Appendix D. The 21-Compartment Model

The 21-Compartment Model is a representation of the CSM at an appropriate level of resolution for communicating the occurrence and distribution of contamination, and can help in making decisions for successful characterization, design, and ultimately remediation toward site remedial objectives. The 21-Compartment Model is intended primarily for fractured bedrock under saturated conditions and can be applied at various stages of characterization and remediation, including, but not limited to:

- communicating the distribution of an individual contaminant or nonaqueous phase liquid (NAPL) between less transmissive (such as rock matrix porosity) and more transmissive zones (such as fractures/bedding planes) within the source zone and down gradient from the source zone
- providing an organized framework to assess contaminant mass flux between the source zone and down gradient from the source zone, and between relevant compartments within the source and down gradient regions
- communicating the distribution of an individual contaminant or NAPL over time between less transmissive and more transmissive zones, and between the source area and down gradient from the source area
- identifying data gaps in site characterization or the remedial investigation
- establishing SMART functional objectives for remediation
- screening remediation technologies
- communicating the rationale for monitoring within the source zone or down gradient from the source zone (whether to monitor more transmissive zones, or to monitor for potential rebound from the matrix, or back-diffusion).

Visual models, based on site characteristics, provide a logical and fundamental basis for discussion and understanding among all parties involved during the development of a remedial strategy. After the initial compartments are filled in with what is known about the site, the need for more characterization to develop an accurate and usable model for decision-making is often the next step. This model is also useful for presentation of site-specific remedial concerns to other interested parties and stakeholders. The 21-Compartment Model, is not a replacement for the CSM but rather a tool that can be used in conjunction with, and help communicate key elements of, the CSM.

For contaminant mixtures in the 21-Compartment Model, such as chlorinated solvents and fuels (such as gasoline or diesel), these can occur in four phases in the source zone (DNAPL or LNAPL, aqueous, sorbed, and vapor) and three phases in the plumes (per NRC 2005, there is no DNAPL or LNAPL in plumes). Each of these phases can occur in subsurface zones that can be classified as “transmissive” (mobile) or “lower permeability” (immobile).

Table C-1 shows the 21-Compartment Model in blank tabular form. One way to use the 21-Compartment Model is to use qualitative estimates, or ranges, of the potential chemical concentration (or potential) in each compartment as relevant to a particular site. Colors may additionally be assigned to the ranges. Then, mass transfers between compartments can be anticipated as contaminants flow from zones of higher chemical potential to zones of lower chemical potential. The transfers may be advective or diffusive. Table C-2 shows the transfers that are possible among the various compartments.

Table D-1. The 21-Compartment Model in blank tabular format

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor*						
NAPL*				NA	NA	NA
Dissolved						
Sorbed						

*Would not apply to contaminants (such as metals) for which there is no liquid or vapor phase.

Table D-2. The 21-Compartment Model with common contaminant fluxes between compartments (Solid arrows are reversible fluxes; dashed arrows are irreversible fluxes.)

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor						
NAPL				NA	NA	NA
Dissolved						
Sorbed						

Note that flux lines shown are intended to convey the qualitative direction of flux, but not the quantitative value of the flux

In the Integrated DNAPL Source Strategy (ITRC 2011) guidance, a 14-Compartment Model, for application to unconsolidated media, was introduced. For a more thorough discussion for how the 14-Compartment Model, and by extension this 21-Compartment Model can be applied, refer to that document. This document highlights a few key applications of the 21-Compartment Model for saturated fractured bedrock, including applying the 21- Compartment Model to development of the CSM for a contaminated fractured bedrock site, and an example for using the 21-Compartment Model to screen remedial technologies for sites with contaminated saturated fractured bedrock. The examples shown are mostly sites with DNAPL release to illustrate the use of the 21-Compartment Model, but the same concepts can be applied to individual contaminants or to other mixed contaminants such as LNAPL, based on their unique fate and transport characteristics.

