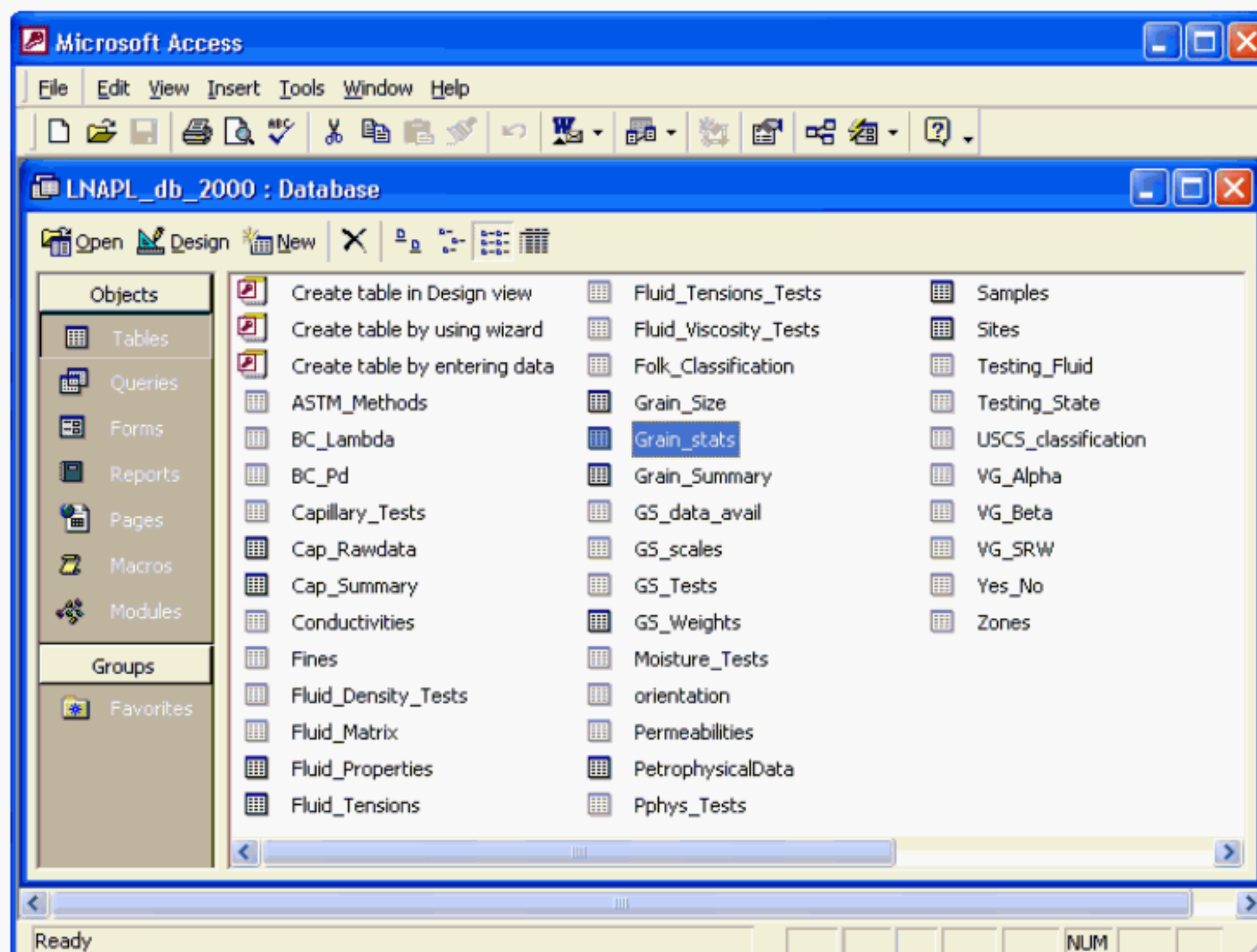


Light Non-Aqueous Phase Liquid (LNAPL) Parameters Database

Version 2.0 Users Guide

Regulatory Analysis & Scientific Affairs Department

Publication Number 4731
December 2003



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FORWARD

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PREFACE

The Light Non-aqueous Phase Liquid (LNAPL) Parameters Database is a collection of information about samples that have had their capillary parameters determined, as well as other physical parameters measured. Capillary properties are critical in multiphase calculations, and those results have very high sensitivity to these properties. The primary purpose of this database is to provide information to users who are trying to characterize the movement and distribution of LNAPL within a site that has a limited set of direct observations of the capillary properties of the site. Other databases of related parameters have typically been derived from measurements in the agricultural or the petroleum extraction industries; neither being necessarily representative of near-surface environmental conditions. This database give the user the opportunity to understand the range of capillary characteristics observed at sites that are geologically similar, but where there are more direct and laboratory observations available.

This document is broken up into 4 primary sections: Data Retrieval, Data Entry, Database Design, and Database Maintenance. Most users have interest in the first topic.

- The Data Retrieval section describes the types of data that are contained in the database and how a user can quickly retrieve subsets of the database that match various user input filters or selection criteria. This section includes several user scenarios with user inputs and database outputs conveyed through a series of sample screens and text.
- The Data Entry section describes how a user can add new data to the database using two primary data entry methods: 1) manual data entry through data entry forms, and 2) data import from electronic sources. Both methods are described and examples are provided. API recommends that only individuals and organizations with a high level of technical and database expertise attempt to add data to the database.
- Appendices A-C are written for database developers. A detailed description of the database design is provided in the first appendix. This section describes the structure of the database and the relationships between its tables, queries, forms, reports, and macros. The database maintenance section describes areas within the database that will require periodic maintenance and how to perform that maintenance, data validation, removing data from the database, etc.

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1 Getting information out of the database: Data Retrieval

The most basic use of this database of LNAPL parameters involves retrieving a subset of data records that match a particular set of selection criteria. In database jargon, this process is called “querying the database”. Users specify what subset of information they would like to retrieve, and the set of criteria by which matching records should be determined. However, before one can get started retrieving data, one must know a little bit about the types of data stored in the database.

1.1 Database contents

The LNAPL Parameters Database is a collection of information about samples that have had their capillary parameters determined, as well as other physical parameters measured. Capillary properties are critical in multiphase calculations, and those results have very high sensitivity to these properties. Capillary properties are sparsely documented in technical literature, and the documentation that exists is generally for other fields of study. Thus, they are not as applicable to environmental release conditions. There are significant property differences between the environmental samples in the subject database and those found in the historic literature. The purpose of this manual is not to discuss these differences, but rather document the construction and content of the API LNAPL parameters database.

The data (samples) contained in this database come from a number of different sources and sites (refineries, fuel storage facilities, military bases, etc.); information now in the public domain. The data that have been included in this database were not collected for the purpose of populating a database of useful parameters. The samples were collected to answer site-specific questions and to aid in the mitigation and remediation of site-specific problems. Given this diverse sample background, it is not surprising that the range of tests performed on each sample and the testing procedures used during the tests differ in many cases. Nevertheless, this is currently the most complete set of laboratory measurements of samples whose properties have been analyzed for the purpose of understanding LNAPL remediation in near-surface aquifers.

The database contains the following types of information:

- Sample capillary parameters and the raw data from which they were derived. This information is available for nearly all samples in the database.
- Petrophysical data including density (bulk/grain), porosity, permeability, conductivity, water and hydrocarbon saturations, etc.
- Grain size data. Grain size data are collected and presented in several ways.
 - Raw grain size distribution data (weight fraction vs. grain size)
 - Grain size at various percentages of the cumulative sample weight (i.e. the grain size at the 10th, 50th, and 90th percentiles).
 - Grain size distribution statistics (mean, median, standard deviation)
 - Fraction of the sample in various grain size classifications (% sand, % silt, etc.)

Typically, if the full raw grain size distribution is available, then all of the summary parameters are also available. For some samples, only summary data is available, while others have no data available.

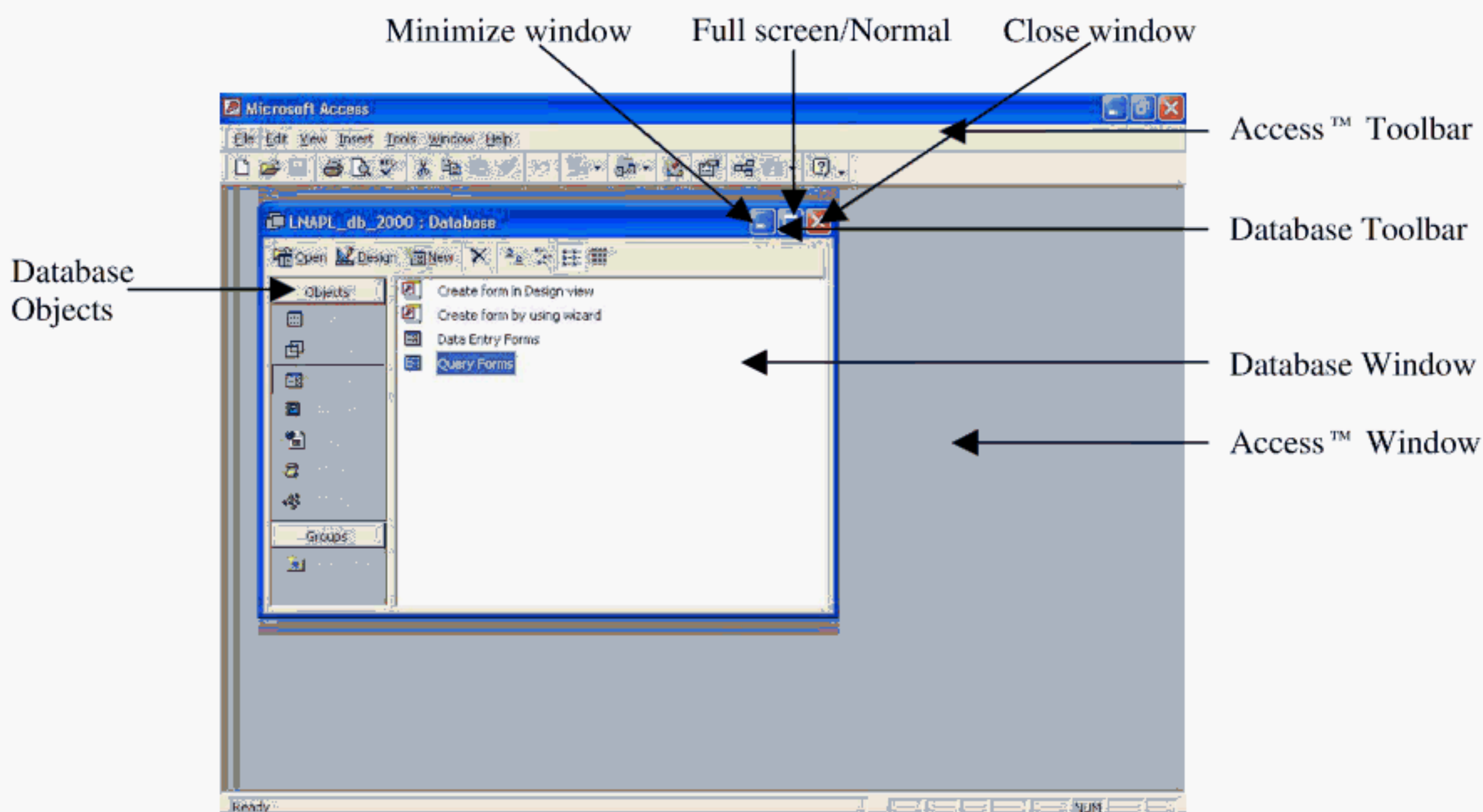
- Fluid properties (viscosity, density, interfacial tensions). Typically, fluid properties samples are not taken from the same samples where rock properties are measured. Fluid properties samples are provided as a form of site characterization, rather than for direct comparison with other samples within the site.

In many cases, the process of measuring one set of sample properties (grain size) makes the sample useless for measuring other properties (e.g., porosity). In general, the collection of measurements attributed to a single sample is obtained from slices of a single core not separated by more than 6 vertical inches from the slice where the sample capillarity was determined.

1.2 Getting Started

The first step is to open the database in Microsoft Access™. Locate the database file *LNAPL_db_2000.mdb* and then double click the left mouse button on the file. After opening the database, your screen should look like the screen in Figure 1.

Figure 1: Basic Access screen with annotations



The database should open with the *Forms* object open and the *Query Forms* option highlighted. However, the database will open in the state that it was in when it was last closed. If the last user did not leave the database in normal state, then some set-up might be necessary prior to getting started. On the left hand side of the screen, under the heading *Objects* (see figure 1), select *Forms* (single or double left-mouse click). The screen should now look like the screen in figure 1. Double click the left mouse button to on *Query Forms* to bring up the various query forms.

Helpful Hint: The query forms are displayed in the most user-friendly manner when the database window is maximized (full screen).

Figure 2: Query Forms

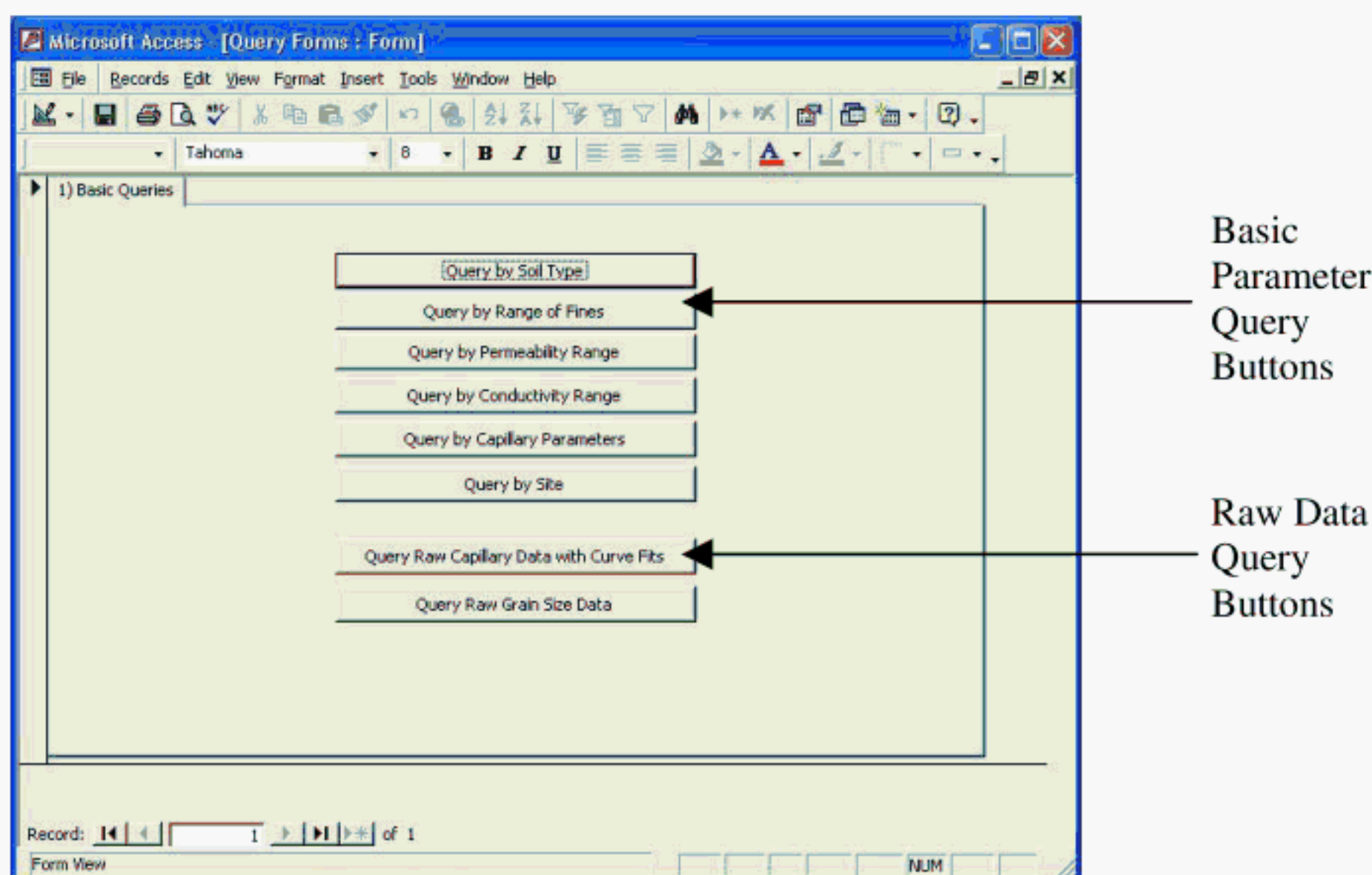
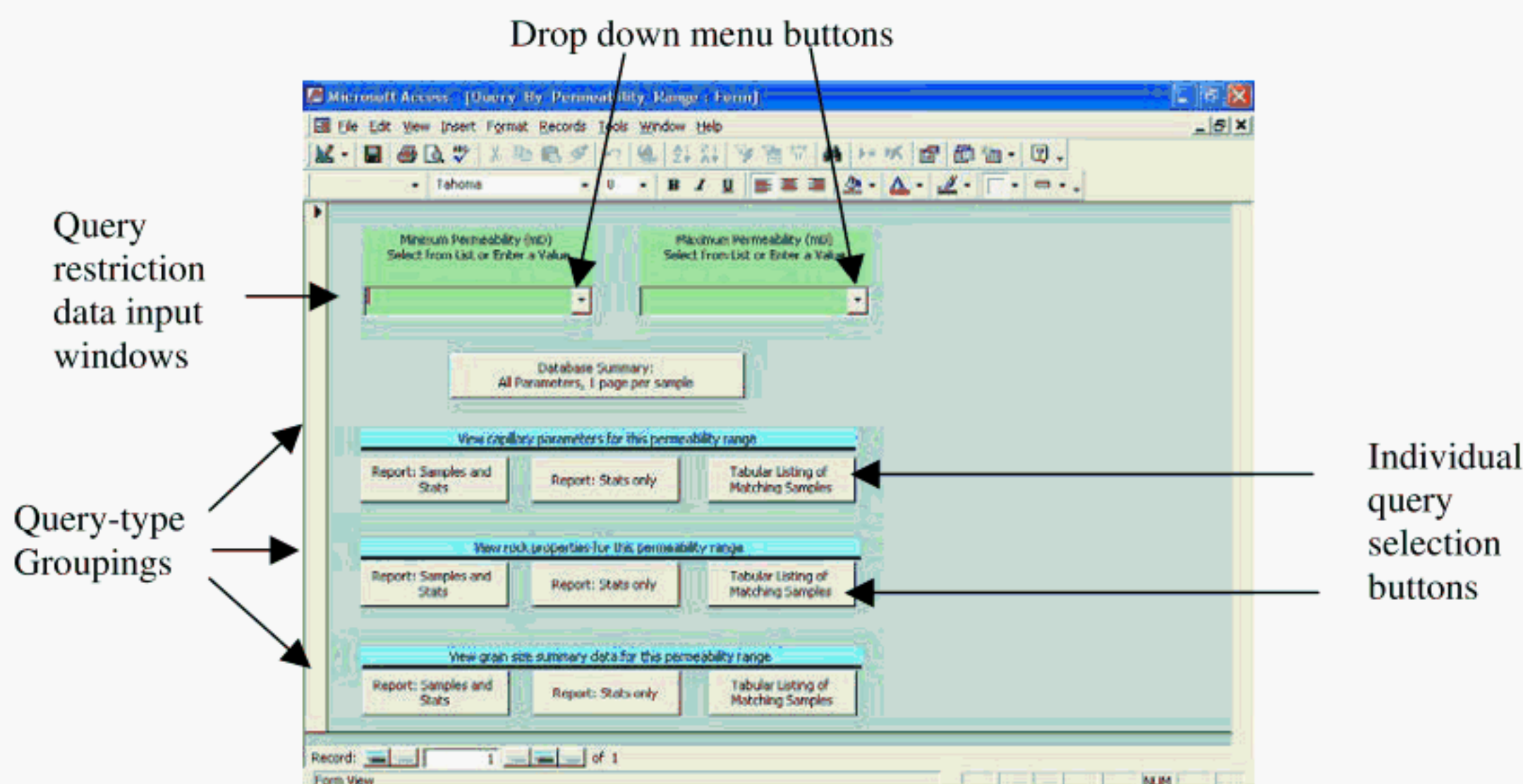


Figure 2 shows the *Query Forms* screen. At the top of the form are 5 buttons that provide access to the basic parameter queries. At the bottom of the screen are 2 buttons that provide access to raw data for individual samples.

For now, we will concentrate on the basic parameter queries and results; raw data queries/results will be discussed later. All of the basic parameter query screens look similar to each other, and provide output in the same formats. The only difference between the 5 queries is how the data are selected for display. We will use *Query by Permeability Range* for our examples, and discussion of the various types of query results and displays. Select any query options by clicking (left mouse) on the desired button.

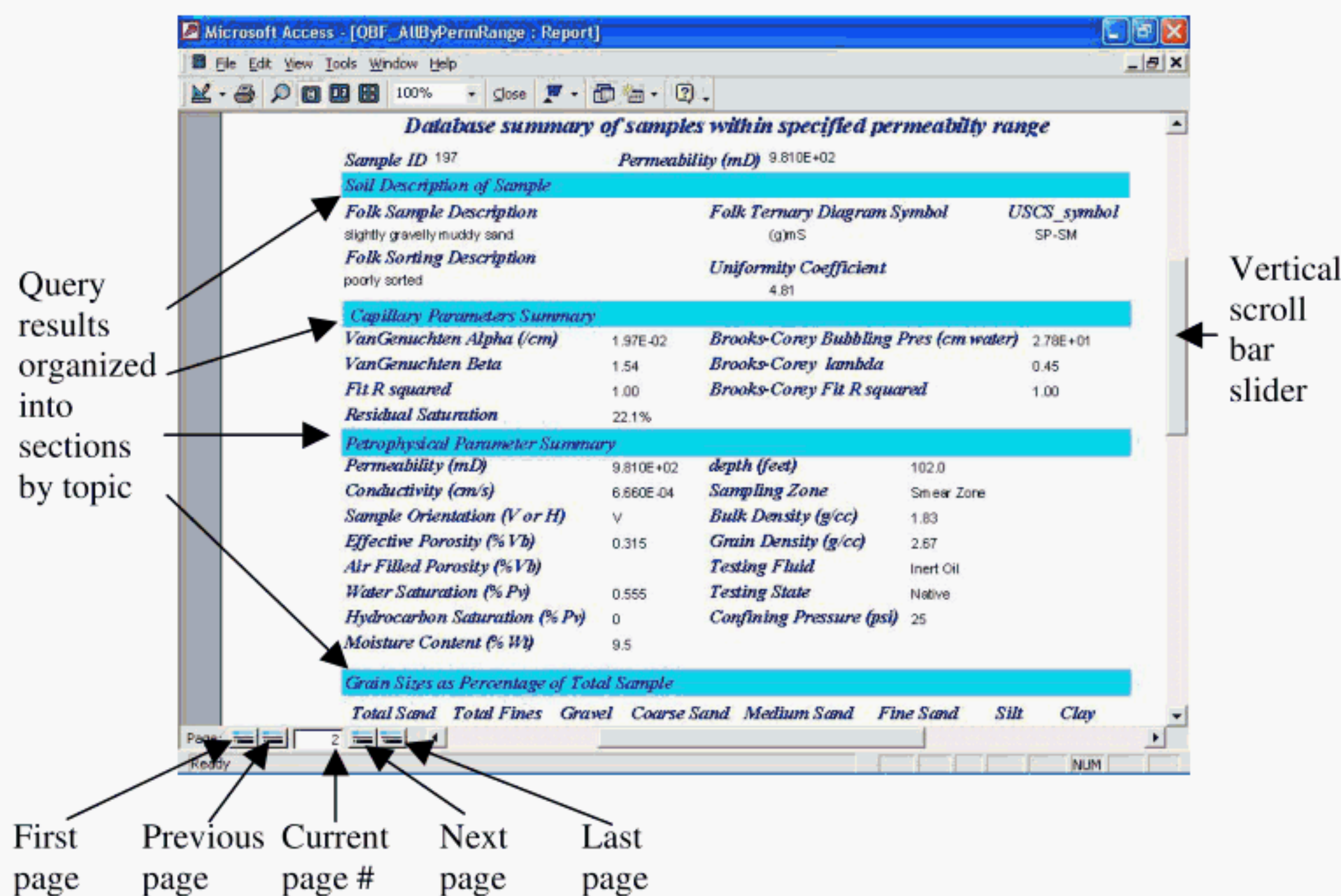
Figure 3: Query by Permeability Range screen (maximized) with annotations



When the *Query by Permeability Range* option is selected the screen should look like the example in Figure 3. At the top of the screen is the user input area. At the bottom of the screen is a collection of data return and display options. The user must first specify a minimum and maximum permeability. You can either type values into each of the entry forms or you can select from the options provided in the menu (click on down arrow next to the data entry area. The options provided in the menu characterize the statistical distribution of the parameter that is controlling the query. These include the parameter minimum, maximum, average, median (50th percentile), first quartile (25th percentile), and third quartile (75th percentile). Even if you decide to enter a specific value, you should probably check the menu items to get a feel for the database content. Make sure that the maximum value selected/entered is greater than the minimum value selected/entered!

