

Section 5.0
LNAST USER'S GUIDE

This chapter provides guidance on how to use the toolkit software utility (LNAST; **LNAPL Dissolution and Transport Screening Tool**) to evaluate LNAPL impacts to groundwater under a range of conditions. First, an overview of the program menus and structure will be given. The reader will then be guided through data input, with a discussion of the parameter selection process. Chapter 6 will provide some example problems and recommendations will be given for execution of a site screening.

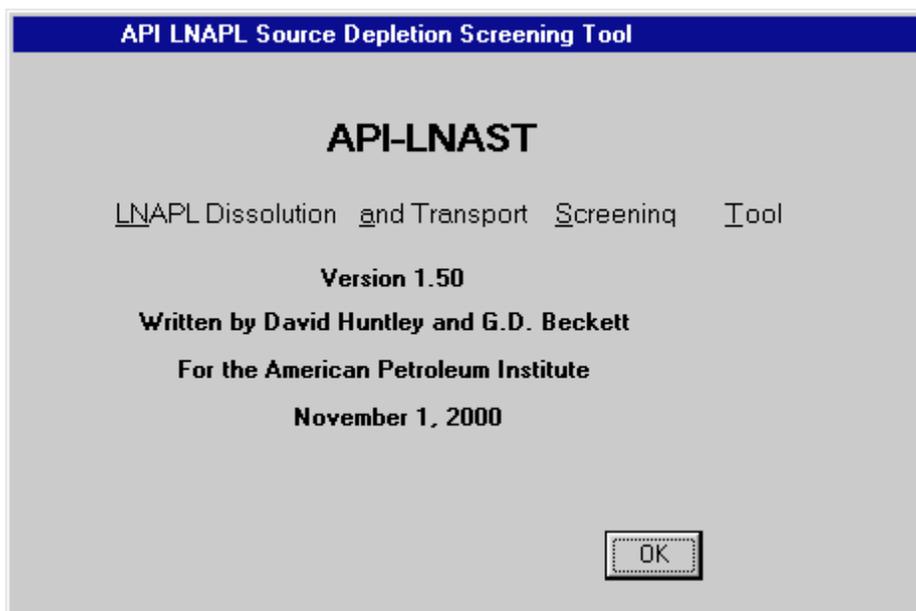


Figure 5-1, LNAST introduction screen. Select **OK** to start the program.

It is recommended that you open up the LNAST software utility for viewing as you read this section. The first window displayed is a software title screen giving version and date information (Figure 5-1). Clicking the **OK** button will take the user to the input and execution menus of the utility (Figure 5-2). Again, details of the entries and execution will be given after the general overview below.

5.1 SOFTWARE UTILITY OVERVIEW

As discussed above, the LNAST software utility was written to calculate (1) the depletion of soluble or volatile components from a multicomponent LNAPL source area, followed by (2) the downgradient movement of a dissolved phase, subject to biodegradation and dispersion. The sequence of steps the user must undertake is critical to the successful use of the program.

First, the user must select and input the appropriate soil, groundwater, and LNAPL physical and chemical properties. This is done through a series of five input tabs in the LNAPL utility, identified as "Soil Properties", "Groundwater Conditions", "Source Area Parameters", "LNAPL Properties", and "Solute Transport Properties".

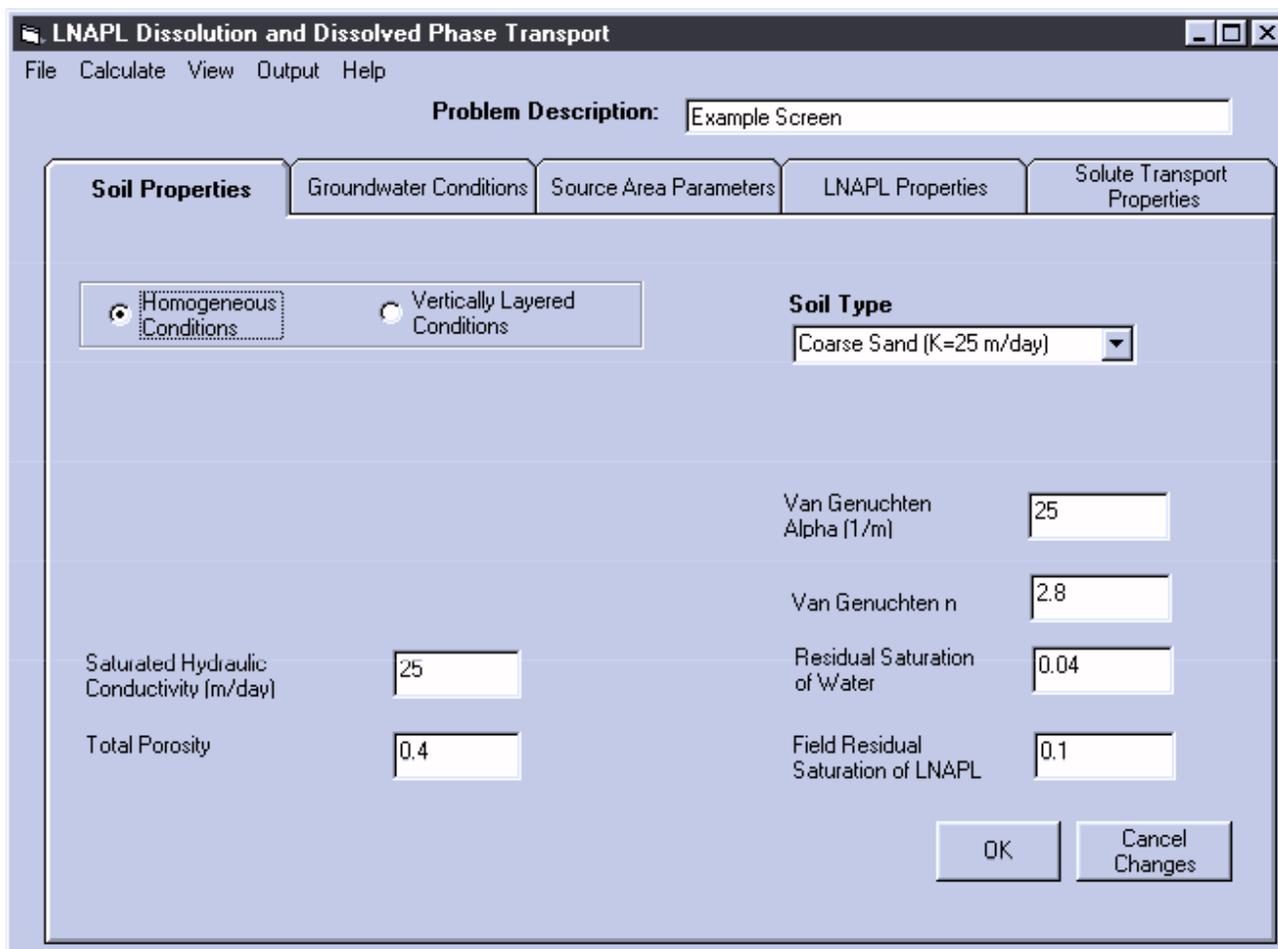


Figure 5-2. The **Soil Properties** Tab, with a homogeneous conditions and coarse sand selected.

Second, the user must direct the program to calculate the depletion of LNAPL source through dissolution and/or volatilization. This is done by selecting LNAPL Source Depletion found under the CALCULATE menu option. Based on the data previously input, the software utility first calculates LNAPL mass, distribution, and the fractions of chemicals of concern. Multiphase fluid mechanics are used to calculate the groundwater flow through the LNAPL zone, and chemical transport principles are linked to estimate advective and dispersive chemical losses from the LNAPL source. The result of this series of calculations is the dissolved phase concentration of each of the specified LNAPL components in the source area (i.e. in contact with the LNAPL) as a function of time. These results may be displayed, printed, or copied as either a table of values, a graph, or both.

Third, the results of the LNAPL source depletion calculation are used to calculate the resulting downgradient dissolved phase concentrations for each of the soluble components using the Domenico (1987) analytic solution to the three-dimensional solute transport equation under one-dimensional groundwater flow conditions. The user initiates this step by selecting Downgradient Dissolved Phase, again found under the CALCULATE menu option. It is important to note that the user must first select calculation of the LNAPL source depletion before the downgradient dissolved

phase calculations can be done. In addition, if any soil, groundwater condition, source area parameter, or LNAPL property is changed, the LNAPL source depletion calculations must be completed before any downgradient dissolved phase calculations are undertaken. The output from the source area depletion calculations are used as input to the downgradient dissolved phase calculations. As for the LNAPL source depletion calculations, the downgradient dissolved phase calculations may be displayed, printed, or copied as either a table of values, a graph, or both.

5.2 LNAOST MENU OPTIONS

The LNAOST software utility is organized as a standard Microsoft Windows program. Five pull-down menu options (**File**, **Calculate**, **View**, **Output**, and **Help**) are found along the top of the active window (Figures 5-2 and 5-3). The **File** menu (Figure 5-3) selection allows the user to start a **New Project**, to **Open** (an existing) **Project**, to **Save Project** using the existing file name, to **Save Project As** a new file name, or to **Exit** the program. Starting a **New Project** sets all of the parameters to their default values. This is automatically done when the user starts the program, but the user may wish to do this after completion of a series of calculations as a fast way to re-initialize everything before entering a new data set. **Open Project** will initiate a standard file open window, which allows the user to find and open a project file that has been previously saved. It is not necessary or appropriate to do this when initiating a new project. **Save Project** and **Save Project As** are the standard file save menu options in the Windows environment. **Save Project As** opens a file directory window, that allows you to specify a new file name (and directory location) to save your project information. The option **Save Project** simply saves the project under the last filename used. Finally, the **Exit** menu option is self-explanatory.

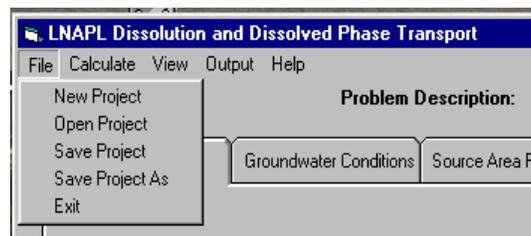


Figure 5-3. The **File** pulldown menu has several options for managing and saving calculation input files.

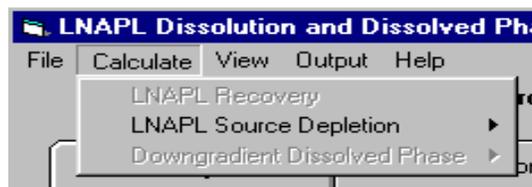


Figure 5-4. The **Calculate** menu.

