Table_S3_supplement. Screening tools with their input and output data

Model	Input	Outcomes

BioBalance Toolkit	• General information:
	  • Hydrogeologic parameters: concentration goal, precipitation, seepage velocity, porosity, soil bulk density, organic carbon partitioning coefficient
	  • Source geometry: type of source (submerged/vadose zone), width, length, thickness
	  • Geochemical data: importance of reductive dechlorination
	• Source module:
	  • Vadose zone:
	  • COC data: average source concentration
	  • Vadose zone source data: distance from the top of contaminated zone to the top of water-bearing unit, volumetric water content of source zone, organic fraction of soil
	  • Reduction factor: remaining mass factor, remaining mass flux
	  • Submerged zone:
	  • COC data: average soil concentration in source, average groundwater concentration in source
	  • Reduction factor: remaining mass factor, remaining mass flux
	  • Change in concentration of competing electron acceptors across the source zone
	  • Change in concentration of reaction byproducts across the source zone
	  • Concentration of daughter products in the source zone
	• Donor module
		• General:
		  • Calculated concentration goal
		  • Thickness of plume
		• Source module
		  • Vadose zone: groundwater flow model, mass flux goal, mass flux, concentration in groundwater under source, mass in source zone, source decay coefficient, remediation timeframe with MNA, remediation timeframe with MNA +source flux mass reduction
		  • Submerged zone: mass flux, mass flux goal, mass in source zone, source decay coefficient, remediation timeframe with MNA +source flux mass reduction
		  • % donor going to solvent during initial stages of source remediation
		• Donor module: donor to chlorinated solvent mass ratio
		• Plume module: centreline concentration/mass flux versus distance calculated for time, % reduction in flux due to source removal
		• Summary report: evaluates sustainability of the source zone prior to and after addition of an external donor, summarizes overall plume stability

	• Donor A: fraction of CVOCs in NAPL, fraction of electron donor in NAPL, adjustment factor • Donor B: fraction of CVOCs in NAPL, fraction of electron donor in NAPL, adjustment factor • Plume module: fraction of organic carbon, 1st order decay coefficient • Summary report: amount of external donor added to the source zone (enhanced bioremediation)	
BIOCHLOR	• Hydrogeologic data: seepage velocity; hydraulic conductivity; hydraulic gradient; effective porosity; • Dispersivity: longitudinal dispersivity, transverse dispersivity, vertical dispersivity • Adsorption: retardation factor, aquifer matrix bulk density, organic carbon partition coefficient, fraction organic carbon; • Biotransformation data: first-order decay coefficients, dissolved solvent half-life, abiotic first order rate coefficient, yield; • General data: area length and width, simulation time, redox zones length; • Source data: source area concentrations, source area width, source thickness in saturated zone; • Field data for comparison	• Concentrations either along the centreline concentrations or as an array. • Mass of organics in the plume array for two models:1) No Degradation and 2) Sequential First Order Decay. • Mass removed that is the difference between the mass of contaminant if no biotransformation occurs and the mass of contaminant if biotransformation/productions occurs. • Flow rate of groundwater
BIOSCREEN	• Hydrogeologic data: seepage velocity; hydraulic conductivity; hydraulic gradient; effective porosity; • Dispersivity: longitudinal dispersivity, transverse dispersivity, vertical dispersivity, estimated plume length, • Adsorption: retardation factor, soil bulk density, organic carbon partition coefficient, fraction organic carbon; • Biodegradation data: first-order decay coefficient, dissolved plume solute half-life, delta oxygen, delta nitrate, observed ferrous iron, delta sulphate, observed methane, • General data: area length and width, simulation time;	• Concentrations either along the centreline concentrations or as an array. • Plume mass if no biodegradation. • Actual plume mass for three models: no degradation, 1st order decay and instantaneous reaction. • Plume mass removed by biodegradation. • Change in electron acceptor/byproduct masses. • Original mass in source • Mass in source now • Current volume of groundwater in plume

