Table S1_supplement. Summary of the models used for the transport of hydrocarbons

Name of the model	Capabilities	Developer/author/Source
SCREENING TOOLS		
Bio1D	Simulation of biodegradation and sorption of hydrocarbons	GeoTrans, Inc, IGWMC, CertainTech, (Srinivasan and Mercer 1989): https://bio1d1.software.informer.com/11.0/
Biobalance Toolkit	Tool provides Remediation Time Frame (RTF). The module has the capacity to address the impact of different remediation strategies on the source mass and the mass flux from the source.	GSI Environmental Inc., (Kamath et al. 2007), https://www.gsienv.com/product/natural-attenuation-tool/
Biochlor	Simulation of remediation by natural attenuation of chlorinated solvents.	EPA 2000, https://www.epa.gov/water-research/biochlor-natural-attenuation-decision-support-system
Bioscreen	Simulation of natural attenuation of dissolved hydrocarbons at petroleum fuel release sites.	EPA 1996, (Newell et al., 1996) https://www.epa.gov/water-research/bioscreen-natural-attenuation-decision-support-system
CapSim	Simulation of 1D reactive transport through multi-layered soil, including non-generic processes such as bioturbation or deposition	(Shen et al. 2018) https://github.com/EnvironmentalSoftware/CapSim.
CDISCO	The Excel interface tool for modelling of in situ chemical oxidation of hydrocarbons using permanganate.	Environmental Technology Certification Program project, (Borden et al. 2010),
HSSM	Model simulates flow of LNAPL and transport of a chemical constituent of the LNAPL from the surface to the water table	EPA, 1995 (Weaver et al., 1994) https://www.epa.gov/water-research/hydrocarbon-spill-screening-model-hssm-windows-version
NAS	Tool used to estimate remediation timeframes for monitored natural attenuation (MNA) to decrease	VirginiaTech, USGS and NAVFAC, (Mendez 2008)

	concentrations of the contaminant and meet the standards.	
REMchlor	Model simulates the transient effects of groundwater source and plume remediation.	EPA 2007, (Falta et al. 2007) https://www.gsienv.com/product/remchlor-md/
REMFuel	Model simulates the transient effects of groundwater source and plume remediation for fuel hydrocarbons.	EPA 2012 (Falta et al., 2012) https://www.epa.gov/water-research/remediation-evaluation-model-fuel-hydrocarbons-remfuel
RT1D	Model simulates chemical and kinetic reactions	(Torlapati and Clement 2013)
SourceDK	Model is a computer decision support tool for estimating remediation timeframes and assessing the uncertainty associated with those estimates.	GSI Environmental Inc. for the Air Force Civil Engineering Center (AFCEC) https://www.gsienv.com/product/natural-attenuation-tool/
STOCHASTIC MODELS		
ART3D	This reactive transport model considers retardation, advection, dispersion, and the reactions of multiple species.	Brigham Young University (Jones et al. 2006), http://www.et.byu.edu/~njones/share/art3d/
Factorial-design-based stochastic approach	The approach integrates a solute transport model, factorial analysis, and Monte Carlo technique.	(Qin et al. 2008)
Fuzzy stochastic approach	The approach quantifies probabilistic and fuzzy uncertainties associated with the site contamination assessment	(Zhang and Huang 2011)
HPS-PROBAN	An integrated approach coupling the horizontal plane source model and the package aims to conduct of probabilistic analyses	Proban – Veritas Research 1992 (Hamed et al. 1995)
Null Space Monte Carlo (NSMC)	It integrates the deterministic model that is calibrated by stochastically generated fields of parameters	(Doherty, 2015).
Lasar-Phreeqc approach	This solution couples two elements, Lasar approach for incorporation of the statistical uncertainty and Phreeqc for modelling of the geochemical processes	(Malmström et al. 2004)
Premchlor	Model can be used for simultaneously evaluating the effectiveness of source and plume remediation, taking into account of	ESTCP project, (Liang et al. 2010)