D.1 CSM and the 21-Compartment Model

After generating an initial CSM for a bedrock site, but prior to performing site characterization, the 21-Compartment Model can be applied to further develop the CSM in subsequent iterations, and then be used as a tool during remediation alternative screening. The 21-Compartment Model applies generally to three common fractured bedrock settings: uncemented sandstone, shale, and granite. In these settings, a contaminant mass may be distributed among the various compartments and the mass distribution can change over time, which can be taken into account in the site characterization objectives. The 21-Compartment Model may then be revisited following the site characterization and refinement of the CSM to determine how the site understanding may have changed because of characterization activity.

Table D-3a fills in the 21-Compartment Model to represent a hypothetical site underlain by uncemented sandstone just after a DNAPL spill occurred. At this stage, the chemical potential in the DNAPL phase is high, and there has been little mass transfer into other compartments. At this early stage of spill site maturation, the mass transfers are primarily from the DNAPL into other compartments. Note for uncemented sandstone that contaminant mass is shown to be present in matrix storage and fracture flow, but also to be present in matrix flow (flow through the relatively porous/transmissive rock matrix associated with uncemented sandstone).

In transmissive zones (within secondary porosity features such as fractures and bedding planes) aqueous- or vapor-phase contaminants (here, chlorinated solvents) are carried with the flow of water or soil gas. In contrast, low-permeability zones (primary porosity) are largely stagnant from a flow perspective. Critically, low-permeability zones store and release contaminants via diffusion (Freeze 1979; Sudicky 1986; Parker 1994; Chapman 2005; Sale 2008).

Table D-3a. The 21-Compartment Model for the early-stage DNAPL spill site underlain by sedimentary bedrock (uncemented sandstone).

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Low	Medium	Medium	Medium	Medium	Low
NAPL	Low	Low	High	NA	NA	NA
Dissolved	Low	Medium	Medium	Medium	Medium	Low
Sorbed	Low	Low	Medium	Medium	Medium	Low

Table D-3b shows the same hypothetical site underlain by uncemented sandstone, but after a period where the contaminants, and in particular the DNAPL, have partitioned to other compartments. This is a middle stage representation characterized by an absence of DNAPL, and increase dissolved phase concentrations. In addition, this middle stage is characterized by matrix diffusion whereby high dissolved concentrations are diffusing into the rock matrix, which later acts as a reservoir of sustained dissolved contamination through back-diffusion.

Table D-3b. The 21-Compartment Model for the mid-stage DNAPL spill site underlain by sedimentary bedrock (uncemented sandstone).

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Medium	Medium	Medium	Medium	Medium	Medium
NAPL	Medium	Medium	Medium	NA	NA	NA
Dissolved	Medium	Medium	Medium	Medium	Medium	Medium
Sorbed	Medium	Medium	Medium	Medium	Medium	Medium

Table D-3c shows the same hypothetical site underlain by uncemented sandstone, but after a longer period where the contaminants, and in particular the DNAPL, have partitioned to other compartments, and high concentrations of dissolved contaminant have attenuated. This late stage is characterized by an absence of DNAPL and a decrease in previously high dissolved phase concentrations. This late stage is also characterized by back-diffusion, with dissolved concentrations diffusing from the rock matrix back into fractures, which may sustain concentrations above cleanup levels.

Table D-3c. The 21-Compartment Model for the late-stage spill site underlain by uncemented sandstone.

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Low	Low	Low	Low	Low	Low
NAPL	Low	Low	Low	NA	NA	NA
Dissolved	Low	Low	Low	Low	Low	Low
Sorbed	Low	Low	Low	Low	Low	Low

Tables D-4a through D-4c illustrate the same three stages as applied to a site underlain by shale bedrock. Note for shale bedrock that matrix flow is not present, and these compartments are shaded out as not applicable. Otherwise the progressive partitioning of contaminant mass is similar over time to the uncemented sandstone.

Table D-4a. The 21 Compartment Model for the early-stage DNAPL spill site underlain by shale.