	• Source data: source thickness in saturated zone; source zone width, source zone concentration, source half-life (calculated by model), soluble mass in NAPL; • Field data for comparison	• Flow rate of groundwater
CapSim	• Chemical and physical parameters (name, modelcular weight, concentration, temperature) • Adsorption coefficient, sorption isotherm • Matrices data: properties, layers • Properties of overlying water column • Reaction module (rate, coefficients, kinetic model)	• Concentration, flux, solid concentration, total concentration, water concentration, material fraction
CDISCO	• Model set up: modelling duration, time step model length, target number of days to calc. ROI, minimum oxidant concentration; • Hydrogeologic characteristics: top of injection intervals, bottom of injection interval, aquifer thickness, thickness of mobile zone, porosity, longitudinal dispersivity, hydraulic conductivity, depth to water table; • Soil and NOD characteristics: bulk density, total NOD, fraction instantaneous, second order slow NOD consumption rate; • Oxidants information: name of oxidant, molecular weight of oxidant, initial oxidant concentrations Contaminants information: name of contaminant, molecular weight of contaminant, initial contaminant concentration, molar ration of oxidant to contaminant consumed, contaminant retardation factor; Injection parameters: injection duration per well or point, contaminant concentration, oxidant concentration; Injection rate: injection rate to be used for model and design, in addition	• Concentration of oxidant versus radial distance, concentration of contaminant • Total costs for oxidant, injection, well installation and other

	For well: well screen diameter, effective diameter of sand pack, injection pressure, well loss coefficient, theoretical estimate of injection rate per well, hours per day injected, For direct push probe: injection rate, hours per day injected; Injection design factor: injection ROI overlap factor, total additional injection events planned; Personal, equipment, oxidant costs	
HSSM	• Hydrologic parameters: water dynamic viscosity, water density, water surface tension, maximum relative permeability to water during infiltration, capillary pressure curve model, vertical hydraulic conductivity, ratio horizontal to vertical conductivity, porosity, bulk density, aquifer saturated thickness, depth to water table, capillary thickness parameter, groundwater gradient, longitudinal dispersivity, transverse dispersivity, vertical dispersivity, average annual recharge, saturation • NAPL phase data: NAPL density, NAPL dynamic viscosity, hydrocarbon solubility, aquifer residual NAPL saturation, vadose zone residual NAPL saturation, soil/water partition coefficient, NAPL surface tension, initial constituent concentration in NAPL, NAPL/water partition coefficient, soil/water partition coefficient, constituent solubility, constituent half-life in aquifer, hydrocarbon release options (specified flux, specified area, constant head ponding, variable ponding, NAPL flux, beginning time, ending time, ponding depth, oil volume, lower depth of NAPL zone) • Model simulation data: radius of oil lens source, radius multiplication factor, maximum NAPL saturation in NAPL lens, simulation ending time, maximum solution time step, minimum time between printed time steps and mass balance	• Fluid distribution in vadose zone • NAPL lens profiles • Contaminant mass flux history • NAPL radius history • NAPL lens contaminant mass balance

