Appendix B. Summary of Tools For Site Characterization

Table 22 summarizes potential tools to support site characterization and evaluation. Only limited number of characterization tools are provided in Table 22 because these have been compiled in other ITRC resources. Relevant tools for characterization and evaluation information can be found in the following ITRC documents (itrcweb.org). In particular, the *Integrated DNAPL Site Characterization and Tools Selection* (ITRC 2015b) provides a useful compilation of relevant tools and is a recommended resource for characterization tools. Table 22 provides additional information for evaluation tools compiled from team input.

- *Integrated DNAPL Site Characterization and Tools Selection (ISC-1)*
- *Use and Measurement of Mass Flux and Mass Discharge (MASSFLUX-1)*
- *The Use of Direct-push Well Technology for Long-term Environmental Monitoring in Groundwater Investigations (SCM-2)*
- *Environmental Molecular Diagnostics Fact Sheets (EMD-1)*
- *EMD – New Site Characterization and Remediation Enhancement Tools (EMD-2)*
- *Groundwater Statistics and Monitoring Compliance Website (GSMC-1)*
- *Incremental Sampling Methodology (ISM-1)*
- *User's Guide for Polyethylene-Based Passive Diffusion Bag Samplers to Obtain Volatile Organic Compound Concentrations in Wells (DSP-1)*
- *Technical and Regulatory Guidance for Using Polyethylene Diffusion Bag Samplers to Monitor Volatile Organic Compounds in Groundwater (DSP-3)*
- *Technology Overview of Passive Sampler Technologies (DSP-4*
- *Protocol for Use of Five Passive Samplers to Sample for a Variety of Contaminants in Groundwater (DSP-5)*
- *Decision Making at Contaminated Sites: Issues and Options in Human Health Risk Assessment (RISK-3)*
- *Incorporating Bioavailability Considerations into the Evaluation of Contaminated Sediment Sites Website (CS-1)*
- *Technical and Regulatory Guidance for the Triad Approach: A New Paradigm for Environmental Project Management (SCM-1)*
- *Triad Implementation Guide (SCM-3)*
- *Vapor Intrusion Pathway: A Practical Guideline (VI-1)*
- *Vapor Intrusion Pathway: Investigative Approaches for Typical Scenarios (A Supplement to VI-1)*

Table 22. Compilation of Potential Tools to Support Site Characterization and Evaluation

Tool	Description	Link/Reference
Characterization Tools		
High Resolution Characterization	Multiple characterization tools	https://www.serdp-estcp.org/Tools-and-Training/Environmental-Restoration
MAROS	Tool to assist in monitoring network optimization	http://www.gsi-net.com/en/software/free-software.html
3TMO	The 3-Tiered Monitoring Optimization Tool (3TMO) is a long-term monitoring optimization (LTMO) decision support tool.	Nobel, C. and Anthony, J.A. 2004. "Three-Tiered Approach to Long-Term Monitoring Program Optimization." *Bioremediation Journal* 8 (3-4): 147-165.
Visual Sampling Plan (VSP)	Tool for guiding sampling design with consideration of statistical analyses.	http://vsp.pnnl.gov/
Evaluation Tools		
Risk		
GOLDSIM	GoldSim simulation software allows you to model complex, real-world multimedia environmental systems and assess the risk of those environmental systems.	http://www.goldsim.com/Home/
RESRAD	The RESRAD has been widely used in the US and internationally for calculating doses and risks from exposure to radioactively contaminated soils.	http://web.evs.anl.gov/resrad/
GWSCREEN	GWSCREEN was developed for assessment of the groundwater pathway from leaching of radioactive and nonradioactive substances from surface or buried sources and release to percolation ponds.	https://www.osti.gov/scitech/servlets/purl/10176916 Rood, AS. 2003. *GWSCREEN: A Semi-Analytical Model for Assessment of the Groundwater Pathway from Surface or Buried Contamination, Theory and User's Manual, Version 2.5*. INEEL/EXT-98-00750 Rev 1b, Idaho National Laboratory.