The **Calculate** menu option (Figure 5-4), as discussed above, is where the user initiates calculation of the LNAPL source depletion and the downgradient dissolved phase calculations. In addition, if the user wants to calculate LNAPL source depletion (by dissolution and/or volatilization) after LNAPL recovery, the user will first select **LNAPL Recovery** from the **CALCULATE** menu option prior to calculating LNAPL source depletion. Both the **LNAPL Source Depletion** and the **Downgradient Dissolved Phase** menu items provide further choices for the user. The **LNAPL**

Source Depletion calculation may be done with or without volatilization. Under **Downgradient Dissolved Phase**, the user has the choice of either calculating **Downgradient Extent** or **Concentrations at Selected Distances**. In the first case (**Downgradient Extent**), LNAST calculates the maximum downgradient distance where each dissolved phase compound exceeds a *target concentration*, which is a user-input variable, as a function of time. In the second case (**Concentrations at Selected Distances**) the concentration/time history is calculated at up to 20 user-selected distances from the source area. In both cases, concentrations are calculated along the centerline directly downgradient of the center of the source area at the water table. Because of this, the concentrations and downgradient distances calculated by the software utility are often higher than concentrations typically observed in the field because those are often measured in wells screened across intervals that exceed the thickness of the source area and may or may not be located exactly along the axis of the plume.

The **View** menu option (Figure 5-5) allows the user to go back and view the results of the active calculations. These results are displayed as tables, but graphs may also be created from the **Graph** menu selection found at the top of each table. The user may view **Hydrocarbon Saturation Distribution** and/or **Source Depletion** results only after calculation of the **LNAPL Source Depletion** calculations (under the **Calculate** menu option). The user may view **Downgradient Dissolved Phase** results only after the downgradient dissolved phase calculations are complete.

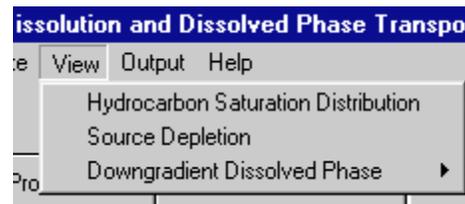


Fig. 5-5. The **View** Menu

The **Output** menu (Figure 5-6) option allows the user to save tabulated results of either the LNAPL source depletion calculations or the downgradient dissolved phase calculations as a tab-delimited file.

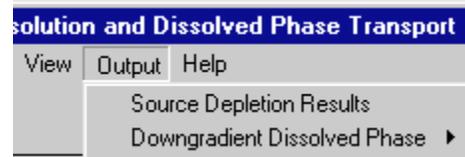


Fig. 5-6. The **Output** Menu

For the current LNAST version (1.50), the **Help** menu option only brings up the starting screen, the window that supplies the date and version number of the program, for reference (Figure 5-1).

5.3 DATA INPUT

Users familiar with multiphase fluid mechanics and fate and transport principles may not require much guidance, but we still recommend reviewing parameter definitions used here as they may be slightly different from those you have used in the past. Screening models like this toolkit can simplify the evaluation of complex multiphase flow, multicomponent partitioning and associated chemical transport. It should be kept in mind, however, that highly erroneous results can be generated if you fail to account for parameter uncertainty and the sensitivity of the results to your input assumptions and site conceptual model. Almost certainly you will need to consider a range of site conditions to gain a full spectrum of reasonable results. Similarly, you will need to think carefully about the applicability of certain assumptions inherent in the definition of the LNAPL source term and all the other related factors. We will do our best to give you a feeling for the most critical aspects in general, but it is most important that you recognize how to place results in site context. For instance, if site groundwater concentrations exhibit characteristics indicative of a depleting LNAPL source, it would be inappropriate to select a source term that results in a large mass and correspondingly extensive long-term impacts. In other words, always ask “Does this make any sense at all with what we see at the site?” If the answer is no, it does not mean physics and chemistry have failed you, it means that one of the critical assumptions or interpretation of the results are not representative and require reevaluation.

Lastly, you will clearly have a better idea of where to start and how to assign input parameters if you measure key data at the site. A first cut of screening evaluations can certainly be performed using judgment and inferential information, and this is often a good step to defining the data most important for more refined evaluations. Given the large number of linked parameters, one may be able to generate a site conceptual model that appears representative, only to find on measurement that some key factors require revision. Solutions from multivariate models are usually non-unique, meaning more than one set of parameters can result in similar results.

As with any scientific calculation, use of consistent units is mandatory. A shareware program called “UNITS” is available on the World Wide Web that can assist in unit conversions (<http://www.steamestem.com>, select the units conversion frame).

As noted above, the software utility calculations are based on the assignment of five linked categories of data: 1) Soil petrophysical characteristics; 2) Prevailing groundwater flow conditions; 3) Description of the LNAPL source distribution in the formation; 4) Chemical and physical properties of the LNAPL and its components of risk concern; 5) Solute transport properties. The user tabs of LNAST coincide with the 5 parameters groups defined above, and will be described in order in the sections that follow.

5.3.1 Soil Properties

Soil parameters may be input assuming either that the soil is homogeneous, or by subdividing the vertical LNAPL impacted zone into up to five layers. The user makes this choice by selecting either the *Homogeneous Conditions* (Figure 5-7) or the *Vertically Layered Conditions* (Figure 5-8) option button on the **Soil Properties** tab. If the user selects *Homogeneous Conditions*, a single value of *Soil Type*, *Saturated Hydraulic Conductivity*, *Total Porosity*, *Van Genuchten Alpha*, *Van Genuchten n*, *Residual Saturation of Water*, and *Field Residual Saturation of LNAPL* (Figure 5-7) are entered.

The image shows a software dialog box titled "Soil Properties" with five tabs: "Soil Properties", "Groundwater Conditions", "Source Area Parameters", "LNAPL Properties", and "Solute Transport Properties". The "Soil Properties" tab is active. It contains two radio buttons: "Homogeneous Conditions" (selected) and "Vertically Layered Conditions". To the right is a "Soil Type" dropdown menu showing "Fine Sand (K= 1 m/day)". Below these are several input fields: "Saturated Hydraulic Conductivity (m/day)" with value "1", "Total Porosity" with value "0.4", "Van Genuchten Alpha (1/m)" with value "7.5", "Van Genuchten n" with value "1.9", "Residual Saturation of Water" with value "0.15", and "Field Residual Saturation of LNAPL" with value "0.14". At the bottom right are "OK" and "Cancel Changes" buttons.

Figure 5-7. The **Soil Properties** Tab, with *Homogeneous Conditions* selected for a fine sand.

If the **Vertically Layered Conditions** option is selected (Figure 5-8), values for each of these parameters must be selected for each of the different layers. Prior to entering the parameters for each layer, the number of layers and the thickness of each layer must be entered. This is done by first entering a value between 2 and 5 under *Number of Soil Layers*. Then, in the adjacent box, each layer number is selected sequentially, starting with layer 1, the lower-most layer, and ending with the upper-most layer. As each layer is selected, the thickness of that layer is entered. Note that the elevation of the bottom of layer 1 is fixed at 0.0 (Figure 5-8) and that the elevation of the bottom of each subsequent layer is the sum of the bottom elevation and the thickness of the previous layer. The soil parameters *Soil Type*, *Saturated Hydraulic Conductivity*, *Total Porosity*, *Van Genuchten Alpha*, *Van Genuchten n*, *Residual Saturation of Water*, and *Field Residual Saturation of LNAPL* may be

Soil Properties	Groundwater Conditions	Source Area Parameters	LNAPL Properties	Solute Trans Properties
<input type="radio"/> Homogeneous Conditions <input checked="" type="radio"/> Vertically Layered Conditions		Soil Type Fine Sand (K= 1 m/day)		
Number of Soil Layers (Max. = 5) <input type="text" value="2"/>	<input type="button" value="Layer 1 (Lowermost)"/> <input type="button" value="Layer 2 (Uppermost)"/>			
Elevation of Bottom of Layer (m above oil/water)	<input type="text" value="0.0"/>	Van Genuchten Alpha (1/m)	<input type="text" value="7.5"/>	
Thickness of Layer (m)	<input type="text" value="0"/>	Van Genuchten n	<input type="text" value="1.9"/>	
Saturated Hydraulic Conductivity (m/day)	<input type="text" value="1"/>	Residual Saturation of Water	<input type="text" value="0.15"/>	
Total Porosity	<input type="text" value="0.4"/>	Field Residual Saturation of LNAPL	<input type="text" value="0.14"/>	
Oscillation Damping <input checked="" type="radio"/> No Oscillation Damping <input type="radio"/> Moderate Oscillation Damping <input type="radio"/> Maximum Oscillation Damping				

Figure 5-8. The **Soil Properties** Tab with *Vertically Layered Conditions* selected for 2 layers.

entered at the same time the thickness of each layer is entered, or the user may scroll through the layer numbers and enter those parameters separately.

The user needs to be aware that source area LNAPL depletion by groundwater dissolution only occurs between the oil/water interface and the potentiometric surface, where the piezometric surface elevation is calculated as $\rho_r t$, where t is the thickness of LNAPL and ρ_r is the relative density of the LNAPL. If, for example, the user specifies three layers, each 1 m thick, and the thickness of LNAPL is less than 2.25 m for an LNAPL with a relative density of 0.75, the uppermost layer will be entirely above the potentiometric surface and there will be no depletion by groundwater dissolution. Similarly, any layer which is entirely below the oil/water interface will not be depleted by volatilization. This is a necessary modularization of the problem to keep the solutions analytic.

5.3.1.1 Soil Type. A soil type needs to be selected from amongst the choices available under the list box identified as **Soil Type** (Figures 5-7 & 5-8). Included within those choices is the soil type “Custom” which, after selecting, can be edited and characterized by any description desired. The soil types are provided as a descriptive indicator of changing soil texture, resulting in a range of conductive and capillary properties. The LNASt utility has been programmed with example soil

conditions from literature (Carsel & Parrish, 1988) that depend on the initial soil type selected. Though selection of a **Soil Type** results in example values of *Saturated Hydraulic Conductivity*, *Total Porosity*, *Van Genuchten Alpha*, *Van Genuchten n*, *Residual Saturation of Water*, and *Field Residual Saturation of LNAPL* in the **Soil Properties** tab, each of those values can be changed by the user by simply typing a new value in the appropriate input box and clicking on another box of on the **OK** button. As on all of the screens that contain **OK** and **Cancel Changes** buttons, changes in soil parameters can be canceled by clicking on the **Cancel Changes** button, which causes all values to revert to the last value entered since before clicking on the **OK** button. As prior discussions have suggested, use of site specific parameters is always preferred, whether derived through measurement or interpretation.

