source area and contaminant contributor, and thus was used to define the source area. Soil gas data was also used to estimate the soil gas concentration that best describes the source area. In this case, the average was used to represent the “most likely” scenario and the maximum and minimum values were used as the bounds for the sensitivity analysis. Previous efforts at the site defined areas with elevated VOC levels using Thiessen polygons. While the actual source area is not a square of known width (w) and thickness (z), these values were estimated based on the site maps and the assigned areas for the Thiessen polygons. The estimated area within the polygons of interest was recalculated to assume the shape of a square with known width. Depth profiles were used to estimate the source area thickness and location within the vadose zone. For all the estimated parameters, either minimum and maximum values were identified from the data or a percent uncertainty was applied to the most likely value to bound the possible input range for scenario testing.

## 9.2 Technology Transfer

Technology transfer activities were part of this ESTCP project to publicize the SVEET2 software capabilities and provide users with insight on software use. Awareness amongst site managers, practitioners, and regulators is critical for the application of the SVEET2 software to evaluate SVE performance and opportunities for cost savings. Though constrained by the COVID-19 pandemic from early 2020, the project team has engaged in technology transfer through a journal article, conference presentation, and webinars (Johnson et al. 2019, 2021a, 2021b; Johnson and Byrnes, 2021). Three additional journal articles are in preparation. Additional interactions with Navy and Army Corps of Engineers site managers are planned through participation in workshops/meetings. With respect to Navy-specific audiences, future knowledge dissemination will occur through the Remediation Innovative Technology Seminar (RITS) and the Environmental Restoration (ER) Managers Training. For the Corps of Engineers in support of the Army, the SVEET2 tool will be mentioned and promoted for use in recurring technical training on remediation options for soil, and at least one virtual demonstration workshop will be arranged and made available for Army personnel. Further, a presentation/workshop is being pursued though U.S. EPA for Federal Remediation Technologies Roundtable (FRTR) members and interested personnel.

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## 10.1 Manuscripts in Preparation

"Practical Management of Big Data for a Spreadsheet Software Tool." In preparation for *Computers and Geosciences* (or possibly *Communications of the ACM*, *SIAM Journal on Applied Mathematics*, or *Journal of Computational and Applied Mathematics*).

"Numerical Modelling as the Foundation for the SVEET Decision Support Software." In preparation for *Environmental Modelling and Software*.

"Using an Equivalent Flux Condition Approach for Soil Vapor Extraction Simulations." In preparation for *Vadose Zone Journal* (or similar).

# Appendix A

# SVE Survey Form

## Survey on Soil Vapor Extraction for Vadose Zone Contaminant Remediation

Responses from this voluntary survey will facilitate expansion of SVEET software applicability, undertaken as part of ESTCP project ER-201731. Provide what answers you can by circling responses and filling in values (estimates are fine), responding with "unknown," "N/A," or "confidential," if appropriate.

1. Please provide the site name, location (installation, city, state), and contact name (DoD PM or other site owner) for your site(s). If you have multiple sites, provide responses/values for each site (here & below). You need not fill in confidential information, simply note "confidential" in your response.

   ______________________________________________

   ______________________________________________

2. Do all of the contaminants of concern located in the vadose zone at your site(s) fall into one or more of the three categories listed below? If not, please specify your additional contaminants of concern.
   - Chlorinated ethenes (e.g., PCE, TCE, and/or daughters)
   - Chlorinated ethanes (e.g., 1,1,2,2-PCA, or 1,1,1-TCA, and/or daughters)
   - Chlorinated methanes (e.g., CT and/or daughters)

   **Yes** ☐ **No** ☐

   Other contaminants of interest: ______________________

   ______________________ ______________________

3. Is there now, or has there ever been, an SVE system operating at this site? **Yes** ☐ **No** ☐

   If 'Yes', then for how long (indicate years or months) has the SVE system…

   …been operated in nominally a continuous mode? ____________ **units?**

   …been operated in a cyclic mode? ____________ **units?**
   *(i.e., on for a certain duration, then off for a certain duration)*

   …been shut down for the long-term? ____________ **units?**

   If SVE has not been applied, is SVE or another vadose zone remedy being considered? **Yes** ☐ **No** ☐

4. Is information about the SVE system publicly available? **Yes** ☐ **No** ☐
   If available, please provide a pointer to relevant documents or web sites:

   ______________________________________________

5. What is the depth to groundwater? ____________ **units?**
6. If known, describe location/size for zone of residual NAPL or highly contaminated soil above water table:
   Depth to ...top of zone? ______ ...bottom of zone? ______ **units?** Areal footprint? _______ **units?**
7. What is the distance to a groundwater compliance point or receptor? ____________ **units?**
8. Is there a surface-infiltration/low-permeability cap at the site? **Yes** ☐ **No** ☐
   If yes, what type of cap? ______________________________
9. If known, what is the nominal recharge rate at the site? ____________ **units?**
10. Is vapor intrusion an issue at the site? **Yes** ☐ **No** ☐
11. Have you previously used, or investigated using, SVEET (or VIETUS) for your site(s)? **Yes** ☐ **No** ☐
12. Are you interested in exchanging additional information and/or trying a beta version of the expanded SVEET tool? **Yes** ☐ **No** ☐