Tool	Description	Link/Reference
CAP88	The CAP88 (Clean Air Act Assessment Package – 1988) computer model is a set of computer programs, databases and associated utility programs for estimation of dose and risk from radionuclide emissions to air.	https://www.epa.gov/radiation/cap-88-pc
@RISK	@RISK is a spreadsheet based tool to perform risk analysis using Monte Carlo Simulation. It also has optimization tools. It is designed to analyze risk and uncertainty in a wide variety of industries, including groundwater remediation.	http://www.palisade.com/risk/ Byrd III, Daniel and C. Richard Cothern, "Introduction to Risk Analysis: A Systematic Approach to Science Based Decision Making, "Government Institutes Publishing, August 2000 (ISBN 0865876967)
Flow and Transport Models		
MODFLOW	MODFLOW is a three-dimensional (3D) finite-difference groundwater flow model. MODFLOW is considered an international standard for simulating and predicting groundwater conditions and groundwater/surface-water interactions.	http://water.usgs.gov/ogw/modflow/ http://pubs.usgs.gov/tm/2005/tm6A16/PDF/TM6A16.pdf
MT3D codes	Numerical modeling tool for transport assessment using MODFLOW for the groundwater flow component. There are a number of subsidiary codes (such as RT3D, SEAM3D, PHT3D, and SEAWAT) and graphical user interfaces available.	https://water.usgs.gov/ogw/modflow/index.html http://bioprocess.pnnl.gov/ https://water.usgs.gov/ogw/mt3d-usgs/ https://water.usgs.gov/ogw/seawat/
RT3D guides and RTFlux	Numerical modeling tool that enables customized reaction processes. Includes a tool to extract flux data from the numerical simulations. Primarily targeted at chlorinated solvent sites, but applicable to other contaminants.	http://bioprocess.pnnl.gov/
REMCHLOR, BIOCHLOR, BIOSCREEN, FOOTPRINT, REMFUEL	Screening-level transport models	https://www.epa.gov/water-research/remediation-evaluation-model-chlorinated-solvents-remchlor https://www.epa.gov/water-research/biochlor-natural-attenuation-decision-support-system https://www.epa.gov/water-research/bioscreen-natural-attenuation-decision-support-system https://www.epa.gov/water-research/footprint-screening-model-estimating-area-plume-produced-gasoline-containing-ethanol https://www.epa.gov/water-research/remediation-evaluation-model-fuel-hydrocarbons-remfuel
PREMChlor	PREMChlor is developed by linking the analytical model REMChlor to a Monte Carlo modeling package GoldSimTM via a FORTRAN Dynamic Link Library (DLL) application. REMChlor, or Remediation Evaluation Model for Chlorinated Solvents, is an analytical solution for simulating the transient effects of groundwater source and plume remediation. In the analytical method, the contaminant source model is based on a power-function relationship between source mass and source discharge, and it can consider partial source remediation at any time after the initial release. The source model serves as a time dependent, mass-flux boundary condition to the analytical plume model, where flow is assumed to be one dimensional. The plume model simulates first-order sequential decay and production of several species, and the decay rates and parent/daughter yield coefficients are variable functions of time and distance. This approach allows for flexible simulation of enhanced plume degradation that may be temporary, limited in space, and have different effects on different contaminant species in the decay chain. Health risks posed by carcinogenic species in the plume are calculated that the contaminated water is used in a house for drinking, bathing, and other household activities.	https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Persistent-Contamination/ER-200704
STOMP	STOMP is a multiphase computer model with capabilities to address a variety of subsurface environments, including nonisothermal conditions, fractured media, multiplephase systems, nonwetting fluid entrapment, soil freezing conditions, nonaqueous phase liquids, first-order chemical reactions, radioactive decay, solute transport, dense brines, non-equilibrium dissolution, and surfactant-enhanced dissolution and mobilization of organics	http://stomp.pnnl.gov/
TOUGH	The TOUGH ("Transport of Unsaturated Groundwater and Heat") suite of software codes are multidimensional numerical models for simulating the coupled transport of water, vapor, noncondensible gas, and heat in porous and fractured media. Has been used for applications to nuclear waste disposal, environmental remediation problems, energy production from geothermal, oil and gas reservoirs as well as gas hydrate deposits, geological carbon sequestration, vadose zone hydrology, and other uses that involve coupled thermal, hydrological, geochemical, and mechanical processes in permeable media.	http://esd.lbl.gov/research/projects/tough/
HYDRUS	HYDRUS is a Microsoft Windows based modeling environment for the analysis of water flow and solute transport in variably saturated porous media.	http://www.pc-progress.com/en/Default.aspx?h3d-ver2