After the controlling parameter(s) is (are) set, the next user should select the data that should be returned and the format of the display from the options provided in the bottom two-thirds of the screen. The following pages show the types of screens that are returned for each of the available options.

Figure 4: Database Summary: All parameters, 1 page per sample



The retrieval/display option at the top/center of the options list is the *Database Summary: All parameters, 1 page per sample* option. As the title indicates, this option will display in *Report* format the complete set of database parameters available for all samples that fall within the user specified parameter range. The results for each sample are provided on separate pages in the report. To “flip” the pages in the report, select one of the page turning options as outlined in Figure 4 (first page, back one page, ahead one page, last page). As noted in the Database Contents section (1.1), not all samples have all possible forms of data included in the database. A blank field in the report indicates that this data type is unavailable for this sample. For example, in Figure 4, the Air Filled Porosity (%Vb) field is blank while the other values within the *Petrophysical Parameter Summary* are all present. This indicates

that the petrophysical properties of sample 197 were measured but this particular parameter was not. In many cases, whole sections of the report (*Soil Description, Capillary Parameters, Petrophysical Summary, Grain Sizes, Grain Weight Percentages, Grain Size Statistics*) may be blank for a given sample if those tests were not performed on the sample. At the bottom of the report (not shown), both the page number and the total number of pages are provided. The number of pages is the same as the number of samples in the database that match the query input.

Helpful Hint: To return to the Query by Permeability Range screen, close the report screen (click the close screen box in the upper right-hand corner).

The remaining query options provide access to a subset of the entire database holdings that match the basic parameter query. There are three subsections: *Capillary Parameters* (this section is not present in the *Query by Capillary Parameters* basic parameter query area), (petrophysical) *Rock Properties*, and *Grain Size Parameters*. Each subsection has three options. To minimize the redundancy, only the individual options from the *Capillary Parameters* section will be shown here. The screens from the other options mimic the capillary parameter output in format but not content. The content of the other items was shown in the *All Parameters* example above.

Figure 5: Report: Samples and Stats

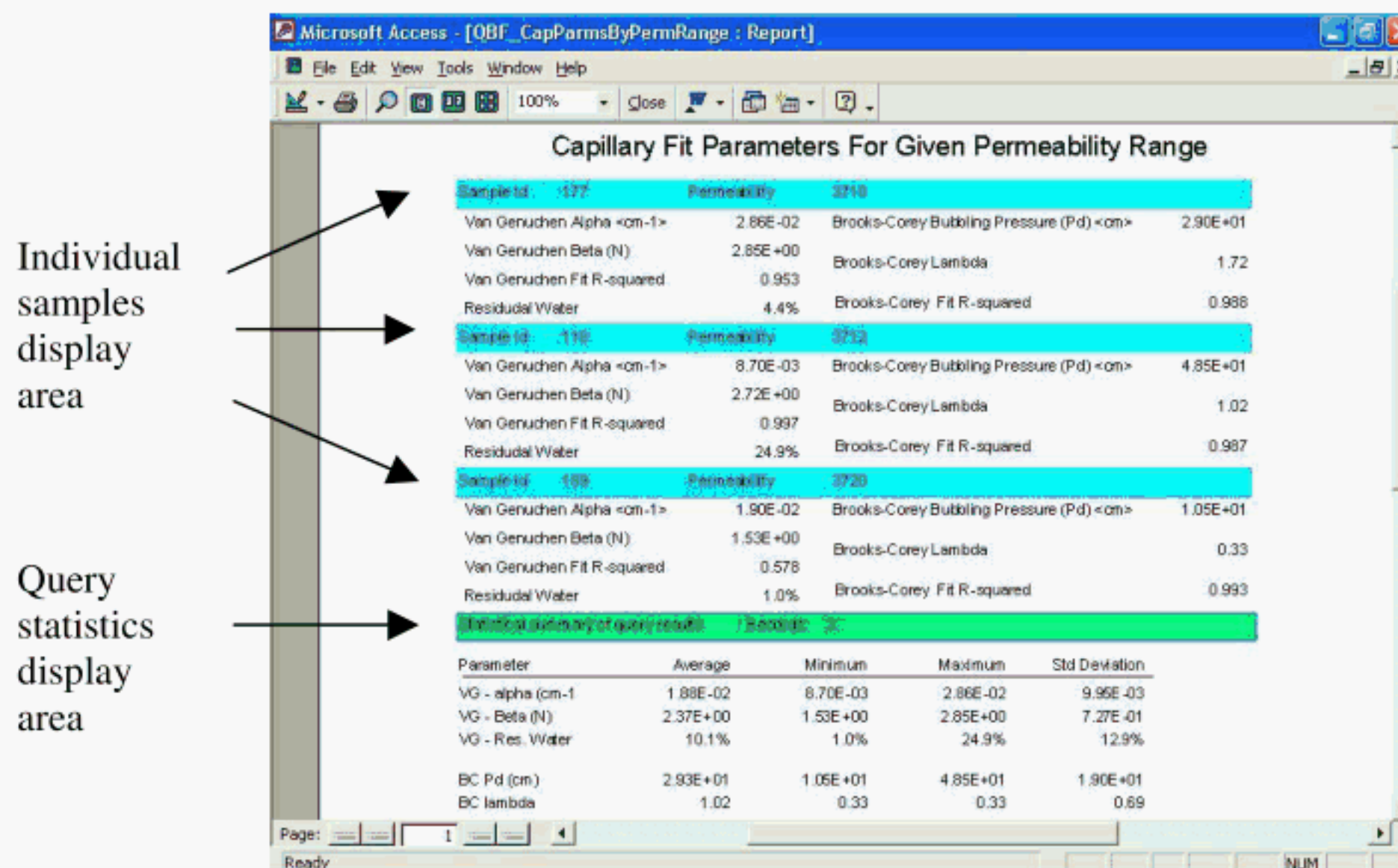


Figure 5 shows the result of a Capillary Parameters Report: Samples and Stats query for a permeability range of 3700-3750 mD. The capillary fit (van Genuchten and Brooks-Corey) parameters for each matching sample are displayed in report format. A statistical summary (average [mean], minimum, maximum, standard deviation, and number of matching samples) of the matching records is provided at the end of the report. If the number of matching samples is large, the report will span many pages. Selecting the *Report: Stats only* option produces just the stats portion of the report from the previous query. No information about the individual samples is returned.

Figure 6: Tabular Listing of Matching Samples

sample_id	VG_alpha (cm-1)	VG_beta	VG_Srv	VG_fit_Rsq	BC_Pd (cm)	BC_lambda	BC_fit_Rsq	permeability (mD)
149	2.77E-02	1.68	44.0%	0.983	2.71E+01	0.63	0.990	1.081E+03
120	1.27E-02	2.41	23.9%	0.987	4.80E+01	1.16	0.996	1.263E+03
156	1.13E-02	2.14	31.0%	0.999	6.55E+01	0.96	0.993	1.432E+03
2	4.50E-03	2.64	13.0%	0.998	1.62E+02	1.43	0.993	1.472E+03
155	2.40E-02	1.62	34.0%	0.997	2.76E+01	0.55	0.985	1.609E+03
195	1.30E-02	2.57	12.2%	0.996	4.64E+01	0.96	0.995	1.621E+03
103	1.23E-02	2.53	25.4%	0.999	2.45E+01	1.69	0.967	1.625E+03
12	1.06E-02	2.06	30.0%	0.998	6.85E+01	0.93	0.987	1.645E+03
15	6.29E-03	1.55	68.0%	0.993	5.65E+01	0.34	0.938	1.678E+03
123	7.55E-03	1.95	33.3%	0.999	6.55E+01	0.67	0.961	1.737E+03
7	9.20E-03	2.45	11.0%	0.999	7.09E+01	1.11	0.987	1.765E+03
114	1.64E-02	1.69	33.8%	0.994	2.71E+01	0.42	0.992	1.913E+03
232	1.66E-03	2.20	6.0%	0.993	1.64E+02	0.24	0.954	2.060E+03
196	3.17E-02	1.53	23.5%	0.989	3.69E+01	0.57	0.998	2.072E+03
102	6.00E-03	1.57	23.8%	0.999	2.30E+01	0.35	0.997	2.106E+03
121	1.72E-02	1.96	30.9%	0.997	4.47E+01	0.90	0.984	2.249E+03
115	1.69E-02	2.06	26.0%	0.990	3.19E+01	0.36	0.962	2.270E+03
127	1.30E-02	2.25	13.0%	0.998	5.31E+01	0.72	0.928	2.285E+03
4	6.50E-02	1.42	40.0%	0.998	1.52E+01	0.41	0.947	2.295E+03
180	5.54E-02	2.66	4.9%	0.994	1.49E+01	2.21	0.981	2.360E+03

The final query display option is to display the query results as a simple spreadsheet table. Column headings are displayed at the top of each column. Values are formatted for display according to the representation (decimal, scientific, percentage) and precision rules that are defined within the database.

1.3 Retrieve samples for a given soil type

The database can be queried to return all samples for a user-specified soil type by selecting the *Query by Soil Type* option from the main query screen (see Figure 2).

Figure 7: Soil Type Selection Menu

USCS Symbol list

USCS Classification Criteria

Select Soil Type

ML: silt (fines > 50%, silt > clay, sand < 20%)

SM: sandy silt (fines > 50%, silt > clay, sand > 20%)

SP: silty sand (fines > 12%, coarse > 50%, sand > gravel, silt > clay)

SP-SM: poorly graded sand (fines < 5%, coarse > 50%, sand > gravel)

SW: silty sand, poorly graded (5% < fines < 12%, coarse > 50%, sand > gravel)

SW-SM: well graded sand (fines < 5%, coarse > 50%, sand > gravel)

SW-SM: silty sand, well graded (5% < fines < 12%, coarse > 50%, sand > gravel)

View capillary parameters for this soil type

Report: Samples and Stats

Report: Stats only

Tabular Listing of Matching Samples

View rock properties for this soil type

Report: Samples and Stats

Report: Stats only

Tabular Listing of Matching Samples

View grain size summary data for this soil type

Report: Samples and Stats

Report: Stats only

Tabular Listing of Matching Samples

The user is provided with a drag-down menu of Unified Soil Classification System ([USCS symbols](#)), and their definitions in terms of the fraction of fines (silt + clay), sands, and gravels, within a sample. Once the user selects a soil type, all of the queries described in [section 1.2](#) are available to the user.

The drag-down menu does not include all possible USCS symbols. There are two reasons for this: 1) The database does include samples of all soil types, and only the soil types present within the database are shown, and 2) the laboratory that performed the grain size analysis on the bulk of samples in the database does not separate clay fractions by organic content. All clays are assumed to be inorganic within the database.

1.4 Retrieve samples within a range of fine (silt + clay) percentages

The database can be queried to return only samples that fall within a user specified range of fine particles. Fines are defined to include the sum of the silt and clay fractions. Many samples, particularly those whose grain size distributions were determined by screening, do not distinguish between fine silt and clay. Setting a low limit on the fine fraction boundary is equivalent to requiring primarily sand size (or greater) particles. Figure 8 shows the data input window for this type of query.

Figure 8: Query by Range of Fines Menu and Options

1.5 Retrieve samples within a permeability range

The retrieval of samples matching a user specified range of permeability was used as the primary example of database usage and will not be repeated here. Please see section 1.2 ([Getting Started](#)) and Figure 3 for additional information.

1.6 Retrieve samples within a conductivity range

Retrieving samples by specifying a range of matching sample conductivities is exactly analogous to retrieving data by specifying a permeability range. The only real differences are the units of conductivity and the valid ranges for the minimum and maximum values.

The units of conductivity are cm/s and the valid range is 0-100 cm/s (generous upper limit). Please refer to sections 1.2 ([Getting Started](#)) and [Figure 3](#) for additional information.

1.7 Retrieve samples with capillary parameters that match search criteria

Retrieving samples where the capillary parameters (van Genuchten and Brooks-Corey) match user specified limits is slightly different from the types of queries that have previously been discussed.

Figure 9: Querying by Capillary Parameters

Parameter Name	Minimum	Maximum
VanGenuchten Alpha (cm ⁻¹) Range = (0-1)	0	1
VanGenuchten Pore Uniformity (Beta) Range = (1-100)	1	100
Residual Water Saturation (S _{rw}) Range=(0-1)	0	1
Brooks-Corey Bubbling Pressure (Pd- cm H ₂ O) Range = (0-50000)	0	50000
Brooks-Corey Pore Uniformity (lambda) Range = (0-10)	0	10

Database Summary:
All Parameters, 1 page per sample

View rock properties for this conductivity range

Report: Samples and Stats Report: Stats only Tabular Listing of Matching Samples

View grain size summary data for this conductivity range

Report: Samples and Stats Report: Stats only Tabular Listing of Matching Samples

Record: 1 of 1
Form View

The most important distinction is in the number parameters that are available to restrict the output. It is very easy for a user to over specify restriction criteria such that no samples are returned. Parameter minima, maxima, and other menu items are not dynamically generated to match the subset of parameters available given previously specified selection criteria. These

values reflect the database as a whole. Users are cautioned to add restriction criteria one at a time. For example, if you want to restrict returned values to a range of VG Alpha values and VG Beta, it would be prudent to run the query first with only the VG Alpha restriction and examine the results to see if any samples match your desired VG Beta restriction criteria. If so, add the second restriction and run the query again.

Note that the *Capillary Parameters* section of the query form (see [Figure 3](#)) is missing.

1.8 Retrieve samples from a particular site

There are times when a user would like to examine all of the samples from a given site (location), to understand the amount of variability in the sites. In addition, some database parameters, such as the various fluid properties, are really site characteristics not associated with individual samples. The *Query by Site* function provides this capability. In this query, the user is asked to select a site from a list of available sites (Figure 10). Not all sites have associated fluid properties data so the user is presented with two options: a list of all available sites and a list of sites where fluid data is available. Note that this query form looks slightly different than the normal basic query forms in that there is an extra category set at the bottom where fluid properties data can be queried. Also note that there is no “query statistics only” function available for the fluids query. Fluid properties are typically measured over a range of temperatures and it does not make sense to “average” these values.

Figure 10: Query by site form

User can select a site from a pick-list of available sites

Fluid properties data can be retrieved for a given site – assuming such data are available

1.9 Raw data retrieval

Raw capillary and grain size data differ from other sorts of data in the database in that many values are associated with a single sample. Permeabilities, capillary parameters, mean grain sizes, etc. are all single valued for a given sample. To extract raw distribution data from the database, a specific sample must be identified. Unfortunately, there are no simple ways to provide the user with much information about a sample in the sample selection menu. Users are encouraged to perform other queries prior to querying the database for raw data. If you find a sample of particular interest, and you would like to know more about the raw data, write down (or remember) the sample ID number and then begin your raw data query.

1.9.1 Raw capillary data for a given sample

Raw capillary data for a given sample can be displayed in three ways: 1) Report format with a plot of the van Genuchten parameter fit, 2) Report format with the Brooks-Corey parameter fit, 3) Table view.

Figure 11: Raw capillary data report with van Genuchten parameter fit

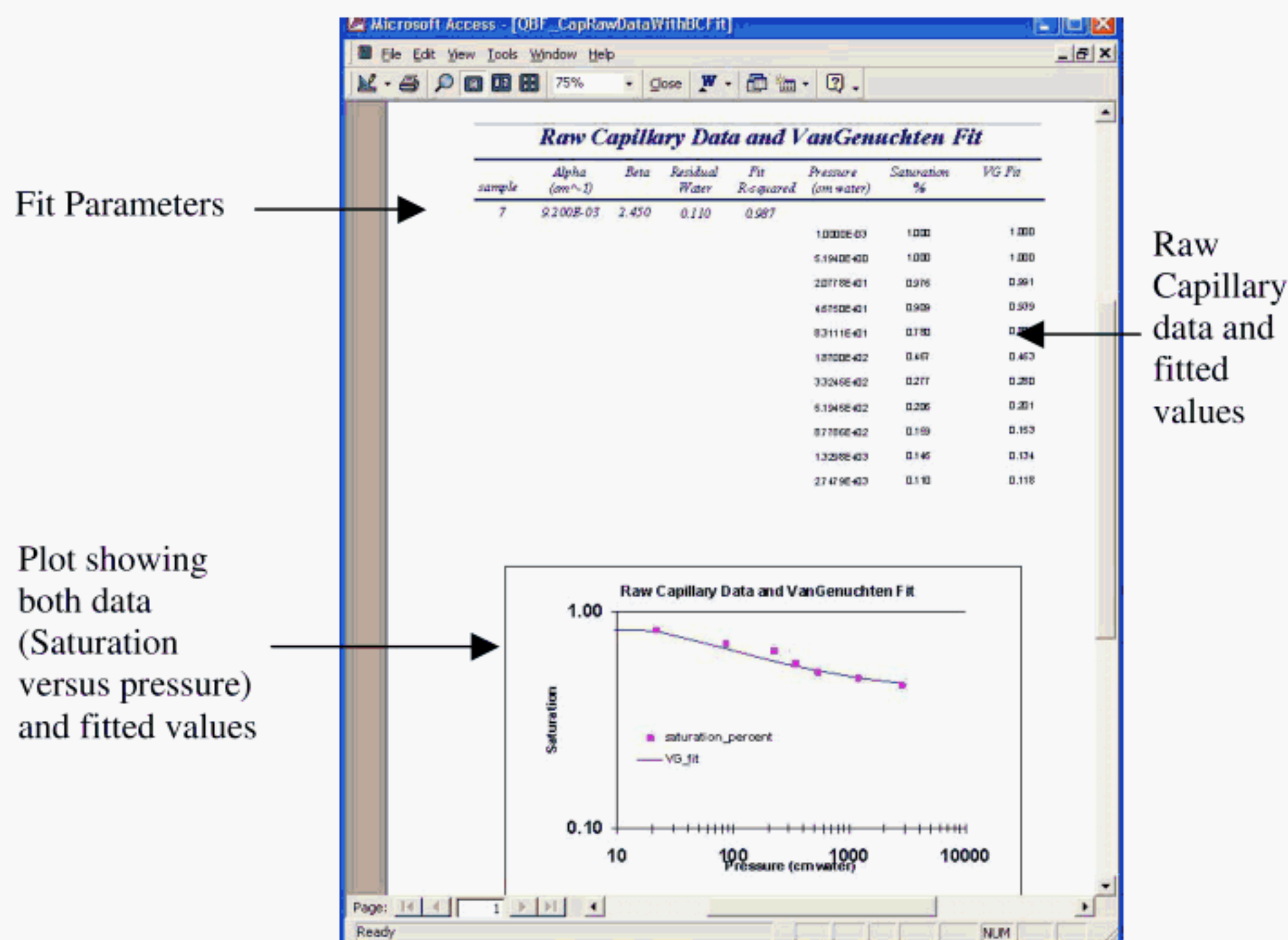
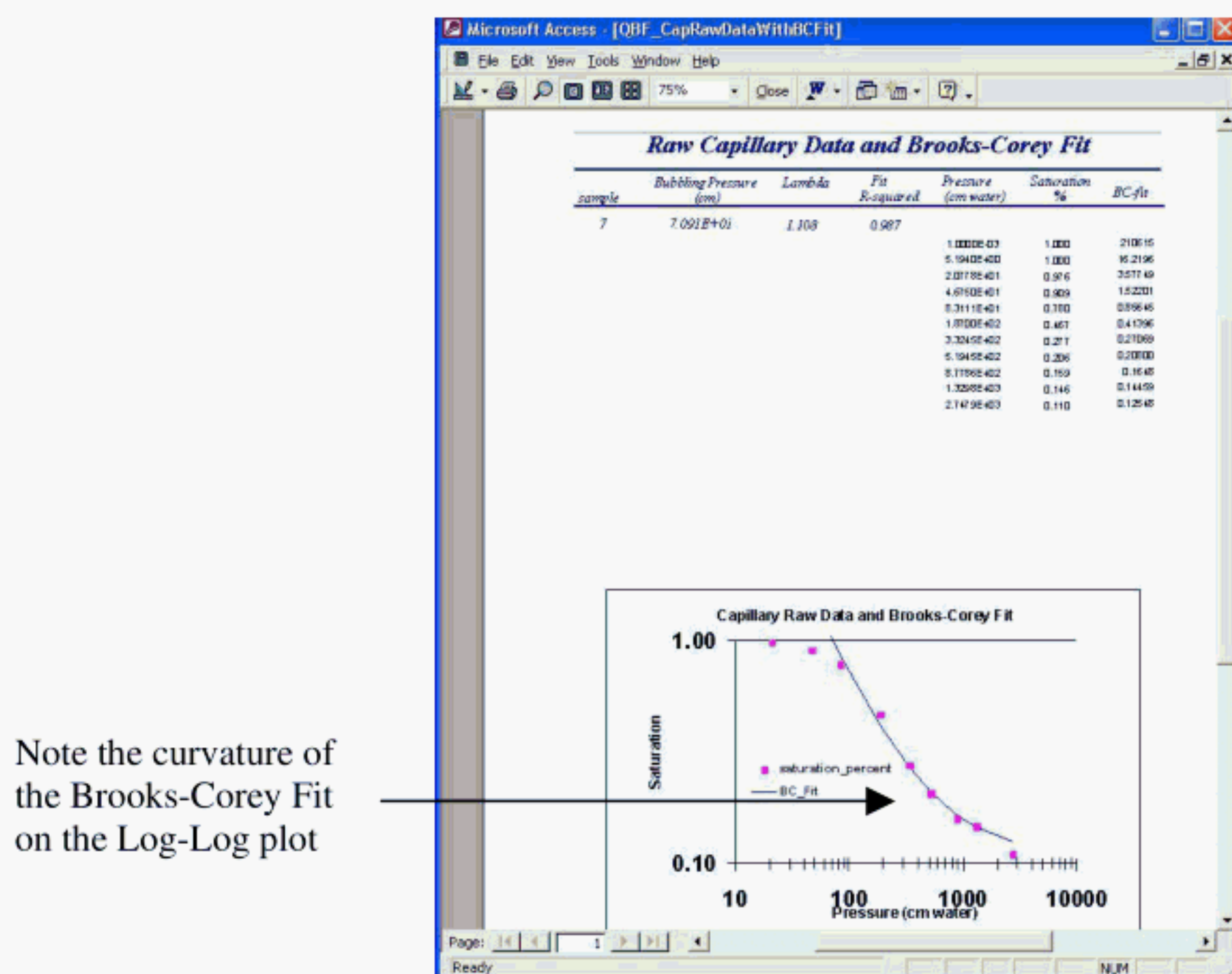


Figure 12: Raw capillary data with Brooks-Corey fit



Some of the raw capillary data with Brooks-Corey analysis and fit plots may look a bit unusual to users familiar with this form of analysis. The Brooks-Corey technique fits a linear function of the logarithm of pressure to the logarithm of effective saturation. Clearly the curve shown in Figure 12 for sample 7 above is not linear and the plot is provided on a log-log scale. The curvature is the result of plotting total saturation (S) versus pressure on a log-log scale. Effective saturation (S_e) is related to total saturation (S) by the expression:

$$S_e = \frac{S - S_{rw}}{1 - S_{rw}}$$

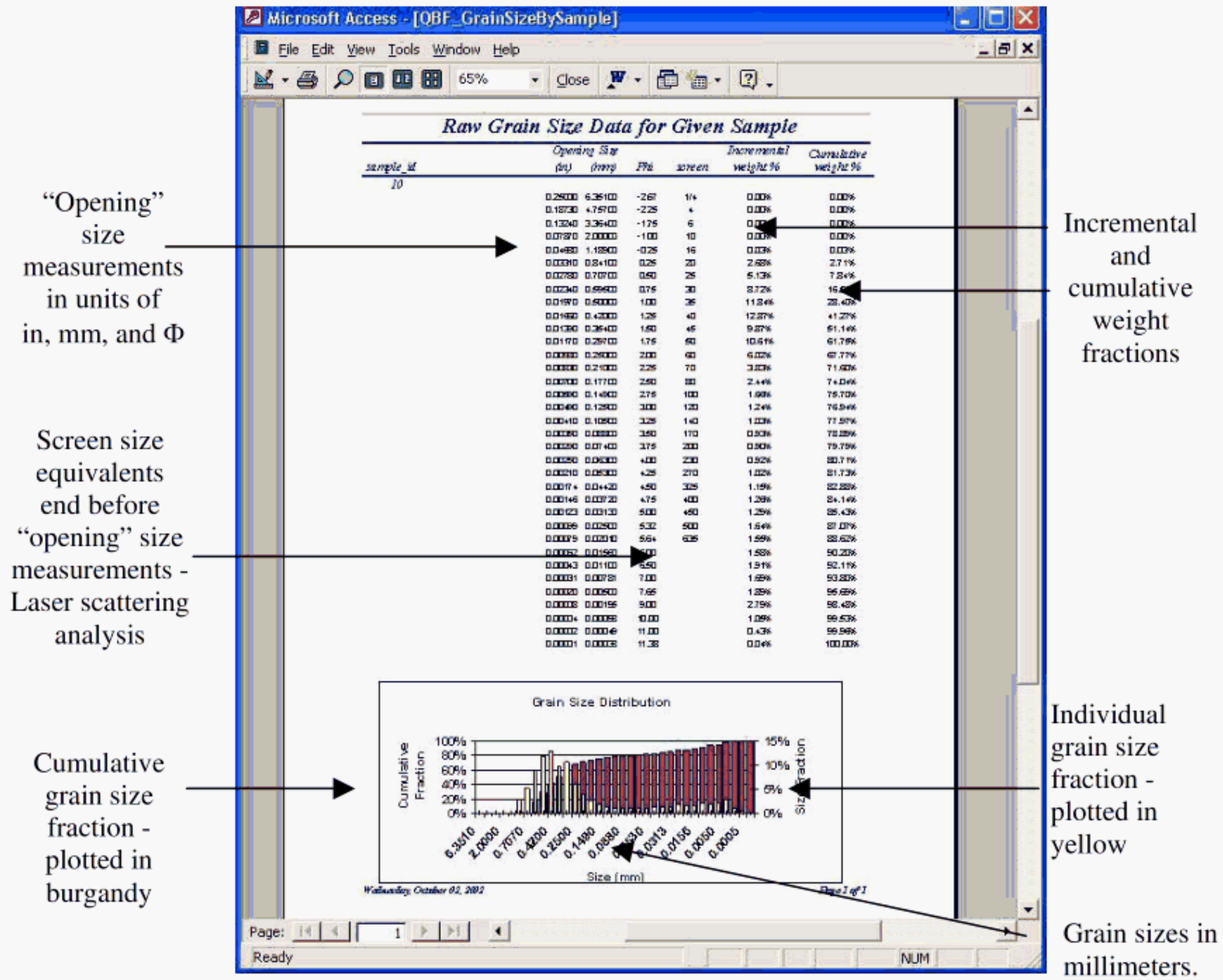
where S_{rw} is the residual saturation.