	checks, OILENS simulation ending criterion (user-specified time, NAPL lens spreading stops, maximum contaminant mass flux into aquifer, contaminant leached from lens drops, fraction of mass remaining), percent maximum contaminant radius, minimum output concentration, beginning time, ending time, time increment, NAPL lens profiles	
NAS	• General data: facility name, site name, additional description, length, mass, time, concentration • Hydrogeologic data: hydraulic conductivity, hydraulic gradient, weight % organic carbon, total porosity, effective porosity, source length, source width, contaminated aquifer thickness • Source data: type of contaminants (chlorinated ethenes or petroleum hydrocarbons), concentration of contaminants, • Field data for comparison: concentrations along the plume sampling date and number wells along the centreline of the plume, redox data • Source reduction and time of stabilization: point of compliance, point of compliance at well, regulatory compliance concentration • Time of remediation: NAPL properties, NAPL solution options, NAPL mass options, Source removal options, velocity range, simulation time, pump and treat options	• Groundwater contaminant velocity • Sorption data • Redox zonation • Natural attenuation capacity • Dispersivity • Decay rate • Target source concentration • Time of stabilization • Graphical view of the reduction in source concentration • Source compliance concentration
REMChlor	• Source Zone Parameters: concentration, mass, gamma, source dimensions (depth, height), Darcy velocity, porosity, source remediation (fraction removed, remediation time, source decay), • Transport Parameters: velocity parameters, number of stream tubes, retardation factors • Plume decay rates and yield coefficients: 9 decay rates for 4 species • Plume reaction zones: two times and two distances	• Changes of CoCs in time • Mass discharge versus distance • Plume visualization

	• Cancer risk parameters • Output options	
REMFuel	• Source Zone Parameters: gamma – power function, source width, length and height, initial source zone concentration, type of NAPL, retardation factor • Flow Parameters: Darcy velocity, porosity • Source remediation: fraction removed, source remediation time • Transport parameters: velocity parameters, number of stream tubes • Component name and reaction types, zero order, first order or Monod's reaction • Output plotting parameters in x, y, z directions and time intervals	• Changes of CoCs in time regarding daughter products
RT1D	• Transport: length, total time, pulse time, grid size, time step, velocity, dispersion coefficient, advection-dispersion options, simulation option (batch kinetics, reactive transport, batch geochemistry, geochemistry coupled with transport) • Kinetic module: mobile components, immobile components, reaction package, ODE solver type, reaction parameters • Geochemistry equilibrium module: components, species, fixed component concentrations, aqueous components, sorbed concentrations, type of surface complexation • Kinetic reaction parameters: component name, retardation factor, initial concentrations of species, boundary, reaction terms • Geochemistry equilibrium parameters: mobile species, stoichiometric relations, sorbed species ID, boundary, total residual concentration, sorbed phase concentrations, sorbed phase composition	• Concentrations of modelled species

SourceDK	Module 1: historical data (concentration and date), option plot , desired clean-up level Module 2: hydrogeology (Darcy velocity, hydraulic conductivity, hydraulic gradient, source characteristics (source groundwater concentration, length, width, thickness, specific discharge, source decay constant, mass), average constituent concentration in saturated zone, soil bulk density, porosity, soil density, retardation factor, layer shape and dimension calculation (layer thickness, layer length, layer width, affected area, soil concentration, groundwater concentration, NAPL saturation, constituent mass fraction, density of source NAPL, biodegradation data (no decay, biodegradation rate constant, biodegradation capacity, delta oxygen, delta nitrate, observed ferrous iron, delta sulphate, observed methane, percentage of biodegradation capacity), output option (number of years, time when decay starts), uncertainty range, field time data for comparison, field concentration data for comparison Module 3: original constituent concentration, desired clen-up level, length of source zone, groundwater seepage velocity, retardation factor, soil bulk density, partition coefficient, fraction organic carbon, effective porosity, type of media (well-sorted, uniform), initial aqueous-phase concentration in source, density NAPL fluid, initial NAPL saturation and its uncertainty, the pumping scenario (Y or N), pore volumes, time to flush out, concentration in pumped water,	Module 1: The model uses exponential extrapolation to calculate the most probable date and the 90% or 95% prediction levels when the desired clean-up level (entered in Section 2) for the chosen constituent will be reached. The model uses a first-order decay relationship to describe how quickly the dissolved concentrations in the source zone (i.e., concentrations that are directly controlled by the rate of NAPL dissolution and/or the rate of desorption from the aquifer material) decline over time. Module2: Concentration vs time plots, mass vs time plot, concentration/time calculator, Module 3: Concentration vs time,