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Low	NA	Medium	Medium	NA	Low
NAPL	Low	NA	High	NA	NA	NA
Dissolved	Low	NA	Medium	Medium	NA	Low
Sorbed	Low	NA	Medium	Medium	NA	Low

Table D-4b. The 21 Compartment Model for the mid-stage DNAPL spill site underlain by shale.

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Medium	NA	Medium	Medium	NA	Low
NAPL	Low	NA	Medium	NA	NA	NA
Dissolved	Medium	NA	Medium	Medium	NA	Low
Sorbed	Medium	NA	Medium	Medium	NA	Low

Table D-4c. The 21 Compartment Model for the late-stage spill site underlain by shale.

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Low	NA	Low	Low	NA	Low
NAPL	Low	NA	Low	NA	NA	NA
Dissolved	Low	NA	Low	Low	NA	Low
Sorbed	Low	NA	Low	Low	NA	Low

Tables 5a through 5c illustrate the same three stages as applied to a site underlain by granite bedrock. Note for granite bedrock that matrix flow is not present, and matrix storage is considered negligible. Otherwise the progressive partitioning of contaminant mass is similar over time as compared with the uncemented sandstone.

Table D-5a. The 21 Compartment Model for the early-stage DNAPL spill site underlain by granite.

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Negligible	NA	Medium	Medium	NA	Negligible
NAPL	Negligible	NA	High	NA	NA	NA
Dissolved	Negligible	NA	Medium	Medium	NA	Negligible
Sorbed	Negligible	NA	Medium	Medium	NA	Negligible

Table D-5b. The 21 Compartment Model filled in for the mid-stage DNAPL spill site underlain by granite.

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Negligible	NA	Medium	Medium	NA	Negligible
NAPL	Negligible	NA	Medium	NA	NA	NA
Dissolved	Negligible	NA	Medium	Medium	NA	Negligible
Sorbed	Negligible	NA	Medium	Medium	NA	Negligible

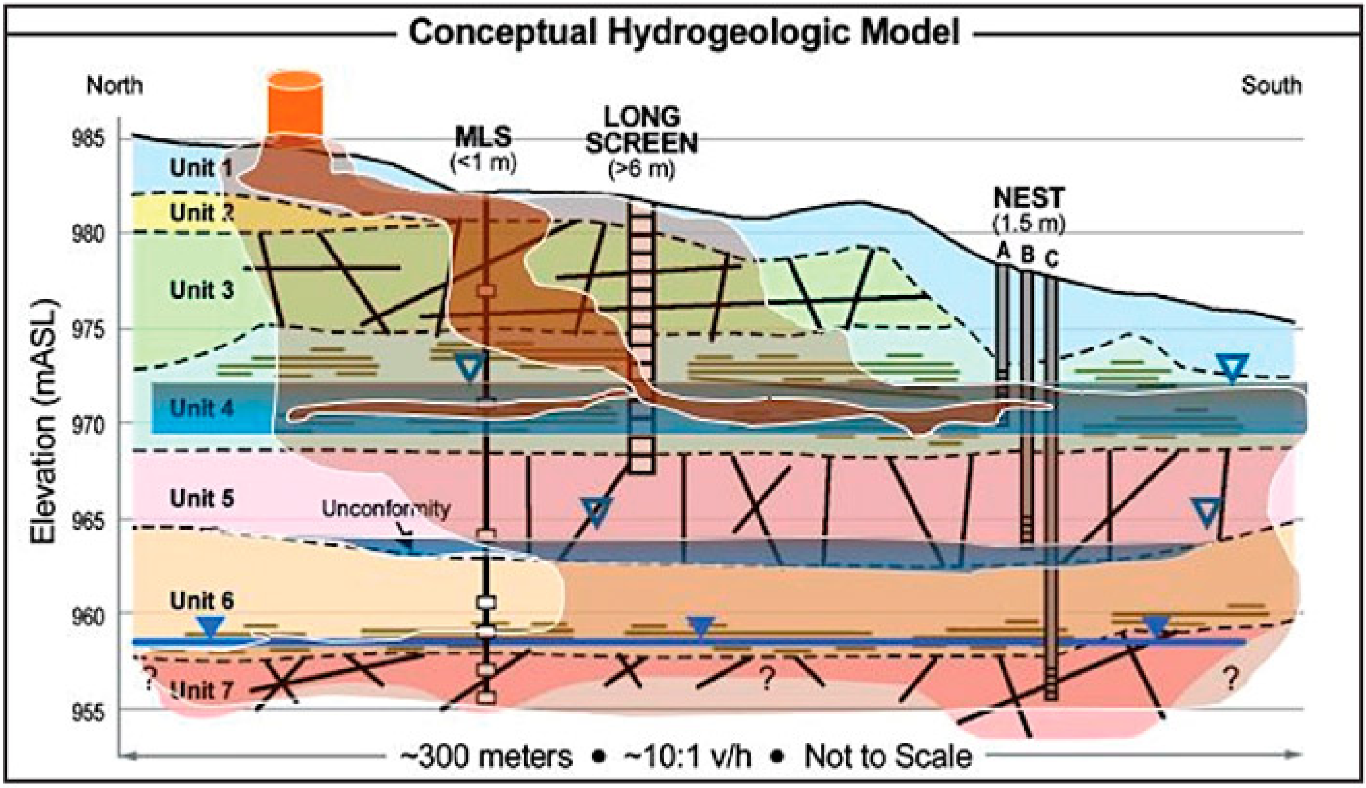
Table D-5c. The 21 Compartment Model filled in for the late-stage DNAPL spill site underlain by granite.

