

# TRFD Fitting Software

## *User's Guide*

*with Reference Manual*



TRFD Fitting Software  
version 2.0 (build 2)

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## Content

<b>Content .....</b>	<b>2</b>
<b>Introduction .....</b>	<b>4</b>
Reading the manual .....	4
System requirements .....	4
Installation .....	4
Technical support .....	4
<b>TRFD Fitting Software – Main Application.....</b>	<b>5</b>
A tour of the environment .....	5
Starting TRFD Fitting Software .....	5
Menu.....	6
Using toolbars, menus, and keyboard shortcuts .....	6
Experiment window.....	6
Main Window Tabs Panel .....	8
Application Windows.....	11
Quick Data Analysis Start .....	13
Single Curve Analysis .....	13
Global Analysis .....	14
Managing Parameters .....	15
Building User-Defined models.....	15
Confidence Intervals.....	15
Fit Quality Criteria .....	16
Data Export.....	16
Managing Experiments.....	17
Saving and Restoring Experiments .....	17
Current Experiment .....	18
Working with Templates .....	18
<b>TRFD Analysis Database.....</b>	<b>20</b>
A tour of the environment .....	20
Starting Analysis Database.....	20
Menu.....	21
Using toolbars, menus, and keyboard shortcuts .....	21
Analysis page.....	22
Parameters page.....	23
Data Preview.....	25
Experiment Preview .....	25
FQ Criterion Preview .....	26
Parameters Dependence Preview.....	27
Analysis Report .....	27
Report Options dialog.....	28
Print Preview window .....	29
Data Management.....	29
Searching .....	29
Sorting .....	30
Filtering .....	30
Data Export.....	30
Database Tables Tools.....	33
Options .....	33
Tables Tools .....	33
Tables Checking .....	34

Tables Check and Repairing.....	34
<b>TRFD Measurements Database.....</b>	<b>34</b>
A tour of the environment .....	34
Starting Measurements Database .....	34
Menu.....	35
Using toolbars, menus, and keyboard shortcuts .....	35
Data Sets panel .....	36
Data Block panel .....	37
Parameters panel.....	39
Application Windows .....	39
Data Import.....	40
Data Management.....	42
Searching .....	42
Sorting .....	42
Filtering .....	43
Data Preview and Data Report .....	43
Data Preview.....	43
Reports.....	43
Database Tables Management.....	45
Creating new set of tables.....	45
Link tables .....	45
Import/Export Database.....	46
Database Tables Tools.....	47
Options .....	47
Select Table Window .....	48
Tables Packing.....	48
Tables Emptying.....	49
Tables Checking .....	49
Tables Repairing.....	49
<b>TRFD Shared Tools .....</b>	<b>50</b>
Filter .....	50
Filter dialog box .....	50
<b>Appendix .....</b>	<b>53</b>
Fitting Procedure .....	53
Global Analysis .....	53
Data Analysis Models.....	53
Fit quality criteria .....	53
<b>Tips and Frequently Asked Questions .....</b>	<b>53</b>
<b>Glossary .....</b>	<b>53</b>
<b>Index .....</b>	<b>53</b>

## Introduction

### ***Reading the manual***

In developing the TRFD Fitting Software one of our primary goals was to make the interface as easy to use as possible. However, some features may not be immediately apparent, so we hope you take some time to at least page quickly through the manual. That way, you won't miss any of TRFD Fitting Software potentials.

The structure of the developed software tools is consisted of three parts: interface part (TRFD Fitting Software – Main Application), analytical part (TRFD Analysis Database) and database (TRFD Measurements Database). There sections in the manual devoted to the use of each part. Also there are some parts (e.g. Filter) that are connected to few manual sections and so they are placed at the end of the manual.

### **System requirements**

In order to use the TRFD Fitting Software package you will need the following:

Required

- 200 MHz processor
- 16 MB RAM

Recommended

- 400 MHz processor
- 64 MB RAM

Common

- Windows 9x or Windows NT 4.0 or later
- 20 MB hard-disk space for the software installation

### **Installation**

Open the TRFD Fitting Software installation folder and start *setup.exe* file. Follow installation wizard request and change the program directory if necessary.

When the installation is completed run TRFD Fitting Software application. When running the application for the first time you will be asked to enter the key.

### ***Technical support***

If you experience problems or have questions while using TRFD Fitting Software, there are a few ways to get the information that you need from Scientific Software Technologies Center: web site support, email support, fax support, and telephone support.

## TRFD Fitting Software – Main Application

The TRFD Fitting Software allows performing the parameters fits based on the multiexponential representation using any number of exponentials from 1 to 10. Any system based on the multiexponential decay can be analyzed. Exponential parameters  $p_j$  and  $\tau_j$  can be fixed to predefined values or can be constrained by corresponding intervals. The software also allows to link parameters into the user-definable groups, so that all parameters of the group have the same value. This feature is especially useful if the contribution of different lifetimes to the decay function is assumed to be equal. Besides single curve analysis the software also allows to perform global analysis of multiple phase vs. frequency traces. In global analysis several experimental data traces are combined and fitted simultaneously.

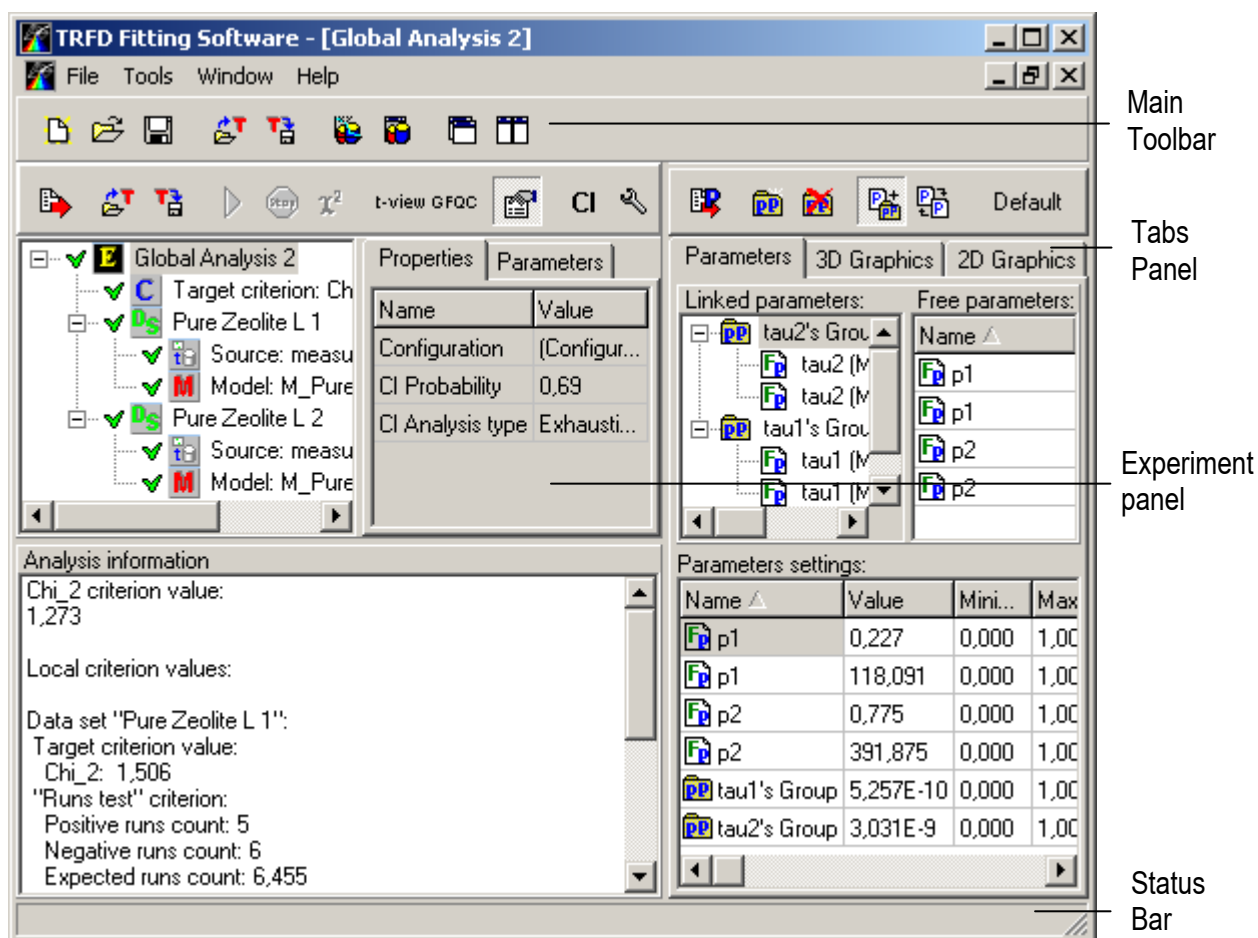
### A tour of the environment

#### Starting TRFD Fitting Software

You can start TRFD Fitting Software Main Application in several ways:

- From the main TRFD Fitting Software program (F3 or clicking Toolbar button).
- Choose Programs | TRFD Fitting Software | Fitting Software 2.0 from the Windows Start menu.
- Choose Run from the Windows Start menu, and then enter TRFDfs.exe.
- Double-click \Program Files\SSTC\TRFD Fitting Software\Bin\ TRFDfs.exe.

