

# ATTACHMENT 19: Guidance for Additional Modeling Needs

[Conceptual Design Process 6](#) involves consideration of additional modeling needs, and includes both narrative guidance and an associated flow diagram. [Figure A19-1](#) includes a decision process to help determine if it is appropriate or feasible to perform more complex ISCO design modeling to help predict oxidant delivery effectiveness, treatment effectiveness, and design costs. The following describes each step of the modeling decision process:

- **Define data objectives** – The primary goal of complex modeling at this stage of the Conceptual Design process should be to increase performance and/or cost certainty. The specific design elements driving uncertainty should be determined prior to considering and selecting a model.
- **Amenability of hydrogeologic / geochemical conditions to modeling** – The site-specific hydrogeologic/geochemical conditions should be considered. Guidelines for certain hypothetical aquifer/source zone conditions have been developed; however these hypothetical studies may or may not be sufficiently adaptable to site-specific conditions.
- **Budget** – Is the project budget able to support an intensive modeling effort and what is the cost-benefit of performing modeling during the conceptual design phase? The project team should consider that additional site data will also be obtained during initial ISCO implementation if the Observational Method is adopted. However, the up-front labor and cost invested in setting up a model can be leveraged during later phases of a remediation project if the ISCO system is to be expanded (which do not require fully calibrated models). The scale of the ISCO design will ultimately be a large factor in evaluating the benefits of modeling during the conceptual design phase.
- **Conceptual Site Model (CSM) completeness** – The CSM should be revisited, taking into consideration data collected as part of [Conceptual Design Process 5](#) to help make sure that model input will be adequately refined to meet data objectives. The [A3. CSM Certainty Evaluation Tool](#) can be used to re- assess the current level and detail of understanding site conditions as they pertain to developing model inputs.

At this stage, it is possible that a numerical model can be used, utilizing data from additional site investigations, bench-scale treatability studies, and/or pilot studies that have been completed at this stage of ISCO Conceptual Design. Simulations specific to the site conditions can be conducted using all the available site data. However, it is necessary to recognize that the available data may not be sufficient to properly calibrate the model. Consequently, the utility of the model may be limited to preliminary analyses, to include: comparing and evaluating alternative strategies (this does not need fully calibrated models) and evaluating the feasibility of delivery schemes.

While a number of numerical model codes exist for simulating both groundwater flow and contaminant transport, there have been few efforts to develop a code for simulating ISCO. Early efforts by Hood (2000), Hood and Thomson (2000), and Zhang and Schwartz (2000) incorporated some of the important processes (second order oxidation, rate-limited or kinetic sorption, and Gilland-Sherwood type DNAPL dissolution mass transfer correlations), but did not incorporate permeability effects of oxidation or oxidant diffusion. Also, these codes are not in the public domain, or based on publicly available flow or transport codes, and so are not readily available for use or modification. Additionally, although reported to incorporate kinetic NOD oxidation, published simulations have treated NOD as an instantaneous sink. In essence, this information means oxidant within a model cell is not available for destroying contaminant until all NOD within that cell has been oxidized. More recently, Heiderscheidt (2005) developed the Chemical Oxidation and Reactive Transport in 3-D (CORT3D) computer code ([S4. CORT3D User's Guide, Install the S5. CORT3D Model Program](#)). CORT3D is based on the publicly available 3-D finite difference multi-component reactive contaminant transport code RT3D version 2.5 (Clement 1997 and 2002) and the publicly available groundwater flow code MODFLOW-2000 (McDonald and Harbaugh

1988, Harbaugh et al. 2000). CORT3D expands the diffusion process to handle each aqueous component independently, adds a chemical oxidation reaction package incorporating second-order contaminant and first-order multi-component NOD oxidation, and adds modules to simulate non-equilibrium DNAPL dissolution and changing permeability from DNAPL dissolution and manganese oxide formation. Development, testing, and documentation of CORT3D (including verification against analytical solutions and other model codes to ensure it properly represents important ISCO-related processes) are fully described by Heiderscheidt (2005). Each of these computer codes was developed for oxidation using permanganate, and a review of available literature has not identified readily available numerical models for other oxidants at the time of this printing. As an example, Heiderscheidt et al. (2008) describe the use of CORT3D in optimizing the injection of permanganate to remediate PCE at the Navy Training Center (NTC) site in Orlando, Florida. [Follow this link to install the CORT3D Model Program.](#)