Each soil type is described primarily through the hydraulic conductivity, which is the basis for comparison with other selected parameters. In general, a high conductivity is correlated with coarser-grained materials and a small capillary rise. Although conductivity is a reasonable and often available correlative parameter, recognize that the calculation outcome is actually more sensitive to capillary parameters. We recommend ignoring visual or texture descriptions in favor of measured or inferred capillarity or hydraulic conductivity whenever possible. Physical soil descriptions from boring logs can be highly misleading with respect to the controlling parameters. For instance, a predominantly coarse-grained material may in fact have a large capillary rise if there is a significant fraction of interstitial fine-grained materials. Similarly, partially cemented materials will typically have both smaller porosity and pore throat size (higher capillary rise).

5.3.1.2 Saturated Hydraulic Conductivity. The hydraulic conductivity of the soil is a measurement of the relative ability of a particular fluid to flow under a prevailing gradient. As discussed previously, the hydraulic conductivity is proportional to the intrinsic permeability and the specific fluid properties (Section 3, Appendix A). LNAST requires a saturated conductivity value for water, which is ultimately used in the groundwater transport calculations both inside and outside the source zone, as well as in certain liquid recovery estimates. Example values for the textural descriptions of various soils are provided from literature.

The hydraulic conductivity for water can be estimated by various lab and field tests. Single well and aquifer pump tests provide hydraulic conductivity values at a field scale and are probably the best measurements one can obtain. In certain situations, hydraulic conductivity measurements from core samples may be viable values. Laboratory measurements of intrinsic permeability or hydraulic conductivity are essentially interchangeable since the standard properties of water are known and apply at most environmental sites. However, lab measurements can suffer from three inherent difficulties. First, small discrete samples may not be representative of the majority of the formation. This potential impact can be minimized by collecting several measurements and by using good

selection judgment in the sampling process. Second, some test methods are run at conditions not analogous to field conditions and one must use caution in interpreting and using results. For instance, a constant head permeameter test may give misleading results if not run at a confining pressure similar to where the sample was collected. Third, and perhaps most important, it can be difficult to collect undisturbed samples in many environments. These primary lab limitations generally apply to any petrophysical test. However, as will be discussed, for some parameters lab testing is often the only realistic option.

5.3.1.3 Total Porosity, Effective Porosity, Residual Water Saturation. The total porosity, effective porosity, and residual water saturation are related terms with respect to the volume of the pore space and the fraction occupied by fluids. All are entered in the program as decimal quantities, taking on values from something greater than zero but usually much less than one (never greater than one). Total porosity is the total volume of voids divided by the total sample volume. The total porosity may be calculated if one knows the bulk and dry grain density. Since many sediments are quartz rich, the grain density can often be assumed to be approximately 2.65 g/cc, leaving bulk density as the only unknown, which is a common measurement.

The effective porosity is that portion of the pore space available for transmission of fluids. It is discussed here because of its relationship to porosity and residual water, but is an input in the last LNAST tab **Solute Transport Properties**. It is smaller than total porosity because some fraction of pore water is usually held as an immobile layer adjacent to pore walls (Hillel, 1982; Corey, 1986) and some pores may be unconnected. The effective porosity is used in calculation of the dissolved-phase solute transport. LNAST allows input of the effective porosity term or approximates it by subtracting the product of the residual water saturation times the total porosity from the total porosity (Stephens, 1996). In general, this underestimates the effective porosity, as it assumes all water retained at residual saturation is a result isolated pores which will not reach chemical equilibrium with fluids moving through the remainder of the pore space.

Residual water saturation is the fraction of water held to be irreducible under natural conditions. Residual saturation is related to residual moisture content and total porosity by $S_r = \theta_r/\theta_t$ (Appendix A). Unfortunately, there are several ways to define residual water saturation, depending on the geologic specialization using the information. In agriculture, residual water content is often taken to be the retained fraction below the wilting point, or the saturation threshold below which plant roots cannot acquire further moisture from the soil (~ 15 bars capillary pressure; Stephens, 1995). For some applications, residual water content is taken to be the retained water under field drainage conditions, also called specific retention or field capacity, which is a higher value (~ 1/3 bar capillary pressure; Stephens, 1995). Regardless of the definition used, the residual water fraction generally increases as the fraction of fine-grained materials increases. We recommend using a residual water

content larger than the wilting point because capillary pressures in the field in the LNAPL zone are far below the order 15 bars. The residual water saturation, in occupying volume in the pores, affects the volume of LNAPL that might be present for any particular set of conditions. The higher the residual water saturation, the smaller the LNAPL volume, all other things being equal.

5.3.1.4 Van Genuchten Capillary Parameters. The van Genuchten (VG) capillary function (1980) is used for all toolkit calculations except for the hydraulic recovery approximations where that function is converted to the Brooks-Corey (BC) capillary function (1964) (Appendices A & B). There are 2 primary parameters associated with the VG function, the parameter α that is inversely related to the capillary fringe height, with coarse materials generally having large α values and fine-grained soils having small values; the n parameter, which is a function of the pore throat distribution, with high values indicating high pore size uniformity. The residual water saturation (described above) is related to capillarity in calculations of pore volumes and saturation.

When capillary values must be assumed, literature values may be used (Appendix C) as qualitatively correlated to hydraulic conductivity. Note that many literature values for unconsolidated materials are from agricultural studies and that native soils might not have the same properties. Agricultural soils are usually disaggregated, tilled, and not in native depositional state. If there was an error in assuming those values based on soil class description, it would usually be to overestimate the pore throat sizing (i.e., capillary α too large), in turn resulting in overestimation of LNAPL mass, longevity, and related conditions.

One may infer some capillary generalities from pore distribution and conductivity. High conductivity often implies a larger pore throat sizing and therefore larger α value. Exceptions to this rule of thumb are formations of well-sorted materials (i.e., having similar grain sizes) that have a high conductivity and simultaneously a small α value. In general, the capillary parameters will be skewed toward the fine-grained fraction in many mixed soils when the fraction of fine material exceeds 15 to 20%. There are also methods of

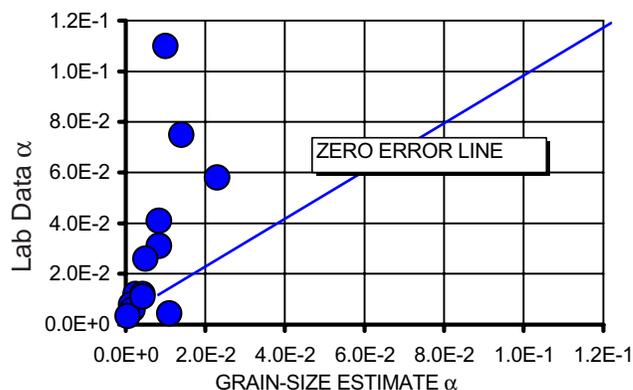


Figure 5-9. Lab versus grain-size estimated α values.

analytically constructing capillary approximations from grain-size distributions (Arya & Paris, 1981; Mishra et al., 1989). These methods can assist in making a preliminary determination of the possible range of capillary values. However, experience has shown that these methods are usually inaccurate and, because of the LNAPL sensitivity to capillary properties, should not be arbitrarily used for refined analyses (e.g., Figure 5-9).

5.3.1.5 LNAPL Field Residual Saturation. This term is analogous to residual water saturation, except it pertains to the LNAPL phase. As discussed in Section 3.4, the residual LNAPL saturation is caused by hysteresis and pore entrapment. The *field residual LNAPL saturation* is the minimum saturation that will remain at the endpoint of hydraulic LNAPL recovery. As such, it is a primary control over the residual risk impacts after hydraulic recovery has gone as far as possible. It is also important because it effectively determines the relative benefit of various hydraulic recovery strategies. For instance, if initial LNAPL saturation averaged 30% at a site and the field LNAPL residual saturation was 20%, then one can immediately see that a best-case mass recovery is about 1/3 of the original mass and 2/3 will remain in place. As will be shown subsequently, the risk magnitude will not have changed and the risk longevity will have been reduced by a similar factor (approximately 33%).

Because the field residual LNAPL mass is so important in the screening calculations, one must use caution in applying lab values that are not really measurements of residual due to hysteresis (see discussion in Section 3). There are several potential methods of approximating field residual saturation values. One is to review soil sampling data from the LNAPL impacted zone at several locations in an area near the known occurrence of free phase product. The greatest saturations not associated with the occurrence of free product in a nearby well would be an indicator of the field residual saturation. For instance, in downtown San Diego, a diesel #1 plume was investigated and it was determined that at field LNAPL saturations below about 10 to 15%, no free product was observed in adjacent monitoring wells for those particular soils (Huntley et al., 1991).

Another method of estimating residual saturation is with water displacement tests whereby a soil core is first drained to residual water by forcing LNAPL through the core under pressure. Then, the LNAPL is redisplaced by water forced into the core. The oil remaining after this test is the lab residual saturation of the LNAPL smear zone. Extrapolation of lab values to field scale is always difficult and must be done with good geologic judgment. As discussed previously, lab residual saturation values will almost always be less than field residual saturation due to heterogeneities and other field scale conditions. Lacking either of the data sets above, one must rely on literature values (Appendix C) as a starting point. Recall that the LNAPL residual saturation is often related to the type of hydrocarbon spilled, with more viscous products often having greater residual saturation. Soil type and pore sorting is also important. In addition, the residual saturation in the vadose zone is often smaller than in the aquifer zone (Mercer & Cohen, 1990), and it is the aquifer zone with which we are concerned in this work. Remember that

the calculations do not apply to a mobile NAPL plume, though certain aspects may be useful in evaluation. Choose the residual saturation parameter carefully or misleading results will occur.

5.3.2 Groundwater Flow Conditions

Following the **Soil Properties**, the next user Tab in the LNAST utility is **Groundwater Conditions**, which identifies the regional groundwater flow rate. The groundwater flow rate is necessary for the calculation of the depletion of the LNAPL source and for the downgradient dissolved phase transport calculations.

For a single material, the groundwater flow rate can be determined by several methods, all based on Darcy's law (Figure 5-10a). For multiple soil types, the regional flow through each unit is based on a single regional gradient and the conductivity for each layer (Figure 5-3b). The flow and transport conditions are constrained by the single selected regional groundwater flow parameter. For example, if specific discharge is selected and entered, the utility uses previously entered values of hydraulic conductivity and effective porosity to calculate gradient and pore velocity. If pore velocity is selected and entered, previously entered values of effective porosity and hydraulic conductivity are used to calculate specific discharge and gradient. Finally, if hydraulic gradient is selected and entered (as it must be for multilayer conditions), previously entered values of effective porosity and hydraulic conductivity are used by the utility to calculate the regional specific discharge and groundwater pore velocity.