The raw capillary data table view looks like the result in [Figure 6](#) but with different columns. Both the raw capillary data and the two fit results (VG, B-C) are shown.

1.9.2 Raw grain size data for a given sample

Raw grain size data can be retrieved either as a table of values or formatted as a report with a plot showing the grain size distribution. The table format looks like the result shown in [Figure 6](#) but with different columns. The report format for the raw grain size data is similar to the format for the raw capillary data in that the report tabulates the distribution and includes a plot of the data ([Figure 13](#)). Raw grain size distributions are measured in one of two ways, screening or by laser scattering. A user can quickly determine which method was used for a given sample by viewing the raw data. If the distribution extends to sizes below the minimum screen size, laser scattering analysis must have been performed. Conversely, if grain sizes extend only to the limits available to screening analysis, then this must be the analysis technique.

Figure 13: Raw grain size data with grain size distribution plot



2 Data Entry

This version of the database has input data for 235 samples from 24 different sites. While this is a good start, many more data sets can and should be entered into the database. This chapter describes the various methods for adding new data to the database. Data that could be entered into the database exist in two common formats, electronic files and paper documents. [Section 2.2](#) describes the tools developed to aid in the transcription of data stored in hardcopy documents. [Section 2.3](#) describes the tools provided for the reformatting of electronic data sets into forms that are easily imported into the database. However, before we describe how to add data to the database we should comment on what data should be added to the database.

2.1 Selecting data for entry into the database

The primary purpose of this database is to provide information to users who are trying to characterize the flow of LNAPL within a site that has a limited set of direct observations of the capillary properties of the site. The basic idea is to try and understand the range of capillary characteristics observed at sites that are geologically similar, but where there are more direct and laboratory observations available. Given this objective, the availability capillary data and analysis should be the principal requirement for the inclusion of a data set (sample) in the database. However, capillary analysis alone is insufficient. Without any other sample characterization (grain size analysis, petrophysical analysis, fluid analysis), the capillary data is not useful in terms of understanding other sites.

There are no features of this database that restrict which data can be entered into the database. It is up to the database user to decide what additional data gets entered. However, if the initial objectives of the database are to be maintained, then only samples that have contain capillary analysis and at least one other form of analysis should be considered for inclusion in the database.

2.2 Manual data entry using data entry forms

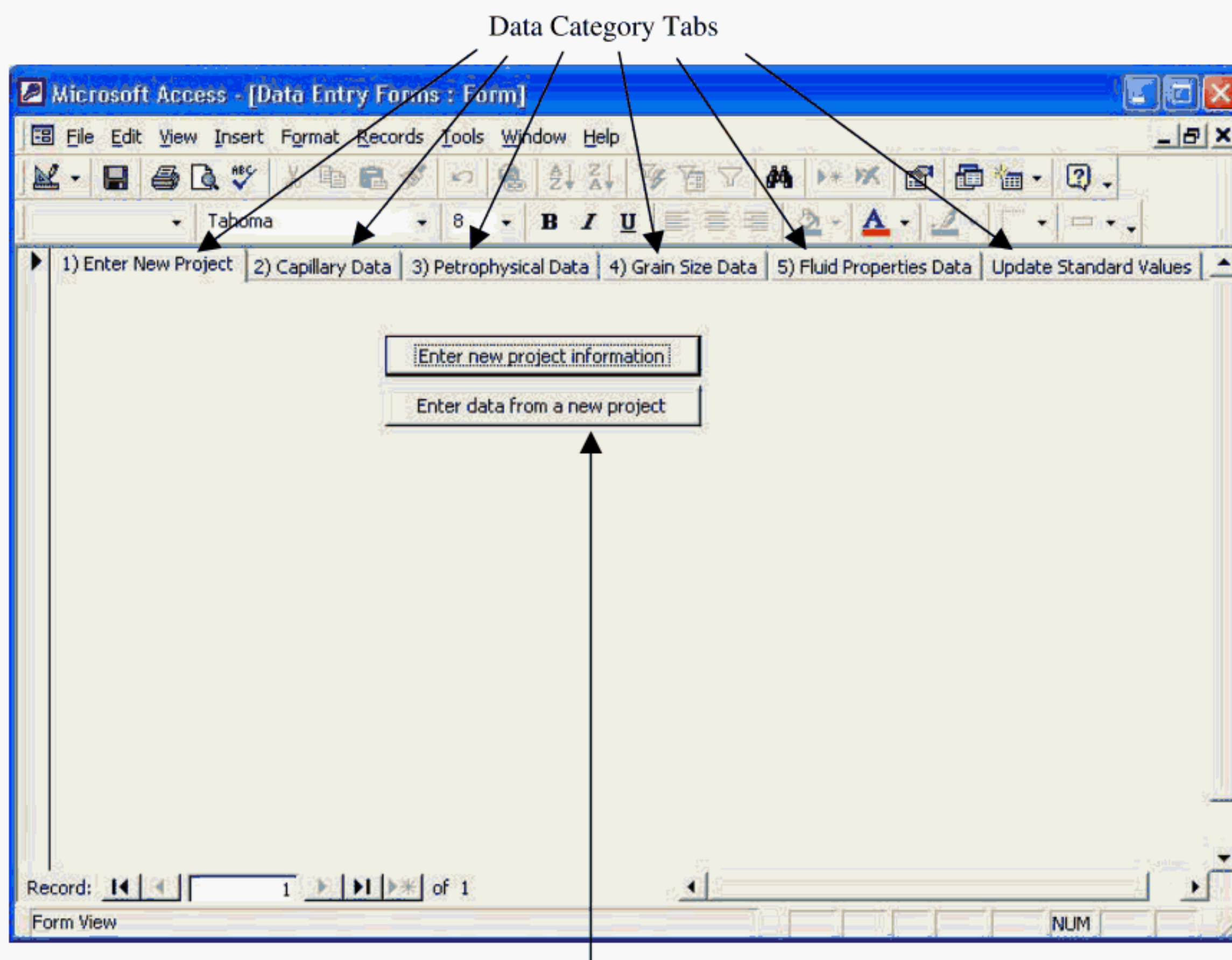
The person entering data needs to have the data well organized prior to getting started. In particular, the user must have determined which samples are going to be represented as a single sample within the database. As described earlier in this document, labs often cannot make multiple measurement types (capillary analysis, petrophysical analysis, grain size analysis) on a single physical sample. The data entered into the database thus far associates data into a single sample record values that were acquired within 6 vertical inches (same well) of the sample analyzed for capillary properties. In other words, the grain size data for a sample collected in well MW17 at 20.5 ft below grade could be associated with a capillary sample collected anywhere between 20 and 21 ft below grade from MW17. Samples from sites where the strata are very finely layered might require more restrictive sample correlation criteria.

In addition to knowing which samples are going to be associated within the database using a single sample identifier, all of the sample analysis methods (ATSM methods) need to be known for each sample and data type (capillary, grain size, fluid viscosity, etc.). This information is included in the database in the **Samples** table.

Data entry will be far more efficient and less prone to mistakes if the data are well organized and documented prior to beginning the data entry process.

To start the data entry process, open the database and select the *Data Entry Forms* from the *Forms* object by double clicking the left mouse button on this item (see Figure 1). This will bring up the basic data entry form (Figure 14). Across the top of the form are a number of tabs. Each tab provides access to a set of data entry forms for similar types of data. Typically the data entry process begins by entering information about the site and its samples. This information must be entered before any further information about the samples can be added to the database.

Figure 14: Basic data entry form



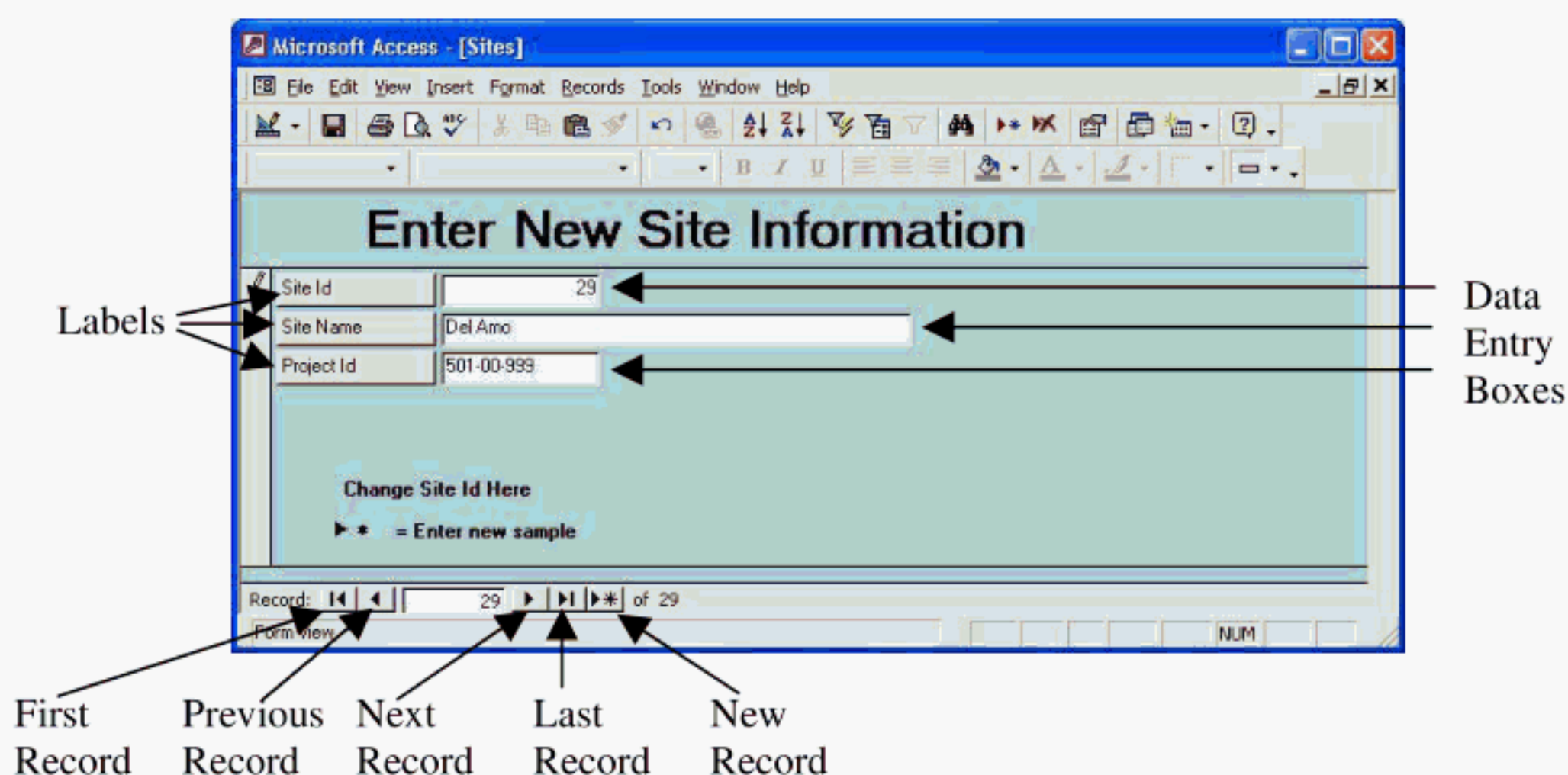
Data Entry forms within the selected
data category (Enter New Project)

2.2.1 Site Entry Form (*Enter New Project Information*)

A site is a small geographic area where one or more samples have been collected. Commonly, sites are places like refineries, military bases, or service stations. Only the most basic information about a site is stored in the database. This includes a site number, name, and project number (see figure 15). The site number is required value; the other values can be left blank, if desired. Some sites are identified within an organization by a project number. Project numbers can provide a mechanism for identifying a site within the database in a

manner that is only identifiable to members of the organization that provided the data. New site data is entered in the blank fields beside the field identifiers. A user can advance to the end of the list of sites by clicking on the “last value in list” icon at the bottom of the screen (▶▶). Figure 15 shows the current last record in the **Sites** table. This lets the user know the highest site number that currently exists in the database. The new **site_id** should be 30 or one more than the last value currently in the database. The user needs to remember the site number when entering new samples into the database (next section). To advance the form to a “new record”, either select (left mouse click) the new record (▶*) icon or the next record (▶) icon.

Figure 15: Site data entry form



2.2.2 Samples Entry Form (*Enter Data From a New Project*)

The samples data entry form is the most complex of the data entry forms. Basic information about the analysis techniques performed on the sample must be added to the database for completeness. To simplify data entry, most input parameters have standard value pick-lists available (Figure 16). All of the samples for a given site must be entered into the **Samples** tables (using this form) prior to entering further information about the sample into the database.

As with the **Sites** table, the first step in the data entry process is to determine the **sample_id** of the last sample entered into the database. Click on the “last record” icon and read the **sample_id** number. The **sample_id** values should increase by one for each new sample. As shown in Figure 16, the last **sample_id** is 235. The **sample_id** entered for the next new sample should be 236 and the **site_id** should be 30 (from the previous section). Each sample that a user enters into the database already has some name by which it is referred to by the organization and/or testing facility that analyzed the sample. To preserve this name it must be entered into the database and associated with the **sample_id**.

Figure 16: Samples data entry form - last completed record

Sample Id area

Data Types Available for Sample

Record Navigation Area

Sample Analysis Method Pick-lists

More Sample Analysis Methods

For each sample, the user must identify the available types of data. The types of data possible include capillary data (should be present), petrophysical (rock properties) data (density, porosity, permeability, saturation, etc.), grain size data, fluid viscosity data, and fluid interfacial tensions data. Samples analyzed for properties of the fluids they contain are commonly not analyzed for other properties. In most cases, fluid properties data are related to a site rather than to individual samples from that site. Each of the data availability values has a Yes/No pick-list except for the grain size data availability box. Grain size data may either be “complete” - meaning that the full grain size distribution is available, or may include only “summary” information – size fractions of sands, silts, and clays or statistical parameters of the grain size distribution, or may not be available at all (“none”).

The data analysis method used in the analysis of each data sample should be entered into the database if the information is available. Each of the basic data analysis procedures has a well-defined ASTM (American Society for Testing and Materials) test method (or similar standards organization, i.e., API, etc.) that prescribes how a particular test is to be performed in a standardized manner. Pick-lists of test methods are provided to assist the user in assigning the appropriate testing method to each sample. Pick-lists include both the test name or identifier and a terse description of the test (Figure 17)

Figure 17: Samples data entry form - new blank record

ASTM Method and Description
Grain size test method pick-list

The default values for each new sample entered into the database are “no data available” and the test methods are “not applicable (N/A)”. Once the `site_id`, `sample_id`, and `sample_name` are entered in the sample ID area, the data availability and testing methods section should be completed. Leave the test method set to “N/A” if the particular data type is not available for that sample (i.e. if there are no fluid tensions data, the test method is “N/A”). If a particular data type is available for the sample, but the testing method is unknown, set test method to a blank string (i.e., “”). If the test procedure used in the analysis is known but is not one of the values in the pick-list, note the sample number and leave the test method blank or with the default “N/A” value. In this situation, the user needs to add a new value to the pick-list return to this sample, and then change the test method to the appropriate value. Adding new standard values to the pick-lists is described in the next section.

2.2.3 Adding new standard values to pick-lists

The pick-lists values that are available in the database describe all of the parameters that have been entered to date. It is likely that as new data are added to the database, additional standard pick-list values will need to be included. To update one of the numerous pick-list sets, select the “Update Standard Values” tab ([see Figure 14](#)) with a left mouse-click on the tab area. This will bring up the standard values data entry menu shown in Figure 18.

Figure 18: Update standard values data entry menu

Each of the test method data entry forms has two values that must be entered; a test name and a brief test description. Figure 19a shows the data input form for capillary test procedures. Figure 19b shows the data entry form for fluid matrix values. This menu requires three input parameters: name, description, and sort order. The sort order sets the order in which to display each entry in the pick-list menu. The default display order is alphabetical, which is somewhat inconvenient for this pick-list. If a user adds a new value to this list, and does not want it to be displayed at the end of the list, the user must select an appropriate display order and then renumber all pick-list items of lower display priority. In other words, if you want a new entry to appear as item 5 in the pick-list, items 6-15 will need their sort order values increased by one. Testing states (Intrinsic, Effective, Native) and testing fluids (Air, Inert Oil, Mercury, Water) are single valued. New values can easily be entered using the appropriate data entry forms (not shown).

Note: The most common inert oil used in permeability testing is kerosene; however other inert oils could be used. The inert oil used in all data currently in the database is kerosene. If users wish to distinguish between various inert oils within the database, inert oil should be globally replaced with kerosene in the **Samples** table. Inert oil should then be replaced in the pick-list with kerosene.

Figure 19: Updating standard values, a) Capillary test method, b) Fluid matrix

a

b

2.2.4 Capillary Data Entry

Two types of capillary data are stored in the database: raw saturation versus pressure values and capillary fit parameters. The capillary data entry menu is brought forward by selecting the “Capillary Data” tab in the main data entry form menu (see Figure 14) and then specifying the type of data that are to be entered (raw, fit parameters). Prior to entering any capillary data in the database, the sample information must have been previously entered into the database using the samples data entry form.

The user must be very careful not to change any of the existing information in the database when entering new data into the system. Protection mechanisms are not in place to prevent a user from overwriting existing system data with new values. In particular, a user could overwrite the capillary parameters for sample 1 with values appropriate to sample 236 by failing to notice data was entered for the wrong sample id/name.

2.2.4.1. Capillary fit parameter data entry form

Two types of capillary fits have been performed on all samples in the database where raw capillary data are available: van Genuchten and Brooks-Corey. The Brooks-Corey method is a two-parameter fit to the linear portion of the residual saturation response to increasing pore pressure. The parameters are the bubbling pressure (P_d <cm H₂O>) and a term that is related

to the pore size/shape uniformity (λ <unitless>). The van Genuchten (VG) method fits the entire saturation response function by using a three-parameter fit. Alpha cm^{-1} is an inverse length scale parameter. Beta (sometimes called N), a unitless parameter, is similar to the pore uniformity parameter of the Brooks-Corey technique. The last parameter of the VG fit is the residual saturation <unitless saturation> parameter. Finally, any fitting technique will provide a measure of the goodness of the fit; in the case, R-squared (R^2). The value can be interpreted as the proportion of the variance in Y attributable to the variance in X. In simplified terms, R^2 squared is a measure of the “goodness” of the fit, where a perfect X-Y correlation has a value of 1.0. Any measure of goodness of fit (χ^2 , etc.) can be entered, so long as its values are normalized such that 1.0 is a perfect fit and 0.0 indicates that the fit is unrelated to the data being fit.

Figure 20: Capillary fit parameters data entry form

Record navigation area

To enter capillary fit parameter data into the database, go to the last record¹ in the database. Then go back a few records to the first new record that was entered into the Samples table that was reported to have capillary data available. Capillary fit parameters cannot be entered into the database if the samples information indicates that there are no capillary data.

2.2.4.2. Raw capillary data entry

Raw capillary data are just measurements of saturation versus capillary pressure. There are many measurements for a single sample. The data entry form for data where there are multiple values to enter for a single sample are somewhat different in appearance than the forms where only a single value (collection of values) is entered for a given sample. Figure 21 shows the *Raw Capillary Data Entry* form.

¹ Record navigation buttons are described in [Figure 14](#)

Figure 21: Raw capillary data entry form

The screenshot shows a Microsoft Access form titled '[8_CapillaryRawDataEntry]'. At the top, there are text boxes for 'Sample Name' (containing 'dummy example'), 'sample_id' (containing '236'), and 'site_id' (containing '30'). Below these is a label 'Enter as many values as needed for this sample!'. The main data entry area is a table with two columns: 'Capillary Pressure cm water' and 'Saturation (0 - 1)'. The table contains three rows of data: (1.000E-03, 100.0%), (4.300E+01, 99.0%), and (6.500E+01, 0.97). Below the table is a 'Record' navigation bar showing 'Record: 3 of 3'. At the bottom of the form, there is a 'Change Samples Here' button and a 'Go To Last sample' button. The bottom status bar shows 'Record: 160 of 160' and 'Form View'.

Applied capillary pressure values in units of cm H₂O

Pressure must be > 0.0

Saturation values are entered in the range of 0.0 - 1.0 and displayed as percentages.

Sample Navigation

Table row navigation

As with any data entry form other than samples, the first step is to navigate to the last record in the database and then back-up to the last sample where data needs to be entered. When new samples first appear, only one row is visible in the data entry table. New rows are automatically added at the bottom of the table each time a row is completed.

Capillary pressure data must be entered in units of centimeters of water and the values must be greater than 0.0. The value 0.001 is entered in place of zero to indicate the initial saturation. Saturation data is stored in the database as fractions (between 0.0 and 1.0) and is displayed as percentages. If the data to be input is not available in these units, a unit conversion must be performed before data entry. It may be easier to calculate the unit conversions in the Excel spreadsheet and then import the data into the database afterward. [See section 2.3.5](#) for a discussion of how to enter data in this way.

2.2.5 Petrophysical data entry form

The basic rock (petrophysical) properties of the samples are important components of this database. These parameters include information about the sampling conditions (depth, zone, and sample orientation) as well as properties that can directly influence the capillary response (saturation, porosity, permeability, etc.). To view the form, bring the “Petrophysical Data” folder forward by clicking on the tab in the basic data entry form (see Figure 14) and then click the *Enter Petrophysical Data* button. The data entry form (see Figure 22) includes both drag-down menus (pick-lists) and fill-in values. All parameters indicate the appropriate units for the database. Parameters such as porosity and saturation are stored in database as fractions (values from 0.0 to 1.0) and are displayed as percentages.