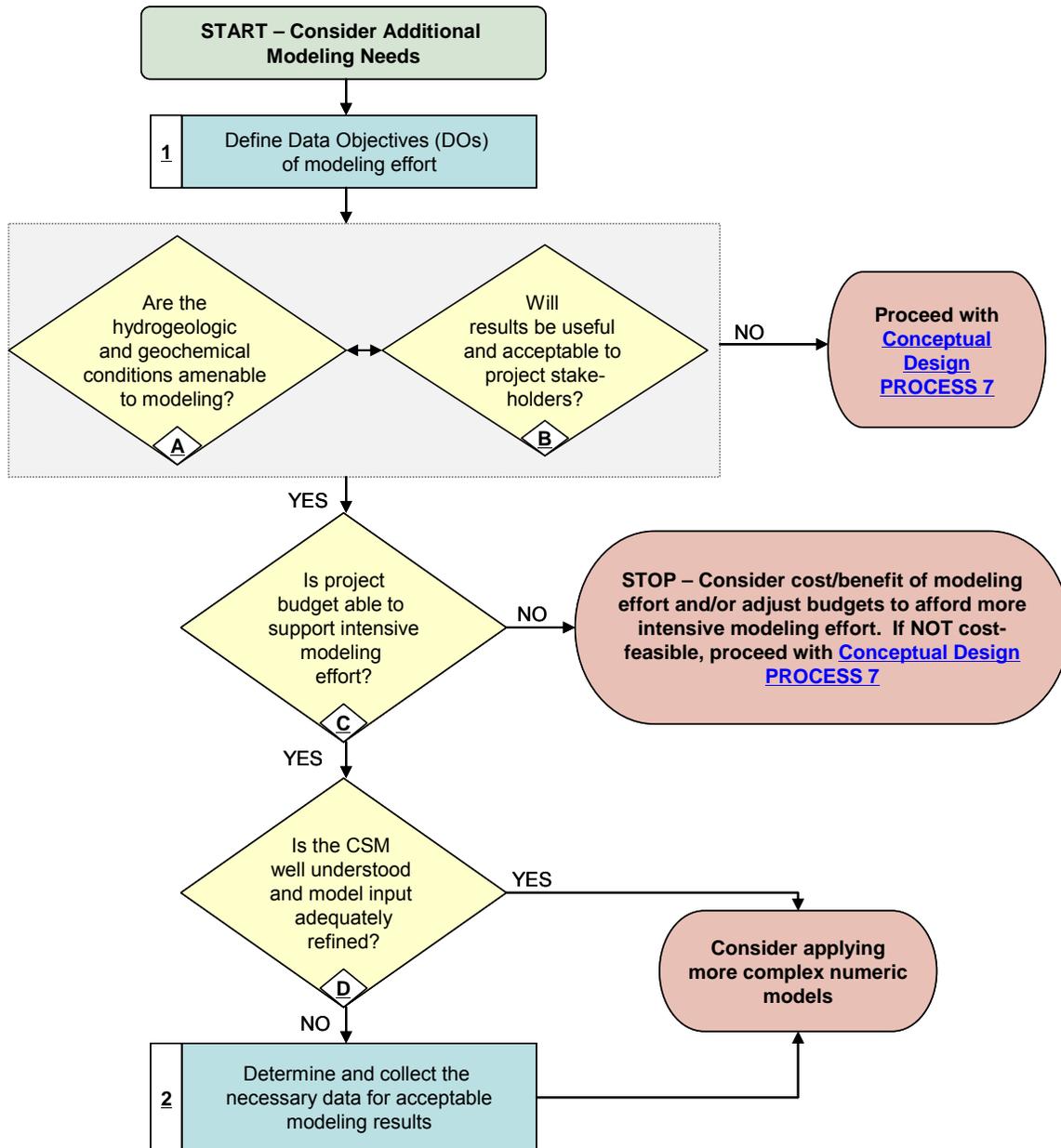


Figure A19-1. Consideration of Additional Modeling Needs Flow Diagram.

The CORT3D-specific input/output parameters are provided in [Tables A19-1](#) and [A19-2](#). Note, the normal flow and transport parameters defining the model discretization in time and space, flow stresses (wells, recharge, drains, rivers, constant head, general head, evapotranspiration), flow model solver, transport processes (advection, dispersion, sinks/sources), and transport solver must also be input.

