Savannah River National Laboratory
Clemson University
GSI Environmental Inc.

SUPPLEMENTARY TABLE
DATA ANALYSIS AND MODELING RESOURCES

Model	Key Input Data Requirements (approx number of parameters, typical)	Model Type	Output	Advantages	Disadvantages	Best Uses
Scenarios (Chlorinated Solvents)	Site data (<10 with representative data from site)	Screening tool	Conceptual model, downstream inputs	Quick and easy, provides insight into key processes and potential site specific remediation opportunities. Free	Qualitative and insufficient to support final decision and system design.	Early site planning activities, developing consensus among regulators, stakeholders, contractors, and site owners.
Scenarios (Metals and Radionuclide)	Site data. Primary focus is geochemical trends to predict impacts of alternative actions on one or more contaminants	Screening tool	Conceptual model, predicted trends	Quick and easy, provides insight into key processes and potential site specific remediation opportunities. Free	Qualitative and insufficient to support final decision and system design.	Early site planning activities, developing consensus among regulators, stakeholders, contractors, and site owners.
GW Sensitivity Toolkit	Site Data . The user supplies site-specific information and the toolkit returns a scorecard addressing resource value and sensitivity to contamination. Primary contaminants are hydrocarbons.	Screening tool	Conceptual model, downstream inputs, limited site specific and aquifer vulnerability factors included.	Quick and easy, provides insight into key processes and potential site specific issues. Free	Qualitative and insufficient to support final decision and system design.	Early site planning activities, developing consensus among regulators, stakeholders, contractors, and site owners.
Source Depletion Decision Support System	Site data and information about historical performance of various treatment technologies on similar sites. Designed to aid the decision-making process for remediation of dense non-aqueous phase liquid (DNAPL) source zones.	Screening tool	Conceptual model, remediation strategy development	Quick and easy, provides insight into key processes and potential site specific issues. Based on real performance and has some information on costs. Free	Qualitative and insufficient to support final decision and system design. Highly dependent on past data and does not fully account for performance improvement through time.	Early site planning activities, developing consensus among regulators, stakeholders, contractors, and site owners.
MAROS	Concentration vs. time , spatial and hydrogeologic data (porosity, groundwater flow direction, seepage velocity, plume thickness), regulatory screening levels. (<10 with data from several locations and times)	Data analysis tool	Trends, statistics, spatial uncertainty, temporal optimization, attainment of cleanup goals, estimates of total dissolved mass over time.	Provides straightforward and disciplined implementation of environmental statistics for data from a monitoring network and documentation of results. Free	Assumes single groundwater flow direction, discreet source and tail zones, requires a minimum dataset of six monitoring locations and four sampling events. Variance in groundwater data and monitoring locations can result in inconclusive or confusing results -- data types limited to traditional (e.g., groundwater well) media and analysis methods -- does not directly handle geophysics data, site operational history, variation in hydrological parameters, anisotropy etc.	Interpreting monitoring data, designing monitoring strategy, evaluating plume stability, identifying locations attaining cleanup goals, updating monitoring network or sampling periods.
SourceDK	Concentration vs. time; source dimensions; soil concentrations; NAPL saturation; NAPL and dissolved phase concentrations (<10 with data from several locations and times)	Data analysis tool	Source mass, source decay rates, remediation timeframe, uncertainty limits	Provides straightforward and disciplined interpretation of source zone data and documentation of results. Free	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires significant judgment to account for geological controls, heterogeneity, etc.	Calculating key parameters associated with a contaminant source. Results can be incorporated in subsequent plume models (below).
Sustainable Remediation Tool	Site Data Information related to the site and the planned (or existing) remediation	Data analysis tool	Estimates of "green metrics", e.g., carbon footprint, resource utilization, etc.	Has built in calculators to provide standardized estimates for specific types of remediation (e.g., pump and treat).	Limited list of remediation options and less flexible (but less complex than) SiteWise	Developing relative understanding or sustainability of different options -- can assist in remediation strategy development.
SiteWise	Site Data Information related to the site and the planned (or existing remediation)	Data analysis tool	Estimates of "green metrics", e.g., carbon footprint, resource utilization, etc.	Flexible data analysis tool that has been widely used in DoD.	Requires more detailed information than SRT (but has more flexibility)	Developing relative understanding or sustainability of different options -- can assist in remediation strategy development.
RACER	Site Data Information related to the site and the planned (or existing remediation)	Data analysis tool	Estimates of costs.	Relatively straightforward and simple to run.	Requires very detailed information.	Developing cost estimates according to a disciplined and rigorous process.
Mass Flux Toolkit	Darcy velocity, sampling interval, concentrations, plume thickness (<10 with data from several locations and/or times)	Data analysis tool	Mass flux, mass discharge, uncertainty analysis	Provides straightforward and disciplined interpretation of concentration transects and trends to estimate flux and documentation of results. Free	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires significant judgment to account for geological controls, heterogeneity, etc.	Determining the significance of a plume and how it is changing through time. Results can be incorporated in subsequent plume models (below).
BIOBALANCE	Seepage velocity, porosity, infiltration, plume thickness, source dimensions and characteristics, electron acceptor/donor concentrations, degradation rates, conceptual performance profiles of potential source remediation technologies (<20 with representative data from site)	Simplified "analytical" model	Concentration predictions, remedial design and decision support, remediation timeframe	Output focused on plume length and timeframe to stabilization/shrinkage (the model iterates to identify the plume stabilization time for the user) -- provides mass flux and mass balance for contaminant, electron donor/acceptor -- scoping estimate of the potential impacts of source remediation on plume. Free	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires significant judgment to account for geological controls, heterogeneity, etc. -- plume calculation for parent compound only -- source remediation implemented at time 0 (plume development prior to remediation not accounted for -- can not simulate remediation in the plume (parameters are fixed for entire model run) -- electron donor/acceptor modules highly simplified -- difficult to simulate complicated and/or changing conditions.	Scoping calculation of plume dynamics (plume growth and timeframe), scoping calculation of the relative importance of different attenuation mechanisms, scoping calculation on sustainability of reductive processes -- scoping calculation of the potential impacts of source remediation alternatives.
BIOCHLOR and BIOSCREEN	Source dimensions and characteristics; dispersion parameters; Darcy velocity; porosity; decay rates and yield coefficients, etc. (<20 with representative data from site)	Simplified "analytical" model	Concentration predictions, remedial design and decision support, remediation timeframe	Output focused on plume concentration and model provides information for parent and daughter compounds -- widely used and accepted model. Free	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires significant judgment to account for geological controls, heterogeneity, etc. -- user selects output times (does not provide plume stabilization timeframe or size without several runs) -- source remediation implemented at time 0 (plume development prior to remediation not accounted for -- can not simulate remediation in the plume (parameters are fixed for entire model run) -- no simulation of electron donor/acceptor -- difficult to simulate complicated and/or changing conditions.	Scoping calculation of plume concentration patterns, scoping calculation of the relative importance of different attenuation mechanisms, scoping calculation of the potential impacts of source remediation alternatives.
REMChlor and REMFuel	Source concentration, mass, dimensions; Darcy velocity; porosity; dispersion; decay rates (<20 with representative data defined for various key zones and times)	Simplified "analytical" model	Concentration and risk predictions, remedial design and decision support, remediation timeframe	Provides ability to simulate site with flexible configuration for source treatment and plume remediation -- provides ability to let plume develop prior to source remediation start, provides ability to alter parameters for plume remediation -- provides ability to simulate PRB -- simple to identify plume stabilization size and timeframe by scrolling through output. Free	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires significant judgment to account for geological controls, heterogeneity, etc. -- difficult to simulate complicated and/or changing conditions --no simulation of electron donor/acceptor.	This model provides key capabilities that rival more complex numerical models -- provides fairly robust scoping calculations (as above) and reasonable support for remedial decisions and designs.
RBCA Toolkit	Source concentration, mass, dimensions; Darcy velocity; porosity; dispersion; decay rates and other factors as needed to account for vapor intrusion or other pathways.	Simplified "analytical" model for pathway and risk analysis	Concentration and risk predictions, remedial design and decision support, remediation timeframe	The RBCA Tool Kit modeling and risk characterization software package designed to meet the requirements of the ASTM Standard Guide for Risk-Based Corrective Action (E-2081) for Tier 1 and Tier 2 evaluations. The software combines contaminant transport models and risk assessment tools to calculate baseline risk levels and derive risk-based cleanup standards for a full array of soil, groundwater, surface water, and air exposure pathways – versions available for hydrocarbons and other hazardous contaminants.	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires significant judgment to account for geological controls, heterogeneity, etc. -- difficult to simulate complicated and/or changing conditions -- no simulation of electron donor/acceptor -- powerful model that accounts for many exposure pathways and calculates risk (but has the associated learning curve for operation).	This model provides key capabilities that rival more complex numerical models -- provides fairly robust scoping calculations (as above) and reasonable support for remedial decisions and designs -- output follows standard risk assessment protocols and model includes most major exposure pathways..
Matrix Diffusion Toolkit	Site Data Typical parameters (Darcy velocity, etc.) and additional estimates of parameters related to matrix diffusion	Simplified "analytical" model for estimating effects of matrix diffusion	Estimates of concentration, mass, and mass discharge in transmissive layer; concentration and mass in the low-k zone	Straightforward and simple to run. Pseudo analytical solution that provides a reasonable estimate of the impacts of matrix diffusion	Order of magnitude estimate. Reliability of results can be variable and depend on availability of data -- requires significant judgment to quantify geological controls, heterogeneity, etc.	Developing understanding of the potential impacts of matrix diffusion -- can assist in remediation strategy development.