    Contact info: ______________________________________
    *(Name, phone/e-mail)*

# Appendix B

# Calculation of Equivalent Flux Conditions

The STOMP simulations underlying SVEET version 1.0 used a bulk density of 1.855 g/mL and a porosity of 30%. To allow a user-specified bulk density and/or porosity, one approach would be to define these characteristics as variable parameters, significantly increasing the number of numerical simulations required. An alternate approach is to calculate equivalent diffusive flux conditions and use results from existing simulations. The primary effect of changing the bulk density and/or porosity is on the residual saturation, which is a key aspect influencing vapor-phase contaminant transport. The following discussion elaborates on the mathematical basis for calculating equivalent flux conditions.

## B.1 Mathematical Foundation

The fundamental equation for diffusion of a volatile organic compound (VOC; denoted with a superscript *o* on variables in the following equations) in the gas phase (subscript *g*) is given in Equation B.1 in terms of mole fraction gradients. Defining $n \cdot s_g = \theta_g$, Equation B.1 becomes Equation B.2.

$$J_g^o = -\tau_g n s_g \rho_g \frac{M^o}{M_g} D_g^o \nabla \chi_g^o \tag{B.1 }$$

$$J_g^o = -\tau_g \theta_g \rho_g \frac{M^o}{M_g} D_g^o \nabla \chi_g^o \tag{B.2 }$$

In the above equations, $J_g^o$ is the diffusive flux, $\tau_g$ is the tortuosity, $n$ is the porosity, $s_g$ is the gas phase saturation, $\rho_g$ is the gas density, $M^o$ is the VOC molecular weight, $M_g$ is the gas phase average molecular weight, $D_g^o$ is the VOC diffusion coefficient in gas, $\chi_g^o$ is the VOC mole fraction in the gas phase, and $\theta_g$ is the gas phase volumetric fraction.

Equation B.2 can be simplified to Equation B.3 by using a gas-phase concentration ($C_g$) gradient.

$$J_g^o = -\tau_g \theta_g D_g^o \nabla C_g^o \tag{B.3 }$$

Other pertinent relations (with subscript *w* for the aqueous phase) are shown in Equations B.4 and B.5, where, $\theta_w$ is the aqueous phase volumetric fraction, $s_w$ is the aqueous phase saturation, $\omega_w$ is the weight fraction moisture content, $\rho_d$ is the dry bulk density, and $\rho_w$ is the density of water. Note that the $S_r$ used in the SVEET terminology is the same as the $s_w$ variable used here.

$$\theta_g + \theta_w = n \cdot s_g + n \cdot s_w = n \qquad \text{(i.e., } s_g + s_w = 1\text{)} \tag{B.4 }$$

$$\theta_w = \frac{\omega_w \rho_d}{\rho_w} \tag{B.5 }$$

### Diffusive Flux Equivalency

Considering Equation B.2, equivalency for diffusive contaminant transport in two different sediments (superscripts *a* and *b*) can be obtained through Equation B.6.

$$\tau_g^a \theta_g^a = \tau_g^b \theta_g^b \tag{B.6}$$

Using the Millington and Quirk correlation [e.g., Ho and Webb, 2006], tortuosity may be expressed by Equation B.7.

$$\tau_g = n^{1/3}\left(s_g\right)^{7/3} = n^{1/3}\left(\frac{\theta_g}{n}\right)^{7/3} = \frac{\left(\theta_g\right)^{7/3}}{n^2} \tag{B.7}$$

Inserting Equation B.7 into Equation B.6 gives Equation B.8.

$$\frac{\left(\theta_g^a\right)^{10/3}}{\left(n^a\right)^2} = \frac{\left(\theta_g^b\right)^{10/3}}{\left(n^b\right)^2} \tag{B.8}$$

Given that the properties for one sediment (say, soil *b*) are available at a field site, Equation B.8 can be rearranged to solve for $\theta_g^a$ of the other sediment (i.e., soil *a*, which would represent the SVEET base case sediment), as shown in Equation B.9.

$$\theta_g^a = \left[\frac{\left(\theta_g^b\right)^{10/3}\left(n^a\right)^2}{\left(n^b\right)^2}\right]^{3/10} \tag{B.9}$$

With this value of $\theta_g^a$, the corresponding values of $\theta_w^a$ and $s_w^a$ can be computed, as shown in Equation B.10.

$$s_w^a n^a = \theta_w^a = n^a - \theta_g^a = n^a - \left[\frac{\left(\theta_g^b\right)^{10/3}\left(n^a\right)^2}{\left(n^b\right)^2}\right]^{3/10} = n^a - \left[\frac{\left(n^b - \frac{\omega_w^b \cdot \rho_d^b}{\rho_w}\right)^{10/3}\left(n^a\right)^2}{\left(n^b\right)^2}\right]^{3/10} \tag{B.10}$$

## B.2 Example Calculation

Suppose, for example, that the subsurface soil at site *b* has the following properties.