**Table A19-1. CORT3D Input Parameters.**

Description [units]	Spatially constant, variable, or either?
Aqueous solubility limit for contaminant [ML <sup>-3</sup> ]	Constant
Density of contaminant [ML <sup>-3</sup> ]	Constant
Density of the solid phase (soil grain density) [ML <sup>-3</sup> ]	Constant
Effective density of manganese oxide solids (MnO <sub>2(s)</sub> ) [ML <sup>-3</sup> ]	Constant
Exponent ( $\alpha_2$ ) of Reynolds number in Gilland-Sherwood relationship for natural dissolution of NAPL [-]	Constant
Exponent ( $\alpha_3$ ) of Schmidt number in Gilland-Sherwood relationship for natural dissolution of NAPL [-]	Constant
Exponent ( $\alpha_4$ ) of $\left(\frac{\theta_n d_{50}}{\tau L}\right)$ term in Gilland-Sherwood relationship for natural dissolution of NAPL [-]	Constant
First-order kinetic rate constant for oxidation of the fraction of natural oxidant demand (NOD) with a faster rate [T <sup>-1</sup> ]	Constant
First-order kinetic rate constant for oxidation of the fraction of NOD with a slower rate [T <sup>-1</sup> ]	Constant
Initial (fully) water saturated porosity of porous media [-]	Either
Initial (saturated) hydraulic conductivity, K [LT <sup>-1</sup> ]	Either
Linear sorption coefficient [L <sup>3</sup> M <sup>-1</sup> ]	Constant
Median soil grain size (d50) [L]	Either
Molecular diffusion coefficient for aqueous contaminant [L <sup>2</sup> T <sup>-1</sup> ]	Constant
Molecular diffusion coefficient for chloride [L <sup>2</sup> T <sup>-1</sup> ]	Constant
Molecular diffusion coefficient for permanganate [L <sup>2</sup> T <sup>-1</sup> ]	Constant
Molecular weight of contaminant [MMol <sup>-1</sup> ]	Constant
Pre-multiplier ( $\alpha_1$ ) in Gilland-Sherwood relationship for natural dissolution of NAPL [-]	Constant
Rate-limited sorption mass transfer coefficient [T <sup>-1</sup> ]	Constant
Residual water saturation [-]	Either
Second-order kinetic rate constant for oxidation of contaminant by permanganate [L <sup>3</sup> Mol <sup>-1</sup> T <sup>-1</sup> ]	Constant
Soil Bulk density, $\rho_B$ [ML <sup>-3</sup> ]	Either
Soil tortuosity factor ( $\tau$ ); used in Gilland-Sherwood relationship for natural dissolution of NAPL [-]	Constant
Starting concentration of aqueous contaminant [ML <sup>-3</sup> ]	Either
Starting concentration of chloride (Cl <sup>-</sup> ) [ML <sup>-3</sup> ]	Either
Starting concentration of oxidant (MnO <sub>4</sub> <sup>-</sup> ) [ML <sup>-3</sup> ]	Either
Starting NAPL contaminant saturation [-]	Either
Starting mass fraction of fast NOD [MM <sup>-1</sup> ]	Either
Starting mass fraction of manganese oxide solids (MnO <sub>2(s)</sub> ) [MM <sup>-1</sup> ]	Either
Starting mass fraction of slow NOD [MM <sup>-1</sup> ]	Either
Starting mass fraction of sorbed contaminant [MM <sup>-1</sup> ]	Either
Stoichiometric mole ratio, moles chloride created by destroying one mole of contaminant [MolMol <sup>-1</sup> ]	Constant
Stoichiometric mole ratio, moles manganese oxide created from consumption of one mole permanganate [MolMol <sup>-1</sup> ]	Constant
Stoichiometric mole ratio, moles permanganate consumed to destroy one mole of contaminant [MolMol <sup>-1</sup> ]	Constant

**Table A19-2. CORT3D Output Parameters.**

Description [units]	Spatially constant, variable, or either?
Concentration of each mobile component at designated observation points and effluent, along with total aqueous flow rate at effluent, at end of each iteration [ML <sup>-3</sup> ]	Variable
Cumulative concentration for each mobile component [ML <sup>-3</sup> ]	Variable
Cumulative mass fraction for each immobile component [ML <sup>-3</sup> ]	Variable
Hydraulic head at each observation point at end of each iteration [L]	Variable
Mass fraction of each immobile component at designated observation points at end of each iteration [MM <sup>-1</sup> ]	Variable
Total mass of each immobile component in simulated aquifer at end of each iteration [M]	Variable

## REFERENCES

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