Once you are in the Main Application, you see the major tools of the program environment.



Main Window consists of the following components:

- Menu

- Main Toolbar
- Experiment window
- Status Bar

Menu and Toolbar provide quick way to invoke the commands of the application. Experiment window consists of two panels: Experimental panel and Tabs panel.

Experimental panel displays current Experiment structure, parameters and properties of contained models and Experiment itself, and Fitting Software feedback.

Tabs panel is used to view parameters groups, its values, and graphical visualization of the Data and of the Experiment Analysis.

Status bar provides information about the current state of the application.

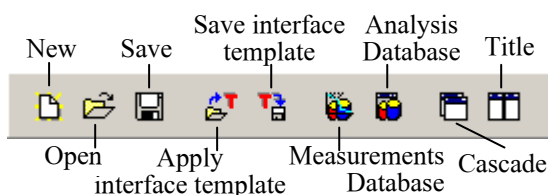
## Menu

General features of the program are available from the application menu. Through the menu you can manage your Experiments: create new Experiment, open existing one, save, close change the configuration of the current Experiment. You can work with few Experiments at the same time, so all window management tools are available.

## Using toolbars, menus, and keyboard shortcuts

Many operations have keyboard shortcuts as well as toolbar buttons. When a keyboard shortcut is available, it is always shown next to the command on the drop-down menu.

TRFD Main Application toolbar provides quick access to frequently used operations and commands that deal with Experiments. Some toolbar operations are duplicated in the drop-down menus. Note that interface template commands are available only on the toolbar.



You can see each button function by pointing the mouse over it. In a second Help Hint appears as a pop-up short text.

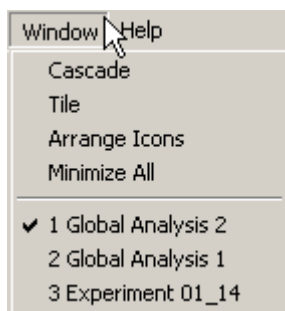
“New”, “Open”, and “Save” commands have to deal with Experiments; next two commands let you Save and Apply templates; then there are two buttons to start additional Fitting Software Database applications and finally the last two buttons customize Experiment windows.

## Experiment window

Experiment window has two parts: Experimental and Tabs panels. Each panel has own toolbar and informative panels.

### *Customizing Experiment windows*

As it was mentioned, you can open few Experiments in one application. Each opened Experiment has own window. That is why it's possible to change the size and position of the Experiment windows. Besides that you can customize opened windows using *Window* option from the application menu.



Using *Window* menu you can view opened Experimental windows in Cascade or Tile way. These commands are duplicated with the corresponding buttons on the application toolbar as well.

With one click you can also minimize all opened windows or switch between windows using the numbered list of opened windows in the *Window* menu.

Each Experimental window can be customized in a proper way. For example, to have the best information view on the screen you can set appropriate sizes for the window components: panels, tabs, informative fields.

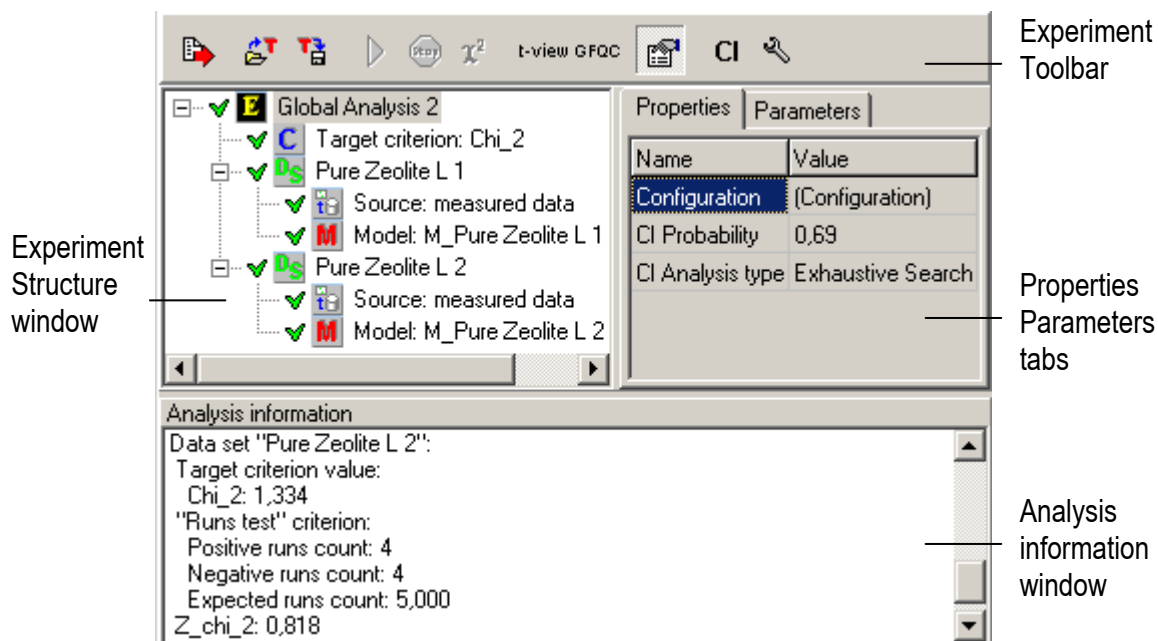
Of course, it would be tedious to repeat customizing procedure every new application start. That is way it is proposed to use interface templates. Interface templates commands: “Apply” and “Save” are available only on the application toolbar.

Don't mix it up Interface templates with Analysis templates. Analysis templates buttons are situated on the Experiment Toolbar.

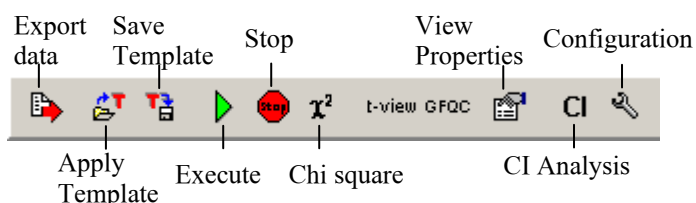
### Experimental Panel

Experimental panel displays the current Experiment structure, parameters and properties, outputs analysis information. It consists of the following components:

- Experiment Structure window
- Experiment toolbar
- Analysis information window



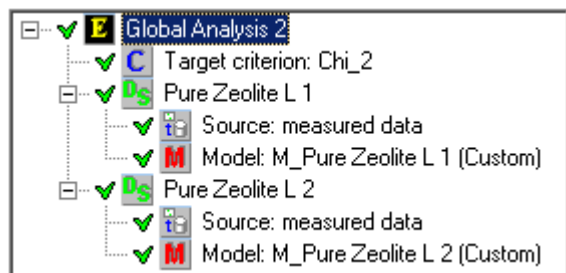
Experiment toolbar provides quick access to frequently used commands that deal with the current Experiment. Some toolbar operations are duplicated in the drop-down menus. Note that some commands are available only on the toolbar.