Figure 22: Petrophysical data entry form

The screenshot shows a Microsoft Access database window titled 'Microsoft Access - [3_Petrophysical_Data]'. The main form is titled 'Petrophysical Data Entry Form'. It contains several sections:

- Samples table info:** Fields for Sample Name (dummy example), Sample ID (236), and Site ID (30). A note states: 'Note: Data can only be entered for samples that have already been defined in the database. If your Sample-ID and Site ID values do not appear, return to the "samples entry" form.'
- Basic sample properties:** Fields for Depth (ft), Sampling Zone, Bulk density (g/cc), Grain density (g/cc), Effective porosity (0-1), Air filled porosity (0-1), Water saturation (0-1), Hydrocarbon saturation (0-1), and Moisture content (0-1).
- Permeability / Conductivity Tests:** Fields for Testing State, Testing fluid, Confining Pressure (PSI), Permeability (mD), Conductivity (cm/sec), and Orientation.
- Navigation:** A 'Change Samples Here' button and a 'GoTo last sample' button. The record navigation bar at the bottom shows 'Record: 183 of 183'.

Annotations on the left side of the form indicate the following sections:

- Samples table info
- Basic sample properties
- Permeability, conductivity, and their testing methods
- Record navigation

As with all data entry forms, the user must navigate to the appropriate records for the new samples prior to entering data.

2.2.6 Grain size data entry forms

Several types of grain size data are stored in the database. Not all types of data are necessarily available for each sample. Bring the "Grain Size Data" folder forward in the basic data entry form (see Figure 14). Figure 23 (below) shows the "Grain Size Data" folder. There are three data entry forms for grain size data. Grain size summary information includes the fractions of sand, silt, and clay, as well as the USCS and Folk Soil descriptions. Grain size statistics include median grain size as well as mean, standard deviation, skew and kurtosis descriptions of the size distribution based on various estimation techniques (Trask, Inman, Folk). Raw grain size distribution data includes the incremental and cumulative weight fraction of the sample retrained in various screens (or screen equivalents when laser scattering technique is used).

Figure 23: Grain Size Data folder

2.2.6.1. Grain size summary data entry

Grain size summary data includes soil descriptions for both the Unified Soils Classification System (USCS) and Folk classification methods. Both soil description methods are based on the relative fraction of grain sizes. The pick-list menus designed to assist users with data entry provide the complete description in terms of the grain size fractions (see [Figure 24](#) on the following page). Grain size fractions are input in the same form. Each size fraction is entered as a value between 0.0 and 1.0. These values are presented back to the user as percentages.

Figure 24: Grain summary data entry form. Panel A illustrates the content of the pick-list menus. Panel B shows a completed form for sample 10.

a

Grain Size Summary Data Entry Form

Sample Name: dummy example
 Sample ID: 236
 site_id: 30

Note: Data can only be entered for samples that have already been defined in the database. If your Sample-ID and Site ID values do not appear, return to the "samples entry" form.

USCS symbol: [dropdown]
 USCS soil group: CL
 Folk symbol: GC
 Folk soil description: GM-GC

Gravel: [dropdown]
 Coarse Sand: [dropdown]
 Medium Sand: [dropdown]
 Fine Sand: [dropdown]
 Silt: [dropdown]
 Clay: [dropdown]

Total Fine Fraction: [text box]
 Total Sand Fraction: [text box]

Record: 94 of 94

USCS soil classification symbol: [text box] NUM: [text box]

b

Grain Size Summary Data Entry Form

Sample Name: TA28@18'
 Sample ID: 10
 site_id: 2

Note: Data can only be entered for samples that have already been defined in the database. If your Sample-ID and Site ID values do not appear, return to the "samples entry" form.

USCS symbol: SM
 USCS soil group: SM
 Folk symbol: zS
 Folk soil description: silty sand

Grain Size Scale: USCS
 Grain size fractions (0-1)

Gravel	Coarse Sand	Medium Sand	Fine Sand	Silt	Clay
0.00%	0.00%	41.27%	38.52%	15.90%	4.31%

Total Fine Fraction: 20.21%
 Total Sand Fraction: 79.79%

Record: 1 of 94

USCS soil classification symbol: [text box] NUM: [text box]

2.2.6.2. Grain size statistics data entry

The statistical moments of the grain size distribution (mean, standard deviation, skew, and kurtosis) and the median size are stored (when available) in the Grain_stats table. All statistical results are reported in units of millimeters. Grain size analysis, and the interpretation of grain size distributions on the transport history of clastic materials, predates modern computing by many decades. Prior to modern computing techniques, several graphical techniques were used to estimate the moments of grain size distribution functions. The methods of Trask, Inman, and Folk are some of the more common methods found in the literature. Grain size statistics reported by many labs typically give these measures. Sometimes computed moments are also provided. Figure 25 shows the grain size statistics data entry form.

Figure 25: Grain size statistics data entry form

The screenshot shows a Microsoft Access window titled '5_GrainStats' with a form titled 'Grain Size Statistics Data Entry Form'. The form contains the following fields and values:

Grain Size Statistics Data Entry Form				
Sample Name	TA28@18'			
Sample ID	10			
Site ID	2			
	Median Grain Size (mm)	0.361		
	Trask Statistics (mm)	Inman Statistics (mm)	Folk Statistics (mm)	Computed Statistics (mm)
Mean	0.343	0.151	0.202	0.329
Standard Deviation (sorting)	0.5520	1.994	2.065	0.223
Skew	0.804	0.630	0.658	0.192
Kurtosis	0.276	0.767	1.682	-0.698

An arrow points from the text 'Grain size distribution moments entered in units of millimeters' to the 'Mean' row in the statistics table.

Record: 1 of 94

2.2.6.3. Raw grain size distribution data entry

Raw grain size distribution data are similar to raw capillary response data in that there are many values associated with a single sample. The data entry form (Figure 26) is an empty table when a new sample is initially accessed. New rows are added to the table as data are entered. Size values can be entered in many different units (millimeters, inches, Phi, and screen number). Millimeters (mm) are the only size values that must be entered into the database. In addition to the grain size measurement, both the incremental sample weight percentage retrained for the grain size and the cumulative grain size fraction need to be entered into the database.

Figure 26: Raw grain size data entry form

Records just added

Current record being added

Access™ window vertical scroll bar

Sample navigation

Table row navigation

opening (in)	opening (m)	Phi_value	US_screen	incrementa	cumulative_w
0.03310	0.84100	0.25	20	0.00%	0.00%
0.02780	0.70700	0.50	25	5.13%	5.13%
0.02340	0.59500	0.75	30	8.72%	13.85%
0.01970	0.50000	1.00	35	11.85%	25.70%
0.01660	0.42000				

Note: If the Access™ window isn't large enough, a user might not see the sample navigation controls when the form first appears. The solution is to either increase the window size, or to use the vertical scroll bar on the right-hand side of the window to move to the bottom of the window until the record navigation control keys are visible.

2.2.7 Fluid properties data entry forms

Two basic sets of fluid properties data are maintained within this database: interfacial tensions (oil/water, oil/air, water/air) data and density/viscosity versus temperature data. Each of these data types has a separate data entry form. To access these forms, click the "Fluid Properties" tab in the basic data entry form (see Figure 14).

2.2.7.1. Fluid density/viscosity data entry form

As with all forms, where multiple data values are entered for a single sample (i.e. raw [capillary data](#) or [grain size](#) data), the blank form appears to contain only a single row. New rows appear in the form when the previous row is complete. Values entered into this table (see Figure 27) include the fluid matrix (pick-list), temperature (degrees Fahrenheit), specific gravity, density (grams/cubic centimeter), dynamic viscosity (centistokes) and static viscosity

(centipoises). If the appropriate fluid matrix value does not appear in the pick-list provided, new standard values can be added ([see section 2.2.3](#)) to the list.

Figure 27: Fluid properties data entry form

Fluid Matrix	Temperature deg F	Specific Gravity	Density g/cc	Dynamic Viscosity cstokes	Static Viscosity cpoise
NAPL	60.0	0.7870	0.7862	0.6970	0.5440
	76.0	0.7805	0.7783	0.6180	0.4780
	100.0	0.7734	0.7681	0.6180	0.4780
	150.0	0.7543	0.7394	0.4930	0.3719

2.2.7.2. Fluid interfacial tensions data entry

Interfacial tensions data are entered into a standard form where multiple values can be entered for a single sample. Temperature is a parameter in this data table. For some samples, interfacial tensions are measured at several temperatures. In other samples, only a single temperature is measured. Sometimes the temperature at which the test was run is unknown. Add as many records to the form for each sample as you need to describe each temperature tested. Temperatures are reported in degrees Fahrenheit. The interfacial tensions are given in units of dynes per centimeter (see [Figure 28](#) on the next page).

Figure 28: Interfacial tensions data entry form

Sample Name: nw20
Sample ID: 182
Site ID: 21

Enter as many rows as needed for this sample!

Interfacial Tensions			
Temperature deg F	Air / Water (dynes/cm)	Air / Oil (dynes/cm)	Oil / Water (dynes/cm)
72.0	58.50	28.50	10.00
0.0	0.00	0.00	0.00

Record: 1 of 1

Change Samples Here
GoTo last sample

Record: 15 of 29

Form View

2.3 Importing data from other sources:

Using the Data Entry (Excel™) Spreadsheet

If data to be added to the database is available in an electronic form, it is often easier to reformat the data to match the database structure and then import the complete data collection at once. The Microsoft Excel™ spreadsheet program is a good intermediary for this purpose. It has excellent compatibility with the Access™ database software, and it is capable of performing the basic transformations necessary during data reformatting. The most common data transformations that occur during reformatting are table and sub-table copy and paste, re-ordering columns within tables, transposing rows and columns, and performing simple mathematical transformations on data like unit conversions. For example, data analyzed by the PTS Labs is typically provided in the form of a collection of worksheets within an Excel™ workbook.

At the beginning of this project, the idea that PTS Labs might be able reformat their standard analysis output to facilitate entry into this database was discussed. Technical issues and database QA/QC issues make this option unworkable. For the foreseeable future, laboratory data will need to be reformatted for entry into this database by people who understand the both the data and the database structure, content, and purpose.

2.3.1 Getting Started

Regardless of whether the data entry person is going to use the manual data entry form or load the database by transferring electronic files formatted into Excel™ worksheets, the user needs to have the data well organized prior to getting started. Data entry will be far more efficient and less prone to mistakes if the data is well organized and documented prior to beginning the data entry process. As discussed in sections [2.1](#) and [2.2](#), particular care must be exercised in making sure that the data entered into the database is appropriate and that **sample_ids** are properly assigned. The **sample_id** value is the primary key that links the various data tables within the database. Before any new data is entered into the database, the highest existing value of the **sample_id** must be determined by examining the last record in the **Samples** table.

Even if the bulk of the data is to be imported from Excel™ files, the Site and Samples data must be entered manually. This information is unique to the database and has no equivalent in the laboratory data. Users are encouraged to use the manual data entry forms (sections [2.2.1](#) and [2.2.2](#)). However, if users decide to enter this data directly into the database tables, they can still make use of the pick-lists as these are table features.

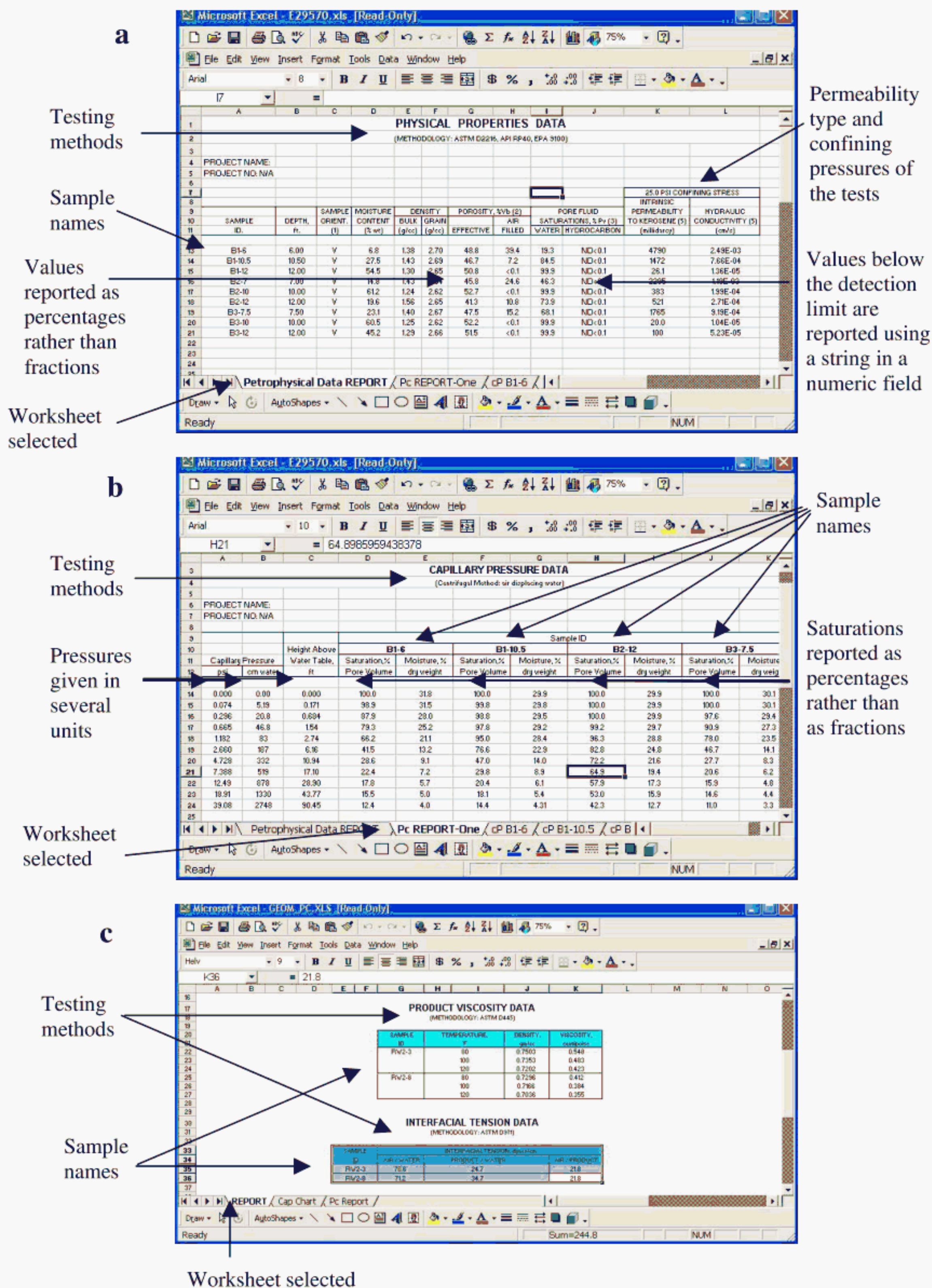
After the data is organized and the mapping from project sample names to **sample_ids** have been determined, the user is ready to begin reformatting data for import into the database.

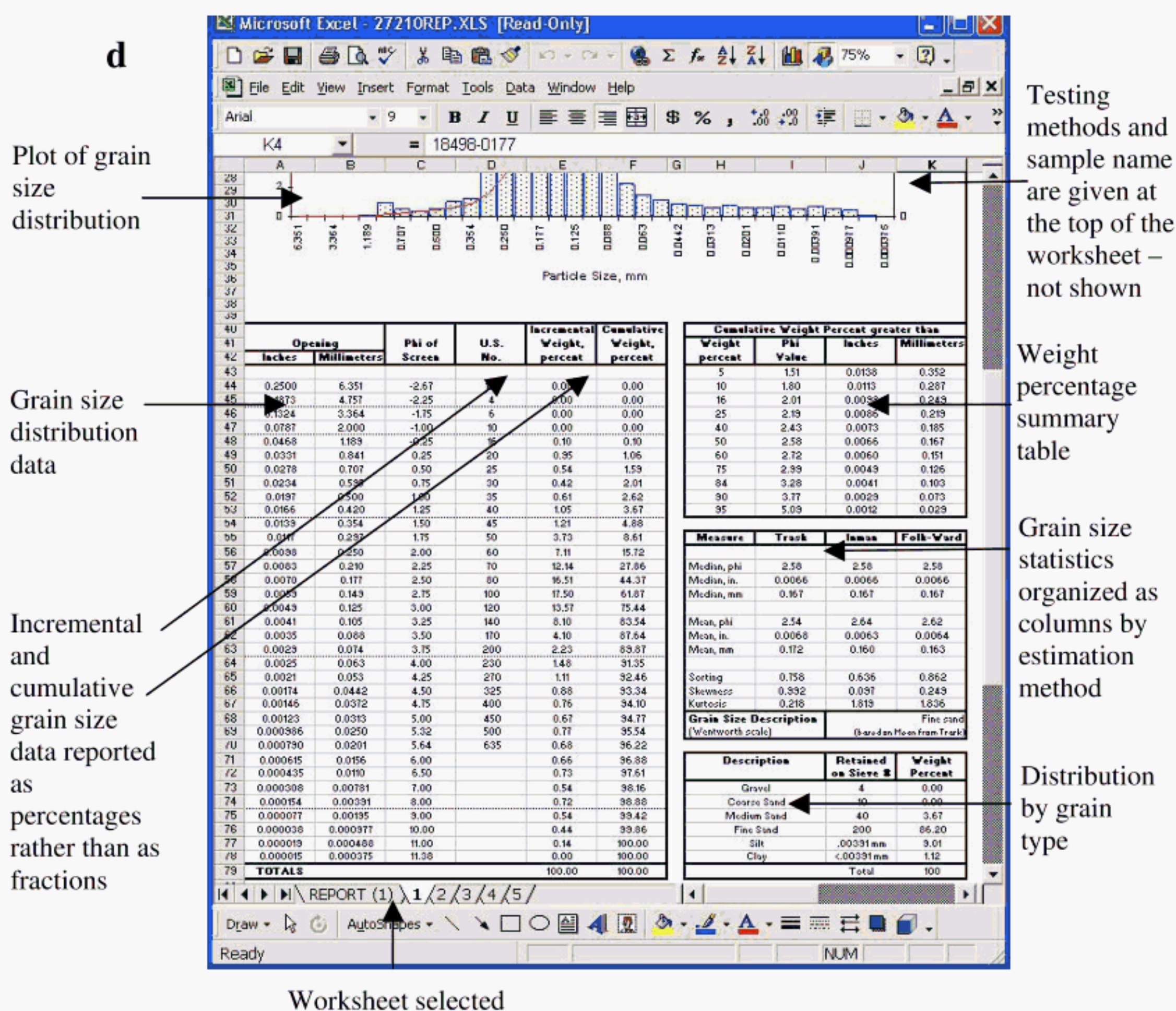
2.3.2 PTS Labs data structures

Most of the data entered into this database were analyzed at the PTS Labs. Accordingly, the database design closely mirrors the current standard output of the PTS Labs. This should not discourage users from entering data analyzed at other laboratories, although it is likely that more work will be involved.

PTS Labs typically produce a single Excel™ workbook that is organized into worksheets with various data types (physical properties, capillary response, grain size, fluids). Typically, physical properties are reported in a single worksheet (Figure 29a) for all samples analyzed in a given site (project). Capillary responses are reported in one or more worksheets (Figure 29b), depending on how many samples are analyzed. All grain size data (distribution, statistics, and summary) are reported on individual worksheets (Figure 29d), one worksheet per sample. Lastly, fluid properties, both interfacial tensions and density/viscosity are typically presented separate tables in a single worksheet (Figure 29c). There is a bit of variability in how PTS Labs formats their analysis results. Some of the variability is attributable to changes in formats over time and other variations are associated with user requests. The discussion that follows regarding the structure of the PTS Labs data formats in no way restricts how the PTS Labs might format their analyses results in the future. The information is presented here strictly as an example of how electronic data might be originally organized prior to being reformatted into forms that can be loaded into this database.

Figure 29: Examples of PTS Labs data formats





2.3.3 Reformatting data for import

Data can be imported directly into Microsoft Access™ from Excel™ by first selecting the data table within Access (in the *Table Object* – see Figure 1) using the import function (File → Get External Data → Import) or through a copy-and-paste operation. There are some significant advantages to using the copy-and-paste method. These include the ability to have columns in the Excel worksheet that are not present in the database, and the ability to import data from any column within the worksheet, not just from column one. It is very handy to be able to have dummy columns in the worksheets that do not get imported in to the database.

Examples of common dummy columns in an import file are the sample name and original data column values (before unit conversions, etc.). The sample name is not included in any database table except the samples table. It is very important that data from different samples does not get mixed together within the database. Keeping the sample name in the import files, in addition to the *sample_id*, can help to prevent mixing of data across samples. Many data columns require fairly simple conversions, such as dividing by 100.0 to convert a percentage into a fraction or similar multiplications by a constant to convert between various units (i.e. millimeters = inches * 0.03937). In cases such as these, preserving the original data column in the worksheet can help to reduce the possibility that data processing errors get propagated into the database.

An Excel workbook (data_template.xls) is provided with multiple worksheets (see Figure 30) to assist users with the task of reformatting electronic data for inclusion the database. Each worksheet within the workbook is designed to support a single data table in the database. In addition, a worksheet provides a number of common unit conversion factors and another worksheet can store notes about the data entry process. Each of the individual worksheets has a blue shaded header region that indicates what data (and units) belong in which columns. In addition, a large area of the worksheet is shaded gray and bounded by a thick black border. The region inside this bounded area is input into the database. Columns outside the bounded area, including the sample name, are not part of the database. Some tables, that are particularly wide, have the sample name column repeated on both ends, just to make it easier to remember what sample is being input within the row.

2.3.3.1. Copying data from Excel into Access

To copy data into an Access table, first copy the data from the Excel worksheet into the paste buffer. Open the appropriate data table in Access, and then select the *Paste Append* option from the Edit menu at the top of the Access window. Any paste errors will be automatically moved to a table called **PasteErrors**. Paste errors typically occur when the database table structure does not match the structure of the data being pasted. Common errors include: paste values out of the valid range of the database column (i.e. value of 0.3 pasted into a field that must be ≥ 1.0), paste values of the wrong data type for database column (i.e. characters in numeric field), etc. These same type of errors occur during an import operation. Table 1 shows common paste errors.

Table 1: Common paste errors when copying data from Excel worksheets to Access tables

Excel Worksheet	Access Table	Common paste errors
PetPhys	PetrophysicalData	Strings such as ND or < 0.1 in the hydrocarbon saturation field (number).
		Saturation / Porosity values out of range – values not converted from percentages (0 - 100) to fractions (0 - 1).
		Invalid <code>sample_id</code> values – PetPhys <code>sample_ids</code> not present in the Samples table.
CapRaw	Cap_Rawdata	Saturation values out of range – values not converted from percentages (0 - 100) to fractions (0 - 1).
		Pressure values out of range – pressure = 0.0
		Invalid <code>sample_id</code> values – CapRaw <code>sample_ids</code> not present in the Samples table.
CapFit	Cap_Summary	Values out of range (Srw, 0 - 1)
		Invalid <code>sample_id</code> values – CapRaw <code>sample_ids</code> not present in the Samples table.
GS-weight%	GS_Weights	Invalid <code>sample_id</code> values – GS-weight% <code>sample_ids</code> not present in the Samples table.
GS-stats	Grain_stats	Invalid <code>sample_id</code> values – GS-stats <code>sample_ids</code> not present in the Samples table.

Excel Worksheet	Access Table	Common paste errors
GS-summ	Grain_Summary	Invalid <code>sample_id</code> values – GS-stats <code>sample_ids</code> not present in the Samples table.
GS-sizes	Grain_Size	Incremental/Cumulative weight values out of range – values not converted from percentages (0 - 100) to fractions (0 - 1).
		Invalid <code>sample_id</code> values – GS-stats <code>sample_ids</code> not present in the Samples table.
Tensions	Fluid_Tensions	Invalid <code>sample_id</code> values – GS-stats <code>sample_ids</code> not present in the Samples table.
Viscosity	Fluid_Properties	Invalid <code>sample_id</code> values – GS-stats <code>sample_ids</code> not present in the Samples table.