$n^b = 0.38$ $\qquad$ $\rho_d = 1.64$ g/cm³

$\omega_w^b = 0.08$ $\qquad$ $\rho_w = 0.9982$ g/cm³ (at 20°C)

Using these values for site *b*, $\theta_w^b$ can be computed using Equation B.5 to yield $\theta_w^b$ = (0.08)(1.64)/0.9982 = 0.1314 (which equates to a water saturation of 0.346). Then calculate $\theta_g^b$ using Equation B.4 to obtain $\theta_g^b$ = 0.38 – 0.1314 = 0.2486.

To find the equivalent properties of the SVEET standard (base case) sediment, which has $n^a$ = 0.30, first plug the value for $\theta_g^b$ into Equation B.9 to determine $\theta_g^a$, as follows.

$$\theta_g^a = \left[ \frac{(0.2486)^{10/3}(0.30)^2}{(0.38)^2} \right]^{3/10} = 0.2157$$

Then, by Equation B.4, $\theta_w^a$ = 0.30 – 0.2157 = 0.0843. Using Equation B.10, $s_w^a$ = 0.0843 / 0.30 = 0.281, which is the equivalent residual water saturation in the SVEET context that corresponds to the field site conditions. This result can be calculated using the single formula from Equation B.10, as follows.

$$s_w^a = \frac{0.3 - \left[ \frac{\left(0.38 - \frac{0.08 \cdot 1.64}{0.9982}\right)^{10/3} (0.3)^2}{(0.38)^2} \right]^{3/10}}{0.3} = 0.281 = effective\ S_r$$

For comparison, if user-specified porosity and bulk density values were not used (i.e., the SVEET base case values of those variables were applied), the site moisture content for this example (0.08) would equate to the following $S_r$ value.

$$S_r = \frac{0.08 \cdot 1.855}{0.3 \cdot 0.9982} = 0.496$$

## References

Ho, C.K., and S.W. Webb. 2006. *Gas Transport in Porous Media*. Springer, Dordrecht, The Netherlands.

# Appendix C

# Monte-Carlo Sample Size Analysis

To determine the appropriate sample size for the Monte-Carlo (MC) analysis, sets of realizations multiple sample sizes (*n* =100 to 5,000) were used for one test case (PCE groundwater concentrations at monitoring well MW-235 at McClellan IC 1). The MC simulation outputs for each sample size are provided in Figures C-1 and C-2. The MC output (i.e., mean, median, standard deviation) stabilizes around *n* = 2,200. However, to ensure output stability, 2,500 MC simulations were run for each SVEET2 case.

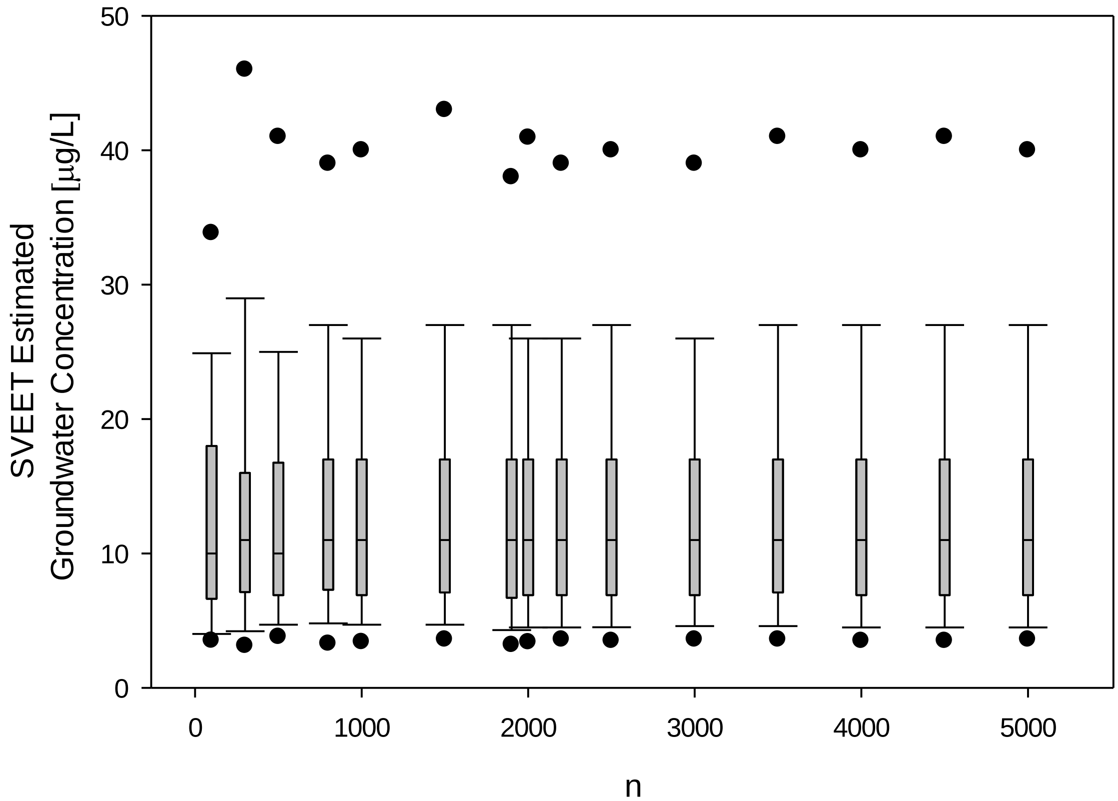


***Figure C-1.*** *Sample size analysis for Monte-Carlo realizations. Boxes indicate the 25$^{th}$ and 75$^{th}$ percentiles, whiskers the 10$^{th}$ and 90$^{th}$ percentiles, dots the 5$^{th}$ and 95$^{th}$ percentiles, and the line is the median value of the dataset.*