Use *t-view* button to “View model decay in time domain”

*GFQS* buttons can be used to “View graphical fit quality criteria”

You can see each button function by pointing the mouse over it. In a second Help Hint appears as a pop-up short text.

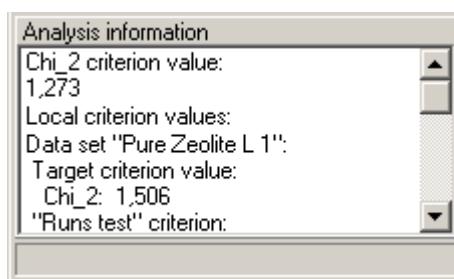


Experiment Structure window may include 5 different types of components:

- ✓ **E** Experiment Name
- ✓ **C** Target Criteria Type
- ✓ **Ds** Data Set Name
- ✓ **t** Source Type
- ✓ **M** Model Name (Type)

You can select any component of the Experiment Structure window and look through its properties and parameters at the Properties and Parameters tabs (if any of them available). It is also possible to change the corresponding values.

Local drop-down tabs menu has only one item “Apply to all similar objects”. This operation can be used to apply the value changes to all other same properties/parameters in the current Experiment.



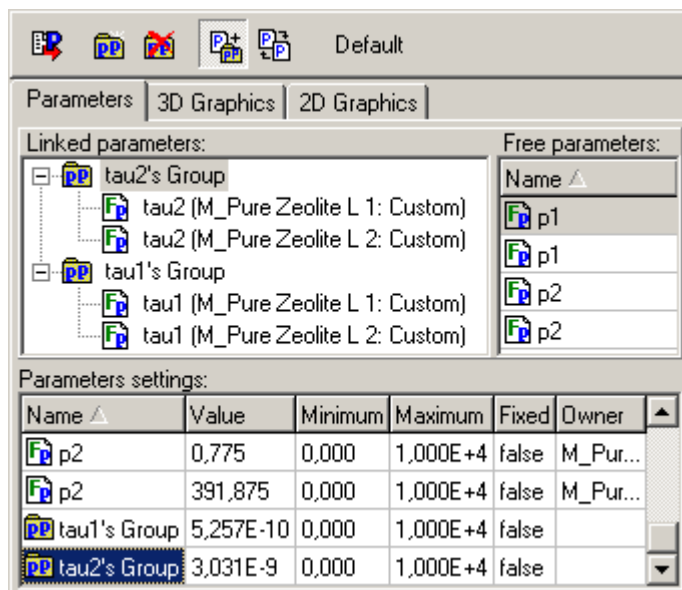
Analysis information window is used to output information for the user. Every time you perform fitting procedure at the end you get evaluated parameters, values of used criteria and etc.

## Main Window Tabs Panel

Tabs panel is used to view parameters groups, its values, and 3d and 2d graphical visualization of the Phase shifts, Residuals and Autocorrelation

### Parameters Tab

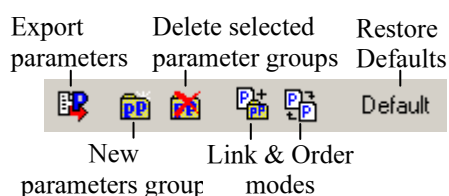
Parameters tab views parameters and its values.



Parameters tab consists of four components:





- Parameters tab toolbar
- Linked parameters window
- Free parameter window
- Parameter settings table



Parameters tab toolbar let you deal with the current Experiment parameters easily. All toolbar operations are duplicated in the drop-down local menus.

You can see each button function by pointing the mouse over it. In a second Help Hint appears as a pop-up short text.

Each record in the Parameters tab has a small icon on the left that shows whether this is some parameter or the name of a certain parameter group:

-  - is the parameters icon;
-  - is the parameters group icon.

Similar parameters in a group have a description in brackets: what Data Set this parameter belongs to and what type the corresponding model is.

Linked parameters window views grouped parameters. Trough the local drop-down menu you can:

- Rename, Delete, Empty selected parameters group.
- Link the parameters of the selected group to another parameters group.
- Change the order of the parameters in the group.
- Create new parameters groups.

You can also use drag and drop operations in the Linked parameters window to move the parameters between groups (select wanted parameter and drag it to the title of the necessary group).

Free parameter window views the list of the free parameters. Trough the local drop-down menu you can:

- Link all similar parameters into new parameter group.
- Link selected parameters to the existing parameter group.
- Find the model to which the selected parameter belongs to.
- View any Fit parameter vs. any external parameter.

Use **Ctrl** and **Shift** keyboard buttons to select few parameters.

Parameter settings table includes all parameters of the current Experiment and corresponding settings. The structure of the Parameter settings table is following:

Field	Explanation
Name	Parameter name
Value	Parameter value
Minimum	Minimum value of the parameter
Maximum	Maximum value of the parameter
Fixed	Let you fix the value of the parameter
CI Left	Left border of the CI (if CI Analysis is turned on)
CI Right	Right border of the CI (if CI Analysis is turned on)
CI Analysis	CI Analysis switch(if CI Analysis is turned on)
Owner	Name of the Data Set to which the parameter belongs to

Trough the local drop-down menu you can:

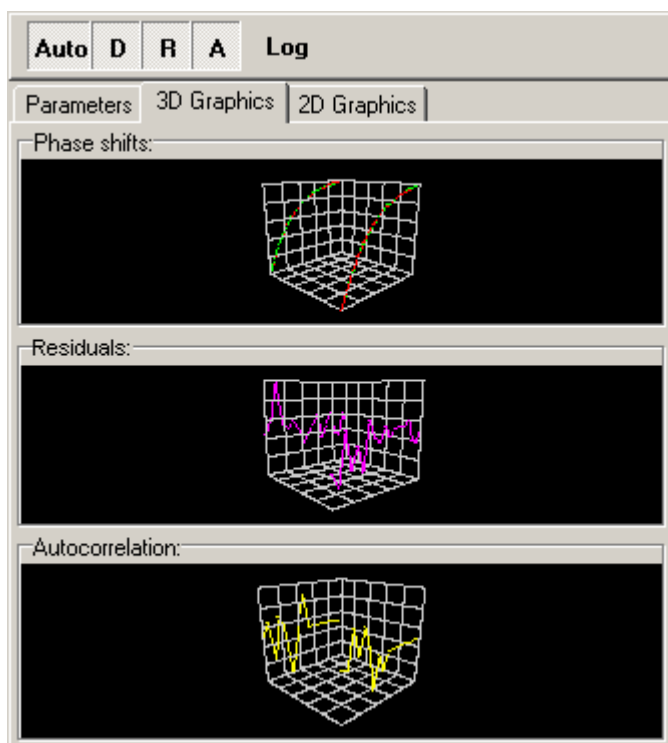
- Rename, Delete or Empty selected parameter.

- Link selected parameters into new parameter group.
- Restore default value for the selected parameter.
- Export current Experiment parameters table into MS Excel file.
- Optimize the view in the parameter table.

Detailed information on how to manage the Experiment parameters is provided down in the “Managing Parameters” section.

### 3d Graphics tab

“3d Graphics” tab is used to display phase shifts, weighted residuals and autocorrelation function in tree-dimensional space.



“3d Graphics” tab includes:

- Tab toolbar
- Up to 3 graphical panels

Use buttons **D**, **R**, **A** on the toolbar to view/hide the corresponding graphs:

- **D** – Phase Shifts
- **R** – Residuals
- **A** – Autocorrelation

**Auto D R A Log**

**Auto** button can be used to share space that graphs take equally.

Press **Log** button to view Phase Shifts in the logarithmic scale.

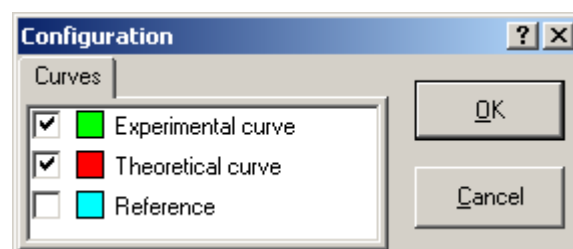
Meanwhile default colors of the Phase Shifts graph are:

- measured curve is green;
- theoretical curve is red.