	the uncertainties in all major parameters	
DETERMINISTIC MODELS		
3DFATMIC	Multidimensional model that simulates flow and transport of contaminants that are subjected to chemical and biological transformations.	EPA, 1997 (Yeh et al.1997) https://www.epa.gov/water-research/three-dimensional-subsurface-flow-fate-and-transport-microbes-and-chemicals-3dfatmic
BIOMOC3D	3D reactive transport model that simulates both aerobic and anaerobic degradation.	USGS, 1997 (Essaid and Benkins 1997) http://water.usgs.gov/software/BIOMOC/
BIOPLUME III	3D finite difference model that simulates reactive transport of hydrocarbon contaminants and its removal due to the natural attenuation.	EPA, 1997 (Rifai et al. 1998) https://www.epa.gov/water-research/bioplume-iii
BIOREDOX-MT3DMS	Multicomponent solute transport model that simulates natural and enhanced bioremediation.	Conestoga Rovers and Associates, (Carey et al. 1999) http://www.porewater.com/software_bioredox.html
BIOSLURP	Finite element model that simulates 3 phase flow and multi-species transport in vadose and saturated zones.	Draper Aden Environmetnal Modeling http://www.mpassociates.gr/software/environment/bioslurp.html
BIOVENTINGplus	Model used for the assessment of the efficiency and costs of the air sparging method.	ES&T (Environmental Services and Technologies) 1996, (Johnson and Parker 1999)
Chain_2D	Model simulates 2D variably saturated water flow and movement of solutes involved in sequential first-order decay reactions	United States Department of Agriculture, US Salinity Laboratory, (Simunek and Genuchten 1994), http://www.ars.usda.gov/services/docs.htm?docid=8914
CORT3D	Chemical oxidation reactive transport, it simulates the interaction of aquifer NOD, oxidant delivery rate, its concentration and transport	(Heiderscheidt 2005; Illangasekare et al. 2006)
CTRAN and SEEP/W	Finite element modelt hat simulates flow and transport of solutes in variable saturated media.	Geo-Slope https://www.geoslope.com/products/ctran-w
FEFLOW	3D finite flow and mass and heat transport model.	DHI-WASY GmbH http://www.feflow.info/

FEHM	3D flow and transport model in variable saturated media	Los Alamos National Laboratory (Zyvoloski 2007) https://fehm.lanl.gov
Hydrus	2 or 3D model that simulates flow and transport of contaminants and heat.	http://www.pc-progress.com/en/Default.aspx?hydrus-3d
MT3D/MT3DMS	Model simulates advection, dispersion and chemical reactions of dissolved compounds in groundwater systems.	MT3D - S.S. Papadopulos & Associates, Inc., and U.S. Environmental Protection Agency (USEPA) MT3DMS - U.S. Army Corps of Engineers Waterways Experiment Station, project of Strategic Environmental Research and Development Program, (Zheng 1990; Zheng and Wang 1999) https://www.usgs.gov/software/mt3d-usgs-groundwater-solute-transport-simulator-modflow
PFLOWTRAN	It is an open source, state-of-the-art massively parallel subsurface flow and multiphase, multicomponent and multiscale reactive transport code.	Lichtner et al., 2015 https://www.pflotran.org/
PHREEQC	Computer program designed to perform a wide variety of low-temperature aqueous geochemical calculations.	USGS, (Parkhurst and Appelo 1999, 2013) http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/
PHT3D	PHT3D couples MODFLOW/MT3DMS models and PHREEQC-2 code. It enables simulating of NAPL dissolution, microbial growth/decay or isotopic fractionation.	Henning Prommer, CSIRO Land and Water Australia and Vincent Post at Flinders University School of the Environment (South Australia) and National Centre for Groundwater Research and Training: (Prommer et al. 1999) http://www.pht3d.org/
RT3D	Software package for simulating 3D, multi-species, reactive transport applicable to simulate natural attenuation and accelerated bioremediation	Scientific Software Group, (Clement 1997) http://bioprocess.pnnl.gov/rt3d.downloads.htm
SEAM3D	Reactive transport model uses to simulate complex biodegradation problems involving multiple	Virginia Polytechnic Institute and State University (Waddill and Widdowson 1998; Waddill and Widdowson 2000)