As discussed previously, this regional groundwater flow rate is used to calculate chemical transport through, below, and beyond the source zone. Within the source zone, the flow rate is scaled by the relative permeability toward water and the resultant effective conductivity throughout the LNAPL source profile.

Figure 5-10a. **Groundwater Conditions** Tab for a homogenous soil.

Figure 5-10b. **Groundwater Conditions** for layered soil problem.

Figure 5-11. **Source Area Parameters** Tab to set LNAPL distribution and geometric conditions.

5.3.3 Source Area Parameters

The next Tab, **Source Area Parameters** (Figure 5-11), form the fundamental basis for the various possible distributions of LNAPL mass considered by the screening model that, when combined with hydrogeologic and chemical properties, result in a quantitative estimate of the potential source depletion and coincident chemical transport in groundwater and soil vapor. The right side of this Tab includes overall geometry that must be specified for all problems. The left side of the Tab determines the methodology used to calculate the vertical distribution of LNAPL within the specified geometry.

Following is a general overview of this properties Tab, followed by a more detailed discussion of each option. Starting with the geometry of the LNAPL, the **Source Area Geometry** menu includes the *Initial Thickness of the LNAPL*, the *Average Depth to the Top of the LNAPL*, the *Length of the LNAPL Zone*, and the *Width of the LNAPL Zone*. For all methods used to calculate the LNAPL saturation distribution except the user-input distribution, the *Initial Thickness of LNAPL* is the equilibrated thickness of LNAPL present or assumed to be present in a representative monitoring well in the plume area under consideration. For the user-input distribution, the *Initial Thickness of LNAPL* will be the total thickness input by the user, as discussed further below. The *Average Depth to the Top of the LNAPL* is used in the estimation of volatile losses to ground surface, when this mechanism is considered by the user. The *Length of the LNAPL Zone* is measured in the direction of (parallel to) groundwater flow. The longevity of the source area is proportional to this length. The *Width of the LNAPL Zone* is the dimension of the source area perpendicular to the direction of

groundwater flow. Though the total mass of LNAPL in a problem is linearly related to the width of the source area for any geometry, so is the groundwater flux and therefore the rate of dissolution. Therefore under the analytic conditions of the calculations, the width of the source area has no impact on the rate of depletion of the source area, and only slightly affects downgradient dissolved phase concentrations through its effect on transverse spreading of the plume. Under “real” conditions, narrow plumes would deplete more quickly because of transverse depletion in the source zone. In these calculations, transverse spreading is not considered until groundwater transport occurs after the leading edge of the LNAPL pool. Therefore the model is conservative in this respect, and underestimates source depletion to some extent with respect to this factor.

It is apparent that the above *Source Area Geometry* describes a box, and since LNAPL plumes are not boxes, one needs to think about how to best prescribe the geometry. The prevalent control over risk and longevity are zones containing the greatest saturations of LNAPL and the longest dimensions of the source area parallel to the direction of groundwater flow. As discussed earlier, under VEQ the LNAPL source mass increases non-linearly with increased observed well thickness. So our first suggestion is to focus on areas of thickest LNAPL impacts as the zone of primary interest. Take a representative observed thickness across that area for input to the calculation. If one wished to be more refined, a contouring algorithm could be run on your observed thickness data points in the “worst-case” area to derive statistical parameters (average, mean, deviation, etc.) to identify a range of selections. Keep in mind that the LNAST utility will generate a source distribution, contaminant mass, and the distributed groundwater flow rate through the LNAPL plume. Because of the focus on conservative averaging and a host of other complications, we strongly suggest not using this mass estimate as a basis for estimating the volume of the spill. To be reasonably representative, a spill volume is estimated by accounting for source area heterogeneity, water level fluctuations, historic LNAPL thicknesses across the area of impact, and the residual saturation under 2-phase and 3-phase conditions. This type of calculation is not the intent of the toolkit screening evaluations. However, if such an estimate has been made, that LNAPL distribution and averaged mass may be input directly by the user as described in Section 5.3.3.5.

Once the source area geometry is defined, you may select from a variety of **Methods Used to Calculate LNAPL Saturation** including *Equilibrium LNAPL Distribution*, *Distribution after a Fixed Period of Remediation*, *Distribution at Minimal Mobility*, *Residual Saturation*, and *User Input Distribution*. These source area stipulations are as important as soil capillary properties in estimating how LNAPL impacts may behave through time, and some careful thought is warranted when selecting the parameters of a particular screening calculation.

5.3.3.1 Equilibrium LNAPL Conditions. One possible LNAPL source approximation is to use the assumption of vertical equilibrium (VEQ) with respect to the LNAPL and water phases. When this is selected, a representative LNAPL thickness is specified and is used along with soil and fluid capillary properties to calculate the vertical distribution of the LNAPL source zone (see section 3.1 for background). It is important to remember that the VEQ assumption, while straightforward, may not be representative for many reasons (recall Section 3.2). VEQ is most likely to be prevalent in homogenous or coarser grained materials where groundwater fluctuations are minimal. There are cases where these assumptions do a good job representing field LNAPL saturation conditions (recall Figures 3-13a-b).

5.3.3.2 Distribution after Fixed Period of Remediation. The LNAST utility has modularized a multiphase recovery estimate method based on several simplifying hydraulic principles, as discussed previously. The multiphase recovery approximation techniques are fully documented by Charbeneau, 1999 (Appendix B). To calculate the *Distribution of LNAPL after a Fixed Period of Remediation*, the user selects the remediation option after specifying the soil, groundwater, and initial source distribution geometry. The selection button is 2nd from the top on the left-hand side of the **Source Area Parameters** Tab (Figure 5-11). When performing a calculation using this option, the user must click on the **LNAPL Recovery** option under the **Calculate** pulldown menu before proceeding to the depletion and downgradient extent calculations. When one executes this calculation, a second user screen will appear (Figure 5-12), and additional inputs will be required depending on the specific LNAPL recovery mechanism selected. The **Calculate** option is only selected after all five primary parameter input tabs have been completed. It is mentioned here because of its order of appearance in the parameter tabs.

As noted previously, LNAPL recovery calculations are estimates of hydraulic recovery only and do not consider the chemical changes that may occur during various cleanup actions. For each cleanup option, there is a specific set of required inputs, such as the radius of capture, drawdown, applied vacuum, screen length, and others depending on the specific option selected (Figure 5-12). Selection of more than one well results only in the multiplication of recovery rates from a single well. It does not consider issues of well interference or any other hydraulic complications or multiphase issues. The LNAPL pool must be bigger than the radius of capture to benefit from evaluating “multiple” well recovery. The selected inputs for each remediation condition, along with the LNAPL distribution and related mobility characteristics, determine the rate of cleanup for a particular option. The recovery calculations can be run for any user selected time to indicate whether a hydraulic recovery action will result in a desired concentration target or timeframe of impacts as a result of that specified period of recovery. As a reminder, all the provided cleanup estimates converge on the specified residual LNAPL saturation selected in the **Soil Properties** Tab, so the endpoint of all the recovery methods will be identical; only the time to reach the endpoint will vary.

Remediation Approach

Interception Trench

Skimmer Well

Single/Dual Pump Recovery

Vacuum Enhanced Skimmer Well

Vacuum Enhanced Single/Dual Pump Recovery

Calculation Options

Water Production Rate

Calculated by Program

Entered by User

Air Production Rate

Calculated by Program

Entered by User

Input Values

Period of recovery (yrs)

Width of Trench (m)

Number of Wells

Fluid (LNAPL and Water) Saturated Screen Length (m)

Screen Length Open to Air Flow

Ratio of Radius of Influence/ Radius of Well (LNAPL)

Ratio of Radius of Influence/ Radius of Well (water)

Ratio of Radius of Influence/ Radius of Well (air)

Applied Air Vacuum (m of water)

Water Pumping Rate (cu m/day/well)

Air Production Rate (cu m/day/well)

Results

Time (yrs)	Thickness (m)	LNAPL Recovery Rate (cu m/day)	LNAPL Volume (cu m) between oil/water and oil/air interface

Figure 5-12. The Calculation of LNAPL Recovery screen that appears when this option is selected from the calculate menu. When recovery is considered, this calculation must be the first completed.

It is important to remember that the screening hydraulic recovery method is based on the Brooks-Corey capillary description of LNAPL distribution (Appendix B; Charbeneau, 1999). In that description, product is theoretically not present or mobile at observed thicknesses less than the corresponding oil entry pressure. This creates a mass calculation discrepancy between the continuous van Genuchten function used in this work for other related calculations as compared to the Brooks-Corey recovery function. In simple terms, the recovery function should be viewed as the recovery of the approximate mobile fraction of free product. The LNAPL recovery estimates are also optimistic and generally underpredict the time of recovery and overestimate the recovery effectiveness because of the assumptions inherent in simplifying the multiphase flow problem to an analytic approach. The suggested use is for comparative evaluations of different strategies under different timeframes.

The specific remediation options are as follows, each requiring different user input. The required input is highlighted automatically by the LNAST utility on selection by the user of the option button corresponding to the specific remediation method. Each of the hydraulic recovery methods is described briefly in the following paragraphs, with the full equations and description provided in Appendix B (Charbeneau et al., 1999).