You can change Phase Shifts curves colors and choose curves you want to display by double-clicking on the graph area to get Configuration dialog.

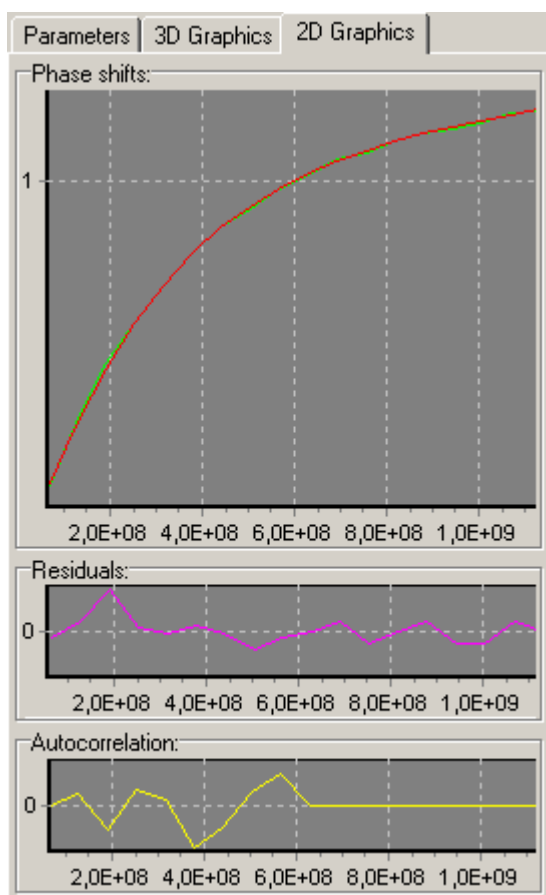
On this dialog you can tick the appropriate curves using corresponding check boxes. Experimental, Theoretical and Reference curves are available.

For each curve you can pick wanted color by pressing on the corresponding colored square.



### 2d Graphics tab

“2d Graphics” tab is used to display phase shifts, weighted residuals and autocorrelation function in two-dimensional space.



“2d Graphics” tab includes:

- Tab toolbar
- Up to 3 graphical panels

Use buttons **D**, **R**, **A** on the toolbar to view/hide the corresponding graphs:

- **D** – Phase Shifts
- **R** – Residuals
- **A** – Autocorrelation

**Auto D R A Log**

**Auto** button can be used to share space that graphs take equally.

Press **Log** button to view Phase Shifts in the logarithmic scale.

Meanwhile default colors of the Phase Shifts graph are:

- measured curve is green;
- theoretical curve is red.

Graph local menu has 3 options:

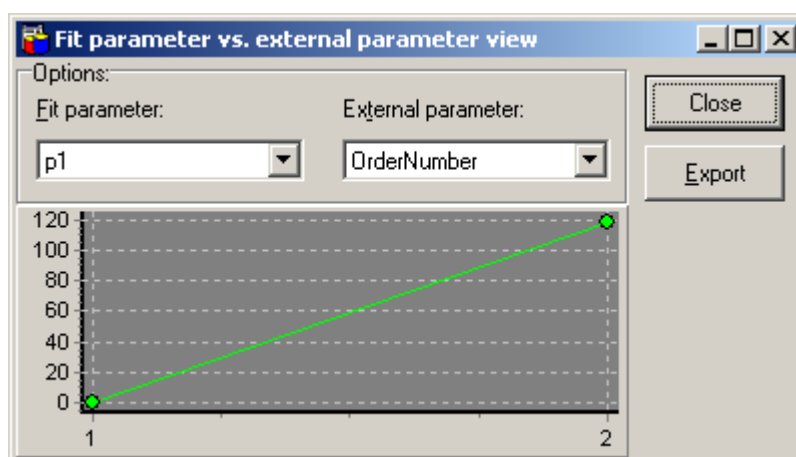
Save graph...  
Copy graph to Clipboard  
Graph configuration...

With the help of the local menu you can Copy the graph to the Clipboard or Save in the BMP file. You can customize the graph components, change colors, set title and axes labels and so on.

## Application Windows

### *Fit parameter vs. external parameter view*

Use “View on graph” option to view Fit parameter vs. External parameter dependence. This option is available in the local menu.



On the graph of this preview window you can see fit parameter dependence vs. any external parameters available from the list. The values of the X axis correspond to the Fit parameter and the values of the Y axis correspond to the External parameter.

You can Fit and External parameters using corresponding combo boxes above the Graph.

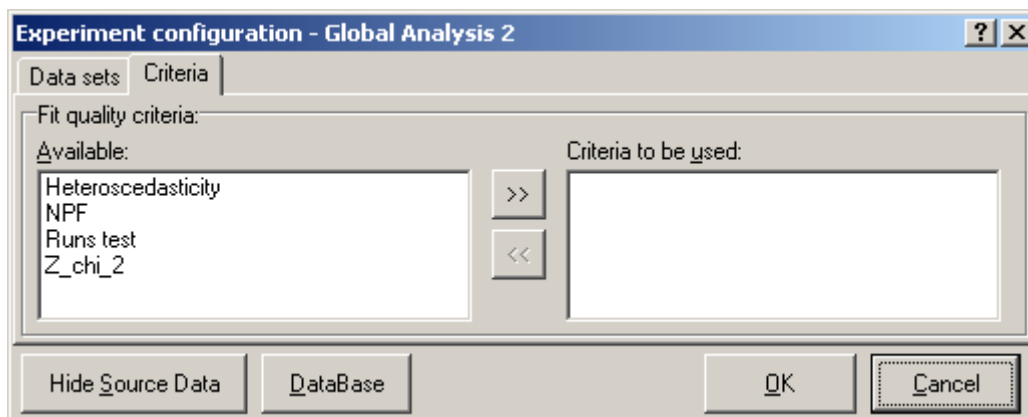
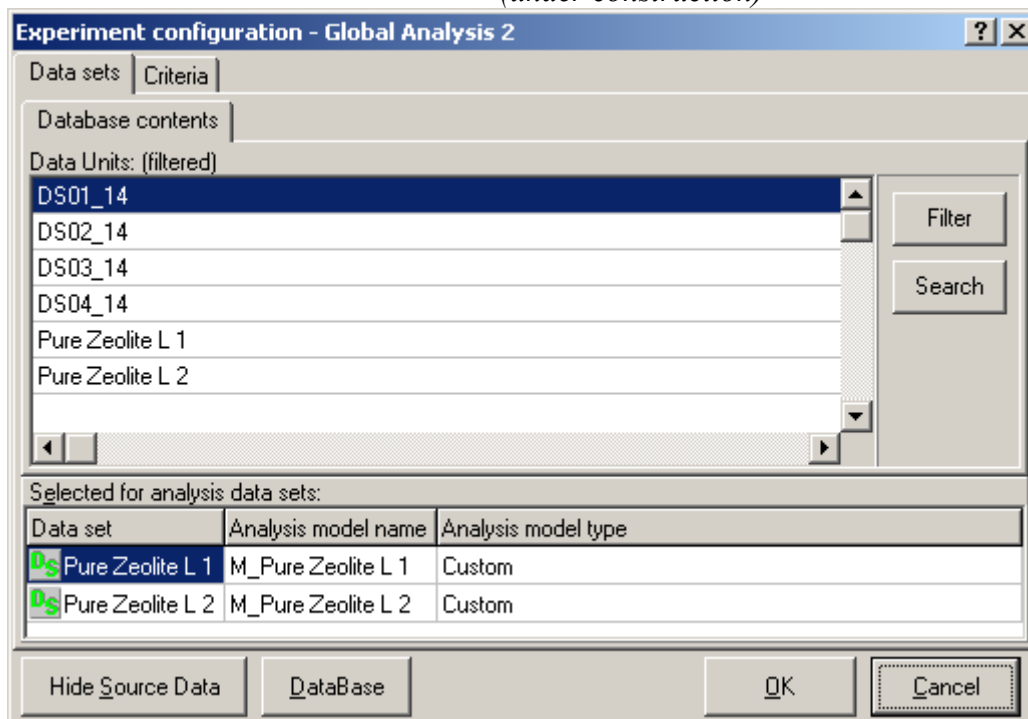
On the Chart using your mouse you can perform any standard action: moving the image, zooming in and out.

