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dSED:
Database for Sediment Early Diagenesis

User Manual

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Last updated: May 3, 2004

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Part I – Database Program Manual

Introduction

The Database for Sediment Early Diagenesis (dSED) is a collection of experimental and theoretical thermodynamic and kinetic data and bibliographic and reference information that is intended as a tool in developing models of early diagenesis in aquatic sediments. While the goals and the philosophy of the database are described in an article (S. Katsev, D.G. Rancourt, and I. L'Heureux, dSED: A database tool for modeling sediment early diagenesis.) that can be downloaded at http://www.science.uottawa.ca/LSSE/dSED, this document is intended to assist users in their work with the database and in learning its programming and search capabilities.

The use of dSED is in most cases simple and straightforward. A large portion of this manual deals with details of dSED implementation that are essential for its customization. Information about the basic use of the database is contained in the sections Retrieving data, Forms and filters, and Examples.

Since, in practice, at this stage, dSED is intended primarily as a collection of kinetic data of greatest use in diagenetic modeling, it may lack many reactions that describe equilibria between various solid and liquid species, as well as speciation reactions for aqueous species. The user is encouraged to seek information on such reactions in one of the programs/databases designed specifically for equilibrium thermodynamic calculations (FITEQL, PHREEQE, etc.) as well as in numerous thermodynamic calculations references. A non-exhaustive list of equilibrium reactions along with the stability constants can be found, for example, in Ref. [7] (see Part II of this manual).

Programming aspects of dSED implementation

Database organization

The dSED database is implemented in Microsoft Access™ 2000. Some aspects of Access data organization that are important for information handling in dSED are outlined below, although an interested user is encouraged to consult that program's manual.

Microsoft Access™ uses a 3-tier approach to information handling through the use of what are called Tables, Queries, and Forms (Figure 1). The information is stored in data Tables in a way that best corresponds to the data structure and minimizes data redundancy. Certain fields in the Tables may be connected by logical links. Search tools called Queries are used as programmable search engines to locate the necessary data in the Tables and to retrieve them according to specified rules. Finally, Forms serve as an interface in which the information is presented in a format convenient for the user.

In dSED, all information can be viewed or entered through the corresponding Forms (Figure 2). For convenience, the Forms are combined in several groups, according to their

functionality, such as forms that display reactions for a particular chemical species or the ones that display reactions of a particular type, e.g. precipitation reactions. The groups of forms are shown in the lower left corner in Figure 2.

An advanced user may add the required functionality by modifying the existing Forms and the corresponding Queries or by writing additional programming routines. The built-in Access filters can also be used for fast information selection, as discussed below.

Figure 1. General database organization in MS Access.