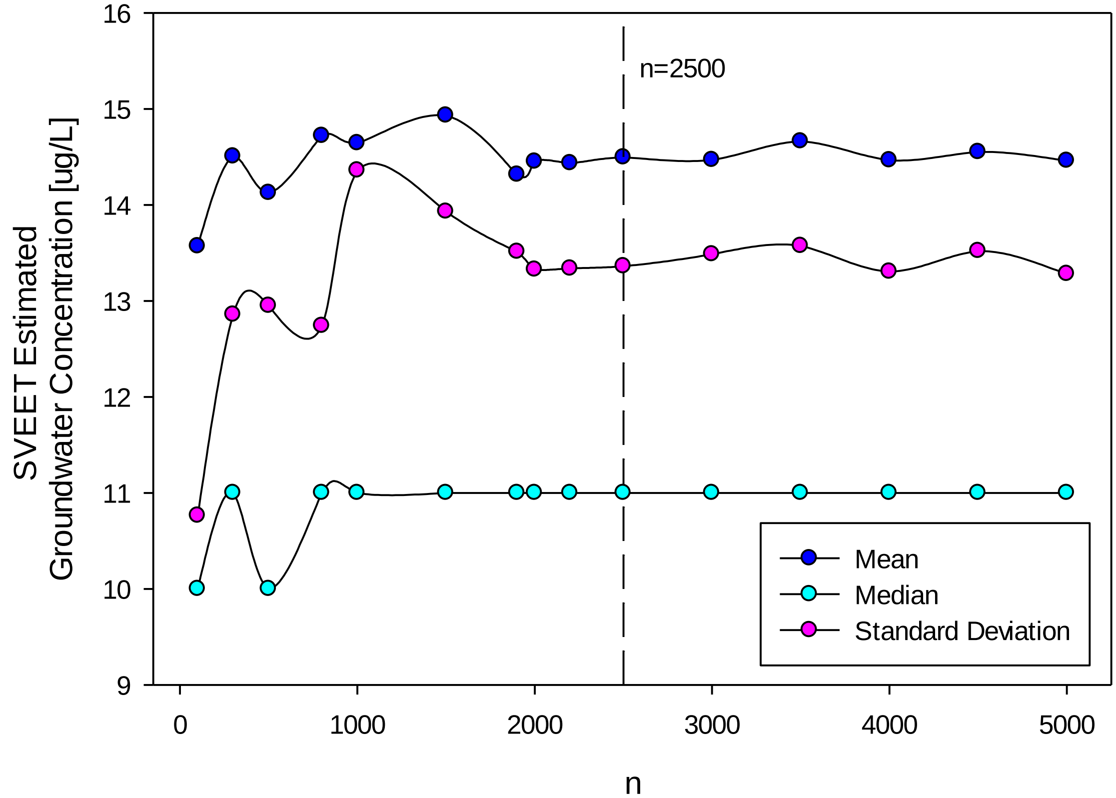


***Figure C-2***. *Sample Size Analysis for Monte-Carlo Realizations.*

# Appendix D

# SVEET2 Ground-truthing Inputs

## D.1 McClellan IC 1

The inputs, and corresponding outputs, of the SVEET2 scenarios for McClellan IC 1 at groundwater monitoring wells MW-235, MW-364 and MW-366 are detailed in tables below. The majority of the site and source area input parameters for McClellan IC-1 are relevant for all three groundwater monitoring wells (Table D-1). The distance to each groundwater well location (*d*) and the measured PCE concentrations ($C_{gw}$) are the only parameters specific to each groundwater monitoring well. When site information was insufficient to estimate uncertainty of an individual parameter, ±15% error was applied to the most likely parameter value as the minimum and maximum inputs.

***Table D-1.*** *SVEET2 Inputs for Estimating PCE Groundwater Concentrations at McClellan IC 1*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely | Relative Uncertainty* |
|---|---|---|---|---|---|---|
| Contaminant | | | | PCE | | |
| Subsurface Temperature | $T$ | °C | 17 | 23 | 20 | 26% |
| Avg. Recharge | $R$ | cm/yr | 0.23 | 15 | 7.13 | 98% |
| Avg. Moisture Content | $\omega$ | wt % | 5 | 14 | 14 | 64% |
| Total Porosity | $\Theta_{total}$ | - | 0.2 | 0.5 | 0.3 | 60% |
| Dry Bulk Density | $\rho_b$ | g/mL | 1.4 | 1.8 | 1.6 | 22% |
| Vadose Zone Thickness | $VZT$ | m | 26.8 | 32.8 | 31.5 | 18% |
| Depth to Top of Source | $L_1$ | m | 2.3 | 5.7 | 3.1 | 60% |
| Source Thickness | $z$ | m | 3.9 | 30.8 | 4.6 | 87% |
| Source Width | $w$ | m | 14.2 | 72.4 | 23.2 | 80% |
| Groundwater Darcy Velocity | $q$ | m/day | 0.01 | 0.1 | 0.02 | 90% |
| Compliance Well Screen Length | $s$ | m | | 3.05 | | 0% |
| Source Gas Concentration | $C_{gs}$ | ppmv | 3.72 | 9.02 | 7.86 | 59% |