1. Interception Trench: The trench is assumed to passively collect LNAPL by ambient drainage. The gradient is the difference between the product/air interface and the groundwater piezometric surface (a.k.a., corrected groundwater elevation). This results in skimming with no groundwater production or drawdown. The solution is based on the analytic solution to a horizontal sink in a rectangular domain and on the width of that sink (Appendix B). Mathematically, the trench length must be less than or equal to the plume width.
2. LNAPL Skimmer Well: This is a radial pumping well solution based on the Thiem equation solution to a line-sink in a radial domain (Appendix B). The drawdown for LNAPL is the difference between the product/air interface and the groundwater piezometric surface (a.k.a., corrected groundwater elevation). The only other parameter required is the ratio of the radius of influence with respect to product to the radius of the well, including filter pack.
3. Single/Dual Pump LNAPL Recovery Well: Like #2 above, except that groundwater production is allowed beneath the LNAPL source zone to induce a larger gradient than under skimming conditions. Both the groundwater and LNAPL respond to that increased gradient. The solution for both groundwater and LNAPL recovery is again based on the Thiem equation solution to a line-sink in a radial domain (Appendix B). The program either calculates the water production rate based on the conductivity and screen length provided (i.e., effective transmissivity), or the rate can be provided directly by the user. In turn, the water production and radii of influence ratios determine the drawdown and gradient for the given hydraulic conductivity. In addition to the input parameters required for a skimmer well, the LNAPL saturated screen length (prior to pumping) is required as is, the ratio of the radius of influence with respect to water to the well radius. The groundwater pumping rate can either be entered by the user or be calculated by the utility. If calculated by the utility, it is assumed that both the piezometric surface and the oil/air interface are drawn down to same position (i.e., product thickness is maintained at zero in the recovery well during pumping).
4. Vacuum-Enhanced Skimmer Well: Like #2 above, except that a vacuum is applied to increase the net gradient. Although groundwater production is not explicitly calculated, there is an implicit assumption that the groundwater piezometric surface will be maintained at its static

level. Since applying a vacuum will cause fluid upwelling, groundwater production is implicitly required in this scenario, though that production rate is not calculated. This is not a comprehensive remediation calculation and only liquid phase recovery is considered. That is, there is no accounting for volatilization from the LNAPL source, which can be significant as discussed previously. The solution for these assumptions is simply a variant on the Thiem equation (Appendix B). Again, the vacuum extraction rate can either be entered directly by the user, or calculated by the program, given the applied air vacuum.

5. Vacuum-Enhanced Single/Dual Pump Recovery: A combination of #3 and #4 above, with no other explanation required.

Once the remediation alternative has been selected and the appropriate parameters entered, the recovery through time is calculated by clicking on the **Calculate Recovery** button. The recovery history table can be saved to a file by selecting the **Save as File** menu option, and as with all other results tables, this can also be plotted by selecting the **Graph** option. It is not necessary, however, to save the results to a file for the transport calculations to occur, as the results are saved in memory for access by the transport calculations. After completing the remediation calculation, return to the main part of the program by closing the LNAPL recovery window. The results and the effect on the LNAPL distribution in the source zone will be stored in memory by the program for use in the subsequent calculations of dissolution and transport, as discussed subsequently.

5.3.3.3 Distribution at Minimal

Mobility. The third possible LNAPL distribution option is the *Distribution at Minimal Mobility* (effective LNAPL conductivity), where the LNAPL saturation corresponding to the specified effective conductivity is determined from the effective conductivity function (Section 3.3; Appendix A). When this option button is selected, the *Criterion for Minimal Mobility* box at the bottom right of the tab will now requires user input of the specific mobility threshold. For instance, one might select a threshold LNAPL conductivity similar to that used for leachate water

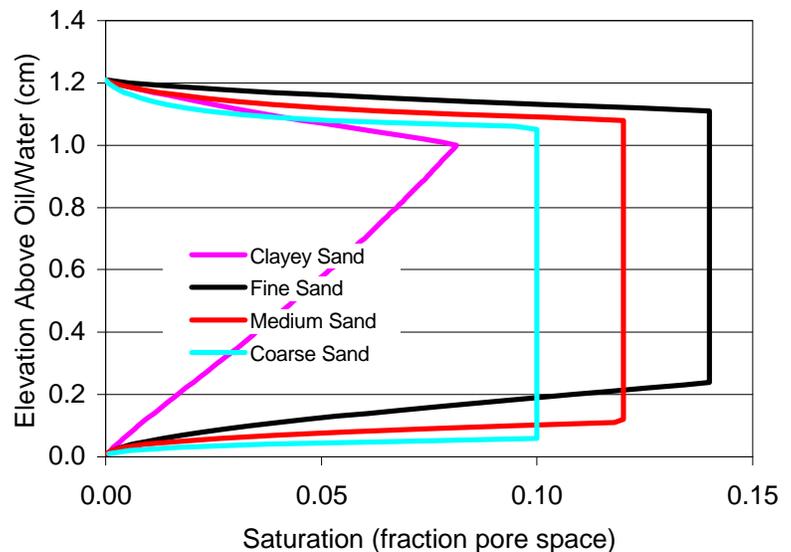


Figure 5-13. LNAPL profiles at minimum mobility, showing truncation once the criterion saturation threshold is reached. Notice that for the clayey material, the threshold is not anywhere exceeded and the profile is unchanged.

in certain regulated landfills, such as the 10^{-6} cm/sec (8.64×10^{-4} m/day). Alternatively, since landfill drainage is vertical and the LNAPL pool gradient is lateral, one could use the LNAPL gradient to scale the effective mobility. Other mobility criteria can be generated by the user based on professional judgment, regulatory requirements, or other relevant factors.

Like all of the **Methods Used to Calculate LNAPL Saturation**, except the user-input distribution, the derivation of the minimum conductivity begins with a VEQ LNAPL saturation profile for the stipulated thickness condition. Then, the profile is truncated at the LNAPL saturation that corresponds to an effective conductivity equal to that specified by the user (Figure 5-13). This estimate method is therefore limited by the same conditions applying to VEQ, and, additionally, assumes that the relative permeability function (Appendix A) is a reasonable approximation of actual conditions.

5.3.3.4 Field Residual Saturation. This option assumes that the maximum LNAPL saturations in a profile are equal to the LNAPL residual saturation specified previously in the **Soil Properties** Tab. As for the other options (except user specified), it operates by first calculating a saturation profile under vertical equilibrium conditions. Where calculated saturations are below field residual, they are left untouched. Where calculated saturations are above residual, they are reduced to the field residual saturation value. This results in a truncated profile similar to those discussed above (see Figure 5-13). The resulting saturation distribution therefore depends upon the soil parameters and the specified thickness of the LNAPL-impacted interval.

Recall also that the endpoint of any hydraulic recovery scheme, given sufficient time, will be the field residual saturation. Therefore, selecting this option will provide a direct estimate of plume longevity and transport after any hydraulic recovery method, but without a time to reach the recovery endpoint. This calculation is useful when the conditions are such that the field residual saturation results in long-lived plume regardless of the hydraulic remediation strategy. In other words, one is able to say something tangible about the best case hydraulic recovery condition without going through the steps to calculate that recovery.

5.3.3.5 User Input LNAPL Distribution. This option allows the user to define the vertical LNAPL saturation profile based on data, interpretations, or other information. When selected, this option allows the user to pull up a submenu (by clicking on the *Edit Saturation Distribution* button) that allows incremental definition of the saturation profile (Figure 5-14). The number of depth intervals is based on your knowledge of the saturation distribution, derived either through assumption or measurement. Application of measured saturation values is self-evident; the user simply inputs results for each interval over which the data apply. The LNAST utility linearizes this data as a step function upward from the lowermost LNAPL/water interface in the formation. A value of zero saturation is assumed by the program at the base of the LNAPL (elevation = 0).

User Input of LNAPL Saturation

Number of Depths of Known LNAPL Saturation:

Elevation (m) of Potentiometric Surface (Corrected Water Table) above base of LNAPL:

Elevation (m) of Uppermost LNAPL above base of LNAPL:

Elevation (m) above Base of LNAPL	LNAPL Saturation
0.25	0.02
0.5	0.05
0.8	0.1
1.7	0.1
1.9	0.15
2	0

Figure 5-14. User defined input of LNAPL distribution for the smear zone example given in the text. Direct measurements can be similarly input.

A smear zone example is given to illustrate data entry. Suppose that the observed thickness in an observation well is currently about 0.3 m, and that the current water/LNAPL interface has risen about 1.7 m over some period. We know that the saturation profile of the current observed thickness does not represent the total zone of LNAPL impact because LNAPL will be stranded in the interval where the LNAPL/water interface rose (Figure 5-15). The LNAPL in that zone will be at residual oil saturation, except for the base of the profile where LNAPL saturation is less than the residual (Figure 5-15). In our example then, the saturation profile would be piecewise specified from the base upward (Figure 5-14). The mass and relative groundwater flow through the profile is calculated by the utility as discussed previously.

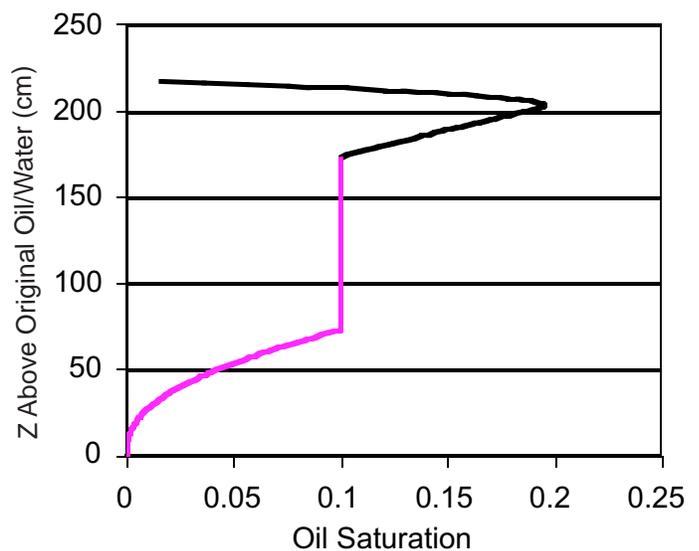


Figure 5-15. LNAPL smearing example due to a rise in the water table, creating a 200 cm (2 m) smear zone.

Soil Properties	Groundwater Conditions	Source Area Parameters	LNAPL Properties	Solute Transport Properties		
LNAPL Phase Properties						
Hydrocarbon Type		Density (gm/cc)	Oil/Water Interfacial Tension (dynes/cm)			
Gasoline		0.73	52			
			Oil/Air Interfacial Tension (dynes/cm)			
			24			
			Viscosity (cp)			
			0.62			
Dissolved Phase Properties						
	Pure Phase Solubility (mg/l)	Pure Phase Vapor Conc. (mg/l)	Mole Fraction of LNAPL	Log(Koc)	Biodegradation Half-Life (days)	Target Concentration (ug/l)
MTBE	48000	1204	0.11	1	9000	40
Benzene	1780	324	0.018	2	90	5
Ethyl Benzene	135	57	0.018	3	65	700
Toluene	515	111	0.079	2.06	60	1000
Xylene	175	38	0.075	2.6	150	10000
		Add Dissolved Constituent	Remove Constituent	OK	Cancel Changes	

Figure 5-16. The LNAPL Properties Tab.

5.3.4 LNAPL Properties

The fourth Tab in the LNASt utility is the **LNAPL Properties** (Figure 5-16) that includes both the physical and chemical attributes of the LNAPL source. The physical aspects combine with soil properties and are important in the mobility, recoverability, and saturation conditions of the source. The physical input values often vary, most particularly the interfacial tension value of the oil/water couplet.