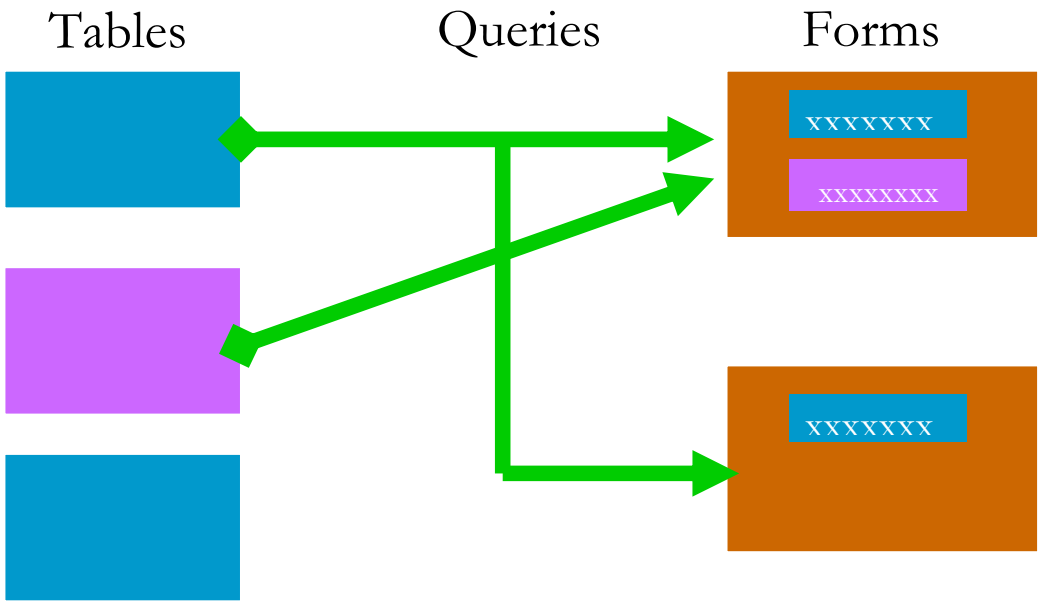
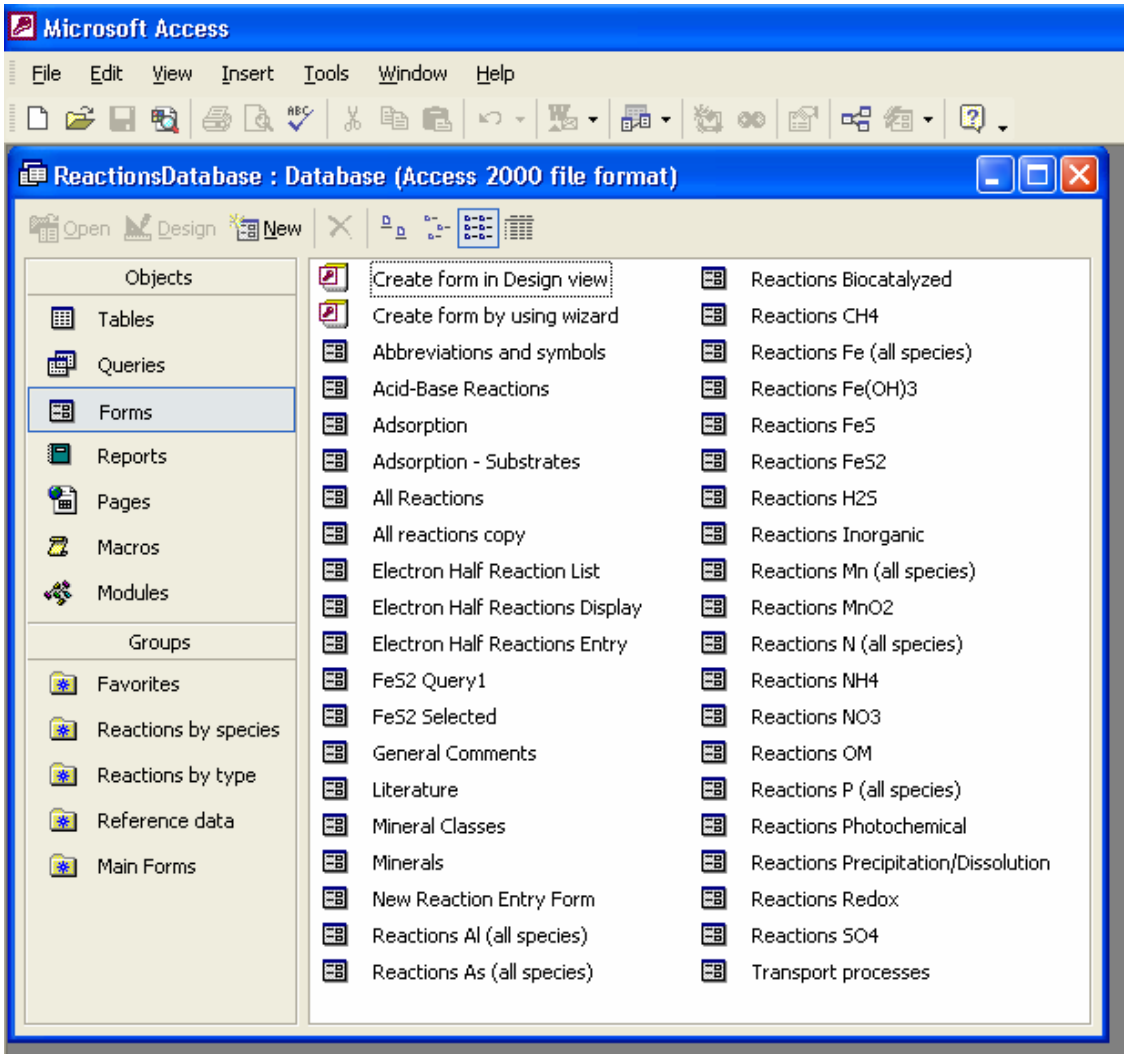


Figure 2 dSED main window showing available Microsoft Access Forms.