* Relative uncertainty is computed as:
Red (high, > 75% ), yellow (intermediate, 25 - 75%), and green (low, < 25%) coloring indicates the level of associated uncertainty for each input parameter. Gray shading indicates there was not enough data available to estimate parameter uncertainty.

## D.2 McClellan IC 19

The inputs, and corresponding outputs, of the SVEET2 scenarios for McClellan IC 19 at groundwater monitoring wells MW-354, EW-379 and MW-355 are detailed in Tables D-2 through D-6. Many of the site input parameters for McClellan IC 19 are relevant for both source areas and individual groundwater monitoring wells. Based on the site data, two potential source areas were identified. Source Area A was assumed to only contain PCE, whereas Source Area B was identified to contain PCE, TCE, and 1-1 DCE. While PCE is measured in the Source Area B, it is not the main component of the soil gas contamination. Based on site maps, groundwater monitoring well MW-354 is located approximately 101 ft (30.4 m) downgradient of Source Area A and 75 ft (22.9 m) laterally off the flow path. MW-354 is screened between 104 and 114 ft (31.7 to 34.7 m) bgs. Two groundwater monitoring wells are located within the vicinity of Source Area B: EW-379 and MW-355. EW-379 is estimated to be 300 ft (91.4 m) directly downgradient from Source Area B and is screened from 102 to 132 ft (31 to 41.2 m) bgs. MW-355 is slightly off the flow path and is located 213 ft (65 m) downgradient and approximately 70 ft (21.3 m) off the flow path centerline. MW-355 is screened between 93.5 and 113.5 ft (28.5 and 34.6 m) bgs.

SVEET2 analyses were completed for each scenario to account for potential site uncertainty, specifically related to the source area and strength parameters. The source area parameters in each scenario include the depth to the top of source ($L_1$), source thickness ($z$), source width ($w$) and soil strength ($C_{gs}$). The distance to each groundwater well location ($d$) and the measured PCE, TCE and 1,1-DCE concentrations ($C_{gw}$) are only parameters specific to each groundwater monitoring well. When site information was insufficient to estimate uncertainty of an individual parameter, ±15% error was applied to the most likely parameter value as the minimum and maximum inputs.

***Table D-2.*** *SVEET2 Inputs for Estimating PCE, TCE, and 1-1 DCE, Groundwater Concentrations at McClellan IC 19*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely | Relative Uncertainty* |
|---|---|---|---|---|---|---|
| Subsurface Temperature | $T$ | °C | 17 | 23 | 20 | 26% |
| Avg. Recharge | $R$ | cm/yr | 0.16 | 0.71 | 0.4 | 77% |
| Avg. Moisture Content | $\omega$ | wt % | 5 | 14 | 14 | 64% |
| Total Porosity | $\Theta_{total}$ | - | 0.3 | 0.5 | 0.3 | 40% |
| Dry Bulk Density | $\rho_b$ | g/mL | 1.4 | 1.6 | 1.6 | 13% |
| Groundwater Darcy Velocity | $q$ | m/day | 0.002 | 0.009 | 0.005 | 80% |
| Vadose Zone Thickness | $VZT$ | m | 28.5 | 38.5 | 33.5 | unknown |

* Relative uncertainty is computed as:
Red (high, > 75% ), yellow (intermediate, 25 - 75%), and green (low, < 25%) coloring indicates the level of associated uncertainty for each input parameter.
Blue shading indicates available site data was insufficient to estimate parameter uncertainty. ±15% uncertainty applied to obtain the listed minimum and maximum values.

***Table D-3.** SVEET2 Inputs for Estimating the PCE Source Area A at McClellan IC 19*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely |
|---|---|---|---|---|---|
| Contaminant | | | | PCE | |
| Depth to Top of Source | $L_1$ | m | 7.7 | 10.4 | 9 |
| Source Thickness | $z$ | m | 14.2 | 19.3 | 16.75 |
| Source Width | $w$ | m | 25.5 | 34.5 | 30 |
| Source Gas Concentration | $C_{gs}$ | ppmv | 7.8 | 15 | 11.70 |
| Blue shading indicates available site data was insufficient to estimate parameter uncertainty. ±15% uncertainty applied to obtain the listed minimum and maximum values | | | | | |

