Dense non-aqueous phase liquids: Site remediation and redevelopment

Conceptual site model development

Purpose

This guidance document provides information on how to develop a conceptual site model (CSM) for sites with dense non-aqueous phase liquid (DNAPL). The document outlines what a CSM is, what the 14 compartment model is and how to use it to develop a CSM, and considerations for integrating geologic properties into the CSM. Note that these principles can be used for any site, not just those with DNAPL.

Developing a CSM

As noted on the Characterization guidance, proper site characterization is necessary because an incomplete CSM leads to having an incomplete understanding of the site. This can lead to developing and implementing solutions that are not effective for site management.

What is a conceptual site model?

A CSM provides a comprehensive description of the release mechanism(s), source, geology, hydrology and distribution of contamination in DNAPL, sorbed, aqueous and vapor phases. It answers three fundamental questions about the site: 1) where does the contamination mostly reside? 2) where is contamination being transported?, and 3) what phase(s) does the contamination exist? Appendix C of ITRC, 2011 has a checklist that can be used to develop a CSM.

The 14-compartment model (discussed below) is a tool used to help visualize a CSM and the importance of chemical transport mechanisms within the CSM. Note that CSMs are continuously updated as new information is obtained.

What about DNAPL source zones as part of the CSM?

DNAPL source zones, as noted on the DNAPL Properties guidance are any area of contaminant mass storage that contributes to the dissolved phase plume. Note that in an early stage DNAPL release, a chemical will diffuse into the low permeability matrix, and these low permeability storage units will “back diffuse” as the DNAPL concentration in high transmissive zones decreases over time (mid to late stage release). These storage units become a secondary release source as they sustain the plume in the high transmissive zones (Sale, 2010). Identifying where “primary” and “secondary” release source(s) exist are important factors for developing a proper CSM.

What is the 14-compartment model?

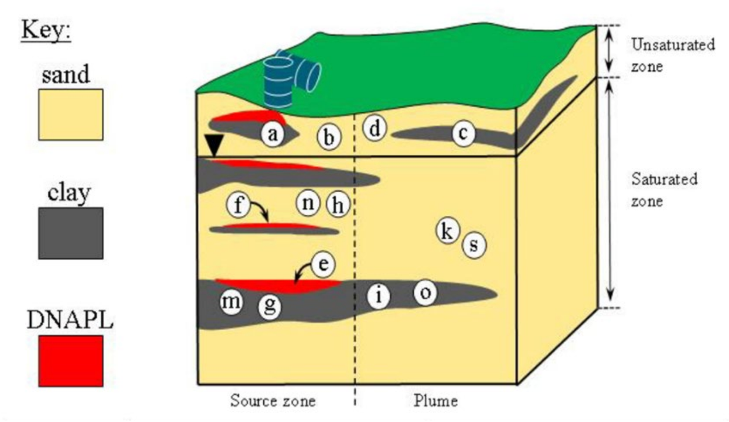
The 14-compartment model (see figure 3-1in ITRC, 2015) is a framework to understand the distribution and movement of contaminants between chemical phases of the source zone and plume at DNAPL sites. Each “compartment” consists of a chemical phase within either the source zone or plume and in either transmissive or low permeability zone. Note that DNAPL, sorbed, and vapor phases exist in the source zone, whereas aqueous and vapor phases are present in both the source zone and plume.

The intent of the model is to show the relative locations of contaminants in each of the 14-compartments as well as the direction in which diffusive mass transfer (i.e. not static mass storage) may be occurring. Diffusive flow is explained on the DNAPL Properties guidance. The model is used to:

- Represent conditions with regard to DNAPL phases and their distribution in transmissive and less permeable zones in the source area and plume.
- Evaluate if mass transfer is advective or diffusive (see DNAPL Properties for an explanation), and if that that transfer is reversible or irreversible
- Conceptualize how the compartments change over time
- Evaluate remedies for specific media by showing how the contaminants may distribute throughout the compartments within the source or the plume.
- Help set remedy goals (Remedy Considerations) by visualizing changes in the compartments over time; this helps evaluate alternatives and their effectiveness.