Information structure (Tables)

The database uses a reactions-centered approach to organizing the information, i.e. the main entries in the database records are individual chemical reactions or, generally speaking, physical, biochemical, or geochemical processes that can be represented as a reaction. Each reaction has its unique ID number that can be used for referencing. The information about reactions is stored in the Reactions Table and can be retrieved in its most complete form through the All Reactions Form.

In addition to the main dataset that characterizes particular reactions, dSED contains additional information that is stored in separate Tables and can be retrieved through the corresponding Forms. This information includes such data as adsorption parameters for different species on various substrates, half-reaction representation for redox reactions,

transport processes in sediments, list of minerals present in sediments, bibliographic references, and other information.

Below is the description of dSED data Tables. This information is needed if new functionality is to be added to the database through programming Queries and Forms. A user interested in only retrieving the information can skip to the next section. In the descriptions below, some Tables are described as auxiliary, which means that their content is used in other tables, for example, as a look-up list in a drop-down box.

dSED Table	Description	Relationships
Abbreviations and symbols	A list of abbreviations and symbols used in dSED is provided as a reference.	
Acid-base reactions	A list of common acid-base reactions is provided as a reference. Equilibrium constants are given.	
Adsorption	Data on adsorption of various aqueous dissolved species on common solid substrate surfaces is provided. The list of possible aqueous species for a drop-down box is specified as an internal list inside the Table while the list of substrates is taken from the Adsorption-substrates table.	Uses Adsorption-substrates table as a data source
Adsorption-substrates	Solid phase surfaces and their properties with respect to sorption are listed as well as typical sorption properties of dead or alive organic matter. This table is an auxiliary data source for the Adsorption table.	Used in Adsorption table
General comments	General comments about the database and its implementation. They are intended to clarify conventions, definitions, etc.	
Half-reaction list	A list of redox electron half-reactions and their equilibrium constants is provided. It is used as an auxiliary data source for the Half Reactions table.	Used by the Half Reactions table.
Half reactions	Electron half-reaction representations for the redox reactions in the main (Reactions) table are stored in this table. The list of half-reactions for the drop-down box is taken from the Half-Reaction List table. The reactions in the main table are referenced by their IDs. Those IDs are used as a primary key for the table. A similar table is planned for proton half-reactions.	Linked to the ID field in Reactions table. Uses Half-Reaction List as data source.
Literature	Bibliographic information on cited references.	
LUT Adsorption-Literature	This is an auxiliary look-up table that matches sorption processes with the corresponding bibliographic references. It contains sorption	Linked to Adsorption and Literature

	process IDs and literature reference IDs.	tables
LUT Rate-Literature	This is an auxiliary look-up table that matches reactions with bibliographic references for reaction rates. It contains reaction IDs and literature reference IDs.	Linked to Reactions and Literature tables
LUT Reaction-Literature	This is an auxiliary look-up table that matches reactions with the corresponding bibliographic references. It contains reaction IDs and literature reference IDs.	Linked to Reactions and Literature tables
LUT Reaction-Model	This is an auxiliary look-up table that matches reactions with the corresponding diagenetic models in which those reactions were used. The table contains reaction IDs and model IDs.	Linked to Reactions and Models tables
LUT Substrate-Literature	This is an auxiliary look-up table that matches adsorption substrates with the corresponding bibliographic references. It contains substrate IDs and literature reference IDs.	Linked to Adsorption-substrates and Literature tables
LUT Transport-Literature	This is an auxiliary look-up table that matches transport processes with the corresponding bibliographic references. It contains transport process IDs and literature reference IDs.	Linked to Transport and Literature tables
Mineral classes	A list of mineral classes that correspond to standard mineral classification. This table is used as an auxiliary data source for the Minerals table.	Used in Minerals table as a data source.
Minerals	A list of various minerals alone with their properties. The mineral group drop-down box uses the Mineral Classes table as a source.	Uses Mineral Classes table as a source.
Models	A list of diagenetic models with the corresponding bibliographic references is provided.	Uses Literature table as source for citations.
Reactions	The main data table. It contains chemical and biogeochemical reactions alone with equilibrium, kinetic, and other information pertaining to them.	
Transport	Common processes that contribute to transport of solid, liquid and gas species in sediments are listed. The table describes the properties of those processes and common approximations taken in their modeling.	