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Negligible	NA	Low	Low	NA	Negligible
NAPL	Negligible	NA	Low	NA	NA	NA
Dissolved	Negligible	NA	Low	Low	NA	Negligible
Sorbed	Negligible	NA	Low	Low	NA	Negligible

For both the sedimentary and igneous examples above, the transmissive zones of early stage plumes contain the highest VOC concentrations in their sources, particularity near the DNAPL phase. For sedimentary rock with significant primary porosity, over time the early-stage DNAPL phase, based on aqueous-phase equivalent concentration, is diminished by advection, biotic and abiotic degradation, and mass transfer into lower-permeability regions (the matrix porosity) and other chemical phases within the source as well as the plume. In a middle stage, the aqueous-phase equivalent concentrations across affected phases and zones are relatively equal. In late-stage plumes, contaminant concentrations have attenuated in the more permeable (transmissive) zones, and the larger remaining concentrations (again only in the sedimentary bedrock example, but not the case with the granite example that has little or no appreciable matrix porosity) remain in the lower-permeability zones within both the source and the plume.

These concepts are a useful tool to develop objectives for site characterization planning and ultimately can be revisited and refined as with the CSM for later remediation and monitoring.

After completing the site characterization, and subsequently refining the CSM, the 21-Compartment Model can be revisited and refined for better decision making. Figure D-6 shows an example of what the 21-Compartment Model might look like following site characterization and refinement of the CSM. For this example, a site illustration is superimposed above the 21-Compartment Model. The table below is filled in to present the CSM at level of resolution that can be communicated to those involved in project planning. Specifically, the first table below the site illustration shows the understanding of the relative distribution of contaminants after site characterization. An additional table presents an interpolation of where the contaminant mass may be over time. This version of the 21-Compartent Model can be used to communicate key information gained from the site characterization for use in decision making during remediation planning followed by monitoring.