Steps to develop a CSM

1. Start investigating/characterizing the site (Characterization guidance). During the course of the investigation, ensure that receptors are identified and any mitigative efforts needed to address immediate exposures are taken. Continue to re-evaluate potential risks to receptors as new data are identified.
2. Construct a plan view map. The plan view map should: depict the source of the release, known contaminant concentration extent, receptors (such as utility lines, supply wells, water bodies, etc.), geologic features, groundwater flow direction, sampling locations, etc.
3. Construct a block diagram, a series of cross sections, or a series of fence diagrams that represent the hydrogeology and contaminant distribution for the site using data collected as part of the site characterization (Characterization guidance). The block diagram (or series of cross sections or series of fence diagrams) should depict the water table, areas of low permeability and high transmissive zones, and contaminant locations (vertically and horizontally, as well as above and below the water table).
4. Construct a representative 14-Compartment Model using a block diagram and the table listed below. While each site needs to depict its own hydrogeology and contaminant distribution, the example site below (from figure 2-11a of ITRC, 2011, for an early to mid-stage release where contaminant mass is starting to diffuse into the low permeability zones) demonstrates this concept; it assigns a letter (all lowercase) for each compartment and places it in the model. Note that this example model only shows DNAPL where it has spread laterally at a spill site and does not show ganglia, aqueous, or vapor phase plumes; other phases should be represented where they exist.

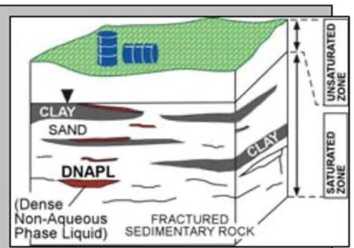


	Source Zone		Plume	
Phase/Zone	**Low Permeability**	**Transmissive**	**Transmissive**	**Low Permeability**
Vapor	a ○	b ○	d ○	c ○
DNAPL	e ○	f ○	**NA**	**NA**
Aqueous	g ○	h ○	k ○	i ○
Sorbed	m ○	n ○	s ○	o ○

5. Depict contaminant concentrations in the 14-compartment model. Place a number in each of the compartments that represents the orders of magnitude (OOM) of contaminant concentration (e.g. a concentration greater than 1 ug /L would be 0, a concentration greater than 10 ug/L would be 1, a concentration greater than 100 ug/L would be 2, etc.). Chemical concentration data obtained from soil, groundwater, and vapor may be used to determine this. Some situations may arise when chemical concentrations are not available (e.g. sorbed in the low permeability in source zone); in these instances values can be estimated by using chemical equilibrium equations (e.g. Raoult's equation, the Ideal Gas equation, Henry's Equation, Instantaneous equilibrium and a constant proportionality). See Sale, 2018 for additional information. Appendix C of ITRC, 2015 describes how to estimate contaminant mass in the 14-compartment model and Appendix B of ITRC, 2011 presents how to apply OOMs at an example site.

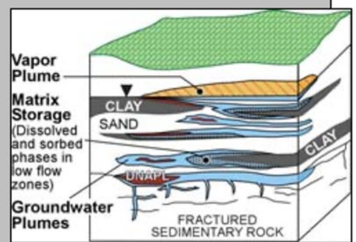
6. Determine the stage of the release based on the actual presence of DNAPL and the amount of mass diffusion into low permeability units and pooling above lower permeability units. Note that DNAPL life cycles at coal tar/creosote sites can be similar to chlorinated solvent sites, but the early stage tends to dominate these sites for long periods of time due to their lower solubility, higher viscosities, and greater hydrophobicity than chlorinated solvents. Use the figure below, which depicts the evolution of a chlorinated solvent release over time,as a guide to determine the stage of the release.

- Early Stage – The majority of the release is present as a DNAPL. Groundwater plumes are just beginning to form and little if any contamination is present in low permeability zones.