Retrieving data (Forms)

The most simple and straightforward way of retrieving information from dSED is by clicking on the corresponding Forms in the main dSED window (Figure 2). Descriptions

of individual forms are given in the section Forms and filters below and the relationships between Tables, Queries, and Forms in dSED are shown in Figure 3a and Figure 3b.

In some cases, the amount of text in a database record is greater than the number of lines that can be seen in the form window (this is usually the case for the Comments fields in the All Reactions table). In this case, the remaining text can be viewed by clicking on the corresponding Form field and scrolling down.

Additional forms (for better viewing) can be opened by clicking on the [>] buttons. These buttons are located next to reaction ID fields (to see all information for the reaction), next to reference list (to see full citation information), or next to model list (to see full citation for the corresponding modeling papers).

The design of the Forms can be easily modified to meet user's requirements. Also, a separate version formatted for printing can be designed by using the Reports tab in the main database window (Figure 2). As these are standard features of Microsoft Access, the corresponding instructions are provided in that program's manual and through the Help menu.

Several standard Microsoft Access search and filtering tools can be used inside the Form windows.

 Database records can be sorted alphabetically by any column in a Form.

 A particular text (mineral name, chemical compound, etc.) can be searched.

 Database records that contain a specified text can be selectively chosen (see examples).

Figure 3a. Relationships between Tables, Queries, and Forms in dSED.