***Table D-4.** SVEET2 Inputs for Estimating the PCE Source Area B at McClellan IC 19.*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely |
|---|---|---|---|---|---|
| Contaminant | | | | PCE | |
| Depth to Top of Source | $L_1$ | m | 1.7 | 2.3 | 2 |
| Source Thickness | $z$ | m | 14.2 | 19.3 | 16.75 |
| Source Width | $w$ | m | 31.5 | 42.6 | 37 |
| Source Gas Concentration | $C_{gs}$ | ppmv | 1.2 | 1.6 | 1.4 |
| Blue shading indicates available site data was insufficient to estimate parameter uncertainty. ±15% uncertainty applied to obtain the listed minimum and maximum values | | | | | |

***Table D-5.** SVEET2 Inputs for Estimating the TCE Source Area B at McClellan IC 19.*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely |
|---|---|---|---|---|---|
| Contaminant | | | | TCE | |
| Depth to Top of Source | $L_1$ | m | 1.7 | 2.3 | 2 |
| Source Thickness | $z$ | m | 14.2 | 19.3 | 16.75 |
| Source Width | $w$ | m | 31.5 | 42.6 | 37 |
| Source Gas Concentration | $C_{gs}$ | ppmv | 306 | 414 | 360 |
| Blue shading indicates available site data was insufficient to estimate parameter uncertainty. ±15% uncertainty applied to obtain the listed minimum and maximum values | | | | | |

***Table D-6.*** *SVEET2 Inputs for Estimating the 1-1 DCE Source Area B at McClellan IC 19.*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely |
|---|---|---|---|---|---|
| Contaminant | | | | 1,1 DCE | |
| Depth to Top of Source | $L_1$ | m | 1.7 | 2.3 | 2 |
| Source Thickness | $z$ | m | 14.2 | 19.3 | 16.75 |
| Source Width | $w$ | m | 31.5 | 42.6 | 37 |
| Source Gas Concentration | $C_{gs}$ | ppmv | 80 | 96 | 94 |
| Blue shading indicates available site data was insufficient to estimate parameter uncertainty. ±15% uncertainty applied to obtain the listed minimum and maximum values | | | | | |

## D.3 CRREL

The inputs, and corresponding outputs, of the SVEET2 scenarios for TCE groundwater concentrations at CRREL's groundwater monitoring well MW 14-107, and TCE vapor concentrations at the Multipurpose room as the result of source area AOC 2 are detailed in Table D-7. When site information was insufficient to estimate uncertainty of an individual parameter, ±15% error was applied to the most likely parameter value as the minimum and maximum inputs.

Based on various site documents, it was assumed that MW 14-107 was located approximately 24 m directly downgradient from source area AOC2 (Table D-8). Through conversations with site personnel, it was noted that the maximum allowable average recharge in SVEET may not be high enough for this site. The maximum average recharge is 15 cm/yr, and the maximum average recharge was set to this upper bound in the various scenarios.

The Multipurpose room was estimated to be located roughly 6.3 m, 23 m, and 4 m (dy, dx, dz) from source area AOC 2. ±15% error was applied to the most likely parameter value for dy and dz as the minimum and maximum inputs (Table D-9).

***Table D-7.** SVEET2 Inputs for Estimating TCE Groundwater and Soil Vapor Concentrations for CRREL AOC 2*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely | Relative Uncertainty* |
|---|---|---|---|---|---|---|
| Contaminant | | | | TCE | | |
| Subsurface Temperature | $T$ | °C | 10 | 13.9 | 10 | 28% |
| Avg. Recharge | $R$ | cm/yr | 1 | 12.7 | 5 | 92% |
| Avg. Moisture Content | $\omega$ | wt % | 9 | 11 | 11 | 18% |
| Total Porosity | $\Theta_{total}$ | - | 0.25 | 0.35 | 0.3 | 29% |
| Dry Bulk Density | $\rho_b$ | g/mL | 1.72 | 1.9 | 1.85 | 9% |
| Vadose Zone Thickness | $VZT$ | m | 24.4 | 41.1 | 41.1 | 41% |
| Depth to Top of Source | $L_1$ | m | 1.5 | 7.6 | 3.0 | 80% |
| Source Thickness | $z$ | m | 10.7 | 22.9 | 10.7 | 53% |
| Source Width | $w$ | m | 15.2 | 17.4 | 15.2 | 13% |
| Groundwater Darcy Velocity | $q$ | m/day | | | 0.05 | |
| Source Gas Concentration | $C_{gs}$ | ppmv | 68 | 4854 | 1855 | 99% |

* Relative uncertainty is computed as:
Red (high, > 75% ), yellow (intermediate, 25 - 75%), and green (low, < 25%) coloring indicates the level of associated uncertainty for each input parameter. Gray shading indicates there was not enough data available to estimate parameter uncertainty.