The chemical parameters are a key element of the fate and transport outcomes of various components from the source, and ultimately of risk. Of all the parameters used in these LNAPL and groundwater transport calculations, the chemistry aspects are the most affected by regulatory guidance, particularly the *Target Concentration*. Further, fuels are chemically variable depending not only on the refined characteristics, which have been variable through time and different manufacturers, but also on the environment and characteristics of the spill itself. It is unlikely that LNASt's default chemical inputs will apply to many sites. Guidance on chemical inputs will be provided, but it is recommended that the appropriate regulatory standards be considered when the final values are selected for chemical screening. Each jurisdiction will likely have specific issues that cannot

Figure 5-17. Hydrocarbon Type.

be addressed in a general document such as this. Examples of LNAPL physical and chemical properties, toxicology, and ranges of fuel compositions are provided in Appendix C. It may also be of interest for the reader to refer to the Total Petroleum Hydrocarbon Criteria Working Group documents for additional information on fuels, chemical fractions, and toxicology (AEHS, 1999).

The LNAST Tab for **LNAPL Properties** has a drop box for the primary description of the *hydrocarbon type* including gasoline, jet fuel, diesel, crude, or custom (Figure 5-17). The LNAPL need not be a petroleum fuel, as long as the physical and chemical properties are known and the basic assumptions made in the toolkit are applicable. Once the LNAPL drop-box item is selected, all the remaining parameter boxes in the tab fill with the suggested “default” parameters. Like all values used in the software utility, the values in the input boxes are user-editable. Do not use the default values if you know them to be non-representative of the site LNAPL of interest. They are intended as a general starting point only, and site specific values should be used whenever available.

The physical and chemical properties entered should be those properties of the LNAPL source as it exists in the subsurface (and in contact with groundwater), not at the fuel pump. Many changes in chemistry occur in NAPLs as they are transported through the vadose zone. The mole fraction of volatile constituents, such as MTBE and benzene, are likely to be much different at depth than in the original surface source (see the example problems in Section 6). In addition, there is sensitivity to the LNAPL physical properties, particularly field interfacial tension values. Chemical and physical analysis of site specific free product, or at a minimum, corresponding evaluations of dissolved-phase concentrations in groundwater is recommended to assist in making more representative calculations of chemical impacts.

5.3.4.1 LNAPL Physical Properties. The physical LNAPL parameters include interfacial tensions, viscosity, and density (in approximate order of relevance). The interfacial fluid tensions (IFT) are used to scale the air/water capillary parameters to the LNAPL/air and LNAPL/water systems (Leverett, 1941; Appendix C), as discussed in Section 3.2. These three capillary couplets are necessary to develop the multiphase description of the source, and these are relatively sensitive values. Note that IFT includes surface tension, a term typically used for liquid in contact with vapor. The viscosity is an important fluid parameter affecting the conductivity of the oil phase (recall prior discussions in Section 3). Density is also a component of conductivity, but is less important because the relative range of variability is small, generally between 0.7 and 0.9 g/cc. Typical ranges for these parameters for a variety of petroleum products can be found in Appendix C.

5.3.4.2 Chemical Properties of LNAPL. Up to this point, factors that control the distribution, mobility, and physical transport of the LNAPL have been discussed. This parameter section takes us into the chemical aspects of the LNAPL. There are three critical factors in this section: 1) Selection of

the chemicals of concern; 2) Selection of the molar fraction of those compounds; 3) Selection of the biodegradation rate. The remaining factors, such as pure phase solubility, organic carbon partitioning coefficient, and vapor concentration are well documented in literature or are easily derived. The target concentration is also straightforward and can be a risk-based standard, a cleanup guideline, an regulatory standard, or other applicable concentration. Federal drinking water standards have been used as the default here, and should not be used site specifically unless consistent with potential water use and applicable regulations. As discussed above, selection of a *Hydrocarbon Type* results in the creation of an example set of soluble compounds of concern. The individual chemical properties of these compounds of concern be edited, and compounds can be added or removed. Any chemical that is not present in your LNAPL source should be removed from the list, by clicking on the **Remove Constituent** button, and selecting the constituent you want removed from the list of constituents in the drop box. Alternatively, if you want to add a constituent, click on the **Add Constituent** button, which adds a blank line on the bottom of the **Chemical Phase Properties** table. The user must now manually enter the required data in that last line of the table.

5.3.4.2.1 Chemicals of Concern. Petroleum fuels are refined from crude oils that have different compositions and the specifications of refining have also varied through time with the changing formulations of the manufacturers (example fuels in Appendix C). Further, the subsurface weathering and degradation of fuels is also sensitive to many environmental variables. Because of this, the component makeup of fuels themselves is variable, therefore the utility user must use caution when selecting both the specific chemical components and their molar fractions within the fuel source. As mentioned earlier, the regulatory agencies associated with a particular site may also have specific guidance and expectations with respect to the specific compounds of concern in various LNAPLs.

In the work presented here, the default chemicals of concern and their maximum expected mole fractions were assimilated from the TPH Criteria Working Group Series (AEHS, 1999). In that work, a wide range of scientific input was sought regarding composition and risk properties of fuels, and a large example database compiled.

In the LNASt LNAPL Properties Tab, one can see that several example gasoline compounds and their physical properties are listed for each fuel type (Figure 5-9; gasoline example). If there are different compounds at the site being screened, the user can insert them for evaluation, as noted above. As mentioned, examples of fuel composition, properties, and toxicity information are provided in Appendix C. Selected parameters requiring user judgment are discussed below. Standard physical properties such as pure phase solubility, vapor concentration, $\log K_{oc}$, and regulatory standards are not discussed as the user can simply input that information from a reliable source.

As an aside, pure phase vapor properties are often reported in terms of partial pressures or volumetrically. These may be converted to the units used in the LNAST utility through the ideal gas law ($pV = nRT$), where p = partial pressure of the compound, V = volume, n = moles, R = ideal gas constant, and T = temperature, all in consistent units. Further, note that ($n/V = p/RT$) is the molar concentration (moles/volume), and knowing the molecular weight of the chemical compound, one can convert to mass per volume units. For readers unfamiliar with these gas law calculations, any basic chemistry text will provide sufficient background.

5.3.4.2.2 Mole Fractions. As discussed, the mole fractions selected for evaluation have a large impact on the results. For instance, pure xylenes would dissolve in water to 175 mg/l, clearly above the federal maximum contaminant limit (MCL) for drinking water of 10 mg/l. However, at a mid-range gasoline mole fraction of 5%, xylenes would only attain an effective solubility of 8.75 mg/l, which is below the MCL. Therefore, whether or not xylenes are a threat above drinking water standards or other mitigation targets depends directly on the mole fraction input. Recalling the previous discussion of Raoult's Law (Section 3.7), it is straightforward to use measured water chemistry in or very near the source to assist in determining the mole fraction in the source (Appendix C). The primary caution in this approach is that dilution can distort the results, and biodecay and sorption can alter the groundwater plume chemistry with distance from the source. Therefore, it is important when gathering mole fraction information that only samples within or very near the source zone be used in the evaluation.

5.3.4.2.3 Organic Carbon Partitioning Coefficient. The organic carbon partitioning coefficient (K_{oc}) is a measure of a chemical's affinity for the organic matter that may be present in soil (Jury et al., 1986). The higher the K_{oc} , the greater the partitioning between the dissolved-phase groundwater and soil matter, all other things being equal. The soil partitioning coefficient (K_d) is the product of the K_{oc} and the fraction of organic carbon (F_{oc}), discussed in the Solute Transport Properties section below). Whereas K_{oc} is a constant for any given compound at standard conditions, the actual partitioning to soil depends on the F_{oc} and other physical soil properties. This factor is used in the groundwater transport calculation and accounts for the slowing (retardation) of compounds having a relatively high affinity for the organic phase.

The organic carbon partitioning coefficient is a common measure for organic compounds. Lacking this information, there are also relationships linking the octanol-water partitioning (K_{ow}) to the K_{oc} (Karickhoff et al., 1979).

5.3.4.2.4 Biodegradation Half-Life. Biodegradation is calculated by a pseudo-first order rate reaction within the groundwater transport module. First order reactions are described by half-lives, or correspondingly by decay constants. As mentioned in Section 3, biodegradation is the most important factor limiting the extent of many dissolved-phase petroleum constituents. While there are many indicators of biodegradation activity, the primary indication is a stagnant or receding dissolved-phase

plume. Literature half-life values for various LNAPL compounds span several orders of magnitude (Howard et al., 1991). The example values provided are in the typically expected range with the understanding that this is a site specific parameter.

To select a biodecay half-life, we recommend the user run several iterations of the calculation method to back into a degradation rate that makes sense for the plume dimensions at your site. Note that as a rate, biodegradation depends on residence time. Under high groundwater flow rates, a smaller half-life is required to result in a plume having the same length as under conditions of lower groundwater flow velocity. So if one evaluates a range of flow rates, an inversely proportional range of biodecay rates would also be needed to fit the same observed plume. As has been discussed, there is an apparent interdependency between groundwater flow rates and biodegradation rates such that this comparative approach is necessary. Based on field observations, one would generally expect higher decay rates at higher rates of flow.

5.3.4.2.5 Target Concentration. The target concentration is that which one would like in groundwater at any spatial point of concern. This could be a regulatory threshold, risk-based target, nuisance-based target, or other concentration based on the specifics of a particular site. When the LNASt program calculates the downgradient extent of a compound of concern, it defines the limit relative to this target concentration goal.

Soil Properties	Groundwater Conditions	Source Area Parameters	LNAPL Properties	Solute Transport Properties
Effective Porosity	<input type="text" value="0.34"/>		Vertical Transverse Dispersivity (m)	<input type="text" value="0.01"/>
Longitudinal Dispersivity (m)	<input type="text" value="3.0"/>		Fractional Carbon Content	<input type="text" value="0.003"/>
Horizontal Transverse Dispersivity (m)	<input type="text" value="0.15"/>		Vapor Diffusion Efficiency Coefficient (0 to 1.0)	<input type="text" value="1.0"/>
Dissolved Phase Calculation Options <input checked="" type="radio"/> Fewest time steps, fastest execution times. <input type="radio"/> Intermediate number of time steps, intermediate execution times. <input type="radio"/> Maximum number of time steps, slowest execution times.				
			<input type="button" value="OK"/>	<input type="button" value="Cancel Changes"/>

Figure 5-18. The **Solute Transport Properties** Tab.