CURRENT						
	Source Zone			Downgradient Extent		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor		low			low	
Napl		low		NA	NA	NA
Dissolved		low			low	
Sorbed		low			low	
5 - 10 YEARS						
	Low or Non Transmissive	Transmissive		Transmissive		Low or Non Transmissive
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor		low			low	
Napl		low		NA	NA	NA
Dissolved		low			low	
Sorbed		low			low	

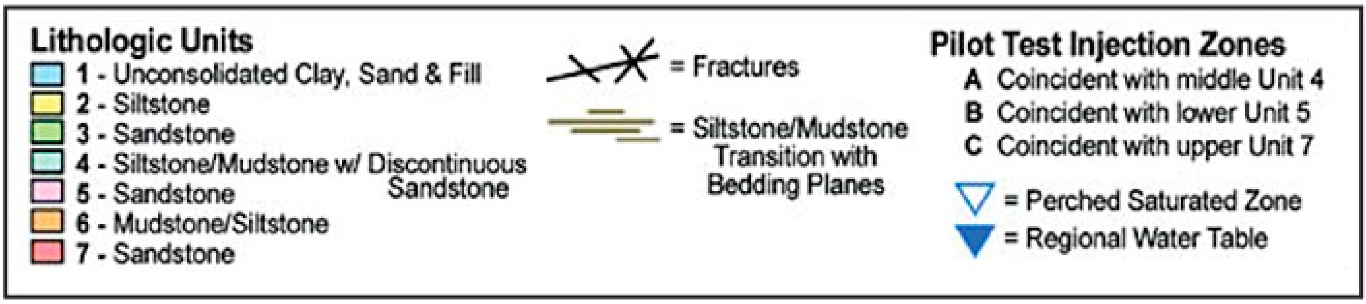


Figure D-6. The 21-Compartment Model combined with site illustration.

Source of Conceptual Hydrogeologic Model: Jim Studer, InfraSUR LLC 4/2/17.

D.2 Technology Screening with the 21-Compartment Model

The 21-Compartment Model presents features of the CSM that aid in understanding and communicating how contaminants are moving and changing over time between the different compartments. This model generally divides the source area and extent of dissolved contaminants into areas of high transmissivity (fracture flow, matrix flow) and areas of low relative transmissivity (matrix porosity). The 21-Compartment Model can also be used for screening alternative remedial approaches, or in the evaluation of individual technologies, and as a tool to communicate combined remedy strategies.

As illustrated in Figures D-7 and D-8 (a through d), the 21-Compartment Model can be applied to evaluating remedial objectives, and for technology screening and for the development and evaluation of alternative remedial approaches. A more quantitative approach to perform this evaluation was discussed in ITRC guidance (ITRC 2011) but is not repeated here. The qualitative approach is applied as follows:

1. Functional objectives are identified and illustrated using the 21-Compartment Model (Figure D-7). For this example, the first absolute objective is protection of human health by reducing the risk of vapor intrusion and the environment by reducing dissolved concentrations below cleanup levels.
2. The remedial strategy under consideration is source area treatment to reduce dissolved contaminant concentrations (PCE DNAPL in this example), which will result in attenuation of dissolved contaminant concentrations down gradient of the source area. The reduction in dissolved concentrations additionally reduces the vapor intrusion risk in the source area and ultimately downgradient from the source area.
3. A remedial approach employing pump and treat technology in the source area is screened first (Figure D-8a). Assuming adequate characterization and mapping of fractures, pump and treat has the potential to significantly reduce dissolved concentrations in the source area, particularly in relatively transmissive fracture flow zones (within the secondary porosity) of the fractured rock. However, even with adequate characterization and mapping of fractures and fracture flow paths, pump and treat may not be effective for addressing contaminant mass present within the matrix porosity of the rock. Upon termination of pump and treat operations, back-diffusion of contaminants from this matrix porosity compartment may result in rebound of dissolved-phase contaminants in groundwater in the transmissive fracture zones. This rebound could lead to an extended remediation life cycle and increased costs compared to more other technologies that may be more effective for contaminants in the rock matrix.
4. Figure D-8b illustrates screening of in situ chemical oxidation (ISCO) using a strong, but relatively short-lived oxidant such as catalyzed hydrogen peroxide. In this case, the strong oxidant can be effectively distributed through the relatively transmissive fracture zones but, due to the short oxidant lifetime, cannot penetrate the rock matrix to address the contaminant mass in the matrix storage compartment. The potential for posttreatment back-diffusion and for not meeting functional objectives can resemble that of pump and treat.
5. Figure D-8c illustrates the screening of ISCO using a longer-lasting oxidant, such as permanganate. In this case (as again assuming adequate characterization and mapping of fractures and groundwater flow paths), the oxidant may effectively destroy contaminants within the transmissive fractures. In addition, due to the longer lifetime of the oxidant and associated chemical gradients, the oxidant persists and can itself diffuse into the matrix porosity. The result may be effective treatment of contaminants in both the transmissive and nontransmissive zones of the fractured rock source area, resulting in mitigation of indoor vapor risks and down gradient dissolved concentrations as therefore meeting the functional objectives more effectively.
6. Figure D-8d illustrates screening of a thermal remediation technology, such as in situ thermal desorption or electrical resistivity heating, for source area treatment. As with the alternative approach using a strong and long lasting ISCO reagent, this alternative also offers the potential to address contaminants in both the transmissive fracture zones as well as less transmissive zones (matrix porosity). Again, the result may be effective treatment of contaminants in both the transmissive and nontransmissive zones of the fractured rock source area, resulting in mitigation of indoor vapor risks and downgradient dissolved concentrations as therefore meeting the functional objectives more effectively.