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Model	Key Input Data Requirements (approx number of parameters, typical)	Model Type	Output	Advantages	Disadvantages	Best Uses
MODFLOW	Detailed site-specific hydrologic parameters (<20 with data from several locations and times)	Numerical model	Same as "Analytical" model, but more integrated and for more complex or dynamic conditions -- primary output is hydrogeologic (water levels and flow).	Provides flexible and robust simulation of hydrogeology -- can be used for steady-state simulations or for dynamic transient simulations -- can be used to simulate complex pump-and-treat systems and zone of capture. Several graphical front end programs are available (e.g., GMS, VisualMODFLOW, etc.)	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires additional programs and modules to simulate contaminant fate and transport, degradation processes, etc. -- does not simulate vadose zone hydrology -- does not simulate source zone contaminant release.	Key exemplar of groundwater models -- widely used and accepted and a powerful tool when used in combination with other models to simulate source and contaminant scenarios and remediation. Many similar models are available.
RT3D	Detailed site-specific parameters including source and plume decay rates (20 to 50 with data from several locations and times)	Numerical model	Same as "Analytical" model, but more integrated and for more complex or dynamic conditions -- primary output is contaminant behavior under varying conditions	Provides flexible and robust simulation of contaminant behavior -- can be used for steady-state simulations or for dynamic transient simulations (e.g., in combination with MODFLOW) -- a large number of contaminant specific modules have been developed to support difference scenarios. Graphical front ends are available (e.g., GMS, VisualMODFLOW, etc.)	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires a large number of inputs and modules can become complicated and expensive to run.	Flexible and powerful tool to simulate sites if detailed evaluation is required and resources are needed. Many similar models are available.
T2VOC	Detailed site-specific parameters including source and plume decay rates (20 to 100 with data from several locations and times)	Numerical model	Same as "Analytical" model, but more integrated and for more complex or dynamic conditions -- provides output for both hydrogeology and contaminant in the vadose zone and groundwater.	Flexible and robust to the most widely ranging scenarios -- but user must provide all of the parameters -- few prestaged modules for contaminants -- provides ability to model thermal remediation and steam -- etc. Currently a graphical front end (PETRASIM) is available that simplified input and output.	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires a large number of inputs and modules can become complicated and expensive to run.	Most powerful tool -- but complicated to run and expensive. Several similar models are available.
SEAM3D	Detailed site-specific parameters including source and plume decay rates (20 to 50 with data from several locations and times)	Numerical model	Same as "Analytical" model, but more integrated and for more complex or dynamic conditions -- primary output is contaminant behavior under varying conditions	Provides flexible and robust simulation of contaminant behavior -- can be used for steady-state simulations or for dynamic transient simulations (e.g., in combination with MODFLOW) -- a well organized sequential electron acceptor and donor approach provides some powerful general capabilities. Graphical front ends are available (e.g., GMS, VisualMODFLOW, etc.)	Reliability of results can be variable and depend on availability of data at proper spacings and/or times -- requires a large number of inputs and modules can become complicated and expensive to run.	Flexible and powerful tool to simulate sites if detailed evaluation is required and resources are needed. Several similar models are available.