**Table D-8.** Groundwater well specific SVEET2 Inputs for Estimating Impacts from CRREL AOC 2

| Groundwater Well | Parameter | Symbol | Units | Most Likely |
|---|---|---|---|---|
| MW 14-107 | Distance to compliance well | $d$ | m | 24.4 |
| | Compliance Well Screen Length | $s$ | m | 3.0 |
| | TCE groundwater concentration at monitoring location | $C_{gw}$ | µg/L | 22,961 |

**Table D-9.** Vapor intrusion monitoring location specific SVEET2 Inputs for Estimating Impacts from CRREL AOC 2

| Vapor Monitoring Location | Parameter | Symbol | Units | Most Likely |
|---|---|---|---|---|
| Multipurpose Room | Longitudinal Distance for Soil Gas | $dy$ | m | 6.3 |
| | Transverse Distance for Soil Gas | $dx$ | m | 23 |
| | Depth of Basement/Foundation | $dz$ | m | 4 |
| | TCE vapor concentration at monitoring location | $VI$ | ppmv | 20,127 |

## D.4 Mather

The inputs, and corresponding outputs, of the SVEET2 scenarios for Mather Site 23C at groundwater monitoring well MAFB-341 are detailed in Table D-10. When site information was insufficient to estimate uncertainty of an individual parameter, ±15% error was applied to the most likely parameter value as the minimum and maximum inputs. Based on site documents and maps, MAFB-341 was estimated to be 91 m downgradient and 53 m laterally from the source area associated with Site 23 C former Bldg. 2587 (Table D-11). Site data indicated a large range in soil gas concentrations in this source area (e.g., from 27 to 260 ppmv), creating uncertainty around both the actual dimensions of the source area, as well as a representative value for soil gas concentrations. The wide range in SVEET estimates stems from the uncertainty related to the source area.

***Table D-10.*** *SVEET2 Inputs for Estimating PCE Groundwater Concentrations at Mather Site 23C*

| Parameter | Symbol | Units | Minimum | Maximum | Most Likely | Relative Uncertainty* |
|---|---|---|---|---|---|---|
| Contaminant | | | PCE | | | |
| Subsurface Temperature | $T$ | °C | 17 | 20 | 18.9 | 15% |
| Avg. Recharge | $R$ | cm/yr | 0.96 | 2.28 | 1.63 | 58% |
| Avg. Moisture Content | $\omega$ | wt % | 9.17 | 10.14 | 9.69 | 10% |
| Total Porosity | $\Theta_{total}$ | - | 0.27 | 0.54 | 0.46 | 50% |
| Dry Bulk Density | $\rho_b$ | g/mL | 1.21 | 1.72 | 1.50 | 30% |
| Vadose Zone Thickness | $VZT$ | m | 29.0 | 29.9 | 29.6 | 3% |
| Depth to Top of Source | $L_1$ | m | 1.31 | 9.14 | 7.62 | 86% |
| Source Thickness | $z$ | m | 6.10 | 16.76 | 12.19 | 64% |
| Source Width | $w$ | m | 30.55 | 62.31 | 39.77 | 51% |
| Groundwater Darcy Velocity | $q$ | m/day | | | 0.10 | |
| Source Gas Concentration | $C_{gs}$ | ppmv | 27.07 | 260.0 | 42.74 | 90% |

* Relative uncertainty is computed as:
Red (high, > 75% ), yellow (intermediate, 25 - 75%), and green (low, < 25%) coloring indicates the level of associated uncertainty for each input parameter. Gray shading indicates there was not enough data available to estimate parameter uncertainty.

***Table D-11.*** *Groundwater well specific SVEET2 Inputs for Estimating Impacts from Mather Site 23C*

| Groundwater Well | Parameter | Symbol | Units | Minimum | Maximum | Most Likely |
|---|---|---|---|---|---|---|
| MAFB-341 | Distance to compliance well (downgradient) | *d* | m | 103.6 | 140.2 | 122 |
| | Distance to compliance well (laterally) | — | m | 45 | 61 | 53 |
| | Compliance Well Screen Length | *s* | m | | | 5.0 |
| | Compliance Well Screen Interval | — | m bgs | | | 2.4 – 3.0 |
| | PCE groundwater concentration at monitoring location | $C_{gw}$ | µg/L | | | 0.16 |

Blue shading indicates available site data was insufficient to estimate parameter uncertainty. ±15% uncertainty applied to obtain the listed minimum and maximum values.

# Appendix E

# Summary of SVEET2 User Feedback

***Table E-1.** Summary of User Feedback Survey Responses*

| Survey Question | Site: CRREL | Site: Tooele | Site: McClellan & Mather | Site: Hill- Landfill 5 |
|---|---|---|---|---|
| SCENARIOS | | | | |
| 1. What type of SVEET2 estimation scenarios did you run? | Ground truthing to site groundwater concentrations; Ground truthing to site vapor concentrations at nearby building (sub-slab) | Determining the stopping point for active SVE | Ground truthing to site groundwater concentrations | Determining the stopping point for active SVE or other source treatment operations |
| 2. What was the end use of the scenarios? | | Assessing if SVE systems could be turned off based on achieving concentrations that are protective of site groundwater cleanup levels | | Scoping calculations for considering options |
| 3. What comparisons did you use in your scenarios? | Comparison to existing groundwater well data. Comparison to existing vapor concentrations. | Comparison to site cleanup levels (MCLs) at a specific receptor location. | Comparison to existing groundwater well data | Comparison to existing groundwater well data |
| SVEET2 INPUTS | | | | |
| 1. Were certain input parameters challenging to define for your site? If so, which ones? | No | Yes. Source zone geometry was difficult to define. Hard to determine where the source ended and where the distributed contamination begins. User guidance could be useful on how to define the source zone and different approaches. | Yes. Source zone geometry. Estimating recharge through a thick vadose zone (100 ft deep). | No. |
| 2. Did you need to use professional judgement when determining the inputs? If so, for what parameters? | No | Yes. Source zone geometry | Yes. Source zone geometry. Estimating recharge through a thick vadose zone (100 ft deep). | Yes. Soil moisture, bulk density, and porosity |

