Table S2_supplement. Screening tools and their limitations

Model	Limitations
BioBalance Toolkit	• The BIOBALANCE Toolkit is able to calculate the overall stability results for the parent concentrations and consider the daughter products in terms of the electron acceptor and electron donor balance. However, the current version of the toolkit does not consider the formation of daughter products and their effect on plume length. • Many of the calculations use observed rates, initial rates and stoichiometry data published in the literature. Therefore, the results should be considered as rough approximations.
BIOCHLOR	• The BIOCHLOR is accurate for simple groundwater flow conditions. It should not be used in systems where pumping can create a complicated hydrodynamic field. • It assumes constant values throughout the model domain • The sequential biotransformation function in Biochlor should not be used for compounds that are not degraded by first-order sequential kinetics.
BIOSCREEN	• The BIOSCREEN is accurate for simple groundwater flow conditions and should not be used in systems where pumping can create a complicated hydrodynamic field, e.g. cone of depression. • The model should not be used where detailed results that closely match site conditions are required.
CapSim	• The CapSim is designed for the in situ capping method, which assumes stratified soil materials, • 1D reactive transport and only first order decay is considered. • The model is written in the Python language, so it seems that the potential user should be trained in this language to be able to run the simulations.
CDISCO	• The CDISCO only allows 1D permanganate/oxidant transport, no flow simulator embedded • Oxidant transport simulated only up to the radius of influence (ROI) • Biodegradation reactions not included
HSSM	• The HSSM assumes constant values throughout the model domain. It therefore greatly simplifies real site conditions • Flow field is uniform (constant velocity) • Biodegradation of contaminants is not considered
NAS	• The timeframe estimated by NAS for full remediation may be long; • Natural attenuation is subject to natural and anthropogenic changes in local hydrogeological conditions, including changes in groundwater flow direction or velocity, concentrations of electron acceptors and donors, and possible future releases;

	• Hydrological and geochemical conditions suitable for MNA are likely to change over time and could lead to renewed mobility of previously stabilised contaminants (e.g. manganese and arsenic) and reduce the effectiveness of remediation; • Aquifer heterogeneity could complicate site characterisation, as with any remediation approach; • Biodegradation intermediates (e.g. vinyl chloride, VC) may be more toxic than the original compound (e.g. trichloroethene, TCE).