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LINKS FOR THE LISTED MODELS AND KEY MODELING FRONT END AND GRAPHICAL OUTPUT TOOLS

Screening Models	Scenarios (Chlorinated Solvents)	http://www.gsi-net.com/files/papers/SRNL-STI-2011-00459.pdf or http://sti.srs.gov/fulltext/SRNL-STI-2011-00459.pdf
	Scenarios (metals and radionuclided)	http://sti.srs.gov/fulltext/WSRC-STI-2006-00096.pdf
	GW Sensitivity Toolkit	http://www.gsi-net.com/en/software/free-software
	Source Depletion Decision Support System	http://www.gsi-net.com/en/software/free-software
Data Analysis Models	MAROS	http://www.gsi-net.com/en/software/free-software
	SourceDK	http://www.gsi-net.com/en/software/free-software
	Sustainable Remediation Tool	U. S. Air Force Civil Engineer Center
	SiteWise	http://www.ert2.org/t2gsrportal/SiteWise.aspx
	Racer	U. S. Air Force Civil Engineer Center
	Mass Flux Toolkit	http://www.gsi-net.com/en/software/free-software
Analytical Models	BIOBALANCE	http://www.gsi-net.com/en/software/free-software
	BIOCHLOR and BIOSCREEN	http://www.epa.gov/ada/csmos/models/biochlor.html or http://www.epa.gov/ada/csmos/models/bioscrn.html
	REMChlor and REMFuel	http://www.epa.gov/ada/csmos/models/remchlor.html or http://www.epa.gov/ada/csmos/models/remfuel.html
	RBCA Toolkit	http://www.gsi-net.com/en/software.html
	Matrix Diffusion Toolkit	http://www.gsi-net.com/en/software/free-software
Numerical / Hybrid Models	MODFLOW	http://water.usgs.gov/nrp/gwsoftware/modflow.html
	RT3D	http://bioprocess.pnnl.gov/
	T2VOC	http://esd.lbl.gov/research/projects/tough/
	SEAM3D	http://el.erdc.usace.army.mil/elpubs/pdf/trel00-18.pdf

GMS	several USGS / Aquaveo / EMS-I e.g., http://www.aquaveo.com/gms
Visual MODFLOW	http://www.swstechnology.com/groundwater-modeling-software/visual-modflow-flex
PETRASIM	http://www.rockware.com/product/overview.php?id=148
TECPLOT	http://www.tecplot.com/
SURFER	http://www.goldensoftware.com/