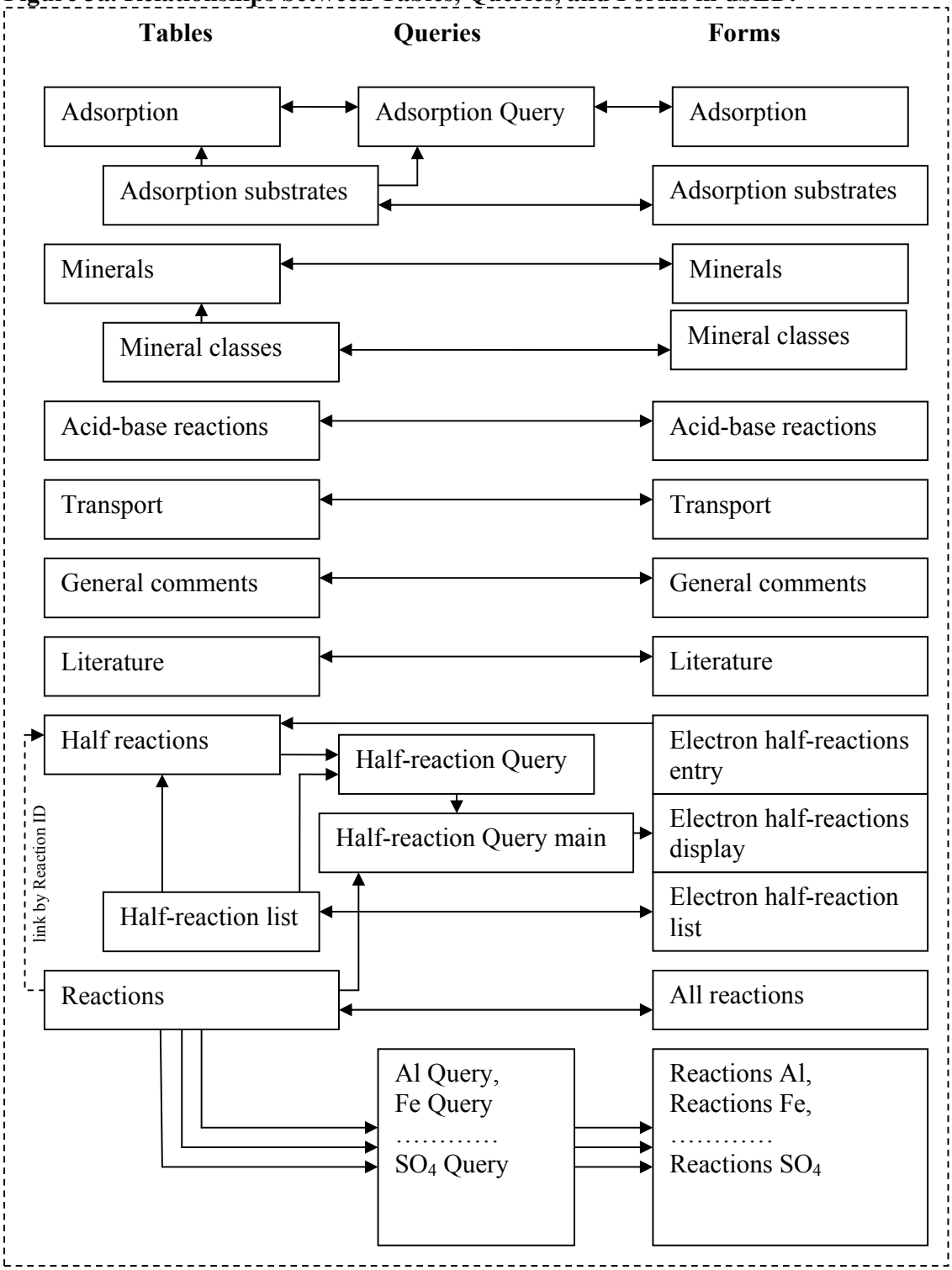
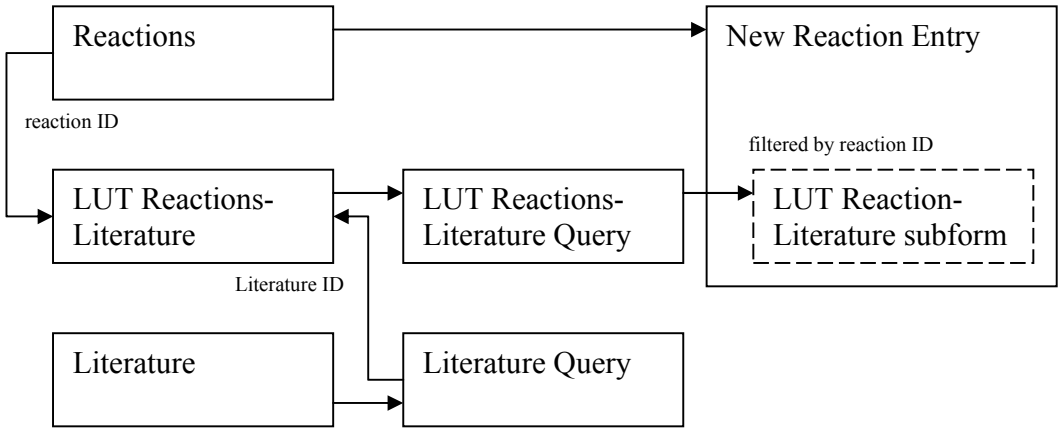


Figure 3b Relationship scheme by which bibliographic references are displayed in a subform of a form (New Reaction Entry) that displays reaction information. Similar schemes are employed to display bibliography for reaction rates, transport processes, sorption processes, and sorption substrates.



Forms and filters

The Forms listed in the main database window (Figure 2) are used to retrieve data from the database and present it in a format convenient for viewing. Many of the Forms are designed to present filtered data, e.g. only reactions involving a particular chemical compound, in which case they are connected to corresponding Queries where the selection criteria are defined. Some Forms can be described as auxiliary in the sense that they are designed as means of entering data into auxiliary tables, while the data entered is best viewed in other Forms.

At the present time, dSED contains the following Forms.

dSED Form	Description	Query
Abbreviations and symbols	Displays the content of the Abbreviations and Symbols table.	
Acid-base reactions	Displays information contained in the Acid-Base Reactions Table. The form is an auxiliary form used only for data entry.	
Adsorption	Displays information contained in the Adsorption Table.	Adsorption Query
Adsorption-substrates	Displays all the information in the Adsorption-Substrates Table. The form is an auxiliary form used only for data entry.	