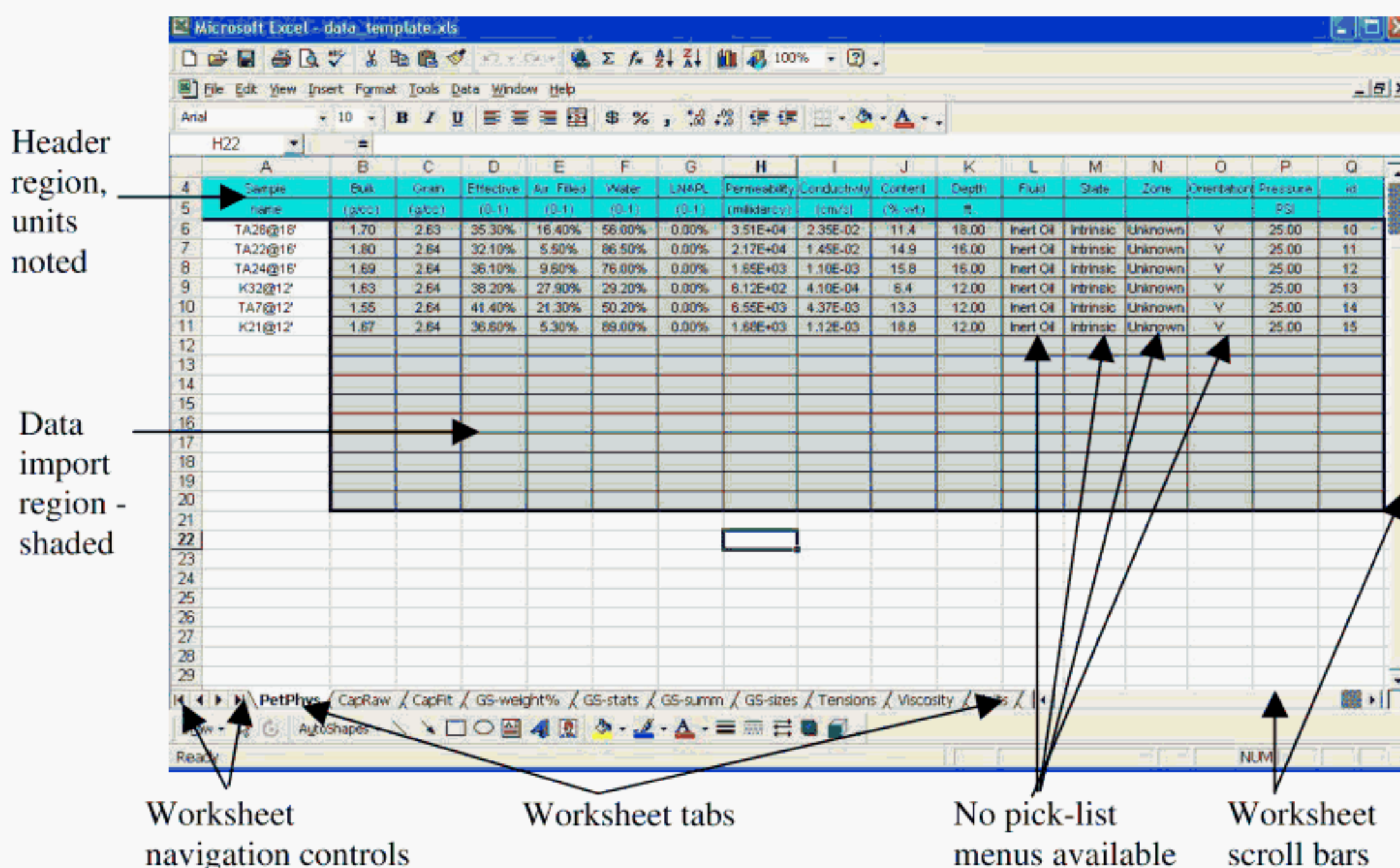
2.3.4 Petrophysical (PphysData) Data worksheet

Data that is included in the petrophysical data table is derived from the Rock Properties worksheet of the PTS Labs analysis results ([Figure 29a](#)). [Figure 30](#) shows the data_template workbook opened up to Petrophysical (PetPhys) data worksheet. At the bottom of the workbook are tabs which contain each of the various individual worksheets. Note that the units of several columns (porosity, saturation) do not match those in the PTS Labs output and some numeric columns contain text strings. Data columns are not necessarily in the same order as the PTS Labs data. The typical process by which data are reformatted for database entry is as follows:

- Copy the entire new data set into the data template in a region of the worksheet that is not going to be imported into the database – keep data rows in their original order.
- Copy/paste columns of data that do not need unit conversions directly into the appropriate columns of the import region.
- Write simple equations that map the original data columns to the import region columns (i.e. `saturation_fraction = saturation_percent/100.0`).
- Input `sample_id` column values to match the sample names. There is no need reorder data rows in order to make the `sample_id` values increment.
- Validate data. Verify that data columns are in the appropriate areas and that `sample_ids` are correctly assigned to samples.

When the data are validated and ready to be loaded into the database, the data can be copied into the database following the procedure described in [section 2.3.3.1](#).

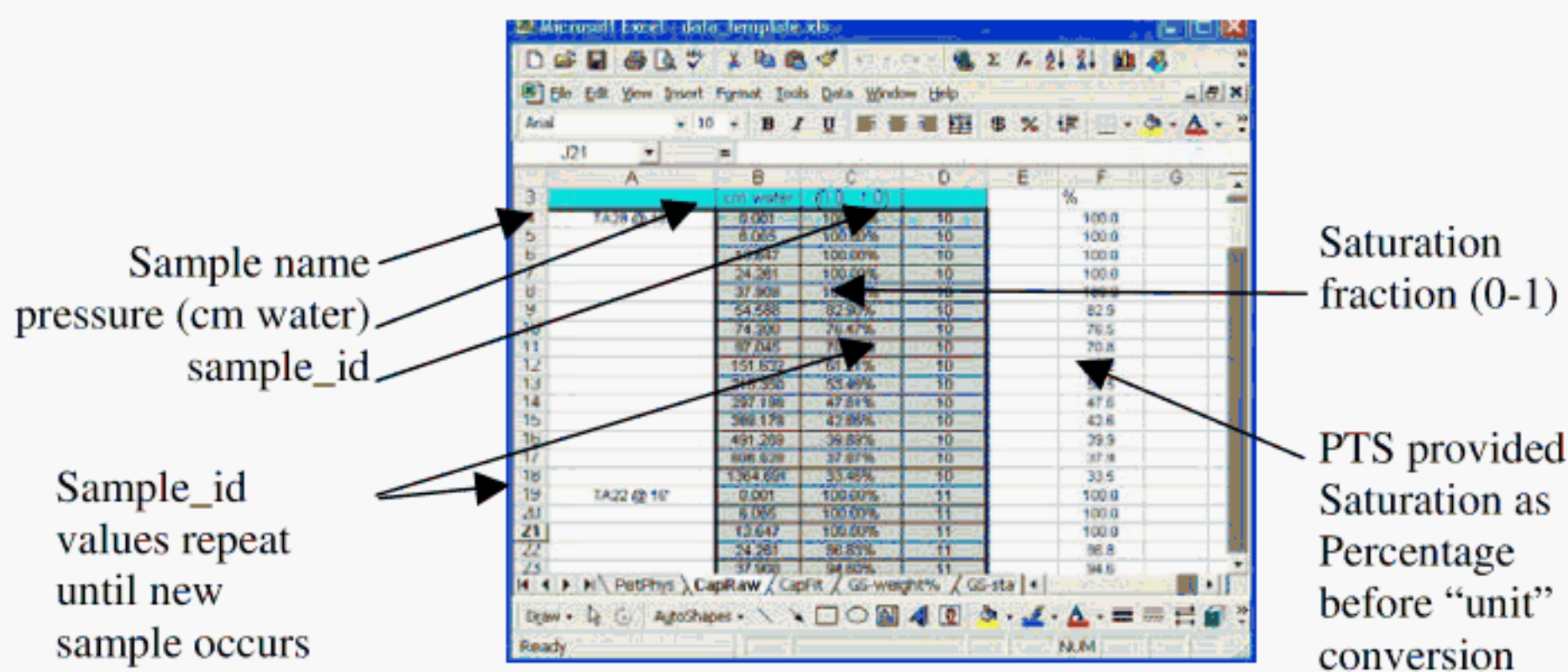
Figure 30: Excel data template workbook - PetPhys worksheet



2.3.5 Raw capillary data (CapRaw) worksheet

Raw saturation versus capillary pressure data can be prepared for import into the database using the CapRaw worksheet (Figure 31) of the data template workbook. PTS Labs typically stores raw capillary analysis data in one or more worksheets called PcReport (see Figure 29b). Pressure data must be input in units of centimeters of water and saturation data are fractions (0 to 1). Typically, PTS Labs will provide pressure data in the units needed but saturation data are provided as percentages. It is common for PTS Labs to provide a saturation value with no pressure applied (pressure = 0). Any zero pressure record must have the pressure restated as a positive value, typically 0.001 cm water. In addition, many values are associated with each sample in this table. Users need to be careful that they correctly reproduce the sample_id field for each record associated with a single sample, and that the sample_id updates when the sample changes.

Figure 31: Excel data template workbook – CapRaw worksheet



2.3.6 Capillary fit parameters (CapFit) worksheet

Capillary curve fitting is not a standard laboratory analysis procedure. All of the capillary analysis data currently included in the database are provided by AVI. There are two standard curve-fitting methods: the van Genuchten (VG) and Brooks-Corey (BC) methods. The VG curve fit is a non-linear fit optimization technique that characterizes the full capillary response at equilibrium as a function of pressure. The BC method is a linear technique that characterizes on the linear portion of the logarithmic response. Both methods are commonly used for aquifer characterization studies. Users who are adding data to the database should fit the raw capillary data to both function and input the fit parameters into the database. Curve fitting software is not included with the database.

The capillary fit data worksheet from data template workbook is shown as Figure 32.

Figure 32: Excel data template workbook - CapFit Worksheet

Sample Name	alpha	beta	Srw	Fit R ²	Pd	Lambda	Fit R ²	Sample_id
TA20 @ 10'	1.415E-02	1.33	0.29	0.989	44.786	0.771	0.984	10
TA22 @ 10'	1.802E-02	1.20	0.45	0.987	20.24594396	0.142	0.954	11
TA24 @ 10'	1.064E-02	2.06	0.30	0.988	61.09172673	0.803	0.978	12
K32 @ 12'	1.111E-02	3.83	0.23	0.988	55.78524238	1.3586	0.99	13
TA7 @ 12'	2.739E-02	2.20	0.15	0.992	27.0337221	1.0111	0.903	14
K21 @ 12'	6.290E-03	1.55	0.675	0.993	86.29097269	0.4266	0.960	15

2.3.7 Grain size weight percentages (GS-weight%) worksheet

Grain size weight percentage data (size of grains at xx% of the total sample weight) are routinely produced by the PTS Labs as part of their grain size analysis ([Figure 29d](#)). Note that the PTS Labs output provides these data as columns where the database stores them in rows. Data must be transposed when (Edit → Paste Special → Transpose) copied from the PTS output file to the data template.

The weight fractions (5%, 10%, 16%, 25%, 40%, 50%, 60%, 75%, 84%, 90%, 95%) are not uniformly distributed but at selected fractions that are used in the distribution moment (mean, standard deviation, skew, kurtosis) estimation methods of Trask, Inman, and Folk. The PTS Labs report these size fractions in several units: Phi, inches, and millimeters. The GS_weight% worksheet allows size fractions to be entered into the database in multiple units by including a units column ([Figure 33](#)). The standard data display forms only show the values in units of millimeters (mm). However, all of the moment estimation techniques (except the mean) are based on units of Phi. In particular, the Folk sorting value (Standard deviation in units of Phi) must be computed in Phi to determine the Folk sorting description. The Folk standard deviation (sorting) is computed as:

$$F_{\text{sorting}} = \frac{\Phi_{16\%} + \Phi_{84\%}}{4} + \frac{\Phi_{5\%} + \Phi_{95\%}}{6.6}$$

and the associated Folk sorting descriptions for F_{sorting} are:

0.00 – 0.24	very well sorted
0.25 – 0.49	well sorted
0.50 – 0.99	moderately sorted
1.0 – 1.99	poorly sorted
2.0 – 3.99	very poorly sorted
> 4	extremely poorly sorted

Figure 33: Excel data template workbook – GS-weight% worksheet

Microsoft Excel - data_template.xls

File Edit View Insert Format Tools Data Window Help

Arial 8

G13 0.389

	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Grain Size Weight Percentages															
2	Size at	Size at	Size at	Size at	Size at	Size at	Size at	Size at	Size at	Size at	Size at	Row				Folk
3	5%	10%	16%	25%	40%	60%	75%	84%	90%	95%		Units	Sample Id	FW std	%40/90	Sorting
4	weight	weight	weight	weight	weight	weight	weight	weight	weight	weight	weight					Description
5	0.778	0.677	0.601	0.525	0.428	0.361	0.306	0.16	0.038	0.016	0.006	mm	10	2.539773	26.75	very poorly sorted
6	0.36	0.56	0.73	0.93	1.23	1.47	1.71	2.65	4.72	5.95	7.41	Phi	10	2.539773	26.75	very poorly sorted
7	5.45	2.182	1.168	0.765	0.524	0.439	0.355	0.238	0.16	0.098	0.054	mm	11	0.871667	5.35	moderately sorted
8	-2.45	-1.13	-0.22	0.39	0.93	1.19	1.5	2.07	2.64	3.35	4.21	Phi	11	0.871667	5.35	moderately sorted
9	0.808	0.703	0.631	0.549	0.448	0.384	0.324	0.216	0.081	0.024	0.008	mm	12	2.167954	18.67	very poorly sorted
10	0.31	0.51	0.66	0.86	1.16	1.38	1.63	2.21	3.63	5.41	6.92	Phi	12	2.167954	18.67	very poorly sorted
11	1.04	0.875	0.775	0.674	0.55	0.477	0.397	0.231	0.062	0.021	0.006	mm	13	2.190454	26.19	very poorly sorted
12	-0.06	0.19	0.37	0.57	0.86	1.07	1.33	2.11	4.01	5.6	7.29	Phi	13	2.190454	26.19	very poorly sorted
13	0.776	0.673	0.595	0.527	0.441	0.389	0.34	0.272	0.207	0.101	0.012	mm	14	1.785303	4.37	poorly sorted
14	0.37	0.57	0.75	0.93	1.18	1.36	1.56	1.88	2.27	3.31	6.43	Phi	14	1.785303	4.37	poorly sorted
15	1.014	0.707	0.554	0.388	0.145	0.072	0.048	0.026	0.014	0.007	0.003	mm	15	3.027727	20.71	very poorly sorted
16	-0.02	0.5	0.85	1.36	2.79	3.79	4.39	5.27	6.17	7.16	8.42	Phi	15	3.027727	20.71	very poorly sorted
17																
18																

Ready

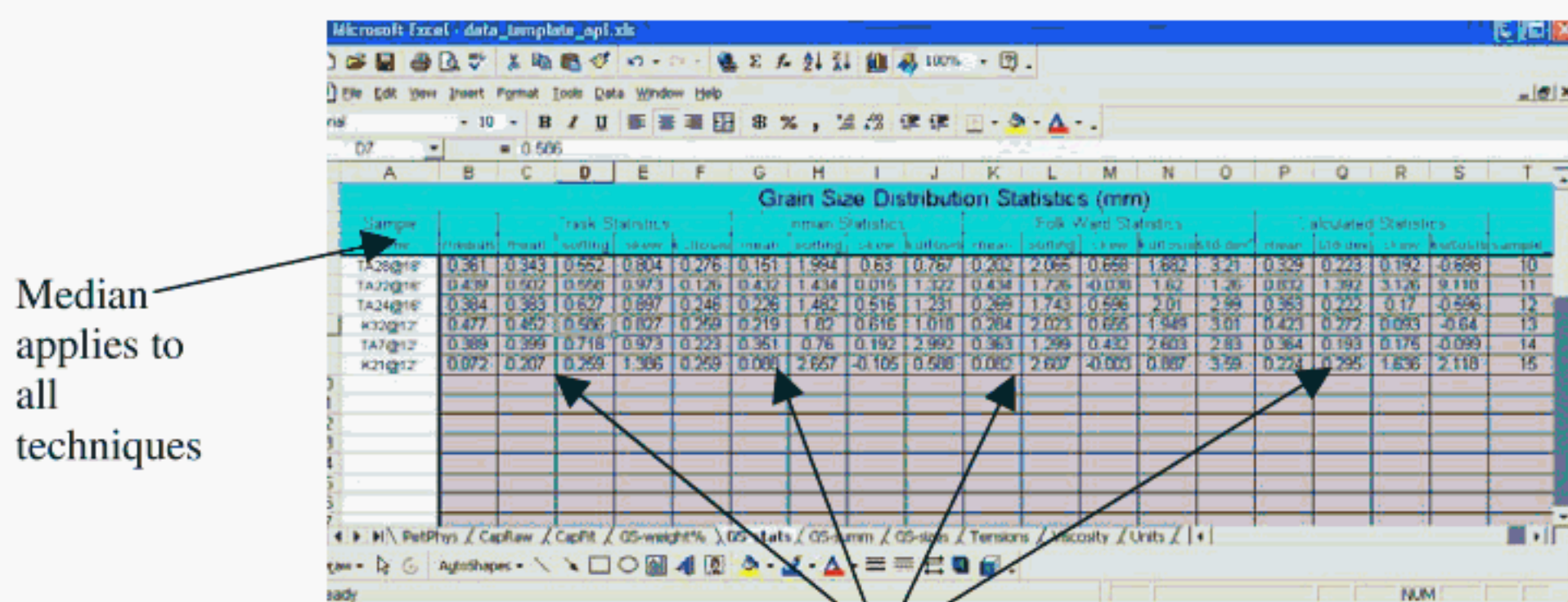
NUM

Sample_id and some of the other parameters repeat when data are entered in both units of Phi and mm

2.3.8 Grain size statistics (GS-stats) worksheet

The moments of the grain size distribution function (mean, sorting, skew, kurtosis) are routinely produced by the PTS Labs as part of their grain size analysis (Figure 29d). Note that the PTS Labs output provides these data as columns where the database stores them in rows. Data must be transposed when (Edit → Paste Special → Transpose) copied from the PTS output file to the data template (Figure 34). In addition, only the statistical moments that are provided in units of millimeters are included in the database - not all of the transposed columns are entered into the database input portion of the worksheet. User's should also note that although the distribution moments vary from one estimation technique to another, and that none of the estimates match the computed moments, the median value is always the same between methods. The median value is a measured parameter – it is not estimated/calculated.

Figure 34: Excel data template workbook – GS-stats worksheet



Various moment estimates and calculated values in units of millimeters

2.3.9 Grain size summary (GS-summ) worksheet

Information about the fraction of each sample that is classified as gravel, sand, silt or clay is prepared for data import in the GS-summ worksheet of the data template (see [Figure 35](#)). The grain size divisions (scales) are determined by the classification system, the two most common of which are the Wentworth scale and the Unified Soils Classification System (USCS). Given the relative amounts of the various grain size fractions ([Figure 29d](#)) in a sample, the data can be further classified into soil types. Again there are competing classification systems, with the Folk and USCS systems being the most common. Both of these systems make use of ternary diagrams. The Folk [ternary diagram](#) and [soil description](#), and the [USCS symbols](#) are included in the Appendix on database design and maintenance. Note that within the database, unindurated samples are assumed when assigning Folk soil descriptions. Similarly, when USCS soil classifications are made, clays have been assumed to be inorganic. In both instances, these assumptions have been made in the absence of either supporting or contradictory data. The organic content of clays, the level of induration, and the fissile properties of the sample are not provided by PTS Labs.

Figure 35: Excel data template workbook – GS-summ worksheet

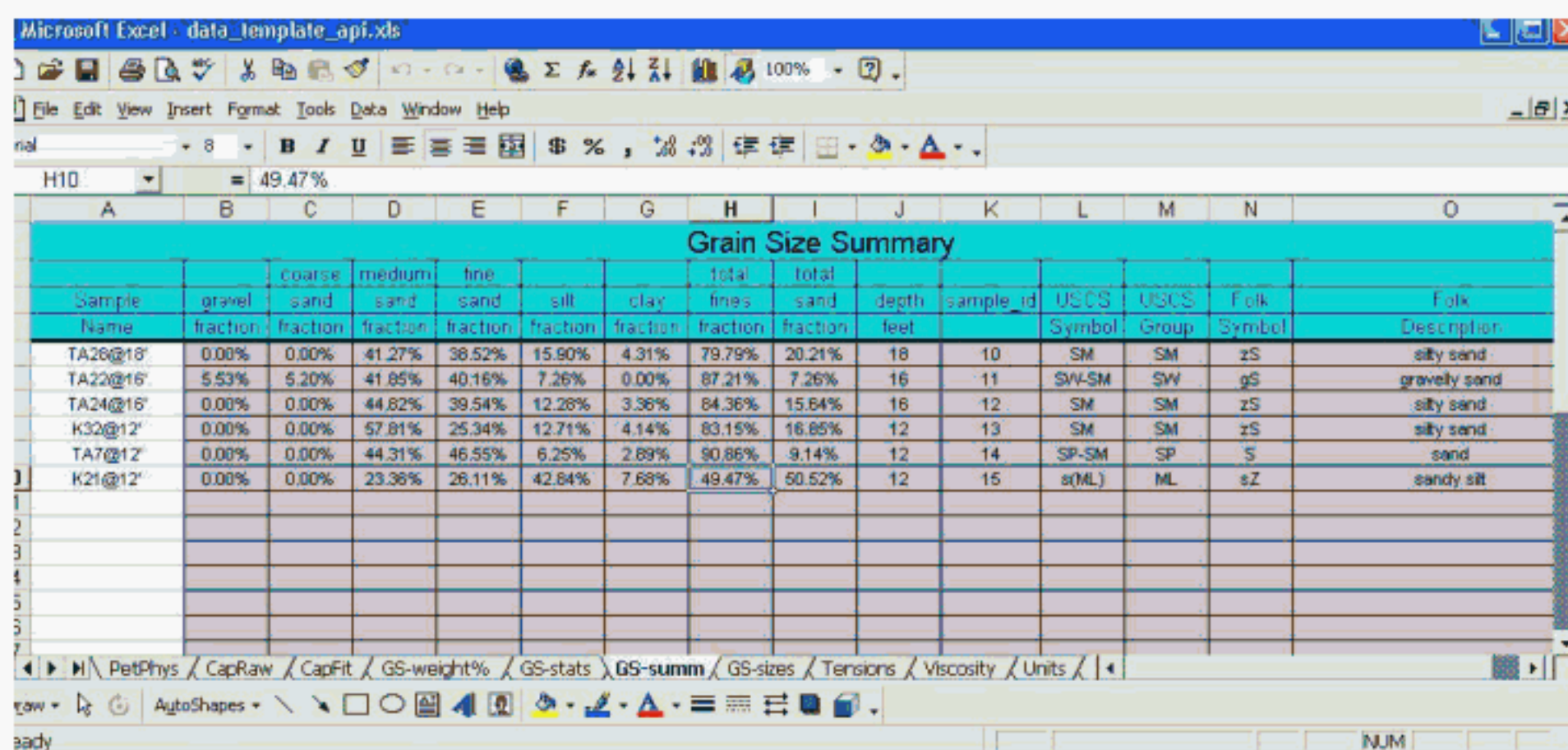


Figure 37: Excel data template workbook – Viscosity worksheet

Viscosity Data								
Sample name	Contaminant Description	Fluid Matrix	Temperature deg F	Specific Gravity	Density g/cc	Kinematic Viscosity cstokes	Absolute Viscosity cpoise	Sample-id
R-9	gasoline		60.00	0.79	0.79			16
	gasoline		76.00	0.78	0.78	0.70	0.54	16
	gasoline		100.00	0.77	0.77	0.62	0.48	16
	gasoline		150.00	0.75	0.74	0.49	0.37	16
W-18	gasoline	Water field	60.00	0.81	0.81			17
	gasoline	Water field	76.00	0.80	0.80	0.82	0.66	17
	gasoline	Water field	100.00	0.79	0.79	0.71	0.56	17
	gasoline	Water field	150.00	0.78	0.76	0.55	0.43	17
W-4	gasoline	Water field	60.00	0.80	0.80			18
	gasoline	Water field	76.00	0.79	0.79	0.80	0.64	18
	gasoline	Water field	100.00	0.79	0.78	0.71	0.55	18
	gasoline	Water field	150.00	0.77	0.76	0.62	0.48	18

2.3.12 Site fluid tensions data (Tensions) worksheet

Fluid interfacial tensions (called surface tensions when one fluid is air) are important parameters in determining multiphase fluid flow characteristics. Tensions are computed for fluid pairs (air-water, oil-water, oil-air). Measurements are typically only made at a single temperature; however, it is worthwhile to preserve information about the temperature at which the test was performed. The PTS Lab data is not well organized for input into the database. [Figure 38](#) shows a typical PTS Lab output beside the data template worksheet for interfacial tensions data. Note that each data value for a given sample in the database input template must be extracted from a different cell in the PTS Labs data file.