Tool	Description	Link/Reference
PORFLOW	PORFLOW is a comprehensive tool to accurately solve problems involving transient or steady state fluid flow, heat, salinity and mass transport in multiphase, variably saturated, porous or fractured media with dynamic phase change. The porous/fractured media may be anisotropic and heterogeneous, arbitrary sources (injection or pumping wells) may be present and, chemical reactions or radioactive decay may take place. It accommodates alternate fluid and media property relations and complex and arbitrary boundary conditions. The geometry may be 2D or 3D, Cartesian or Cylindrical and the mesh may be structured or unstructured, giving maximum flexibility to the user	http://www.acricfd.com/software/porflow/
FEHM	The primary use of FEHM over several years was to assist in the understanding of flow fields and mass transport in the saturated and unsaturated zones below the potential Yucca Mountain repository. Today FEHM is used to simulate groundwater and contaminant flow and transport in deep and shallow, fractured and un-fractured porous media throughout the US DOE complex. The numerical method used in FEHM is the control volume method (CV) for fluid flow and heat transfer equations which allows FEHM to exactly enforce energy/mass conservation; while an option is available to use the finite element (FE) method for displacement equations to obtain more accurate stress calculations. In addition to these standard methods, an option to use FE for flow is available, as well as a simple Finite Difference scheme.	https://fehm.lanl.gov/pdfs/fehm_umV3.pdf
Advanced Simulation Capability for Environmental Management (ASCEM)	Department of Energy simulator/toolset and user interface. It includes a set of tools to support decision making including: data management and analysis, model setup, simulation and evaluation and visualization of results and decision support.	http://esd.lbl.gov/research/projects/ascem/ascemdoe.org
Uncertainty		
R	R provides a wide variety of statistical (linear and nonlinear modelling, classical statistical tests, time-series analysis, classification, clustering) and graphical techniques, and is highly extensible. The S language is often the vehicle of choice for research in statistical methodology, and R provides an Open Source route to participation in that activity.	
PSUADE	PSUADE is an acronym for Problem Solving Environment for Uncertainty Analysis and Design Exploration. It is a software toolkit to facilitate Uncertainty Quantification. PSUADE has a rich set of tools for performing uncertainty analysis, global sensitivity analysis, design optimization, model calibration, etc. PSUADE supports a global sensitivity methodology for models with large number of parameters and complex constraints. PSUADE includes sampling methods, a simulator execution environment, and many different statistical analysis tools.	http://computation.llnl.gov/casc/uncertainty_quantification/
DAKOTA	The DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) toolkit provides a flexible, extensible interface between analysis codes and iterative systems analysis methods. DAKOTA contains algorithms for: • optimization with gradient and non-gradient-based methods; • uncertainty quantification with sampling, reliability, stochastic expansion, and epistemic methods; • parameter estimation with nonlinear least squares methods; and • sensitivity/variance analysis with design of experiments and parameter study methods. These capabilities may be used on their own or as components within advanced strategies such as hybrid optimization, surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty.	https://dakota.sandia.gov/