All reactions	This is the main database Form. It displays all information about all reactions contained in the Reactions Table.	
General comments	Displays information contained in the General Comments Table.	
Electron half-reaction list	Displays information contained in the Half-Reaction List Table. The form is an auxiliary form used only for data entry.	
Electron half-reactions display	Displays the reaction list with redox reactions represented in their half-reaction form. The corresponding data is contained in the Half-Reactions Table.	Half Reactions Query Main
Electron half-reactions Entry	Similar to the Half-Reaction Display Form but is used to enter the half reaction representation for redox reactions. The corresponding data is contained in the Half-Reactions Table.	
Literature	Displays a bibliographic reference list contained in the Literature Table.	
Minerals	Displays the information contained in the Minerals Table, i.e. mineral names, compositions, genesis, etc.	
Models	Displays a list of diagenetic models	
New reaction entry form	Similar to the All Reactions form but displays information in Columnar, instead of Tabular, format so that only one reaction is visible at any time. Contains subforms that display bibliographic reference information and published model reaction sets.	Has subforms that use LUT Queries: Reaction-Literature, Rate-Literature, and Reactions-Models
Reactions Al	Displays a list of reactions that involve aluminum as part of their reactants or products.	Al Query
Reactions biocatalyzed	Displays a list of reactions that are catalyzed or carried out entirely by living organisms.	Biocatalyzed Query
Reactions CH4	Displays a list of reactions that involve methane as part of their reactants or products.	CH4 Query
Reactions Fe	Displays a list of reactions that involve iron (in all iron-bearing compounds) as part of their reactants or products.	Fe Query
Reactions FeS	Displays a list of reactions that involve iron monosulfide as part of their reactants or products.	FeS Query
Reactions FeS2	Displays a list of reactions that involve pyrite as part of their reactants or products.	FeS2 Query
Reactions H2S	Displays a list of reactions that involve hydrogen sulfide as part of their reactants or products.	H2S Query
Reactions	Displays a list of reactions that can proceed	Inorganic Query

inorganic	without participation of living organisms.	
Reactions Mn	Displays a list of reactions that involve manganese (in all Mn-bearing compounds) as part of their reactants or products.	Mn Query
Reactions N	Displays a list of reactions that involve nitrogen (in all forms) as part of their reactants or products.	N Query
Reactions NO3	Displays a list of reactions that involve nitrate as part of their reactants or products.	NO3 Query
Reactions OM	Displays a list of reactions that involve organic matter (solid or dissolved) as part of their reactants.	OM Query
Reactions P	Displays a list of reactions that involve phosphorus as part of their reactants or products.	P Query
Reactions photochemical	Displays a list of reactions that require light.	Photochemical Query
Reactions precipitation/ dissolution	Displays a list of reactions that involve precipitation or dissolution of minerals or amorphous compounds.	Precipitation Query
Reactions SO4	Displays a list of reactions that involve sulfate as part of their reactants or products.	SO4 Query
Reactions redox	Displays a list of reactions in which a change of redox state for some of the reactant or products occurs.	Redox Query
Single adsorption process	Displays all information for one adsorption process in a single window.	Adsorption query, uses LUT Adsorption-Literature Query
Single reaction	Displays all information for one reaction in a single window (same as New Reaction Entry).	
Single transport process	Displays all information for one transport process in a single window.	Uses LUT Transport-Literature Query
Transport processes	Displays all the information on transport processes in sediments that is contained in the Transport table.	

Examples

Example 1. Selecting a set of reactions used in a cited reaction-transport model.

The Reaction Sets column in the dSED Single Reaction Form contains references to various reaction-transport models. Using these references, the reaction sets that are used in those models can be extracted, e.g. for their comparison or analysis.