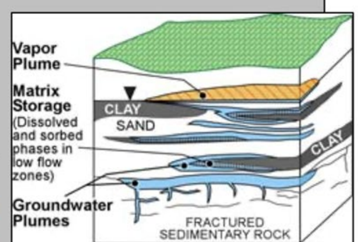
	Source Zone		Plume	
Zone/Phases	Low Permeability	Transmissive	Transmissive	Low Permeability
Vapor	0	2	1	0
DNAPL	0	4		
Aqueous	0	2	1	0
Sorbed	0	2	1	0

- Middle Stage – Much of the original DNAPL release (e.g., 50%) has moved into vapor, aqueous, and/or sorbed phases. Large vapor and/or groundwater plumes may be present and contaminants are present in low permeability zones.



	Source Zone		Plume	
Zone/Phases	Low Permeability	Transmissive	Transmissive	Low Permeability
Vapor	2	2	2	2
DNAPL	2	3		
Aqueous	2	3	3	2
Sorbed	2	3	3	2

- Weathered – DNAPL is absent. Plumes in transmissive zones can be sustained by desorption and/or back diffusion from low permeability layers located in the source zone and plume.



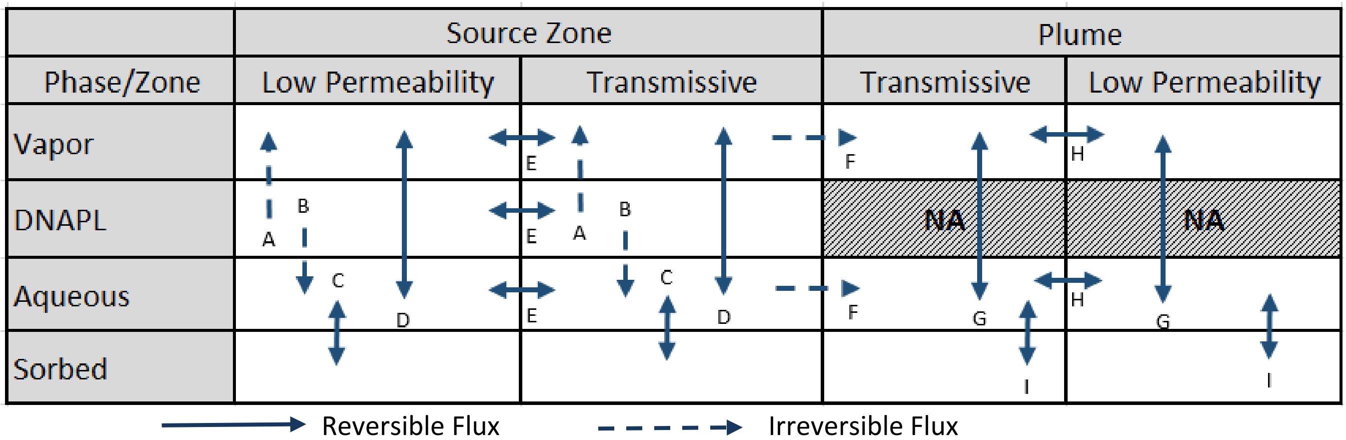
	Source Zone		Plume	
Zone/Phases	Low Permeability	Transmissive	Transmissive	Low Permeability
Vapor	3	2	2	3
DNAPL	1	1		
Aqueous	3	2	2	3
Sorbed	3	2	2	3

From Sale, 2011

7. Evaluate the qualitative transfer of mass flux between compartments by drawing arrows that show reversible and irreversible reactions between compartments. Understanding the mass transfer direction(s) and rate(s) is important to developing a trajectory of the source and plume over time, and this is important to developing a comprehensive CSM.

   All hydrogeologic units are analyzed for their properties and contamination as well as the DNAPL itself. The transmissive units provide advective transport while the lower permeability units initially provide for storage of the DNAPL and pooling above the Lower permeability units. In later stages, DNAPL in the lower permeability units back diffuse into the aquifer and are sources of soil vapor. As a source becomes exhausted and plume structure evolves, compartments that were net recipients of contaminants early in the source/plume development can become net sources of mass transfer late in the plume evolution process.