Tool	Description	Link/Reference
PEST	PEST implements parameter estimation based on the use of only a few parameters, as well as highly parameterized, regularized inversion based on the use of hundreds (or even thousands) of parameters. It implements both linear and nonlinear uncertainty analysis, including its unique, efficient and powerful "null-space Monte Carlo" methodology for rapid generation of many different calibration-constrained parameter fields. PEST provides three options for nonlinear uncertainty analysis: 1. Predictive maximization/minimization 2. "Predictive calibration" 3. Calibration-constrained Monte-Carlo analysis. The last of these is achieved through PEST's unique, and extremely powerful, null space Monte Carlo technique.	http://www.pesthomepage.org/Home.php
UCODE	UCODE_2005 and six post-processors are included. These programs can be used with existing process models to perform sensitivity analysis, data needs assessment, calibration, prediction, and uncertainty analysis. Any process model or set of models can be used; the only requirements are that models have numerical (ASCII or text only) input and output files, that the numbers in these files have sufficient significant digits, that all required models can be run from a single batch file or script, and that simulated values are continuous functions of the parameter values.	http://igwmc.mines.edu/freeware/ucode/?CMSPAGE=igwmc/freeware/ucode/
Visualization		
ParaView	ParaView is an open-source, multiplatform data analysis and visualization application. ParaView users can quickly build visualizations to analyze their data using qualitative and quantitative techniques. The data exploration can be done interactively in 3D or programmatically using ParaView's batch processing capabilities. ParaView was developed to analyze extremely large data sets using distributed memory computing resources. It can be run on supercomputers to analyze data sets of exascale size as well as on laptops for smaller data.	http://www.paraview.org/
VisIt	VisIt is an open source, interactive, scalable, visualization, animation and analysis tool. From Unix, Windows or Mac workstations, users can interactively visualize and analyze data ranging in scale from small (<101 core) desktop-sized projects to large (>105 core) leadership-class computing facility simulation campaigns. Users can quickly generate visualizations, animate them through time, manipulate them with a variety of operators and mathematical expressions, and save the resulting images and animations for presentations. VisIt contains a rich set of visualization features to enable users to view a wide variety of data including scalar and vector fields defined on two- and three-dimensional (2D and 3D) structured, adaptive and unstructured meshes. Owing to its customizable plugin design, VisIt is capable of visualizing data from over 120 different scientific data formats.	https://wci.llnl.gov/simulation/computer-codes/visit
Tecplot	Tecplot 360 is numerical simulation software package used in post-processing and visualization of simulation results. Capabilities include calculating grid quantities (such as aspect ratios, skewness, orthogonality, and stretch factors), normalizing data, verifying solution convergence, interactively exploring data through cut planes, iso-surfaces, and particle paths. Tecplot also supports data import from a wide variety of data formats.	http://www.tecplot.com/

Tool	Description	Link/Reference
Grapher, Surfer and other tools	Grapher is a multipurpose visualization tool capable of producing more than 60 types of graphs. Create 2D or 3D line, scatter, function, class scatter, bubble, step, vector, bar charts, and floating bar chart graphs. Create line, scatter, class scatter, vector, bar, rose, wind, and radar polar plots. Create line, scatter, class scatter, or bubble ternary diagrams. Display high-low-close, candlestick, or stiff diagram specialty plots. Create statistical graphs including box-whisker plots, 2D and 3D histograms, 2D and 3D pie charts, 2D and 3D doughnut plots, Q-Q plots, and normal Q-Q plots. Alter any portion of the graph, axes, or plot for complete control of your display. Surfer is a full-function 3D visualization, contouring and surface modeling package that runs under Microsoft Windows. Surfer is used extensively for terrain modeling, bathymetric modeling, landscape visualization, surface analysis, contour mapping, watershed and 3D surface mapping, gridding, volumetrics, and much more. Golden Software also produces other visualization tools that are described in the brochure at the link below.	http://www.goldensoftware.com/