	substrates and multiple electron acceptors.	
SUTRA	Model for variable saturated and variable density groundwater flow and transport of contaminants and heat	USGS, 1984 (Voss, 1984) http://water.usgs.gov/nrp/gwsoftware/sutra/sutra.html
SWMS 3D	3D flow and transport model in variable saturated media.	U. S. Salinity Laboratory Agricultural Research Service U. S. Department of Agriculture (Simunek et al. 1995) https://data.nal.usda.gov/dataset/swms-3d
TMVOC	Numerical simulator for flow of water, soil gas, and a multicomponent mixture of volatile organic chemicals (VOCs) in multidimensional heterogeneous porous media.	Lawrence Berkley National Laboratory, Earth Sciences Division, (Pruess and Battistelli 2002), https://tough.lbl.gov/software/tmvoc-software/
TOUGH2v2 and TOUGHREACT	Multidimensional finite difference models designed to simulate the coupled transport of water, vapor, non-condensible gas, and heat in porous and fractured media along with chemical processes occurring in the subsurface.	Lawrence Berkley National Laboratory, Earth Sciences Division (Pruess et al. 1999; Xu et al. 2004) https://tough.lbl.gov/
UTCHEM	Model simulates the flow, physical, chemical, and biological processes as a site is remediated.	The University of Texas at Austin (Pope et al. 1999) https://csee.engr.utexas.edu/education/software-and-portals-information

References:

Srinivasan, P., Mercer J.W. (1989). BIO1D — One Dimensional Model for Comparison of Biodegradation and Adsorption Processes in Contaminant Transport, vol. 1.2, GeoTrans, Inc, Herndon, VA (1989).

Kamath, R., Looney, B.B., Newell, C.J., Adamson, D.T., Vangelas, K.M. (2007). BioBalance: A mass balance toolkit.

Newell, C.J., McLeod, R.K., Gonzales, J.R. (1996). BIOSCREEN Natural Attenuation Decision Support System User's Manual Version 1.3, U.S. EPA National Risk Management Research Laboratory, EPA/600/R-96/087.

Shen, X., Lampert, D., Ogle, S., Reible, D. (2018). A software tool for simulating contaminant transport and remedial effectiveness in sediment environments. *Environmental modelling & software*, *109*, 104-113.

Borden, R.C., Simpkin, T., Lieberman, M.T. (2010). User's guide, Design Tool for Planning Permanganate Injection Systems, ESTCP Project ER-0626.

Weaver, J.W., Charbeneau, R.J., Tauxe, J.D., Lien, B.K. and Provost, J.B., (1994). The hydrocarbon spill screening model (HSSM). Vol. 1 User's guide. U.S. EPA. EPA/ 600/R-94/039a. Oklahoma.

Mendez, E., Widdowson, M., Brauner, S., Chapelle, F., Casey, C. (2004). Natural Attenuation Software (NAS): A computer program for estimating remediation times of contaminated groundwater. WIT Transactions on Ecology and the Environment, 69.
Falta, R.W., Stacy, M.B., Noman, A., Ahsanuzzaman, M., Wang, M., Earle, R.C., Brooks, M., Wood, A.L. (2007). REMChlor Remediation Evaluation Model for Chlorinated Solvents User's Manual Version 1.0, Clemson, South Carolina, Ground Water and Ecosystems Restoration Division, U.S. Environmental Protection Agency.
Falta, R.W.,. Ahsanuzzaman, N.M., Stacy, M.B., Earle, R.C. (2012). REMFuel : Remediation Evaluation Model for Fuel Hydrocarbons User's Manual, Version 1.0. U.S. Environmental Protection Agency, Washington, DC, EPA/600/R-12/028, 2012.
Torlapati, J., Clement, T.P. (2013). Benchmarking a Visual-Basic based multi-component one-dimensional reactive transport modeling tool. Computers & Geosciences, 50, 72-83.
Jones, N.R., Clement,T.P., Hansen, C.M. (2006). A Three-Dimensional Analytical Tool for Modeling Reactive Transport. Ground Water, 44, 613-617.