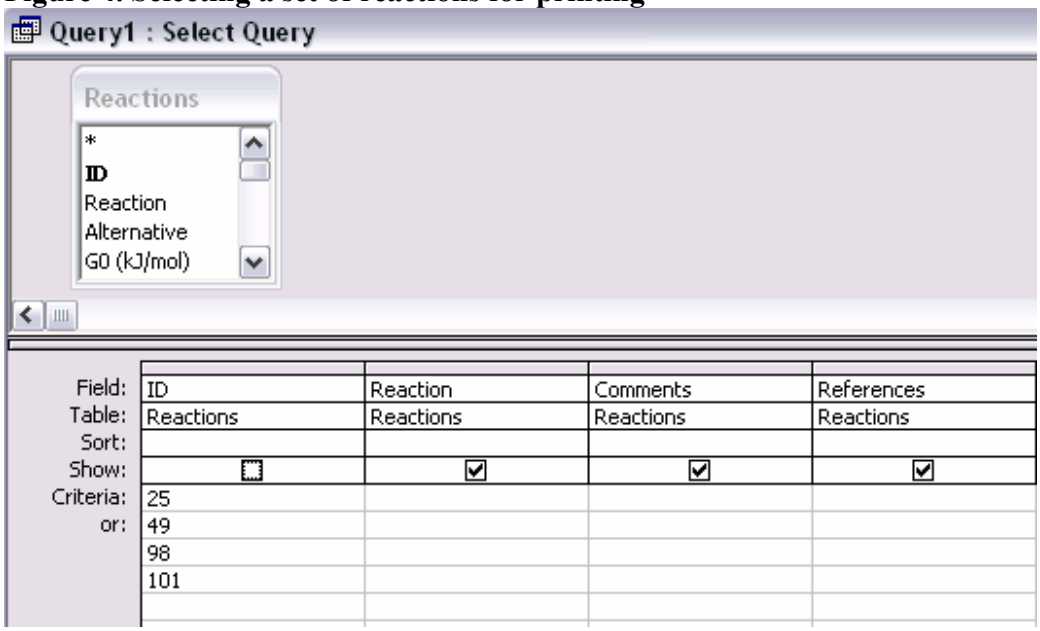
1. Click on the button  in the Single Reaction Form next to the Reaction Sets column. This will open a new Form that contains information about the listed models.
2. Click on the button  next to the model whose reaction set you want to view. A new Form will open that contains reaction processes that have been used in that model.

Example 2. Printing database records for a specific set of reactions.

To print information provided by one or more of the dSED Tables or existing Queries, it is convenient to use the Report feature of Microsoft Access.

1. In the Report tab (Figure 2), click on the New button in the top toolbar and select Report Wizard.
2. Select the fields to be included in the report and follow the prompts to select the report style.
3. Once the report is created, you can modify its layout (e.g. change column width) in the Report Design window by clicking the  button.

Figure 4. Selecting a set of reactions for printing



To print dSED records for an arbitrarily defined set of reactions, that reaction set can be defined in a new Query.

1. In the Queries tab (Figure 2), click on the New button in the top toolbar and select the Design view.
2. In the Show Table window, select the Table(s), from which the information should be derived, e.g. Reactions table.
3. In the Query Design window, select the desired fields from the corresponding drop-down boxes. In the example in Figure 4, the Reaction ID, Reaction formula, Comments, and References have been selected. The checkboxes under the field descriptions indicated whether the information in that field will be included in the query (and report) output.
4. In the Criteria area of the window, specify the reactions for which information should be printed. In Figure 4, the reactions have been specified by their IDs. Specifying criteria in different rows is equivalent to a logical OR operator while entering criteria in different columns of the same row is equivalent to an AND operator (refer to Microsoft Access manual or Help for more details).
5. Close the Query Design window and choose to save it.
6. In the Report tab (Figure 2), click on the New button in the top toolbar.
7. Select Report Wizard and select the name of your query from the drop-down list.
8. Select the fields to be included in the report and follow the prompts to select the report style.

Once the report is created, you can modify its layout (e.g. change column width) in the Report Design window by clicking the  button.

Example 3. Arranging mineral list by mineral classes.

The list of minerals can be viewed alphabetically by mineral names or by mineral class names. To arrange the list by mineral class, click in the Mineral Classes column and then click on one of the  button in the toolbar.

Part II – Modeling and Geochemical Background Information

This section provides reference to published and web resources describing the fundamentals of diagenetic modeling and the essential knowledge related to various aspects of modeling early sediment diagenesis.

General references

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Knowledge Base is maintained by the Marine Geochemistry group at the University of Utrecht, the Netherlands: www.geo.uu.nl/Research/Geochemistry/kb. It is an ongoing project whose goal is to create an updatable knowledge base that could be integrated with numerical early diagenesis simulators also developed by the same group.

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