In this example, the selection of either a strong and long lasting ISCO reagent, or the use of thermal remediation technology, may be able to meet the functional objectives. Other site-specific factors need to be considered before ultimately selecting the remedial approach for a site, but the use of the 21-Compartment Model provides insight into the potential effectiveness, strengths, and weaknesses of individual remedial approaches.

Figure D-7. Identification of functional objectives for remedial approach (uncemented sandstone impacted by an early- to midterm release of PCE DNAPL).

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Medium	Medium	Medium	Medium	Medium	Low
NAPL	Medium	High	High	NA	NA	NA
Dissolved	Medium	Medium	Medium	Medium	Medium	Low
Sorbed	Medium	Medium	Medium	Medium	Medium	Low

Figure D-8a. Remedial approach targeting pump and treat (uncemented sandstone impacted by an early- to midterm release of PCE DNAPL).

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Medium	Medium	Low	Medium	Medium	Low
NAPL	Medium	High	Medium	NA	NA	NA
Dissolved	Medium	Medium	Low	Medium	Medium	Low
Sorbed	Medium	Medium	Low	Medium	Medium	Low

Figure D-8b. Remedial approach targeting ISCO with short lasting reagent (uncemented sandstone impacted by an early- to midterm release of PCE DNAPL).

	SOURCE ZONE			DOWNGRADIENT EXTENT		
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Medium	Medium	Low	Medium	Medium	Low
NAPL	Medium	High	Medium	NA	NA	NA
Dissolved	Medium	Medium	Low	Medium	Medium	Low
Sorbed	Medium	Medium	Low	Medium	Medium	Low

Figure D-8c. Remedial approach targeting ISCO with longer lasting reagent (uncemented sandstone impacted by an early- to midterm release of PCE DNAPL).

	Low or Non Transmissive	Transmissive		Transmissive		Low or Non Transmissive
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Low	Low	Low	Medium	Medium	Low
NAPL	Low	Low	Low	NA	NA	NA
Dissolved	Low	Low	Low	Medium	Medium	Low
Sorbed	Low	Low	Low	Medium	Medium	Low

Figure D-8d. Remedial approach targeting thermal remediation.

	Low or Non Transmissive	Transmissive		Transmissive		Low or Non Transmissive
	Matrix Storage	Matrix Flow	Fracture Flow	Fracture Flow	Matrix Flow	Matrix Storage
Vapor	Low	Low	Low	Medium	Medium	Low
NAPL	Low	Low	Low	NA	NA	NA
Dissolved	Low	Low	Low	Medium	Medium	Low
Sorbed	Low	Low	Low	Medium	Medium	Low