Press **Export** button if you want to export visualized Data to the text file.

Pressing **Close** button you close the window.

### **Configuration window**

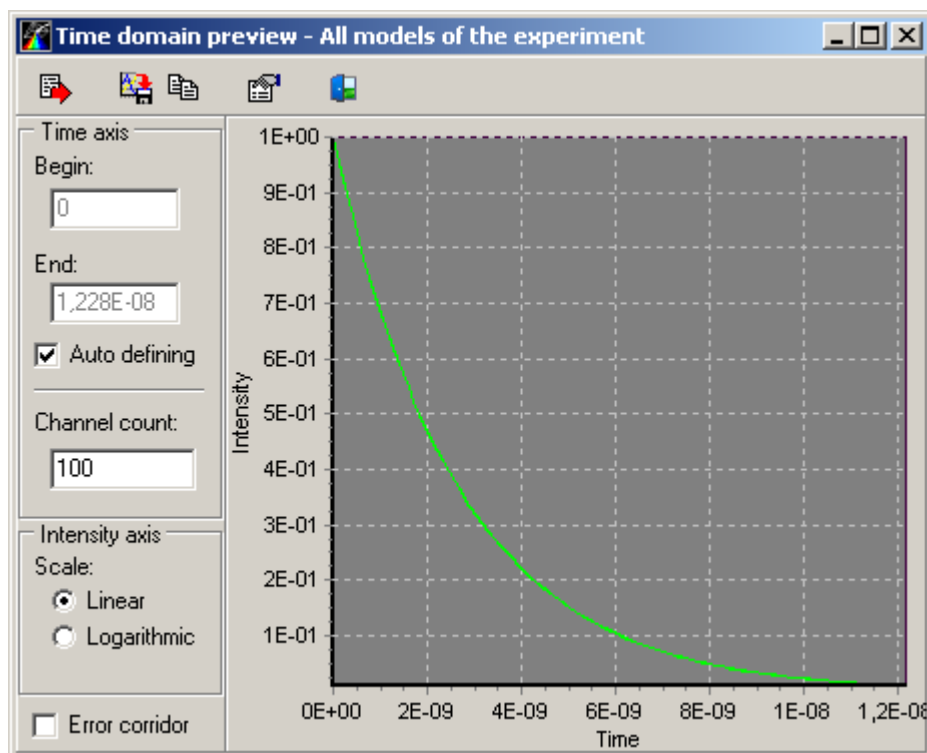
*(under construction)*



### ***i-view window***

*(under construction)*

Once you have performed parameter fitting you can get “Time Domain Preview”. Use ***t-view*** button on the Experiment toolbar.



### Quick Data Analysis Start

Next small example will show how the fitting software works. To perform any analysis first of all you need Data. To create a new Data Set:

1. Start TRFD Measurements Database application (F3 or any other way)
2. Choose File | Import Data Wizard from the main menu to import TRFD data and to create a new Data Set. In the appeared window click *Next* to continue.
3. In the next window fill up all appropriate fields: Data Set name, Operator name, Sample information and the Date.
4. Then in File Dialog drag corresponding files for Reference, Sample and Setup tabs and click *Next*.
5. Finally before you click *Finish* you can add experimental parameters and write additional description.

To get better explanations how to create a new Data Set see “Data Import” chapter at TRFD MD manual part.

Afterwards close TRFD MD application and return to the main application.

6. On the right menu bar press the **Configuration** button to configure the numerical experiment (for the reference see “Configuration window”).
7. Double-click on the name of the newly-created Data Unit, enter Analysis model name, select Analysis model type and press **OK**.

Now everything is ready to press the **Execute** button and when the fitting is completed you can see the result: values of fitted parameters of the model on the Analysis information panel.

To perform detailed analysis start TRFD Analysis Database application (F4 or any other way). Select needed Experiment and conduct further data and results examination.

### Single Curve Analysis

To perform Single Curve Analysis open an appropriate Experiment (using **Open** toolbar button or the main menu *File | Open Ctrl+O*) if the experiment has been saved previously otherwise create a new one (using **New** toolbar or the main menu *File | New Ctrl+N*).

1. On the experiment toolbar press the **Configuration** button to configure the numerical experiment.
2. In the Experiment configuration window double-click on the name of the Data Unit you want to analyze, enter Analysis model name, select Analysis model type and press **OK**.
3. Click on the name of the model in the Experiment tree and change, if necessary, the properties of the objects related to the current numerical experiment.
4. To generate initial guesses for the current parameters of the model press the **Default** button on the parameter tab toolbar menu.
5. When all preparations are performed you can start iterative fit by pressing the **Execute** button.

When execution is finished you can view the results of the fitting procedure:

- final value of  $\chi^2$  criterion in the Analysis information window;
- estimated values of the parameters in the Parameter setting table on the Parameters tab.

You can also see the graphs of the measured and estimated (correspondingly green and red by default) phase shifts, weighted residuals (purple) and autocorrelation function of residuals (yellow) by clicking the “2D Graphics” tab.

To see the graphs of the estimated fluorescence decays in time domain press the “t-view” button on the right menu bar. By using configuration fields you can change the fluorescence decays view.

## Global Analysis

To perform Global Analysis first of all you need to configure the numerical experiment.

1. Open an appropriate Experiment (using **Open** toolbar button or the main menu *File | Open Ctrl+O*) if the experiment has been saved previously otherwise create a new one (using **New** toolbar or the main menu *File | New Ctrl+N*).
2. On the experiment toolbar press the **Configuration** button.
3. In the appeared Experiment configuration window double-click on the name of the Data Unit you want to analyze.
4. In the Data Set window open local menu, select all Data sets (choosing “Select All”) and type of the model that will be used for approximation if it differs from default model.
5. Press the **OK** button to load the configuration.
6. To change the properties of the objects related to the current numerical experiment click Experiment Properties tab, select the component (Model, Data Set or Experiment) and perform changes. Use the “Apply to all similar objects” item from the local menu to apply the value of the current property to all similar objects.
7. To link all parameters with the names identical to the name of the selected one use the “Link all ...” item from the local menu.
8. To generate initial guesses to all parameters press the **Default** button on the parameter tab toolbar menu.
9. When necessary preparations are accomplished and default values of the parameters are generated you can start iterative fit by pressing the **Execute** button.

When execution is finished you can view the results of the fitting procedure:

- final value of  $\chi^2$  criterion in the Analysis information window;
- estimated values of the parameters in the Parameter setting table on the Parameters tab.

Use “View on graph” local menu item to view graphical dependence of the fitted parameters on external parameters. To get required dependence on the graph use fit parameter and external parameter combo boxes.

Click the “3D Graphics” tab to see three dimensional rotational view of the measured and estimated (correspondingly green and red by default) phase shifts, weighted residuals (purple) and autocorrelation function of residuals (yellow).

Click the “2D Graphics” to see phase shifts, weighted residuals and autocorrelation function of residuals on 2D graphs. If you select the Experiment in the Experiment Structure window you will see 2D graphs for all current Experiment Data sets on the same 2D graph. If you select the name of certain Data Set you will see 2D graphs for this particular Data set.

To see the graphs of the estimated fluorescence decays in time domain press the “*t-view*” button on the right menu bar. By using configuration fields you can change the fluorescence decays view.

## **Managing Parameters**

On the Parameters tab in the Parameter setting window:

- To set the initial values of parameters manually use the “Value” fields.
- To set the constraints of parameters use the fields “Minimum” and “Maximum”.
- To fix the value of the given parameter into the predefined value (in the field “Value”) set the “Fixed” field to “true”.
- To switch on the “Confidential interval” analysis press the **CI** button on the right menu bar.
- To enable “Confidential interval” calculation for the certain parameter choose “true” in the “CI Analysis” field.