5.3.5 Solute Transport Properties

The fifth and last Tab is for the **Solute Transport Properties** (Figure 5-18), where the remainder of the parameters needed to calculate groundwater transport of hydrocarbon compounds away from the source are specified. These are just the transport parameters that do not fit in well in the other parameter groups. However, as discussed, all of the properties specified in prior Tabs also influence solute transport outcomes directly or indirectly.

5.3.5.1 Effective Porosity. The effective porosity, as discussed previously, is automatically calculated to be the total porosity minus the residual volumetric water content (direct and indirect inputs in the first Tab, **Soil Properties**). One can also directly input a different effective porosity if desired. The effective porosity is used in the calculation of the average linear groundwater flow velocity, a key input in the groundwater transport equations.

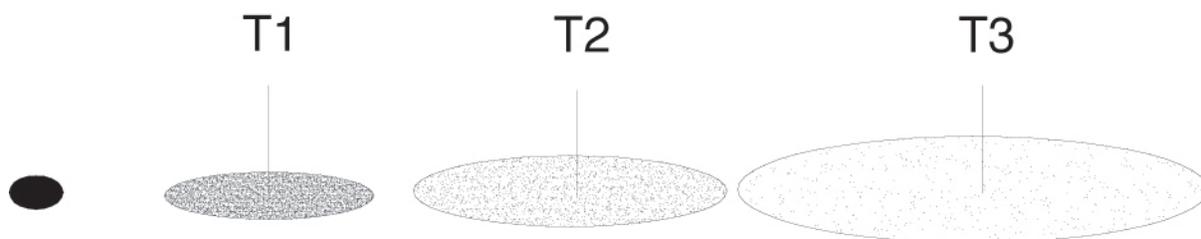


Figure 5-19. Schematic instant point source plume migration downgradient, showing the effects of dispersion, as the plume mass is unchanged but occupies a larger volume through increasing time T1, T2 and T3 (non-degraded conditions).

5.3.5.2 Dispersivity. The dispersion of plumes causes spreading and dilution away from the ideal centerline of movement. For an ideal, nonreactive (i.e., no biodegradation) point source plume, the total solute mass remains unchanged after elimination of the source, but occupies a larger and larger volume as dispersive travel progresses (Figure 5-19). There are three factors influencing dispersion: 1) Mixing in pore channels due to complex pathways; 2) Mixing in individual pore channels due to discrete contrasts in the fluid velocity profile; 3) Mixing from molecular diffusion of compounds following the chemical gradient. Of these, the mechanical mixing aspects are usually the most important, except in low permeability materials where diffusion plays an important role (Sauty, 1980, Pickens & Grisak, 1981). The term dispersivity refers to the coefficient of hydrodynamic mixing, with the total mechanical mixing being proportional to both the dispersivity and the velocity (Appendix A). Therefore, more plume mixing occurs at higher groundwater velocities. The dispersivity can be derived by measuring breakthrough curves for a solute passing through a soil core, and then fitting a type curve. However, several studies have determined that dispersivity is a scale dependent parameter (Pickens & Grisak, 1981; Sudicky, 1986; Xu & Eckstein, 1995). Therefore, applying a lab-derived value may be of little practical value, since the field-scale dispersivity would usually be significantly larger.

While field studies of dispersivity have produced variable results, some general rules of thumb have been identified based on the field scale of the plume: 1) Longitudinal dispersivity [α_L] 10% of plume length; 2) Horizontal or transverse dispersivity [α_T] 10 to 33% of α_L ; 3) and vertical dispersivity 1 to 5% of [α_L]. For more refined estimates, one can calibrate to site observations. A wider plume than predicted might indicate a larger transverse dispersivity, a longer more diffuse plume could suggest a larger value of longitudinal dispersivity. While of general interest, the dispersivity is not the most critical parameter in the calculation results, although it clearly influences the net plume distribution.

5.3.5.3 Fractional Carbon Content. The fractional organic carbon content (Foc) is a measure of natural organic material in soil for which organic contaminant in petroleum have some affinity and will partition to during the spreading stages of dissolved-phase plume genesis. Fine-grained minerals can also act analogously, sorbing some fraction of the passing petroleum plume. When organic material is present, the sorption of individual compounds generally depends on the affinity for the organic phase as compared to the water phase. Usually, sorption of organic compounds increases with increasing molecular weight, polarity, and branched structure.

This parameter can be measured or inferred, as it has low sensitivity in the calculations when LNAPL mass is present. For most alluvial sediments, the value of organic carbon is typically low. However, deposition in many aquatic environments can include a significant organic content, in which case lab measurements are recommended. A caution for lab measurement is that certain ranges of petroleum contamination will be measured as organic carbon unless the lab is aware that the sample may be impacted and treats it accordingly.

5.3.5.4 Vapor Diffusion Efficiency. This vapor diffusion efficiency is a scalar from 0 to 1 (Appendix A) that is multiplied by the vapor flux to reduce the net flux exiting the LNAPL source. One may use this coefficient based on site specific measurement for any condition that can limit vapor transport from the LNAPL to ground surface. One such condition present at many sites is a low vapor permeability surface cover, like concrete or asphalt. Most risk assessment guidelines allow a vapor flux attenuation factor between 0.1 and 0.001 for such conditions (ASTM, 1995). Another condition that will limit vapor flux is any zone of high moisture content. We know from capillary discussions in Section 3 that fine-grained materials interbedded with coarse will usually have a much higher water content and lower effective vapor diffusion efficiency.

We recommend the user input vapor diffusion efficiency for surface cover as suggested in regulatory guidance and/or in a specific risk evaluation method. For soil zones of high moisture, it is recommended that the user determine the effective vapor diffusion coefficient using the moisture content and the Millington-Quirk Equation (Section 3.7). A rough approximation for the vapor efficiency

coefficient is to calculate the “new” effective diffusion coefficient (accounting for the high moisture horizon) and divide that by the original, while accounting for the zone thicknesses (Equation 5-1):

$$D_e^* \approx L_t / (L_m / D_{em} + L_d / D_{ed})$$

$$VE \approx D_e^* / D_{ed}$$

where L is the particular zone thickness where the subscript t indicates total, m and d moist and dry, D_e is the new effective vapor diffusion coefficient, and VE is the vapor efficiency coefficient.

A more thorough method for estimating vapor diffusion efficiency is to first calculate the stratigraphic moisture profile above the capillary zone for the two soil types you are evaluating, the dryer and the more moist. Then, construct a stratigraphic moisture profile by superimposing the moisture from each soil type into the proper elevation sequence (recall Figure 3-42). Calculate the effective diffusion coefficient (D_e^*) using the summation equation in Appendix A, and divide by the original integrated value (D_{ed}) to define the vapor efficiency coefficient.

5.4 PERFORMING CALCULATIONS

This is an overview of the calculation procedure using the LNASt utility. The interested user may gain additional insight by reviewing the example problems in the following chapter where some of the thought processes are provided and the first example problem is a working tutorial. Through the five Tabs in the LNASt utility, the user has input soil, groundwater, source distribution, LNAPL properties, and transport parameters necessary to evaluate the time dependent concentrations within and associated with the LNAPL source under ambient and remediated conditions.

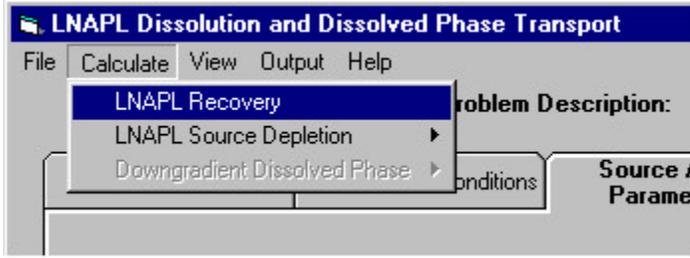


Figure 5-20. The Calculate drop menu. Source depletion is calculated from initial LNAPL conditions directly or, alternatively, the LNAPL distribution after a fixed period of remediation is calculated 1st, depending on the source area selection by the user.

recovery option was not selected, one would proceed directly to the LNAPL Source Depletion calculation. The source depletion calculation *must* occur before downgradient groundwater transport calculations each and every time there is a change in any controlling parameter. The output from the source depletion calculations is the input into groundwater transport estimate, and must therefore be updated each time a new condition is considered. The source depletion estimates are stored in computer memory, and hence must be overwritten by explicit recalculation or old values will be used for the new problem, producing incorrect results.

The user has two source depletion options, with or without volatilization (Figure 5-21). Recall the discussion of the vapor efficiency coefficient that affects volatilization, if selected (see Section 3.7). When the utility is given the command, it will calculate



Figure 5-21. The source depletion calculation options, with or without volatilization from the LNAPL source.

the source depletion by dissolution and, optionally, volatilization. This is the required input to the groundwater fate and transport module. When the calculation of source depletion is complete, a table will be shown (Figure 5-22) that displays the individual component dissolved phase concentrations within the source zone. The user may save the file (**Save as File**), graph (select the **Graph** menu option displayed), or simply close this window; the calculation results are held in memory and

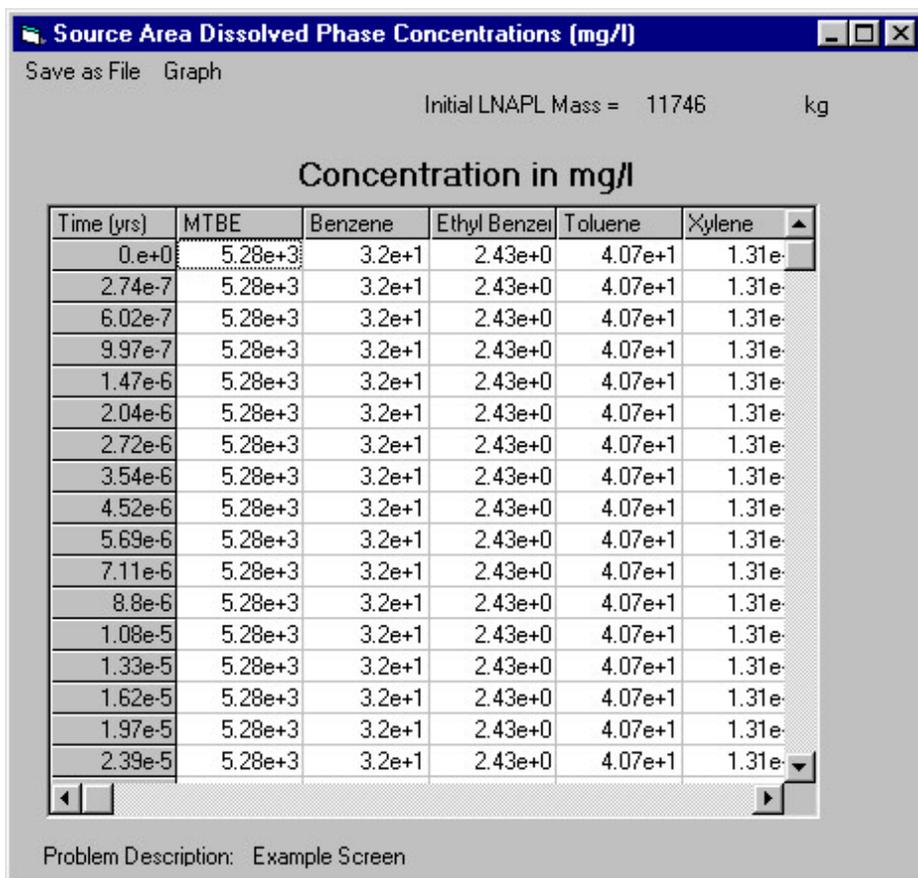


Figure 5-22. Output table that is automatically displayed after calculation of the source zone depletion estimate. The concentration values represent the estimated concentration in groundwater at the leading edge of the LNAPL source zone. Vapor losses are considered, if selected.