Figure 38: Excel workbook – Viscosity worksheet with side-by-side PTS Lab formatted data

The screenshot shows an Excel workbook with the following data:

Tensions Data						PTS Labs			
Sample name	Temperature deg F	Air-Water tension dyne/cm	Air-LNAPL tension dyne/cm	Water-LNAPL tension dyne/cm	Sample Id	PHASE PAIR	TEMP °F	INTERFACIAL TENSION Dynes/cm	SURFACE TENSION Dynes/cm
R-9	76.00	63.50	24.32	17.52	16	R-9 Water	Air	76	63.50
W-18	76.00	62.02	24.52	18.50	17	R-9 Water	R-9 Fuel	76	17.52
W-4	76.00	62.02	23.80	15.60	18	R-9 Fuel	Air	76	24.32
						W-18 Water	Air	76	61.12
						W-18 Water	W-18 Fuel	76	18.50
						W-18 Fuel	Air	76	24.52
						W-4 Water	Air	76	62.02
						W-4 Water	W-4 Fuel	76	15.60
						W-4 Fuel	Air	76	23.80

Appendix A—Database Design and Maintenance

This database is prepared in Microsoft AccessTM. Parameters are stored in individual tables in the database and are linked through common sample identifiers. Data to include in the database, where available, contain:

Petrophysical Data: Moisture content, water saturation, LNAPL saturation, total porosity, effective porosity, intrinsic permeability, native-state permeability, bulk density, grain density, and grain size parameters (mean grain size, median grain size, sorting, skewness, kurtosis, uniformity coefficient), U.S.C.S. group name/symbol, soil ternary diagram designator.

Other Information: Hydrologic zone of sample collection (vadose, capillary, product, or water saturated zone) other descriptive information (cementation, consolidation, etc.).

LNAPL Fluid Properties: Density/specific gravity, interfacial tensions, and viscosity.

Raw capillary-pressure data. Raw capillary-pressure data is provided in separate tables and linked to the database by identifier. Raw data can be used to inspect derivation of van Genuchten and/or Brooks-Corey parameters or to derive parameters for other capillary models, if desired.

Raw grain-size analysis data. Where available, raw grain size data is provided in separate tables and linked to the database by identifier. Raw grain size data can then be used for calculations, plotting, or other analyses.

Data for inclusion in the database come from public domain files in AVI's project records, and from San Diego State University Master's Theses. The original estimate was that approximately 150 data sets could be obtained from these two sources, which turned out to be generally representative of the number of data sets entered.

A.1 Database Design Document Audience

There are two separate aspects to this appendix: 1) database design and maintenance and 2) data parameters, validation, and information extraction. The database design and maintenance sections are written so that any one with a basic understanding of relational data structures will understand the data organization. Most of the data included in the database was originally stored in Microsoft ExcelTM spreadsheets. The database maintenance section assumes a basic knowledge of both the AccessTM and ExcelTM software packages. Data can be extracted from the database by using Structured Query Language (SQL) queries, which is imbedded in the AccessTM software, as well as in other database engines. Some user-knowledge of SQL query formation and/or the organization of queries and reports in AccessTM is assumed.

The data is hydrogeologic and related to multiphase flow theory. As such, the definitions of various data elements, the validation of their values, and the discussion of derivation of the various LNAPL-related parameters assume a general knowledge of multiphase mechanics. Equations pertaining to multiphase evaluations are provided for reference in Appendix D.

A.2 Design Overview

This database has been constructed to assist in selecting parameters needed to evaluate LNAPL mobility, recovery, and source distribution. By bringing together a collection of fully analyzed samples (capillary, petrophysical, grain size, and fluid properties) from a variety of depositional settings and soil types, the correlation between the available parameters can be explored and used as appropriate. At this point, the potential relationships between various sample parameters have not been established. The goal is to collect as much information as possible about samples for which a full suite of LNAPL-related parameter analysis has been performed, organize the data in a logical manner within a database construct. The user may begin to mine the database to establish the potential relationships between parameters and determine a basis for selecting key parameters needed for multiphase evaluations.

The database is designed as a collection of relational tables linked through a single (primary) key element: **sample_id**. This key element allows records in one data table to be associated with records in another table. A simple one-to-one relationship can occur in some cases. In the simplest form of relational database, there is a single **master** table and many **subordinate** tables. Each record in the master table is unique, with only one record for each sample. With other tables, the relationship is one-to-many. Many records in a subordinate table are associated with a single record in the master table. By way of example, a given sample may have one set of petrophysical properties (density, permeability, etc.) but also have many measured pairs of saturation versus pressure to derive capillary fit parameters.

The **sample_id** is a short integer value, assigned at the time of data entry, which can be rapidly compared during queries and joins. There are eleven (11) data tables in the database. The tables themselves follow the format of the typical laboratory data files for the most part, though clearly the exact format is lab dependent. Because many of AVI's projects have had analyses provided by PTS Labs, the data entry was framed to make it easy to assimilate their information to facilitate data entry, validation, and quality control.

Many samples only have a subset of the comprehensive LNAPL data parameters. No entries are created in data fields if the parameter of interest is unmeasured or unavailable for a particular sample. If a partial set of table values is obtained from a sample, those values are entered and the remaining elements are left blank (NULL filled). In some cases, trace amounts of some quantity are present at levels below the reporting detection limit of the laboratory. In these cases, a small numeric flag is input for the value. In general:

NULL:	Indicates no measurement was made,
0:	Indicates that a measurement was made and no quantity was found.
FLAG:	Indicates that a quantity was observed to be present but was present below the laboratory reporting detection limit.

FLAG values vary for different elements and tables. Please see the table and column descriptions that follow for additional information on **FLAG** values. If there is no discussion of **FLAG** values for a table/column then none are present in the database.

A.2.1 Data Type Basics

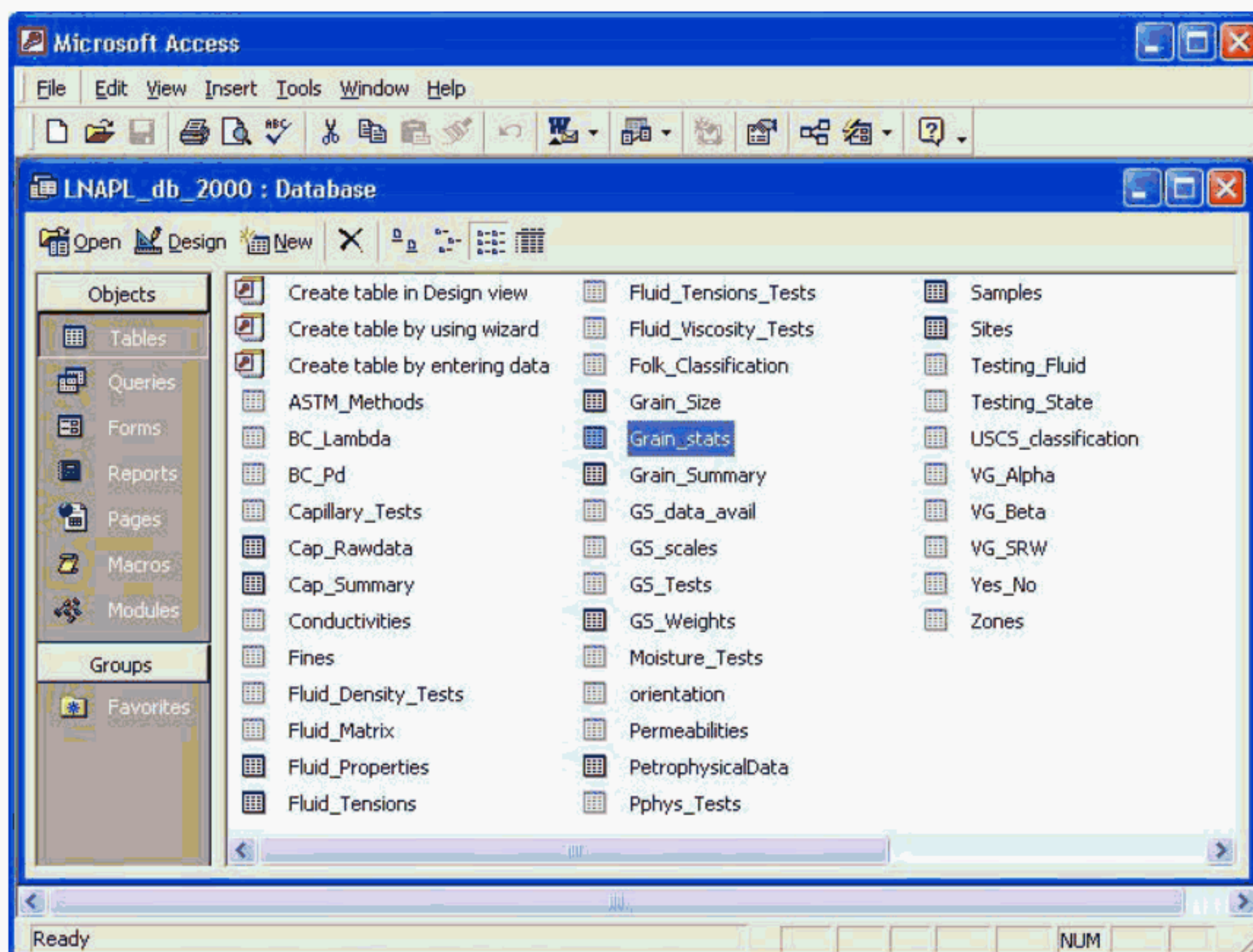
Values that are stored in digital form are given binary representations. The basic data types are integer, floating point, and character. The number of bytes used to represent a parameter affects precision with which the parameter can be stored, the range of values that parameter can have, and the amount of storage (disk space) it takes to store the data. In general, it takes more computer power to compare large numbers of bytes than small numbers of bytes. The number of bytes used in the definition of a parameter needs to be optimized for all of these factors.

Individual characters (1 byte) are commonly grouped together to form text strings. When storing text data, it is important to know the number of characters available (maximum string length). In the discussion that follows, text data types will be followed by the maximum number of characters allowed in that field, e.g. text(10). Integers are typically formed by using 1, 2, or 4 bytes. In general, a 1-byte integer is called a **byte**, a 2-byte integer is called a **short int**, a 4-byte integer is called an **int** or a **long int**. Floating point representations are typically called **singles** (4 bytes) or **doubles** (8 bytes).

A.3 Database Tables

This database could have been substantially simplified in structure. Fewer tables could have been used to store the data parameters. All of the one-to-one relationships could have been collapsed into a single, rather wide, master table. Reducing the complexity of the database would simplify user interface development and testing. However, one of the primary objectives of the database at this stage of its development is to support data entry. The design selected closely mimics the analysis laboratory output for the types of data included in the database. Later, user interfaces may need to be developed to fully exploit the content of the database. A listing of the database tables is shown in [Figure 39](#).

Figure 39: Listing of all database tables



A.3.1 Sites Table

The **Sites** table defines the various projects or sample collections that are contained in the database. In general, this information is not available for output to users but can be handy during data input. The primary application of this table is to allow the correlation of fluid sample data – data that characterize a site more than a single sample – with the group of samples collected from that site. A description of the data in the **Sites** table is presented in Table 2.

Table 2: Sites

Sites			
Column Name	Type	Units	Description
site id	short int	N/A	Site identifier – unique key
site name	text (50)	N/A	Site name
project_id	text(50)	N/A	Site project number – this is a way of identifying sites in a manner that may only be known to the data provider

A.3.2 Samples Table

The **Samples** table is the master table for this database. As indicated in [Figure 41](#), all other tables are designed around, and related through this table. This table defines the **sample_id** (unique) and **site_id** (not unique) keys. Samples from a common site can be assumed to be from a single project. In most cases, this means from a common depositional environment. In addition, this table contains a list of all data types that are available for each sample and the American Society for Testing and Materials (ASTM) sample testing method identifiers. Short integers were selected for the key values because of the relative speed with which they can be compared. There is no immediate concern that the maximum value (32767) of a short int will affect database development. A description of the data in the **Samples** table is provided in Table 3.

Table 3: Samples

Samples Table – Database Master Table			
Column Name	Type	Units	Description
site id	short int	N/A	Site identifier key
CAP_Data	text(10)	N/A	Capillary data available (Yes/No)
CAP_method	text(12)	N/A	ASTM test identifier for raw capillary data – lookup table = Capillary_Tests
Pphys_data	text(10)	N/A	Petrophysical data available (Yes/No)
Pphys_method	text(12)	N/A	ASTM test identifier for petrophysical data – lookup table = Pphys_Tests
Moisture_method	text(12)	N/A	ASTM test identifier for moisture data.- lookup table = Moisture_Tests
GS_Data	text(10)	N/A	Grain size data availability for this sample: None = no grain size data for this sample, Complete = All grain size data tables completed for this sample, Summary = only grain size summary data available for this sample – lookup table = GS_data_avail
GS_method	text(12)	N/A	ASTM test identifier for grain size data – lookup table = GS_Tests
GS_Scale	text(10)	N/A	Grain size scale (Wentworth, USCS). – lookup table = GS_scales
Viscosity_data	text(10)	N/A	Fluid properties data available (Yes/No)
Viscosity_method	text(12)	N/A	ASTM fluid properties testing method – lookup table = Fluid_Viscosity_Tests
Fluid_density_method	text(12)	N/A	ASTM fluid density testing method – lookup table = Fluid_Density_Tests
TensionsDataAvail	text(10)	N/A	Interfacial tensions data available (Yes/No)
Tensions_method	text(12)	N/A	ASTM interfacial tension testing method. Lookup table = Fluid_Tensions_Tests
sample id	short int	N/A	Sample identifier, unique key
sample_name	text(50)	N/A	Sample name (well number and depth)

A.3.3 Capillary Parameters Table

The Capillary Parameters table (Cap_Summary) contains a single set of van Genuchten and Brooks-Corey curve fit parameters to the raw capillary data for each sample (see Capillary Equations in Appendix D). The raw capillary data include the equilibrium pairs of capillary pressure and water saturation. In some cases, instead of saturation (percent of pore space occupied by the wetting phase), lab data was provided as volumetric content (volume of wetting phase divided by volume of sample). This subset of volumetric data was converted to saturation units for database consistency.

The van Genuchten method fits all of the raw capillary data by using three (3) parameters: “Alpha” (α) a parameter inversely related to the capillary rise; “Beta” ($[\beta]$ sometimes called N) is a parameter related to the uniformity of the pore throat size; and Residual Water (S_{rw}), which is a parameter related to the asymptotic limit of fluid evacuation in response to increasing pressure.

The Brooks-Corey method fits only the linear response of the logarithm of the sample saturation to logarithm of the capillary pressure. This method characterizes the capillary response of the sample by using two (2) parameters: the bubbling pressure (P_d) is the pressure (cm H₂O) that is required to initiate fluid evacuation, and Lamda (λ), is a pore uniformity parameter.

For both capillary curve-fitting methods, an R -squared (R^2) value is provided that is a measure of the fit quality. The value can be interpreted as the proportion of the variance in Y attributable to the variance in X . In simplified terms, R^2 squared is a measure of the “goodness” of the fit, where a perfect X - Y correlation has a value of 1.0. A description of the data in the Cap_Summary table is presented in Table 4.

Table 4: Cap_Summary

Derived Capillary Parameters			
Column Name	Type	Units	Description
VG_alpha (cm-1)	single	cm ⁻¹	van Genuchten Alpha parameter
VG_beta	single	N/A	van Genuchten Beta parameter
VG_Srw	single	N/A	van Genuchten residual water parameter
VG_fit_Rsquared	single	N/A	van Genuchten fit R-squared value.
BC_Pd (cm H ₂ O)	single	cm H ₂ O	Brooks-Corey bubbling pressure
BC_lambda	single	N/A	Brooks-Corey pore uniformity parameter
BC_fit_Rsquared	single	N/A	Brooks-Corey fit R-squared value.
sample id	short int	N/A	Sample identifier, unique key

A.3.4 Raw Capillary Data

The Raw Capillary Data table (Cap_Rawdata) contains the basic sample properties (see description – Table 5). The raw capillary data show the change in the saturation (percent) and moisture content (percent dry weight) as capillary pressure (cm H₂O) is increased. Many data rows for each sample are available when capillary data is taken. Table 5 presents a summary of the information in the Cap_Rawdata table.

Table 5: Cap_Rawdata

Raw Capillary Data (Saturation vs Pressure)			
Column Name	Type	Units	Description
cap_pressure	single	cm H ₂ O	Applied pressure, centimeters of water
saturation	single	%Pv	Saturation percentage of pore volume
sample id	short int	N/A	Sample identifier, unique key

A.3.5 Petrophysical Data Table

The petrophysical data table (**PetrophysicalData**) contains information about the basic rock properties of the sample and the test conditions under which those properties were determined. There is a single data row for each sample where the petrophysical properties are available. Sample densities (grain, bulk) are reported in units of grams/cm³. Porosities (effective, air-filled) are shown as a percentage of bulk volume. Saturation (water, hydrocarbon) is provided as a percentage of pore volume. Hydrocarbon saturation levels present some data reporting problems in the database. In many cases, hydrocarbon saturation values are at or below the detectable limits of the testing method, with a typical detection limit of 0.1% (by Dean Stark analysis). Samples with trace hydrocarbons present, detectable by smell or other indirect evidence are reported by using the FLAG value 0.001. Permeability and Conductivity measurements are subject to both test state choices (intrinsic, native, relative) and test fluid (inert oil, water, air) properties. Both the test state and test fluid choices are recorded in addition to the permeability (milliDarcy) and conductivity (cm/s) values. The confining pressure of testing is also entered, although for the samples currently in the database all conductivity and permeability tests were performed at 25.0 psi confining pressure. Information found in the **PetrophysicalData** table is summarized in Table 6.

Table 6: PetrophysicalData

Rock Properties			
Column Name	Type	Units	Description
bulk_density (g/cc)	single	g/cm ³	Bulk density of the sample
grain_density (g/cc)	single	g/cm ³	Density of the matrix grains of the sample
effective_porosity	single	%Vb	Effective porosity as a percentage of bulk volume
porosity_air_filled	single	%Vb	Air filled porosity as a percentage of bulk volume
water saturation	single	%Pv	Percentage of the total pore volume that is water filled
hydrocarbon saturation	single	%Pv	Percentage of pore volume that is hydrocarbon filled
permeability (mD)	single	mD	Sample permeability in milliDarcy
conductivity (cm/sec)	single	cm/s	Sample conductivity
moisture_content	text(50)		% weight
depth (ft)	single	Fbg	Sample depth measured in feet below grade
testing_fluid	text(20)	N/A	Permeability/Conductivity test fluid = { Air, Inert Oil, Water }

Rock Properties			
Column Name	Type	Units	Description
state	text(20)	N/A	Permeability/Conductivity test state = {Intrinsic, Relative, Native}
zone	text(20)	N/A	Hydrologic zone where sample was acquired = {Unknown, Vadose, Capillary, Water Saturated, Product Saturated}
Orientation	text(1)	N/A	Sample orientation during testing = {V=vertical, H=horizontal}
Confining_Pressure (psi)	single	psi	Confining pressure for the permeability test
sample id	short int	N/A	Sample identifier, unique key

A.3.6 Fluid Properties Table

The Fluid Properties table (Fluid_Properties) shows the density and viscosity of the hydrocarbon, often at multiple measurement temperatures. The type of product is identified, where available. However, many lab analyses are run blind, and there is no information on the hydrocarbon makeup. In cases where other information is available, AVI has provided an interpretation as to the fuel classification, if possible.

Because the method and matrix of sampling are different for soils and fluids, there is not a 1-to-1 correspondence between a specific fluid and soil sample. However, the data may be useful when characterizing LNAPL sites and the results of capillary analysis from samples taken therein. A description of the data in the Fluid_Properties table is listed in Table 7.

Table 7: Fluid_Properties

Fluid Properties (Viscosity/Density) Table			
Column Name	Type	Units	Description
NAPL_description	text(50)	N/A	Brief description of the contaminant
Fluid_Matrix	text(50)	N/A	Sample matrix
temp (degF)	single	°F	Sample temperature
specific gravity	single	N/A	Specific gravity of the hydrocarbon
density (g/cm3)	single	g/cm ³	Density of the hydrocarbon.
viscosity (cpoise)	single	cpoise	Hydrocarbon viscosity in centipoise
viscosity (cstokes)	single	cstokes	Hydrocarbon viscosity in centipoise
sample id	short int	N/A	Sample identifier, unique key

A.3.7 Fluid Tensions Table

The fluid tensions table (Fluid_Tensions) contains the interfacial tensions of the air/water/hydrocarbon fluid pairs. Multiple entries (rows) may be shown for a given sample when measurements are made at different temperatures. Information found in the Fluid_Tensions table is summarized in Table 8.

Table 8: Fluid_Tensions

Fluid Interfacial Tensions Table			
Column Name	Type	Units	Description
Temp (F)	single	°F	Sample temperature
IFT_aw (dynes/cm)	single	dynes/cm	Air-Water interfacial (surface) tension
IFT_ao (dynes/cm)	single	dynes/cm	Air-Product interfacial (surface) tension
IFT_ow (dynes/cm)	single	dynes/cm	Water-Product interfacial tension
sample id	short int	N/A	Sample identifier, unique key

A.3.8 Grain Size Summary Table

The Grain Size Summary table (Grain_Summary) shows the soils description of the sample and the summary data that is used to generate that description (see overview presented in Table 9). A single row in the table is shown for each sample where there are grain size data. The columns include the Folk (1954) ([Figure 40](#) and [Table 10](#)) and USCS soil/sediment description symbols ([Table 11](#)), the Folk soil textural and sorting descriptions, the median grain size, and the weight percentage of the various grain size components (gravel, sand, silt, clay) as defined on the USCS or Wentworth scale (Wentworth, 1922).

Table 9: Grain_Summary

Grain Size Summary Table			
Column Name	Type	Units	Description
gravel%	single	Wt%	Weight percent of gravel in the sample
coarse sand%	single	Wt%	Weight percent of coarse sand
medium sand%	single	Wt%	Weight percent of medium sand
fine sand%	single	Wt%	Weight percent of fine sand in the sample
silt%	single	Wt%	Weight percent of silt in the sample
clay%	single	Wt%	Weight percent of clay in the sample
total Sand%	single	Wt%	Total sand weight percent in the sample
total Fines%	single	Wt%	Total fines weight percent in the sample
depth (ft)	single	Fbg	Depth of sample (feet below grade)
sample id	short int	N/A	Sample identifier, unique key
USCS_group	text(10)	N/A	USCS soil group symbol
USCS symbol	text(10)	N/A	USCS soil description symbol
Folk symbol	text(50)	N/A	Folk sediment texture description symbol.
Folk description	text(80)	N/A	Folk sediment texture description.