## **Building User-Defined models**

Instead of using predefined models you can create your own models with the help of built-in script programming language. To use user-defined models press the **Configuration** button on the left menu bar to configure the numerical experiment. Then click on the model type that corresponds to appropriate Data Set and select Custom and press **OK**.

To select user-defined model from the attached database click on the name of the model in the *Experiment tree* and using *Subtype* property apply appropriate custom model type.

All settings are being loaded from database and mapped into the proper panels: the parameters appear in the *Parameter setting* window, the name of the model changes to “Custom”.

If you want to create your own model click on the name of the model in the *Experiment tree* and using Configuration property in the *Experiment tree* enter the *custom model configuration* dialog where you can manage parameters and write your own model using built-in script programming language.

## **Confidence Intervals**

To enable calculation of the Confidence intervals press the **CI** button on the right menu bar. At the same time the fields “CI left”, “CI right” and “CI Analysis” becomes visible in the Parameters settings table.

- To enable confidential interval calculation for the certain parameter choose “true” in the “CI Analysis” field.
- If you want to change the confidence probability select the Experiment title and varying the “CI Probability” property set the necessary value.

Determination of confidence intervals by exhaustive search starts immediately after the fit. The progress is displayed in the “Analysis information” window. Once the fitting procedure is finished the values of the Left and Right bounds of the confidence intervals appears in the “Parameters settings” table.

### **Fit Quality Criteria**

To add additional fit quality criterion to the fitting procedure

- On the left menu bar press the **Configuration** button.
- In the appeared Experiment configuration dialog go to Criteria page and select required criterion name in “Available” list.
- Press “>>” button to add selected criterion to the list of criteria that will be used in the fitting procedure and “<<” button to remove selected criterion from the list

When the fitting procedure is completed the values of additional fit quality criteria for each Data Set are displayed in “Analysis information” window. By pressing the **GFQC** button on the right menu bar you can view the graph of the fit quality criteria.

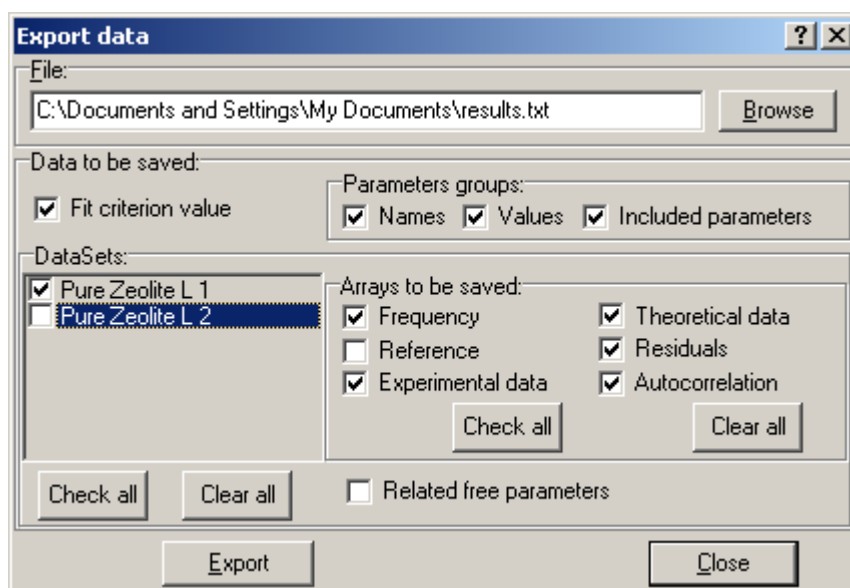
### **Data Export**

Use Export Data option to export current Experiment Data into text file. Use **Export Data** button on the Experiment toolbar to get Data Export dialog box. You can save such information as:

- fit criterion value;
- parameters groups, contained parameters and its values;
- free parameters;
- frequencies;
- reference data;
- experimental and theoretical data;
- arrays of correlation functions and residuals.

To export the Data into the file follow next steps:

1. Choose “Export Data” item from the Experimental local menu.



2. In the appeared Export Data window first of all type the name of the file that will be used to store the Data. Use Browse button to find appropriate folder.



- On the “Data to be saved” panel choose the Data you want to export. You can save fit criterion value, parameters values, frequencies, reference data, experimental and theoretical data, residuals and autocorrelation function.

Use **Check All** and **Clear all** buttons when you work with check boxes.

- Press **Export** button to finish Export operation and then **Close** to close Export Data dialog.

## Managing Experiments

### Saving and Restoring Experiments

“File” application menu contains the commands to manage Experiments. These commands are described in the table bellow.

File	Tools	Window
New		Ctrl+N
Open		Ctrl+O
Save		Ctrl+S
Save As...		
Close		
Exit		Ctrl+X

Field	Explanation
New	To creates a new Experiment
Open	To open an existing Experiment
Save	To save current Experiment for the first time
Save as	To save current Experiment with a specified name
Close	To close current Experiment
Exit	To exit the application

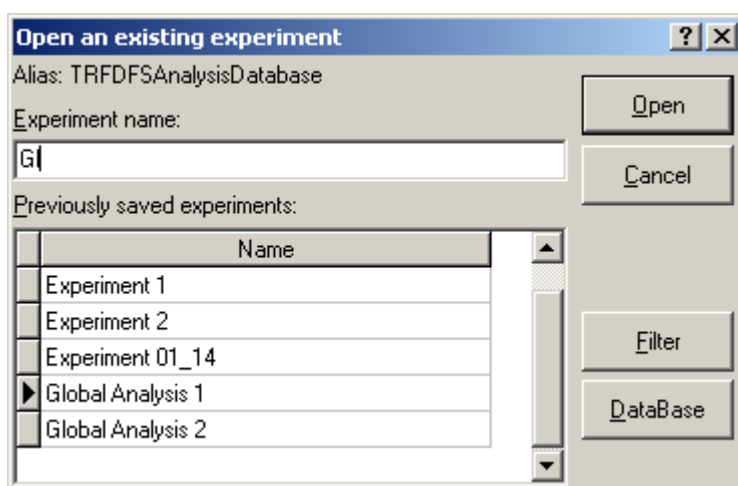
“New”, “Open” and “Save” commands are available on the application toolbar.

Be aware, that if you exit the program without saving open Experiments, you loose all the changes you have made with it. Same happen when you close current Experiment. You will not get any notifying message either. That is why it is suggested to remember to save the current Experiment before closing it and to save all opened Experiments before you exit the application.

You can open few Experiments in one application. To get information about customizing your Experiments refer to the corresponding chapter “Customizing Experiment windows”.

#### Open an existing experiment dialog box

“Open an existing experiment” dialog box is used to load previously saved experiments.



Use “Experiment Name” field to enter the name of the experiment you want to load from the Analysis Database.

You can quickly find the experiment you need by typing the first few characters of its name. In this case the application will automatically select the first experiment which name starts with typed characters.

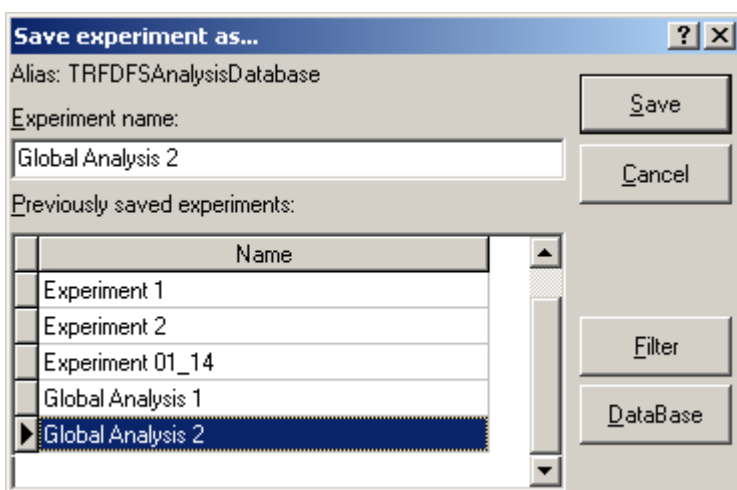
Press **Open** button to open selected experiment. Use **Cancel** button to close this dialog box.

Press **Filter** button to create a filter for “Previously saved experiments” list. If this filter is applied, only those experiment names that correspond to the filter criteria are displayed.