   The following figure (modified from ITRC, 2011)(m) and corresponding text relates contaminant flux between compartments.



(Note that the letters on this figure correspond to the letters in the source zone and plume characteristics discussed below. They do not refer to the lowercase letters dicussed in step 4 of CSM development)

Mass transfer characteristics

- Can be advective or diffusive (see DNAPL Properties guidance. Transport in transmissive zones is primarily advective, while transport in lower permeability zones and between lower permeability and transmissive zones are primarily by diffusion.
- Advective transfers are irreversible. Diffusive transfers are reversible, with the exception of diffusion-controlled dissolution of DNAPL.
- Transfers between lower and higher permeability zones are predominantly diffusive.
- Diffusive transfers flow from higher chemical potential compartments to lower chemical potential compartments.

Source zone characteristics

A. May include irreversible mass transfer between the DNAPL and vapor phase in both the lower permeability and transmissive zones.

B. May include irreversible mass transfer between the DNAPL and aqueous phase.

C. May include reversible mass transfer between the aqueous and sorbed phases.

D. There can also be reversible mass transfers between the aqueous and vapor phases. Note that this does not involve the DNAPL phase.

E. There can be reversible mass transfer between low permeability and transmissive areas within the source zone and the plume.

Plume characteristics

A. There is an irreversible mass transfer from the vapor and aqueous phases of the source zone into the transmissive zone of the plume. In other words, contamination migrates from the source zone to the plume, but not from the plume to the source zone.

B. There also can be reversible mass transfers between the vapor and aqueous phases in the transmissive zone and in the lower permeability zones. Note that this does not involve the DNAPL phase.

C. There may be reversible mass transfers between the transmissive and the lower permeability zones for vapor and aqueous phases.

D. There may be reversible mass transfers between the aqueous and sorbed phases in the transmissive zone and in the lower permeability zone.

   1. Continue to collect data to characterize your site. Collect data as necessary to fill in data gaps.
   2. Evaluate the model in comparison with potential remedies to obtain the most cost effective solutions (see Remedy Considerations guidance).

Additional geological considerations for a CSM

What about considerations for low permeability zones?

While low-permeability materials (e.g. fine silt, clay) can impede vertical DNAPL migration, that does not mean the presence of a low-permeable zone is protecting groundwater beneath it. This is because variations in grain size, composition, and depositional environments create the same heterogeneities observed in coarser materials, and there may be significant secondary permeability (unsaturated zone clays are commonly fractured, plant roots can cause preferential pathways, erosional events, etc.)

What about fractured bedrock?

As the DNAPL migrates downward, it may come into contact with bedrock where it can diffuse into the rock matrix and migrate through fracture networks until the initial driving head is dissipated and the DNAPL becomes immobile. The DNAPL gradually dissolves into the groundwater within fractures as well as within the rock matrix in contact with the DNAPL. This dissolved-phase material then migrates with water flowing through the fractures, forming a down-gradient plume from the release area. As the plume migrates, molecular diffusion occurs from the plume within the fractures into the bedrock matrix (this process is enhanced with significant matrix porosity). Over time, the dissolved-phase contaminants that have diffused into the matrix then act as an area of back-diffusion into groundwater within the fractures. This process is illustrated on Figure 3-5 of ITRC, 2015. If a silty or clay sediment is present in the bedrock fractures, the sediments may also sorb the contamination and slowly desorb over time.

Additional information on fractured bedrock investigations can be found in ITRC, 2017.

Manage site uncertainty

The CSM development process communicates uncertainty/needs (the systematic planning portion of the Triad approach), which leads to developing streamlined work plans for dynamic work strategies. This leads to collecting reliable data at a greater density than is typically economically feasible with conventional methods (real-time measurement technologies of the Triad approach). Further information can be found on the Triad Resources website.