Qin, X.S., Huang, G.H., Chakma, A. (2008). Modeling Groundwater Contamination under Uncertainty: A Factorial-Design-Based Stochastic Approach. Journal of Environmental Informatics, 11(1).
Zhang, X., Huang, G.H. (2011). Assessment of BTEX-induced health risk under multiple uncertainties at a petroleum-contaminated site: An integrated fuzzy stochastic approach. Water Resources Research, 47(12).
Hamed, M.M., Conte, J.P., Bedient, P.B. (1995). Probabilistic screening tool for ground-water contamination assessment. Journal of Environmental Engineering, 121(11), 767-775.
Doherty, J. (2015). Calibration and uncertainty analysis for complex environmental models. Brisbane, Australia: Watermark Numerical Computing.
Malmström, M.E, Destouni, G., Martinet, P. (2004). Modeling expected solute concentration in randomly heterogeneous flow systems with multicomponent reactions. Environmental Science and Technology, 38, 2673–2679.
Liang, H., Falta, R., Newell, C., Farhat, S., Rao, P.S.C., Basu, N. (2010). PREMChlor: Probabilistic Remediation Evaluation Model for Chlorinated Solvents. ESTCP Project ER-0704. Clemson University, Clemson,SC, 76p.
Yeh, G.T., Cheng, J.R., Short, T.E. (1997). 3DFATMIC: User's Manual of a Three-Dimensional Model of Subsurface Flow, Fat and Transport of Microbes and Chemicals. EPA/600/R-97-053. National Risk Management Research Laboratory, USEPA, Ada, OK 74820.
Essaid, H.I., Bekins, B.A. (1997). BIOMOC, a multispecies solute-transport model with biodegradation. Menlo Park, CA: US Department of the Interior, US Geological Survey.
Rifai, H. S. (1998). Bioplume III natural attentuation decision support system user's manual version 1.0.
Carey, G.R., Van Geel, P.J., Murphy, J.R. (1999). BIOREDOX-MT3DMS V2.0: A Coupled Biodegradation-Redox Model for Simulating Natural and Enhanced Bioremediation of Organic Pollutants – User's Guide. Waterloo, Ontario, Canada: Conestoga-Rovers & Associates.
Johnson, J.A., Parker, J.C. (1999). Cost Minimization Strategies for Site Characterization and Remediation Using Design Penalty Cost. Proceedings of the Petroleum Hydrocarbons and Organic Chemicals in Ground Water: Prevention, Detection, and Remediation Conference: November 17-19, 1999, Houston, Texas. National Ground Water Association, 1999.
Šimŭnek, J., van Genuchten, M.Th. (1994). The CHAIN_2D code for simulating two-dimensional movement of water flow, heat, and multiple solutes in variably-saturated porous media. Version 1.1. Res. Rep. 136. U.S. Salinity Lab., Riverside, CA.
Heiderscheidt, J.L. (2005). DNAPL Source Zone Depletion during In Situ Chemical Oxidation (ISCO): Experimental and Modeling Studies. PhD Dissertation. Golden, CO.: Colorado School of Mines.
Illangasekare, T.H., Marr, J.M., Siegrist, R.L., Glover, K.C., Moreno-Barbero, E., Heiderscheidt, J.L., Saenton, S., Matthew, M., Kaplan, A.R., Kim, Y., Dai, D., Gago, J.L., Page, J.W.E. (2006). Mass Transfer from Entrapped DNAPL Sources Undergoing Remediation: Characterization Methods and Prediction Tools SERDP Project No. CU-1294. Golden, CO.