Press **DataBase** button to open selected experiment in the TRFD Analysis Database application.

### Save experiment as... dialog box

“Save experiment as” dialog box is used to save the active experiment.




Use “Experiment Name” field to enter the name of the experiment you want to load from the Analysis Database.


Press **Save** button to save active experiment with the entered name. Use **Cancel** button to close this dialog box.

Press **Filter** button to create a filter for “Previously saved experiments” list. If this filter is applied, only those experiment names that correspond to the filter criteria are displayed.

Press **DataBase** button to open selected experiment in the TRFD Analysis Database application.

### Current Experiment

Once you have opened an Experiment ready for calculations or you have performed all preliminary preparations with the newly-created Experiment it is time to perform fitting procedure. Press **Execute** button  on the Experiment toolbar to fit model parameters.


If you want to stop fitting procedure press **Stop** button .

To export current Experiment data press **Export Data** button .


### Working with Templates

#### Working with Interface Templates

To save current interface settings: the size and position of the windows; colors, lines settings of the graphics and etc. you can use interface templates.


- Press the **Save interface template** button  on the main toolbar to save current interface settings.
- In the appeared “Create and save new interface template” dialog box type the name of the interface template and press **Save**.

Once you have your interface templates stored you can always use them.


- To apply interface template to the application press the **Apply interface template** button  on the main toolbar.
- In the appeared “Load and apply an existing template” dialog box choose the name of the template you want to apply and press **Apply**.

#### Working with Analysis Templates

To save settings in the Experiment Structure window, Linked Parameter window and Parameters settings window you can use templates.

- Press the **Save Template** button  on the Experiment toolbar to save all settings that correspond to the current numerical experiment as template.
- In the appeared “Create and save new template” dialog box type the name of the template and press **Save**.

Once you have your templates stored you can always use them.

- To apply template to the current numerical experiment press the *Apply Template* button  on the Experiment toolbar.
- In the appeared “Load and apply an existing template” dialog box choose the name of the template you want to apply and press *Apply*.

Don't mix up Interface templates with Analysis templates.

Note, that Analysis templates buttons are situated on the Experiment toolbar, and Interface templates are situated on the application toolbar.

## TRFD Analysis Database

Analysis Database program is used for economical storage and convenient control of the analysis results, that were obtained by TRFD Fitting Software. The program provides convenient and fast way of searching and retrieving information and let you get rid of a great amount of paper needed to keep information about the measurements, performed analysis as well as avoid routine manipulation with computer files, folders, etc.

The Database consists of several tables with the automatically supported relationships.

The main features of the database are:

- fast storing the results of analysis often-used model and parameter linkage configurations (Templates) in the Database;
- convenient representation the results of analysis;
- representation the templates configuration;
- extensive possibilities for searching and filtering information;
- build-in two-dimensional graphical pre-viewer of experimental and recovered correlation functions and residuals;
- two-dimensional graphical pre-viewer of estimated parameters dependence
- export data to the ASCII files;
- quick deleting all records from the tables;
- packing tables after deleting in order to reduce the size of the tables;
- checking and repairing the tables;
- generating and printing the user-defined reports on the base of the selected records.

The Database supports data integrity and validity. All information concerning the defined object is stored in one record in table. The mechanism of data integrity forbids deleting a record from one table which is linked to the records in the other tables. Data validity guarantees that values stored in the tables are always valid by the checking of the range and type of the entered data. Database is protected from the accidental changing or deleting of information by the default forbidding of editing.

Database avoids data redundancy: each record has only one instance. It means that it is not required to enter information into the tables, if the same information is already stored in the database. User can just establish the relation between the entered and stored information. This feature is especially useful when one needs to update records in the database. The correction should be done only once at one point (where the changed information is stored) and then this update will take effect in all records which are related to the selected one.

Database provides extensive possibilities for searching information. The fastest way how to find a record by a specific field is by typing first symbols of this field in a special window. Cursor moves to the record with the field, which contains symbols matching the typed ones. The possibility to sort any table by any field is also supported.

User may also interactively create filter with complex conditions in order to decrease the selected number of records.

Such operations as looking through the records, deleting records, editing information are provided by Database Navigator.

In addition to this manual to find out about TRFD AD application you can use Help file that comes separately. The name of the file is **AnalysisDB.hlp**.

### ***A tour of the environment***

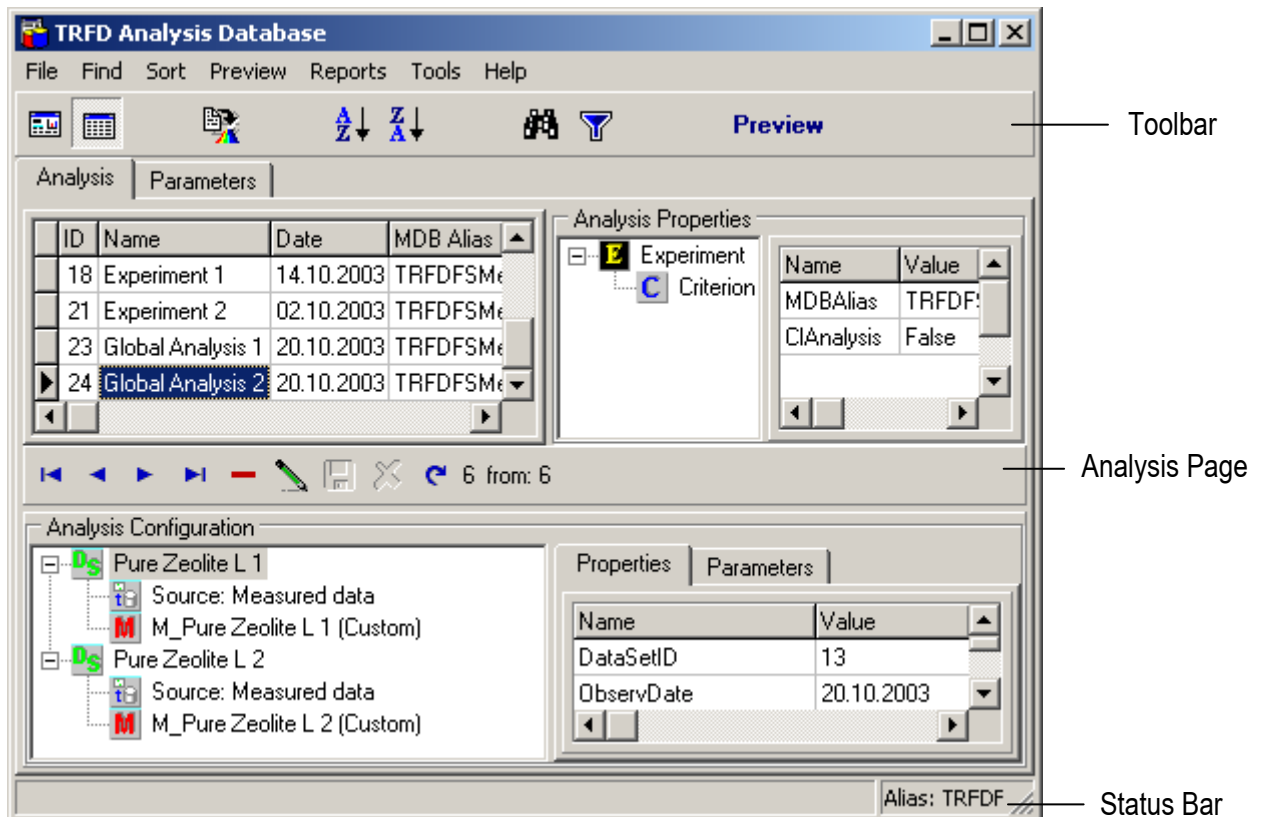
#### **Starting Analysis Database**

You can start TRFD ADB in several ways:

- From the main TRFD Fitting Software program (F4 or clicking the button)

- Choose Programs | TRFD Fitting Software | Analysis Database 2.0 from the Windows Start menu.
- Choose Run from the Windows Start menu, and then enter TRFDADB.exe.
- Double-click \Program Files\SSTC\Fitting Software\Bin\TRFDADB.exe.