the table and graph are available in the **View** menu until another calculation is run. The hydrocarbon mass in the geometric source zone is also provided but, as discussed earlier, should not be viewed as an actual plume mass estimate because of simplifying geometric conditions and because one would typically select worst-case areas for screening purposes. It is best viewed as an averaged mass in a type area. However, if this

LNAPL mass is infeasibly large based on other site knowledge, that would indicate the site

screening parameters need to be reconceptualized by the user. The averaged LNAPL mass is provided as a reality check for this reason. Obviously, this calculation method is constrained by mass and other relationships, and needs an estimated starting mass distribution for the type area as part of the conceptual model.

The simplest way to compare multiple site conceptualizations is to save the source depletion and transport calculation results from each run in separate files and import into a common analysis platform, such as a spreadsheet or database program. Selection of **Save as File** from the top of the output table window saves the output results as tab-delimited files ASCII file, which are easily imported into most analysis routines.

If one chooses to graph from this environment, by selecting **Graph** from the menu options at the top of the table, a plot of the concentration of all of the compounds specified in the **LNAPL Properties – Dissolved Phase Properties** window will be plotted as a function of time. This graph may be manipulated in a number of ways. It may be printed to any of the printers recognized by the users

windows setup (**Print** menu option), the **Legend** may be turned on or off, the graph may be copied to another program, or the graph itself may be edited. To copy the graph to another program, select **Copy/Save** from the

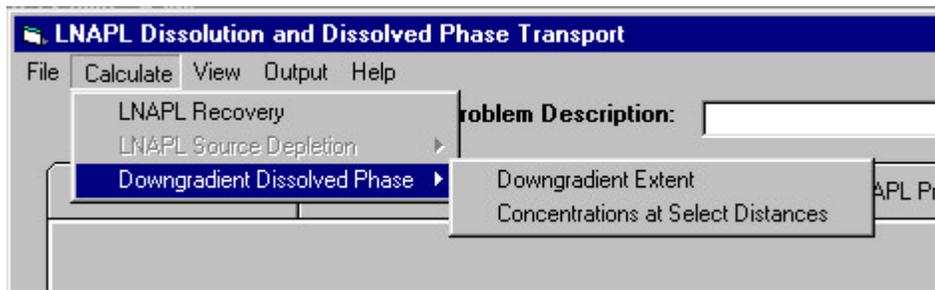


Figure 5-23. After the LNAPL source depletion is run, the Downgradient Dissolved Phase calculation can occur. Two options are provided:
 1) Downgradient extent based on target concentration;
 2) Concentration through time estimated at selected distances.

menu at the top of the graph, which opens a copy/export window. To copy and paste a graph directly to another program, select *Bitmap* as the Export type and *Clipboard* as the **Export Destination**. Executing the **Paste** command in any open program will then copy the graph into that open file. To save the graph as a file for import into another program in the future, select *Metafile* as the Export type and *File* as the **Export Destination**. Then click on the **Browse** button to open up menu that allows you to name the file to be saved. In addition, double-clicking on any of the graphs will bring a window that allows the user to change many of the aspects of the graph, including the title (and subtitle), the way the data sets are plotted (and which data sets are plotted), and the text fonts.

With the source zone depletion calculated, the user can now go on to calculate the time dependent groundwater concentrations associated with the prescribed soil and LNAPL source conditions. This action is also initiated by pulling down the **Calculate** Menu and choosing between a *Downgradient Extent* evaluation and *Concentrations at Selected Distances* (Figure 5-23). The *Downgradient Extent* evaluation calculates the downgradient movement and eventual contraction of dissolved components at their specified target concentration as a function of source depletion through time.

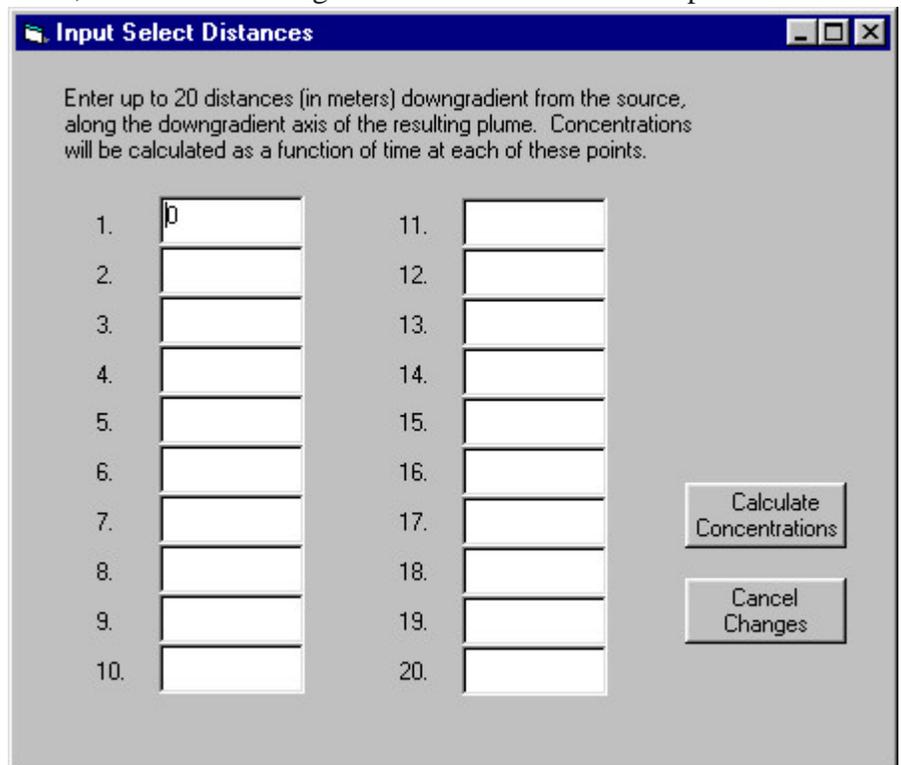


Figure 5-24. When the concentration at selected distances is selected, this screen appears prompting the user for the desired downstream locations along the central axis of the plume.

The *Concentrations At Selected Distances* are commonly known as breakthrough curves and the estimated concentration spectrum through time will be provided at the selected points (Figure 5-24). The user is prompted for the desired locations through a second drop-down menu that appears when that option from the **Downgradient Dissolved Phase** menu is selected. The execution time of the groundwater transport calculations depends on your computer CPU speed, the number of compounds selected, and the number of downgradient distances. For example, with five compounds selected, a 233 MHz computer will take approximately three minutes to execute downgradient extent simulation. A progress bar showing the degree of completion is displayed while the model is running. For any simulation, it is recommended that initial conceptual runs be done with a minimum of compounds and/or distances to “dial in” to reasonable site conditions. Then, the appropriate level of detail with respect to compounds of concern, distances, and other variable factors can be put into the final set of calculations. There is little sense in wasting time (yours and the computer’s) on extensive preliminary runs investigating the probable range of site LNAPL conditions.

Once the groundwater transport is calculated, LNASt automatically displays output tables of interest. Again, these output data can be **Saved** or **Graphed** using the pull-down menu at the top of the output table. Similarly, after the runs are complete, tables and graphs can be regenerated by pulling down the **View** menu and selecting the output of interest.

5.5 KEY ASSUMPTIONS

Several key assumptions are critical in this toolkit (recall, there are several “tools” that are linked in the cleanup and transport evaluations). There are also other potential limitations stemming from unconsidered site specifics or general unknowns in the current base of scientific knowledge. Several technical considerations have been discussed in context with the subject matter of the preceding report sections. Keep the limitations in mind as you use the toolkit and you will generate better answers.

The assumptions in the list given below are ordered in relative importance, based on experience and scientific opinion, but the hierarchy of your particular site may be different. Further, certain limitations apply only when specific evaluation conditions are selected in the toolkit. The key assumptions are: 1) Homogeneous or uniformly layered soil conditions, and homogeneous fluid, and chemical conditions; 2) Capillary hysteresis is not explicitly considered, with only the residual oil factor considered; 3) Static LNAPL conditions with no active transport in the free phase outside the defined geometry; 4) Ideal remediation hydraulics under homogeneous conditions, no well interference, hydraulic inefficiency, etc.; 5) Equilibrium chemical partitioning; 6) First-order biodecay; 7) Macroscopic hydraulic and chemical interactions, no non-ideal conditions such as fingering, cutoff, etc.

Of these main assumptions, the nuances of heterogeneity cannot be overemphasized. We have already developed the primary concepts of multiphase synergy. So it is easy to imagine that aquifer

heterogeneities that cause order of magnitude changes in standard groundwater flow conditions, will now cause several orders of change for multiphase conditions. For instance, we often see field conditions where LNAPL is present in coarse-grained material near VEQ, but LNAPL is nearly absent in the interbedded fine-grained units (recall Figures 3-12 and 3-13). While complicated, it is easily explained in the multiphase context by observing that the time to equilibrium is short in the coarse materials and exponentially longer in the fine-grained zones. When coupled with natural hydrologic variability, this often means that fine-grained units will never come to equilibrium with LNAPL. Under these conditions, if one assumed the LNAPL saturation distribution to be at vertical equilibrium, the assumption would cause a larger source mass to be estimated than actually present, along with a longer source residence time than would be demonstrated in the field. The point is to keep the geologic setting and multiphase concepts in mind when using these screening tools so that the answers are in context with site conditions.