| | Site | | | |
|---|---|---|---|---|
| **Survey Question** | **CRREL** | **Tooele** | **McClellan & Mather** | **Hill- Landfill 5** |
| 3. Did any of your site values fall outside of the acceptable input parameter range of SVEET2? If so, what parameters? | Yes. Recharge (site value of ~ 30 cm/yr exceeds SVEET2 input max of 15 cm/yr) | No | No. | Yes. Source thickness and groundwater velocity were below the minimum SVEET2 values |
| 4. How did you define the source strength parameters (concentration or mass discharge)? | Soil gas concentration | Soil gas concentration | Soil gas concentration | Soil gas concentration |
| 5. What type of data did you use to determine source strength parameters? | Soil gas database | Site monitoring data with regular sampling of SVE wells and vapor monitoring | Site monitoring data | Soil gas concentration collected from site vent wells |
| 6. Did you conduct multiple calculations for ranges of input parameters or just use a single set of parameters? | Multiple. To assess sensitivity. | Multiple. To assess uncertainty of input parameters | Multiple. To assess sensitivity. | Single set of inputs |
| 7. How did you define or assess if/when your site was at equilibrium conditions? | Used data before and after extended SVE pilot testing to ensure site was at equilibrium | Used values from end of rebound period | Defined soil gas equilibrium to be when monthly PID or soil gas concentrations are within 50% of each other for 2 or more consecutive months. | N/A |
| | | GENERAL | | |
| 1. Did you find SVEET2 to be applicable and helpful for your site? | Yes. Would be highly applicable earlier in the site progress. | | No, because sites had already been closed using VLEACH. But did see the potential for SVEET2 to be used instead of VLEACH calculations. Also, interested in using SVEET2 for vapor intrusion estimations. | No |

| | Site | | | |
|---|---|---|---|---|
| **Survey Question** | **CRREL** | **Tooele** | **McClellan & Mather** | **Hill- Landfill 5** |
| 2. Was the SVEET2 documentation sufficient for use of the tool? | No. Felt there was limited user documentation available. | | | Yes |
| 3. Was the SVEET2 documentation sufficient for communication of the results to the project team, regulators, and other stakeholders? | | | | Yes |
| 4. Do you have any other feedback? | Yes. Prefer if gas concentrations were always in the same units (e.g., ppmv or ppbv) | | | None |

# Appendix F

# SVEET2 User Feedback Survey

Below is the user feedback survey form that was provided to all the sites to elicit feedback on SVEET.

**SVEET Beta-Testing User Feedback**

**Thank you for testing SVEET2!**
Please consider the following questions when providing feedback on the use of the beta version of the SVEET2 software.
**Scenarios:**

1. What type of SVEET estimation scenarios did you run?
    a. Determining the stopping point for active SVE or other source treatment operations?
    b. Setting performance requirements for optimization of an SVE system or other type of source treatment?
    c. Determining whether active source remediation was necessary?
2. What was the end use of the scenarios?
    a. Scoping calculations for considering options?
    b. Compiling direct technical support for remedy operations or a remedy decision
3. What comparisons did you use in your scenarios?
    a. Groundwater concentrations?
        i. For comparison to an existing monitoring well?
        ii. To calculate groundwater concentrations at a specific receptor location?
        iii. To calculate groundwater concentrations at selected locations as part of a planning or scoping effort?
        iv. Other?
    b. Vapor concentrations?
        i. For comparison to an existing monitoring location?
        ii. To assess potential for vapor intrusion?
        iii. To calculate vapor concentrations at selected locations as part of a planning or scoping effort?
        iv. Other?

**SVEET2 Inputs:**

1. Were certain input parameters challenging to define for your site? If so, which ones?
2. Did you need to use professional judgement when determining the inputs? If so, for what parameters?
3. Did any of your site values fall outside of the acceptable input parameter range of SVEET? If so, what parameters?
4. How did you define the source strength parameters (concentration or mass discharge)?
5. What type of data did you use to determine source strength parameters?

6. Did you conduct multiple calculations for ranges of input parameters or just use a single set of parameters?
7. How did you define or assess if/when your site was at equilibrium conditions?

**Software:**

1. Was SVEET user friendly?
2. Did you experience any errors or bugs when using SVEET?
3. Any user interface suggestions?

**General:**

1. Did you find SVEET to be applicable and helpful for your site?
2. Was the SVEET documentation sufficient for use of the tool?
3. Was the SVEET documentation sufficient for communication of the results to the project team, regulators, and other stakeholders?
4. Do you have any other feedback?