Zyvoloski, G. (2007). FEHM: A control volume finite element code for simulating subsurface multi-phase multi-fluid heat and mass transfer. Los Alamos Unclassified Report LA-UR-07-3359.
Zheng, C. (1990). MT3D, A modular three-dimensional transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems, Report to the Kerr Environmental Research Laboratory, US Environmental Protection Agency, Ada, OK.
Zheng, C., Wang, P.P. (1999). MT3DMS: A modular three-dimensional multispecies model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems; Documentation and User's Guide, Contract Report SERDP-99-1, U.S. Army Engineer Research and Development Center, Vicksburg, MS.
Lichtner, P.C., Hammond, G.E., Lu, C., Karra, S., Bisht, G., Andre, B., Mills, R., Kumar, J. (2015). PFLOTRAN user manual: A massively parallel reactive flow and transport model for describing surface and subsurface processes (No. LA-UR-15-20403). Los Alamos National Lab.(LANL), Los Alamos, NM (United States); Sandia National Lab.(SNL-NM), Albuquerque, NM (United States); Lawrence Berkeley National Lab.(LBNL), Berkeley, CA (United States); Oak Ridge National Lab.(ORNL), Oak Ridge, TN (United States); OFM Research, Redmond, WA (United States).
Parkhurst, D.L., Appelo, C.A.J. (1999). User's guide to PHREEQC (version 2) - a computer program for speciation, reaction-path, 1D-transport, and inverse geochemical calculations. US Geol. Surv. Water Resour. Inv. Rep. 99-4259. U.S.G.S.
Parkhurst, D.L., Appelo, C.A.J. (2013). Description of input and examples for PHREEQC version 3--A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations: U.S. Geological Survey Techniques and Methods, book 6, chap. A43, 497 p.
Prommer, H., Davis, G.B., Barry, D.A. (1999). PHT3D — A three-dimensional biogeochemical transport model for modelling natural and enhanced remediation. Proc. Contaminated site remediation: Challenges posed by urban and industrial contaminants. Fremantle, WA, 351-358.
Clement, T.P. (1997). RT3D - A Modular Computer Code for Simulating Reactive Multi-Species Transport in 3-Dimensional Groundwater Aquifers. PNNL-11720. Richland, Washington: Pacific Northwest National Laboratory.
Waddill, D.W., Widdowson, M.A. (1998). A three-dimensional model for subsurface transport and biodegradation. ASCE Journal of Environmental Engineering, 24, 336-344.
Waddill, D.W., Widdowson, M.A. (2000) SEAM3D: A numerical model for three-dimensional solute transport and sequential electron acceptor-based bioremediation in groundwater. ERDC/EL TR-00-18, U.S. Army Engineer Research and Development Center, Vicksburg, MS.
Voss, C.I., (1984). SUTRA – A finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport: U.S. Geological Survey Water-Resources Investigations Report 84-4369, 409 p.
Šimůnek, J., Huang, K., van Genuchten, M.T. (1995). The SWMS_3D code for simulating water flow and solute transport in three-dimensional variably-saturated media. US Salinity Laboratory Research Report, 139.
Pruess, K. Battistelli, A., (2002). TMVOC, A Numerical Simulator for Three-Phase Non-isothermal Flows of Multicomponent Hydrocarbon Mixtures in Saturated-Unsaturated Heterogeneous Media. Lawrence Berkeley National Laboratory Report LBNL-49375, Berkeley, CA.
Pruess, K., Oldenburg, C.M., Moridis, G.J. (1999). TOUGH2 user's guide version 2 (No. LBNL-43134). Lawrence Berkeley National Lab.(LBNL), Berkeley, CA (United States).
Xu, T., Sonnenthal, E., Spycher, N., Pruess, K. (2004). TOUGHREACT user's guide: A simulation program for non-isothermal multiphase reactive geochemical transport in variable saturated geologic media (No. LBNL-55460). Lawrence Berkeley National Lab.(LBNL), Berkeley, CA (United States).
Pope, G., Sepehrnoori, K., Sharma, M.M., McKinney, D.C., Speitel, G.E. Jackson, R.E. (1999). Three-dimensional NAPL fate and transport model. EPA Report 600/R-99/011, U.S. Environmental Protection Agency, Cincinnati, OH.