Figure 40: Folk ternary diagrams (Folk, 1954)

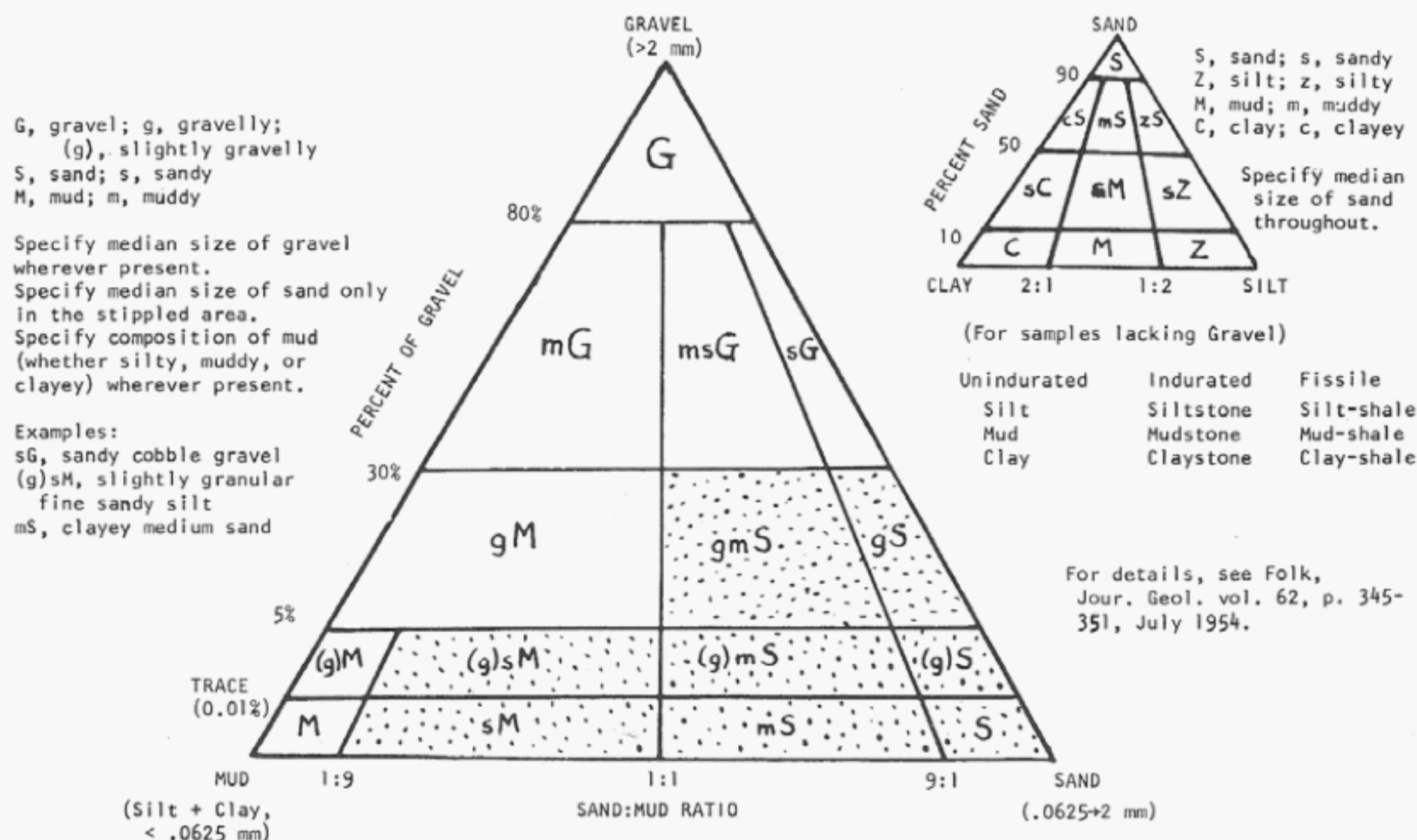


Table 10: Folk soil description formation

Terms applied to mixtures of gravel, sand and mud as depicted in the large triangle in the Figure 40 above		
Symbol	Major Texture Class (description)	Examples of Usage (complete description)
G	Gravel	Cobble gravel, granule gravel
sG	Sandy gravel	Sandy granule gravel
msG	Muddy sandy gravel	Muddy sandy pebble gravel
mG	Muddy gravel	Silty cobble gravel
gS	Gravelly sand	Granular fine sand
gmS	Gravelly muddy sand	Pebbly silty coarse sand
gM	Gravelly mud	Cobbly clay
(g)S	Slightly gravelly sand	Slightly granular medium sand
(g)mS	Slightly gravelly muddy sand	Slightly pebbly muddy medium sand
(g)M	Slightly gravelly mud	Slightly pebbly clay
S	Sand	Well-sorted medium sand
mS	Muddy sand	Silty fine sand
sM	Sandy mud	Fine sandy clay
M	Mud	Silt

Table 11: USCS soil classification

USCS soil classification		
Group	Symbol	Description
CL	CL	Clay (fines > 50%, clay > silt, sand < 20%)
CL	s(CL)	Sandy clay (fines > 50%, clay > silt, sand > 20%)
GC	GC	Clayey gravel (fines > 12%, coarse > 50%, gravel > sand)
GC	GP-GC	Clayey gravel poorly graded (5% < fines, coarse > 50%, gravel > sand)
GC	GW-GC	Clayey gravel well graded (5% < fines > 12%, coarse > 50%, gravel > sand)
GM	GM	Silty gravel (fines > 12%, coarse > 50%, gravel > sand, silt > clay)
GM	GM-GC	Clayey gravel (fines > 12%, coarse > 50%, gravel > sand, silt ~ clay)
GM	GP-GM	Silty gravel poorly graded (5% < fines > 12%, coarse > 50%, gravel > sand)
GP	GP	Gravel, poorly graded (5% < fines, coarse > 50%, gravel > sand)
GW	GW	Gravel, well graded (5% < fines, coarse > 50%, gravel > sand)
ML	ML	Silt (fines > 50% silt > clay, sand < 20%)
ML	ML-CL	Silty clay (fines > 50% silt~clay, sand < 20%)
ML	s(ML)	Sandy silt (fines > 50% silt > clay, sand > 20%)
ML	s(ML-CL)	Sandy silty clay (fines > 50% silt ~ clay, sand > 20%)
PT	Pt	Peat and other highly organic soils
SC	SC	Clayey sands (fines > 12%, coarse > 50%, sand > gravel, clay > silt)
SC	SP-SC	Clayey sand, poorly graded (5% < fines < 12%, coarse > 50%, sand > gravel)
SC	SW-SC	Clayey sand, well graded (5% < fines < 12%, coarse > 50%, sand > gravel)
SM	SM	Silty sand (fines > 12%, coarse > 50%, sand > gravel, silt > clay)
SM	SM-SC	Silty sand (fines > 12%, coarse > 50%, sand > gravel, silt ~ clay)
SM	SP-SM	Silty sand, poorly graded (5% < fines < 12%, coarse > 50%, sand > gravel)
SM	SW-SM	Silty sand, well graded (5% < fines < 12%, coarse > 50%, sand > gravel)
SP	SP	Poorly graded sand (fines < 5%, coarse > 50%, sand > gravel)
SW	SW	Well graded sand (fines < 5%, coarse > 50%, sand > gravel)

A.3.9 Raw Grain Sizes Table

The Raw Grain Sizes table (Grain_Size) shows the incremental and cumulative weight percentages of the material passing through a screen mesh of known size, indicating the limit of the grain size diameter for that smaller than a measuring (screen, opening) size. There are many entries for each sample where grain size data are available. The opening size is provided in two forms: opening millimeters and Phi (a logarithmic transformation of the Wentworth scale devised by Krumbein, 1937). Grain sizes of particles that are several centimeters larger are usually determined by direct measurement (calipers). Silts and clays are sometimes analyzed by pipette or hydrometer methods when the screening technique is used to characterize the larger particles. In some samples where the grain size data is obtained by screening the sample, the cumulative weight percent may not reach 100%. In these cases, the remainder of the sample was retained “in the pan” and is taken to be smaller than the smallest opening size reported. Most of the raw grain size data provided by PTS Labs is analyzed by using laser scattering methods when the largest grain sizes are pea gravel or smaller. In these samples, cumulative weight percentages are provided for the full particle size distribution. The ASTM particle size testing method is stored in the **samples** table. A summary of the type of information found in the Grain_Size table is presented in Table 12.

Table 12: Grain_Size

Raw Grain Size Data Table			
Column Name	Type	Units	Description
opening (in)			
opening (mm)	single	Mm	Retention size in millimeters.
Phi_value	single	Phi	Retention size in Phi
US_screen_number	text(10)		Screen number for opening size
incremental Wt%	single	Wt%	Incremental weight percent retained
cumulative Wt%	single	Wt%	Cumulative weight percent retained
sample_id	short int	N/A	Sample identifier, unique key

A.3.10 Weight Percentages Table

The Weight Percentages table (GS_Weights) shows the size of the sample at which various key (5, 10, 16, 25, 40, 50, 60, 75, 84, 90, 85) cumulative weight percentages are retained, in units of either Φ (phi) or millimeters. (A description of the data in the GS_Weights table can be found in [Table 13](#).) There can be two rows of data for each sample if values are given in both units. The “key” weight percentages are used in various graphical techniques of estimating the statistics of the size distribution without directly measuring it (see Folk, 1954 or Trask, 1938). The first four parameters of a probability distribution function are the mean, standard deviation, skew, and kurtosis. Before computer-assisted calculation of statistical parameters was practical, graphical methods of estimating parameters such as the standard deviation (spread about the average), skew (asymmetry in the spread about the mean) and kurtosis (peakedness or flatness of the distribution) were developed. Statistical estimates derived by graphical techniques are generated typically by comparing ratios of cumulative weight values in units of Φ . Despite the fact that the original limitations on computation power have long since been overcome, there is a wealth of literature where inferences about sediment transport mechanisms and fluvial processes are founded on grain size distribution properties that were graphically derived. These methods continue to be used and are the only estimates of the statistics of the distribution provided by the geotechnical labs for most samples.

In general, statistical estimates of the mean and standard deviation of the size distribution in these samples have been computed using the standard statistical equations for defining the parameters of a weighted size distribution. The grain size uniformity coefficient, defined as the ratio of the 40% grain size and the 90% grain size (40% / 90% in units of mm), is also computed and stored in this table. Because the uniformity coefficient uses the total grain-size spectrum, it is often outside the range typically calculated simply for sand (no fines). The user can calculate this or any other parameter for a subset of the range by running a query on the grain-size table for a certain grain-size range. The Folk standard deviation (sorting) and sorting descriptions in this table are described in [section 2.3.7](#).

Table 13: GS_Weights

Grain Size Weight Percentages Table			
Column Name	Type	Units	Description
5%	single	mm/ phi	Size of 5% cumulative weight retention grain in units of mm or Φ as defined by the Units field.
10%	single	mm/ phi	Size of 10% cumulative weight retention grain in units defined by the Units value.
16%	single	mm/ phi	Size of 16% cumulative weight retention grain in units defined by the Units field.
25%	single	mm/ phi	Size of 25% cumulative weight retention grain in units defined in the Units field.
40%	single	mm/ phi	Size of 40% cumulative weight retention grain in units defined by the Units value.
50%	single	mm/ phi	Size of 50% cumulative weight retention grain in units defined by the Units value.
60%	single	mm/ phi	Size of 60% cumulative weight retention grain in units defined by the Units value.
75%	single	mm/ phi	Size of 75% cumulative weight retention grain in units defined by the Units value.
84%	single	mm/ phi	Size of 84% cumulative weight retention grain in units defined by the Units value.
90%	single	mm/ phi	Size of 90% cumulative weight retention grain in units defined by the Units value.
95%	single	mm/ phi	Size of 95% cumulative weight retention grain in units defined by the Units value.
units	text(10)	N/A	Units for size data in this row of the table. Values are either mm or Phi (Φ). Data for many samples are provided in both units of Phi and millimeters.
sample_id	short int	N/A	Sample identifier, unique key.
FW-stddev	single	Φ	Folk-Ward standard deviation in units of phi.
uniformity	single	N/A	Uniformity coefficient = 40% size/90% size.
sorting_desc	text(50)	N/A	Folk sorting description.

A.3.11 Grain Size Statistics Table

The Grain Size Stats table (Grain_stats) shows the grain size distribution statistics computed by a variety of methods. (See summary – [Table 14](#).) There is a single row for each sample where the size distribution statistics are available. The grain size distribution is provided both as the true characteristics (mean, standard deviation, skew, kurtosis) of the distribution and as estimates of the parameters created by using various estimating techniques (Trask, Inman, and Folk-Ward). The parameter estimates are provided with the lab reports of grain size data. The true characteristics of the distribution were calculated by AVI, which

only computed the first two moments. The Folk-Ward (Folk) sorting values in this table are used to generate the Folk sorting description that is stored in the Grain_stats table. All data is shown in millimeter units.

Table 14: Grain_stats

Grain Size Statistics Table			
Column Name	Type	Units	Description
Median (mm)	single	mm	Median grain size.
Trask_mean (mm)	single	mm	Trask method of estimating the mean.
Trask_sorting	single	mm	Trask method of estimating the stddev.
Trask_skew	single	mm	Trask method of estimating the skew.
Trask_kurtosis	single	mm	Trask method of estimating the kurtosis.
Inman_mean (mm)	single	mm	Inman method of estimating the mean.
Inman_sorting	single	mm	Inman method of estimating the stddev.
Inman_skew	single	mm	Inman method of estimating the skew.
Inman_kurtosis	single	mm	Inman method of estimating the kurtosis.
Folk_mean (mm)	single	mm	Folk-Ward method of estimating the mean.
Folk_sorting	single	mm	Folk-Ward method of estimating the stddev.
Folk_skew	single	mm	Folk-Ward method of estimating the skew.
Folk_kurtosis	single	mm	Folk-Ward method of estimating the kurtosis.
Folk_stddev	single	Φ	Folk-Ward standard deviation (Φ).
Moment_mean (mm)	single	mm	Moment mean of the grain size distribution.
Moment_stddev	single	mm	Moment standard deviation.
Moment_skew	single	mm	Moment method of estimating the skew.
Moment_kurtosis	single	mm	Moment method of estimating the kurtosis.
sample id	short int	N/A	Sample identifier, unique key.

A.3.12 Ancillary Tables

There are two basic types of ancillary support tables: 1) those that facilitate data entry by providing the user with simple pick-lists, and 2) query support tables that provide information about the range of a parameter within the database (i.e. minimum, median and quartiles). Ancillary tables that provide standard values for data entry are primarily linked to the Samples and PetrophysicalData tables where some data must be entered manually. The values in these tables are used to populate drag-down menus that are associated with various data columns.

A.3.12.1 Data Entry Support Tables

- **Yes_No:** Values {"Yes", "No"} are linked to columns CAP_Data, Pphys_data, Viscosity_data, and TensionsDataAvail in the Samples table.
- **GS_Data:** Values {"Complete", "Summary", "None"} are linked to column GS_Data in the Samples table.

- **GS_Scales:** Values {"USCS", "Wentworth"} are linked to the column **GS_Scale** in the **Samples** table.
- **Testing_Fluid:** Values {"Air", "Inert Oil", "Water", "Mercury"} are linked to column **testing_fluid** in the **PetrophysicalData** table.
- **Orientation:** Values {"V", "H"} are linked to the column **Orientation** in the **PetrophysicalData** table.
- **Testing_State:** Values {"Intrinsic", "Native", "Specific"} are linked to the column **testing_state** in the **PetrophysicalData** table.
- **Zones:** Values {"Water Saturated", "Product Saturated", "Capillary", "Vadose", "Unknown"} are linked to column **zone** in the **PetrophysicalData** table.
- **Folk_Classification:** Values{substantial list of values} are linked to the **Folk_symbol** and **Folk_description** columns in the **GS_summary** table.
- **USCS_classification:** Values{substantial list of values} are linked to the **USGC_symbol** and **USCS_group** columns in the **GS_summary** table.
- **NAPL_descr:** Values {"gasoline", "diesel", "gasoline and diesel", "80% gasoline 20% diesel", "jet A", "JP-4", "Av gas, jet, and other", "unknown"}.
- **Fluid_Matrix:** Values{"Water pristine", "Water field", "LNAPL", "Air", "Vapor", "Gasoline", "JP-4", "JP-5", "Jet A", "Diesel #2", "Diesel #1", "Fuel Oil", "Crude light", "Crude heavy", "Bunker C"} are linked to the column **matrix** in the **Fluid_Properties** table.
- **Capillary_Tests:** Values {"ASTM-D425M", "ASTM-D3152", "N/A"} are linked to the column **CAP_method** in the **Samples** table.
- **GS_Tests:** Values {"ASTM-D422M", "ASTM-D4464", "N/A"} are linked to the column **GS_method** in the **Samples** table.
- **Pphys_Tests:** Values {"API-RP40", "N/A"} are linked to the column **Pphys_method** in the **Samples** table.
- **Moisture_Tests:** Values {"ASTM-2216", "N/A"} are linked to the column **Moisture_method** in the **Samples** table.
- **Fluid_Density_Tests:** Values {"ASTM-1481", "N/A"} are linked to the column **Fluid_density_method** in the **Samples** table.
- **Fluid_Viscosity_Tests:** Values {"ASTM-D445", "N/A"} are linked to the column **Viscosity_method** in the **Samples** table.
- **Fluid_Tensions_Tests:** Values {"ASTM-D971", "DuNouy", "N/A"} are linked to the column **Tensions_method** in the **Samples** table.

A.3.12.2 Query Support Tables

Query support tables are linked to query forms to provide users with pick-list options when qualifying a query. These tables contain statistical parameters that describe the valid range of values that should be input into a query. The basic set of parameters provided in these tables

are the minimum, maximum, maximum, average (mean), median, 1st (lower) and 3rd (upper) quartiles. The tables that contain these values are static. As new samples are entered into the system, the data in these tables must be updated. This is a manual task that must be performed by the database administrator. The query support tables (generating queries) are:

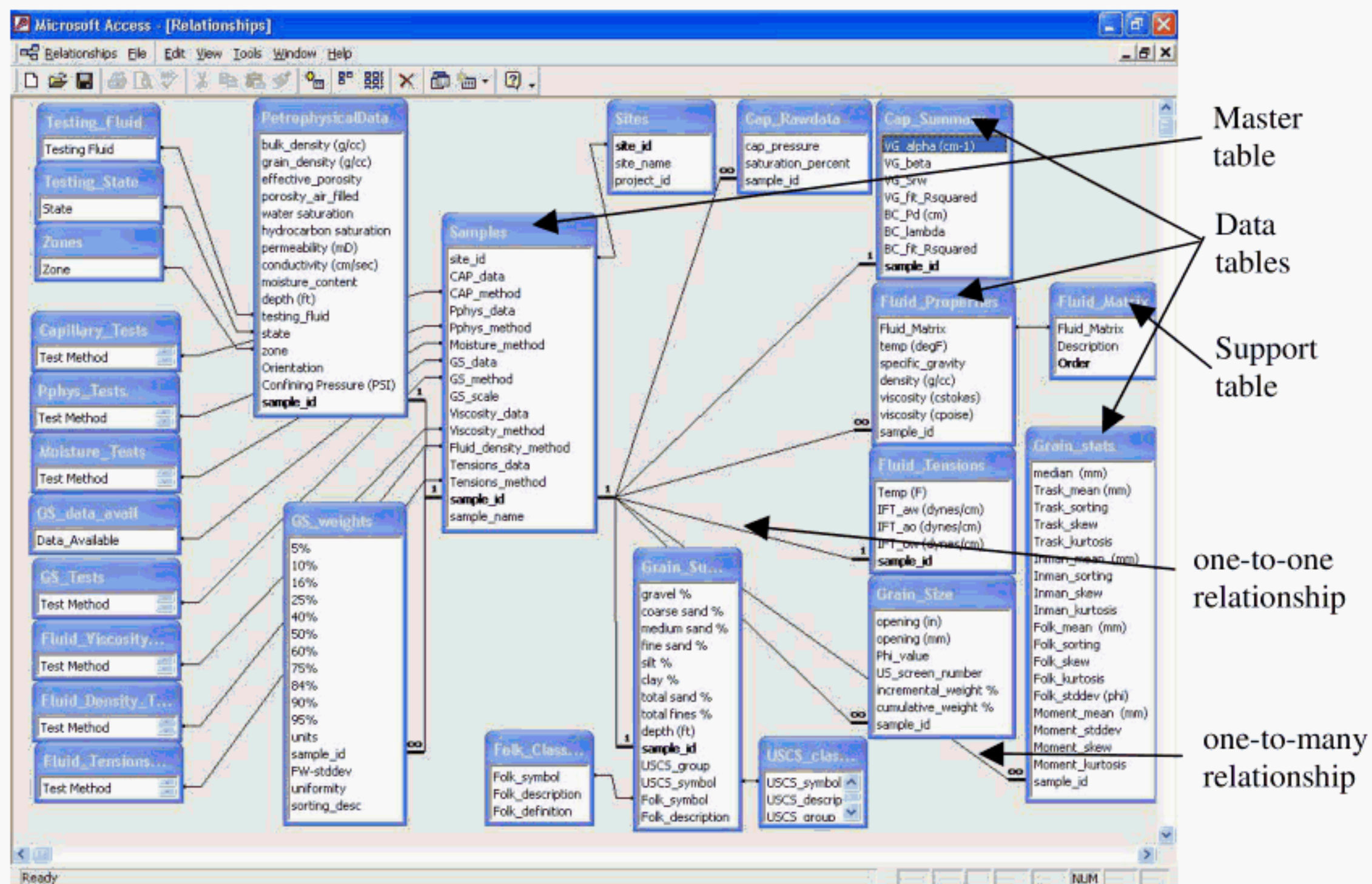
- Conductivities (ConductivityQuery)
- Permeabilities (PermeabilityQuery)
- Fines (FinesQuery)
- VG_Alpha (VG_alpha_query)
- VG_Beta (VG_beta_query)
- VG_SRW (VG_Srw_query)
- BC_Lambda (BC_lambda_query)
- BC_Pd (BC_Pd_query)

Each support table has an associated query that will determine the minimum, maximum, and average value of the appropriate parameter. The median and quartile values are not directly supported within MS Access. To determine these values, sort the data in the appropriate table (PetrophysicalData, Cap_Summary, GS_Summary) into ascending order on the desired value (i.e. permeability). The number of records is shown at the bottom of the table. The GS_Summary table shows 93 records. The median is value in the middle (i.e. the value of 47th record) when sorted on total fines %. There are 46 values less than this value and 46 values that are greater. The lower quartile is found in record 24 (47 – 23) and the upper quartile is in record 70 (47 + 23). Once the full set of values has been determined, data in the appropriate tables can be updated.

A.4 Database Structure

The basic structure of the database, plus all of the relationships between tables, is shown in Figure 40. The **Samples** table is the database centerpiece. The **Samples** table is called the master table and the other data tables are known as slave tables. Each of the other data tables link (lines) to the **Samples** table through the **sample_id** (master key) field. At the **Samples** table, the relationship is always single-valued. This is indicated the “1’s” where the relationship lines meet the **sample_id** field in the **Samples** table. Many of the data tables have one-to-one relationships with the **Samples** table (indicated by a “1” where the relationship line meets the slave table). In these tables, there is only a single data row for a given **sample_id**. Slave (data) tables are not required to have data rows for every value of the master key in the master table. Some tables have one-to-many relationships with the master table as indicated by the ∞ symbol where the relationship line meets the slave table. This means that the slave table has many rows of data associated with a single value of the master key in the master table.

Figure 41: Database structure and relationships



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Appendix B—Data Quality Control

With the development of any database for shared use comes a need for data validation and integrity checking. In general, many common data errors will not be caught by simple screening techniques. However, data errors are routinely caught when the data is used in scientific analysis. Most of the data that have been included in the API LNAPL Parameters database have been analyzed by AVI during routine project work for AVI clients. The only new and original data included in the database are the following: the Brooks-Corey fits to the capillary data, the generation of the statistics of the grain size distribution data, and the assignment of soils/sediments descriptions and symbols based on the grain size data.

B.1 Data Sources

Most of the data that are available in the API LNAPL parameter database have been obtained from three (3) sources: PTS laboratories measurements, AVI measurements, and parameters derived by AVI. In certain cases, however, information from other laboratories, academic institutions, and contractors has been used. Because the methodologies of testing are similar or identical, data from all sources is expected to be comparable, and no discernable differences were noted as a function of the data source. Different analyses methods are tracked in the **Samples** table. AVI historically conducted capillary data tests using the pressure-plate method (ATSM test method D3132). All of the PTS capillary test data are acquired by using the centrifugal method (ASTM D425M). The two data sources can be distinguished by examining the **CAP_method** column in the **Samples** table.

B.2 Measurement Techniques and Standards

All data measurements are consistent with ASTM or other documented standards for that particular measurement type. The ASTM standard analysis method for each measurement type is recorded in the **Samples** table.

The derived capillary parameters (van Genuchten alpha, beta, and residual water; Brooks-Corey bubbling pressure and lambda) are obtained by fitting the raw capillary data to the relevant equations. The van Genuchten equation is non-linear. Curve fitting is performed by successive approximation, holding one parameter fixed and optimizing for the other, then reversing the fixed and optimized parameters. The Brooks-Corey equation is log-linear but the full data set usually is not. The key is selecting the appropriate subset of data points that comprise the linear response of the system modeled in the Brooks-Corey method. In both cases, the data and fit are plotted graphically and reviewed by two hydrogeologists independently prior to inclusion in the database.

The statistics of the grain size distribution are generated from the raw grain size data by incorporating the moment equations into the data entry spreadsheet containing the soil and sediment descriptions for each sample. The weight percentages of gravel, sand, silt, and clay are compared to the values to the Folk and USCS ternary diagrams to arrive at a description and/or symbol.

B.3 Data Validation

Once a data template is fully populated and validated by the data entry technician, the template contents should be reviewed by a hydrogeologist prior to transfer into the database. All data entered into the database by AVI has been through this process. Although all data worksheets are reviewed, most data are merely spot-checked. The exception is the derived capillary parameter data. For these values (based on curve fitting techniques) the hydrogeologist examines the plot of the data and fit before accepting the data for inclusion into the database. After this final level of data validation, the data are copied into the individual database tables as a “copy and paste” operation.

After all available data was entered into the individual data tables by the data entry technician, a final spot-check of the data was performed. In all, a minimum of 2 reviews should be performed on all data, with additional reviews of calculations and other parameter derivations.

B.3.1 Referential Integrity Checking

Database referential integrity is internally enforced by Access™ as part of the database design between the **Samples** table and all data tables. This means that samples in all of the data tables must have a corresponding **sample_id** in the **Samples** table and that the **sample_id** must be a unique key in the **Samples** table. The enforced referential integrity makes it simple to delete a collection of samples from the database. If a row is deleted from the **Samples** table, all occurrences of the **sample_id** deleted in the deleted row, will be automatically deleted from all slave tables. This can be both a time saver and a curse for database administrators (DBA). If the database is updated by an untrustworthy technician, the DBA runs the risk that a technician might accidentally delete or alter significant portions of the database by making rather minor changes in the **Samples** table.

Referential integrity is a relationship property within MS Access™. It can be turned on or off at the DBA's discretion. Currently the relationship between the **Sites** table and the **Samples** table is not turned on. Turning this relationship on would allow a DBA to delete all samples from a given site by simply deleting the site from the **Sites** table. At present, that capability seemed too risky to justify its value.

B.4 Database Backups

The best way for a DBA to protect against the mishaps associated with opening up the database to data entry by untrustworthy technicians is frequent backups. The database is relatively small, just a few Mb, and can easily be backed up to a secure drive or CD-RW in a few minutes. AVI will maintain a copy of the database as delivered to the API but beyond that, database backups are the responsibility of the user.

Appendix C—Database Maintenance

The database is currently, fully populated with all of the data from the AVI files. If no new data is added to the database, the maintenance requirements should be minimal. However, it is likely that new data will need to be added to the database as it becomes available. Data entry is discussed in [Section 2](#) and the need for data quality control is the subject of [Appendix B](#). This section explains the methodology behind the basic query forms and data entry templates contained in this database.

For starters, most of the database is hidden from the users. Rather than confusing the average user with the details all of the tables, queries, forms, reports, and macros that form the basis of this database, these objects have been hidden from view. Whether an object is hidden or not is a property of the object (table, query, etc.). Most of the time, the DBA will want to see everything in the database. To view (or hide) hidden objects, select (deselect) the hidden objects box in the Tools->Options menu within Access™.

C.1 The Query-by-Forms method

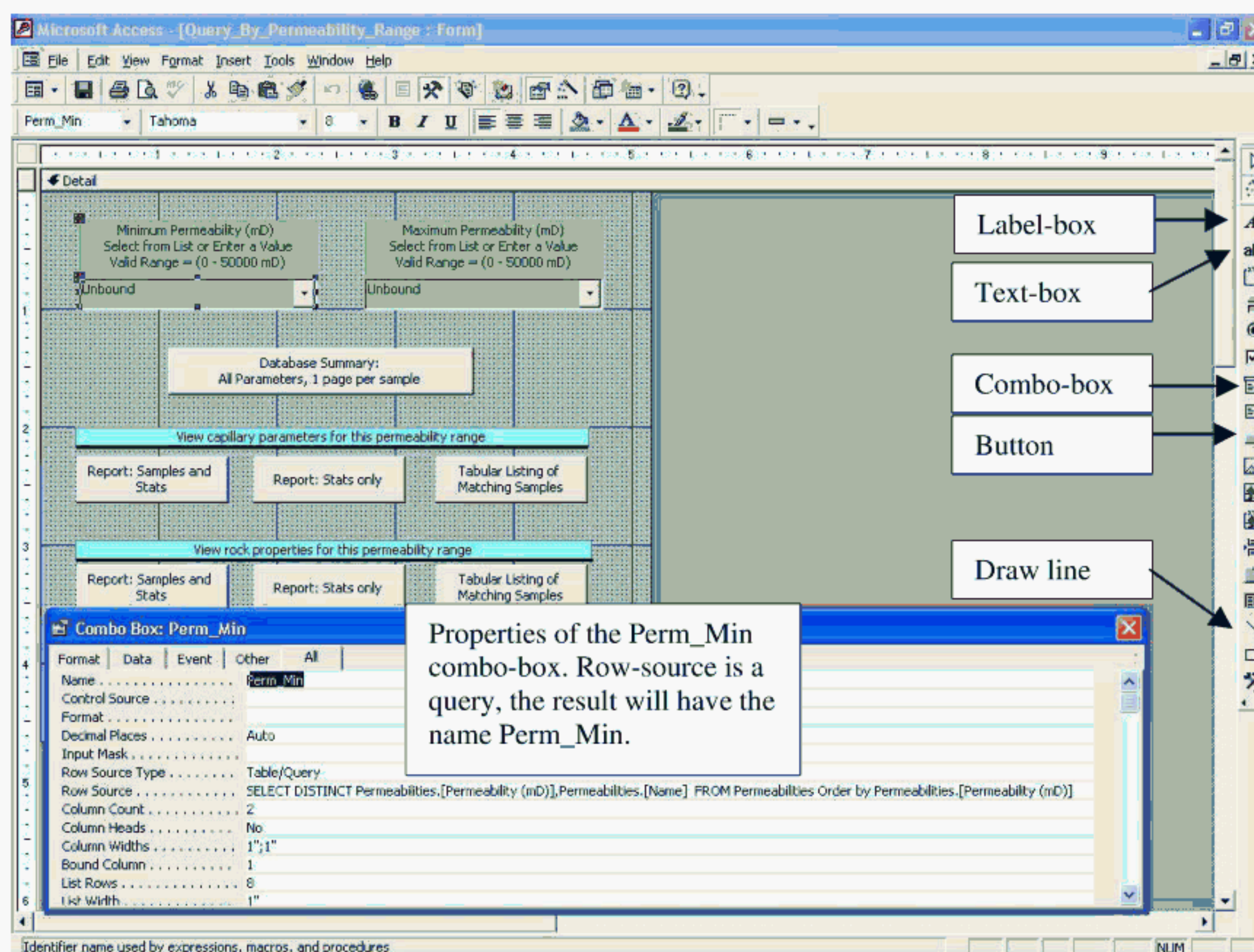
The basic technique used to provide the user with easy to use queries and forms is the “query by form” (QBF) technique. The basic approach is to use a form to provide a user with a pick-list where the values in the pick-list come from a query. In this database, special query support tables (see Appendix A, [section A3.12.2](#)) have been added for just this purpose. Values selected by the user can then be passed to another query by referencing both the form and the name of the value. Each basic form has many query options. The options are presented to the user as buttons on the form. Each button has its “on-click” property set to run a macro. The macro in turn either opens another form, a report, or a query. When data is to be displayed in “datasheet view”, the macro will point to a query with the datasheet view selected; otherwise a report is opened. Reports are linked to queries that automatically execute when the report is opened. The “Query by Permeability Range” form is used as an example below.

- 1) The Query By Permeability Range form is created from scratch. Two combo-boxes (pick-list and title box pairs) are placed at the top of the form. Various buttons are added to provide hooks into reports and queries. Text boxes are used to group buttons together that perform related tasks. Lines are drawn to enhance the grouping. The combo-box row-source is defined to be a query of the Permeabilities table:

```
SELECT DISTINCT Permeabilities.[Permeability (mD)],Permeabilities.[Name]
FROM Permeabilities Order by Permeabilities.[Permeability (mD)];
```

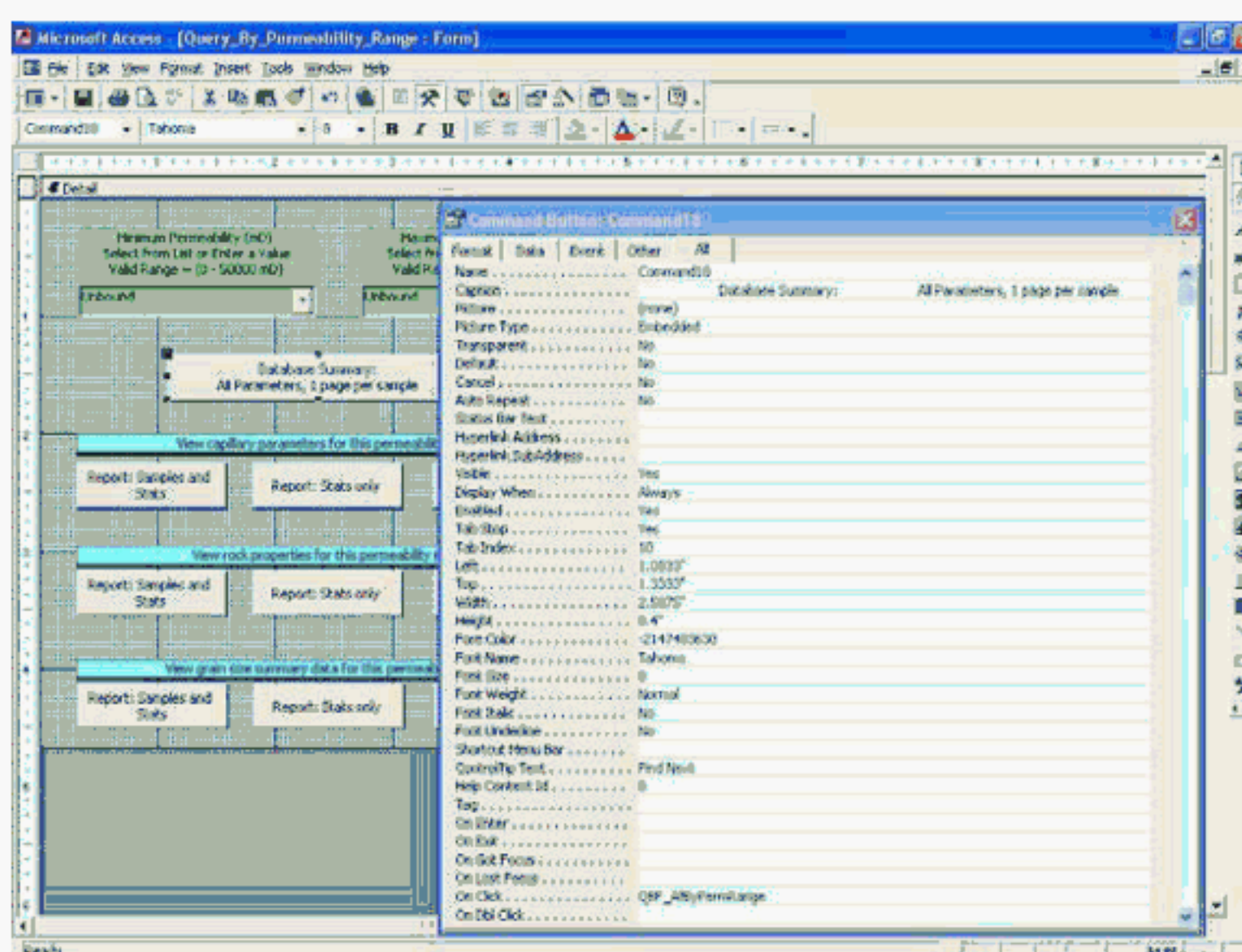
The query returns two values, a permeability and a name (min, median, max, etc.). The column count property is set to 2, the column widths are set at 1” each, and the column bound to the Perm_Min is the first column in the query (*Permeability (mD)*). The procedure is repeated using the identical query to set the Perm_Max parameter in the other combo-box ([Figure 42](#)).

Figure 42: Design view of the Query_By_Permeability_Range form



- 2) The button properties are set including the text as shown (caption) (Figure 43) and the “on click” property is set to a defined macro name (QBF_AllByPermRange).

Figure 43: Database Summary button property settings



- 3) The QBF_AllByPermRange macro is extremely simple and is not shown. The Action is set to “open report”, the report name is set to “QBF_AllByPermRange”, and the display type is set to “Print Preview”.
- 4) To define the QBF_AllByPermRange report, a query (QBF_AllByPermRange) must first be developed to extract the needed information from the database. The “SELECT” clause of the query lists the values that need to be returned. In this case, everything from all of the tables.

The “FROM” clause of the query defines how to join the data from the various tables. Left joins to the **Samples** table ensures that all **sample_id**’s from the **Samples** table will appear, and that nulls will be returned if there are no corresponding values in the slave tables for the given **sample_id**.

The “WHERE” clause identifies restrictions to be placed on the data return. In this case, data is restricted to the permeability range values set as **Perm_Min** and **Perm_Max** in the form **Query_By_Permeability_Range**.

Lastly, the “ORDER BY” clause specifies what order to return the data. In this case, data are returned sorted in ascending order by permeability.

SELECT Samples.sample_id, Cap_Summary., Grain_Summary.*, PetrophysicalData.*, Grain_stats.*, GS_weights_mm.*, GS_weights.units*

FROM (((Samples LEFT JOIN Cap_Summary ON Samples.sample_id = Cap_summary.sample_id) LEFT JOIN Grain_Summary ON Samples.sample_id = Grain_Summary.sample_id) LEFT JOIN PetrophysicalData ON Samples.sample_id = PetrophysicalData.sample_id) LEFT JOIN Grain_stats ON Samples.sample_id = Grain_stats.sample_id) LEFT JOIN GS_weights_mm ON Samples.sample_id = GS_weights_mm.sample_id

WHERE ([PetrophysicalData].[permeability (mD)] between ([Forms]![Query_By_Permeability_Range]![Perm_min]) and ([Forms]![Query_By_Permeability_Range]![Perm_max]))

ORDER BY ([PetrophysicalData].[permeability (mD)]);

- 5) The QBF_AllByPermRange report is created much in the same way that the **Query_By_Permeability_Range** form was created (Figure 43). A blank form is populated with labels, text boxes, and items that help to organize the report (lines, boxes, etc.). Information that is to be displayed once at the top of the page goes in the “report header” section. In this case that includes the **sample_id** and **permeability**. Values that are to be displayed once for every data row retrieved are put into the “detail” section of the report. For this report, that includes nearly everything else. Values that are needed only once per page (date, page number) are put in “page footer” section of the report. Lastly, values that summarize all of the rows returned by the query such as statistical parameters (min, max, average) and record counts are put into the “report footer” section.

The Text Box control source properties must be set to values returned by the query as shown in Figure 44 below.

Figure 44: QBF_AllByPermRange report design view

The screenshot shows the Microsoft Access design view for a report named 'QBF_AllByPermRange : Report'. The report is structured with several sections and fields:

- Report Header**
- Page Header**
- Database summary of samples within specified permeability range**
- Sample ID**: Includes fields for 'Samples.sample_id' and 'Permeability (mD)'.
- Soil Description of Sample**: Includes fields for 'Folk Sample Description', 'Folk Ternary Diagram Symbol', 'USCS Symbol', 'Folk Sorting Description', and 'Uniformity Coefficient'.
- Text Box: Samples.sample_id**: A pop-up window showing the properties of the 'Samples.sample_id' field, including Name, Control Source, Format, Decimal Places, Input Mask, Visible, Vertical, Hide Duplicates, Can Grow, Can Shrink, Running Sum, Left, and Top.
- Hydrocarbon Saturation (%Pv)**: Includes fields for 'hydrocarbon saturation' and 'Confining Pressure (psi)'.
- Moisture Content (%Ww)**: Includes fields for 'moisture content' and 'Confining Pressure'.
- Grain Sizes as Percentage of Total Sample**

The design view shows the layout of the report, including the placement of fields and the use of text boxes for data entry. The status bar at the bottom indicates 'Design View' and 'NUM'.

The user should note the intentional consistency in the naming to the queries, macros, and reports – all items associated with the task have the identical name (i.e. QBF_AllByPermRange). Forcing the query, report, and macro under the same name makes it easier to track down problems as the report is designed and debugged.

C.2 Adding Queries to the Database

The addition of predefined queries to the database is encouraged. Queries can be created either through the query wizard or within the design modes provided with Access™. Users of the database in this form (absence of a complete user interface) will need to develop queries to determine the important relationships between parameters. This process will eventually determine the set of user requirements for the user interface development.

C.3 Adding Reports to the Database

Reports to format and present query results are quite simple to create in Access™. Like queries, reports can be generated either by using the wizard or design view modes of the database. Graphics can added reports if desired. Users should refer to the reports containing graphics (i.e. QBF_GrainSizeBySample_report, QBF_CapDataWithBCFit) for examples of how to include graphics within reports. The graphics capability available with Access™ is somewhat limited.

Appendix D—Basic Equations

D.1 Definitions of head and pressure related to capillary bath and soil pore analogy:

$$H = Z + \frac{P}{\rho g} \quad (1) \quad P_c = P_n - P_w \quad (2) \quad h_c = \frac{P_c}{\rho g} \quad (3) \quad P_c = \frac{2\sigma}{r_c} \quad (4)$$

Where H = total head, Z = elevation, P = pressure, P_c = capillary pressure, P_n = pressure in nonwetting phase, P_w = pressure in wetting phase, σ = the interfacial tension between the fluid pairs, r_c is the radius of curvature of the pore throat, H_c = capillary pressure head, ρ = fluid density 1.0 g/cc when referenced to the water phase as all couplets are for convenience and consistency.

And noting that the capillary rise between each capillary couplet is dependent on the interfacial tension (IFT), we can develop the following scaling relationships between couplets referenced to the water system by equation 4 above.

$$P_c^{aw} = \frac{2\sigma_{ow}}{r} \quad (5) \quad P_c^{ow} = \frac{2\sigma_{ow}}{r} \quad (6) \quad P_c^{ao} = \frac{2\sigma_{ao}}{r} \quad (7)$$

Since the pore radius of curvature and is equal for each of these relationships, we can rewrite to scale the capillary rise of one system (we will assume air/water) to any of the other systems. Recall the definition of capillary head above (Equation 3), with each couplet referenced to the air/water system.

$$\frac{2}{r_c} = \frac{P_c^{ij}}{\sigma_{ij}} \quad (8) \quad P_c^{ao} = P_c^{aw} \frac{\sigma_{ao}}{\sigma_{aw}} \quad (9) \quad P_c^{ow} = P_c^{aw} \frac{\sigma_{ow}}{\sigma_{aw}} \quad (10)$$

This scaling relationship can be used to take the air/water capillary data measured in a lab and scale it to the oil/water or air/oil fluid systems. The new curves are then refit by a capillary function to define the capillary parameters for that new couplet (e.g., equations 12 & 13 below, Van Genuchten [VG] and Brooks Corey [BC] functions). Alternatively, a simpler approach is to note that the pore radius is the key factor for this conversion and, therefore, one should be able to scale the capillary rise or bubbling pressure parameter accordingly (Farr et al., 1990); these are the parameters “ α ” for the VG equation, and “ Ψ_b ” for the BC equation that are discussed below.

D.2 Definitions of saturation, volumetric fluid content, and head in soil:

$$S_e = \frac{\theta - \theta_r}{\theta_m - \theta_r} \quad (11) \quad S_e = \left[1 + (\alpha_{ij} h_{c_{ij}})^n \right]^{-m} \quad (12) \quad S_e = \left[\frac{\Psi_{bij}}{\Psi_{cij}} \right]^\lambda \quad \text{for } \Psi_c > \Psi_b, \text{ else } S_e = 1.0 \quad (13)$$

$$h_{ow} = (1 - \rho_{ro}) Z_{ow} \quad (14)$$

$$h_{ao} = (\rho_{ro}) Z_{ao} \quad (15)$$

Where S_e is the effective water saturation below the oil/air table and the total liquid saturation above the oil/air table; i & j denote the couplet of interest; Ψ_b is the Brooks-Corey bubbling pressure; λ is the

BC pore size index; θ is the volumetric fluid content, with r & m subscripts indicating residual and maximum endpoints; α is a capillary parameter inversely related to the soil capillary rise; N is a capillary parameter related to the uniformity of pore throat distribution; $m = 1 - 1/N$; ρ_{ro} is the relative oil density scaled against water (specific gravity); h_{ow} and h_{ao} are the oil/water and air/oil capillary heads.

Between the oil/water and oil/air interfaces, we have a two-phase system of oil and water controlled by the oil-water capillary parameters. Above the oil/air interface, we have a 3-phase system controlled by the air/oil and oil/water water parameters. And above the oil capillary fringe, we revert back to an air-water capillary system.

$$V_o = \Theta_e \int_0^{surf} S_o dz \quad (16)$$

The oil saturation profile corresponding to some observed oil thickness, is calculated using the capillary relationships above. The total oil volume (V_o - Equation 16) per unit area is simply the vertical integral of the oil saturation profile multiplied by the effective porosity ($\theta_m - \theta_r$). It is also possible to rewrite the VG and BC equations above to explicitly account for the residual water saturation, in which case the total porosity would be used for the volume/area integration. The calculations in the toolkit account for this factor in calculating the total LNAPL and component mass used for the transport calculations. Whether using the VEQ approximation, or some other oil distribution defined by the user or approximated by a recovery calculation (see Appendix B), the evaluation method integrates the volume per area over the area of the plume as defined by the user input.

D.3 Definitions of conductivity, relative permeability, effective conductivity and transmissivity

$$K = k_i \frac{\rho g}{\mu} \quad (17)$$

$$K_{eff} = k_r k_i \frac{\rho g}{\mu} \quad (18)$$

$$T_{eff} = \frac{k_i \rho_n g}{\mu_n} \int_0^{Z_o} k_{rn} \delta z \quad (19)$$

$$k_{ro} = (S_o)^{0.5} \left[(1 - S_w^{1/m})^m - (1 - S_t^{1/m})^m \right]^2 \quad (20)$$

$$k_{rw} = S_w^{1/2} \left[1 - (1 - S_w^{1/m})^m \right]^2 \quad (21)$$

$$k_{ra} = (1 - S_t)^{1/2} (1 - S_t^{1/m})^{2m} \quad (22)$$

Where kr = is relative permeability with respect to w - water, o -oil (LNAPL), a -air phases (Mualem, 1976; Parker, 1989), S = phase saturation (t - total, w - water, o - oil), $m = 1 - 1/N$ where N is a capillary parameter, as defined above.

$$q_p = -K_{eff_p} i_p \quad (23)$$

$$q_{pi} = -\frac{k_{rp} k_{ij}}{\mu_p} \left[\frac{\partial P_p}{\partial x_j} + \rho_p g \frac{\partial z}{\partial x_j} \right] \quad (24)$$

Darcy's Law may be written in 2 forms: where i and j are direction indices with repeated values indicating tensor notation, p is an index indicating fluid phase, q_{pi} is the Darcy velocity, k_{rp} is the relative permeability scalar, k_{ij} is the intrinsic permeability tensor of the soil, μ_p is viscosity, P_p is the pressure, ρ_p is the density, g is gravitational acceleration, z is elevation.

The mass conservation equation is necessary to account for changes in fluid movement in any phase and any direction [eq. D-2]. The equation mathematically states that a change in flux in any given direction must be equaled by a change in fluid storage in the corresponding elemental pore space.

$$\frac{\delta q_{pi}}{\delta x_j} = \frac{\delta}{\delta t} (\theta_e \rho_p S_p) - M_p \quad (25)$$

Where t is time, θ_e is effective porosity, ρ is density, and S is phase saturation, and M_p is a source/sink term with respect to phase p accounting for pumping, injection, or other boundary functions, and x indicates the Cartesian direction of the differential equation.

Groundwater Flux

The volumetric groundwater flux (q) below and within the LNAPL pool varies as a function of the background or regional specific discharge (q_{max}) and the water saturation. Below the LNAPL/water interface, the groundwater flux is equal to the regional specific discharge. Above the groundwater piezometric surface, or corrected water table (defined as elevation where the groundwater pressure is equal to zero), there is no horizontal groundwater flux. Between the LNAPL/water interface and the groundwater piezometric surface, the groundwater specific discharge is given by:

$$q = k_{rw} k_i \frac{\rho_w g}{\mu} i \quad (26)$$

where k_{rw} is the relative permeability of the wetting phase (water), k_i is the intrinsic permeability of the soil, ρ_w is the density of water, μ is the viscosity of water, and i is the hydraulic gradient.

Recognizing that the background or regional specific discharge (q_{max}) is given by:

$$q_{max} = k_i \frac{\rho_w g}{\mu} i \quad (27)$$

equation (26) can be rewritten as $q = k_{rw} q_{max}$, or $\frac{q}{q_{max}} = k_{rw}$, where the relative permeability, k_{rw} was given

above. In a multilayer case, q_{max} through each zone is defined by the permeability or conductivity of that horizon.

The water fluxes from each layer are summed to give the total flux across the zone.

The above equations can be used to calculate the ratio of groundwater flux through the LNAPL zone (q) to the regional flow q_{max} .

Appendix E—References

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