Once you are in TRFD ADB, you see the major tools of the program environment.



Main Window consists of the following components:

- Menu
- Toolbar
- Analysis page
- Parameters page
- Status Bar

Menu and Toolbar provide quick way to invoke the commands of the application.

Analysis and Parameters pages display all information about one particular analysis.

Status bar provides information about the current state of the application.

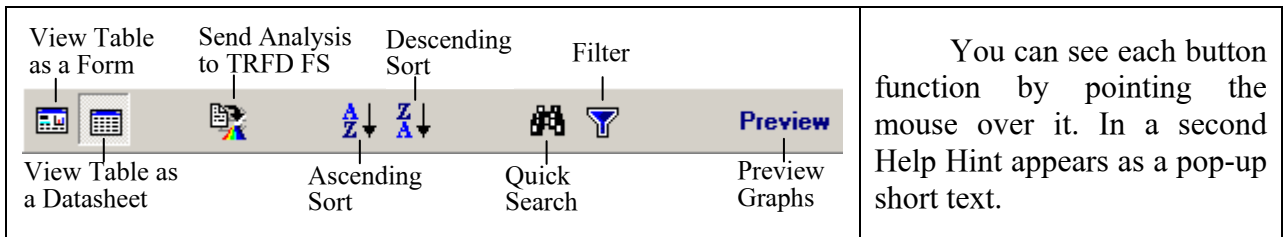
## Menu

All features of the program are available from the main menu. Through the menu you get Database tables control. You can export Data, sort and filter records in the Database, search through the Database, create Analysis reports and get Data preview.

## Using toolbars, menus, and keyboard shortcuts

Many operations have keyboard shortcuts as well as toolbar buttons. When a keyboard shortcut is available, it is always shown next to the command on the drop-down menu.

TRFD MDB toolbar, located in the main window, provides quick access to frequently used operations and commands. All toolbar operations are duplicated in the drop-down menus.



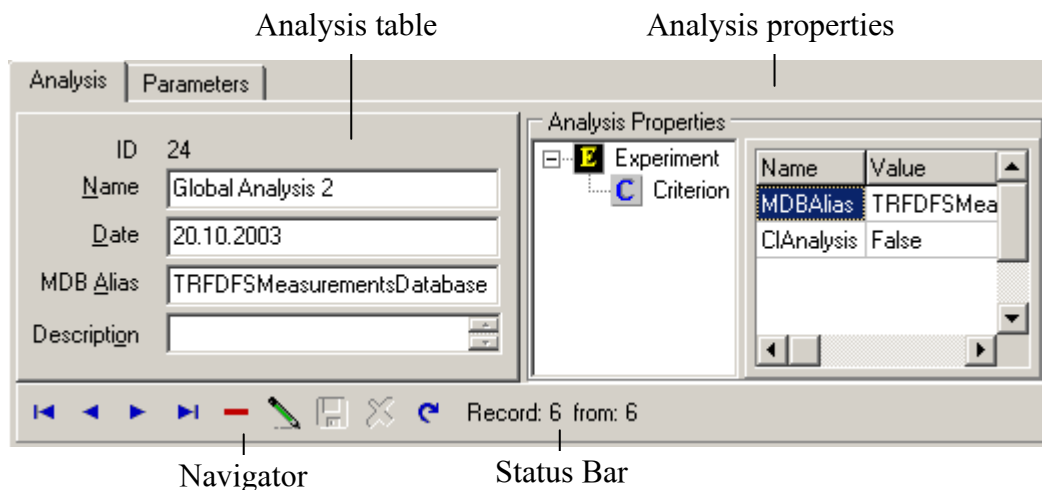
It should be noted that not only main window but all other application windows have similar Toolbars as well as Navigator and Status Bar to work with Database tables.

## Analysis page

Analysis page is used to view the configuration and the properties of the current experiment in the analysis tables. It includes following components:

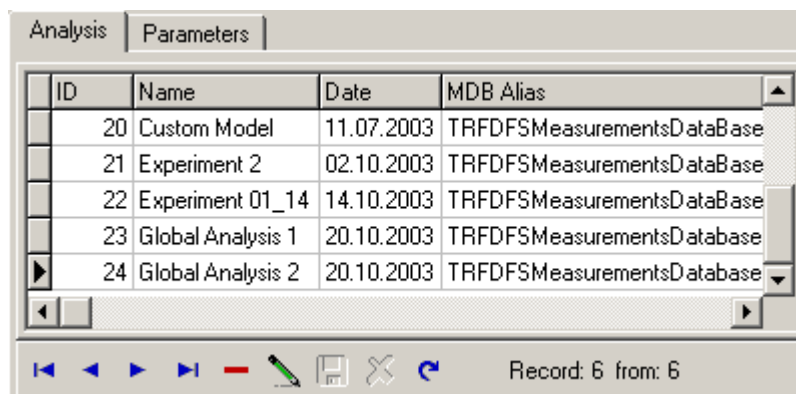
- Analysis table, Navigator and Status Bar
- Analysis properties panel
- Analysis configuration panel

### Analysis table



Analysis table is the central table in the Analysis Database. If you select the record in this table you get all information about the analysis of corresponding experiment. Use Navigator to manage the records of the Analysis table. The tables, which are depended on the Analysis table, contain properties and parameters of the analysis and configuration of the analysis. If you delete the record in the Analysis table, all records that are related to the analysis will be deleted.

Analysis table can be viewed as a form view or datasheet view. To change the view mode use Toolbar buttons or proper items in the menu.

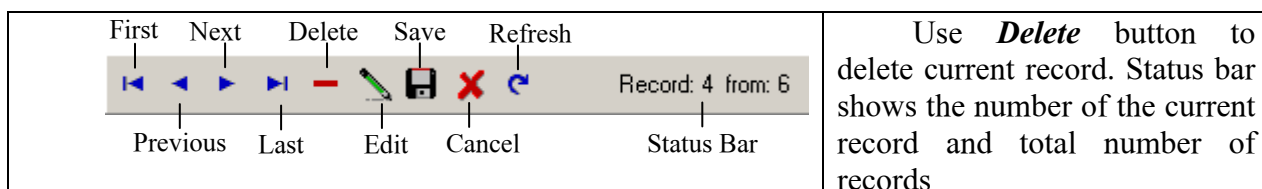


Briefly about the fields of the Analysis table:

Field	Explanation
Name	Analysis name
Date	Date of Analysis
MDA Alias	Alias of the analyzed Measurements Database
Description	Short description of the Analysis

### Navigator and Status Bar

Convenient Navigator which is situated on the bottom of the page will help you to navigate through the Analysis table. Use buttons **First**, **Previous**, **Next**, **Last** to find appropriate Analysis record.



Once you press **Edit** button you can edit Analysis table fields. Press **Post** button to save Analysis table changes or **Cancel** to return previous information back. Press **Refresh** button to refresh data in the table fields.

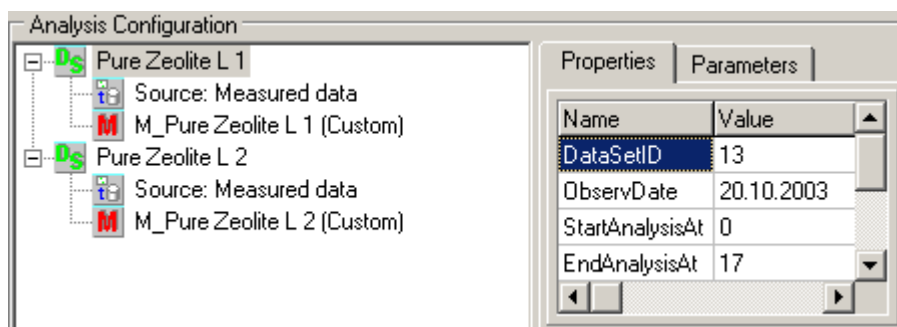
All actions that you can perform with the Analysis table and contained information are available in the local and main menu. To open the local menu, right-click on the Analysis table.

### Analysis properties panel

Analysis properties panel shows current Experiment structure and the properties of the selected element of the Experiment.

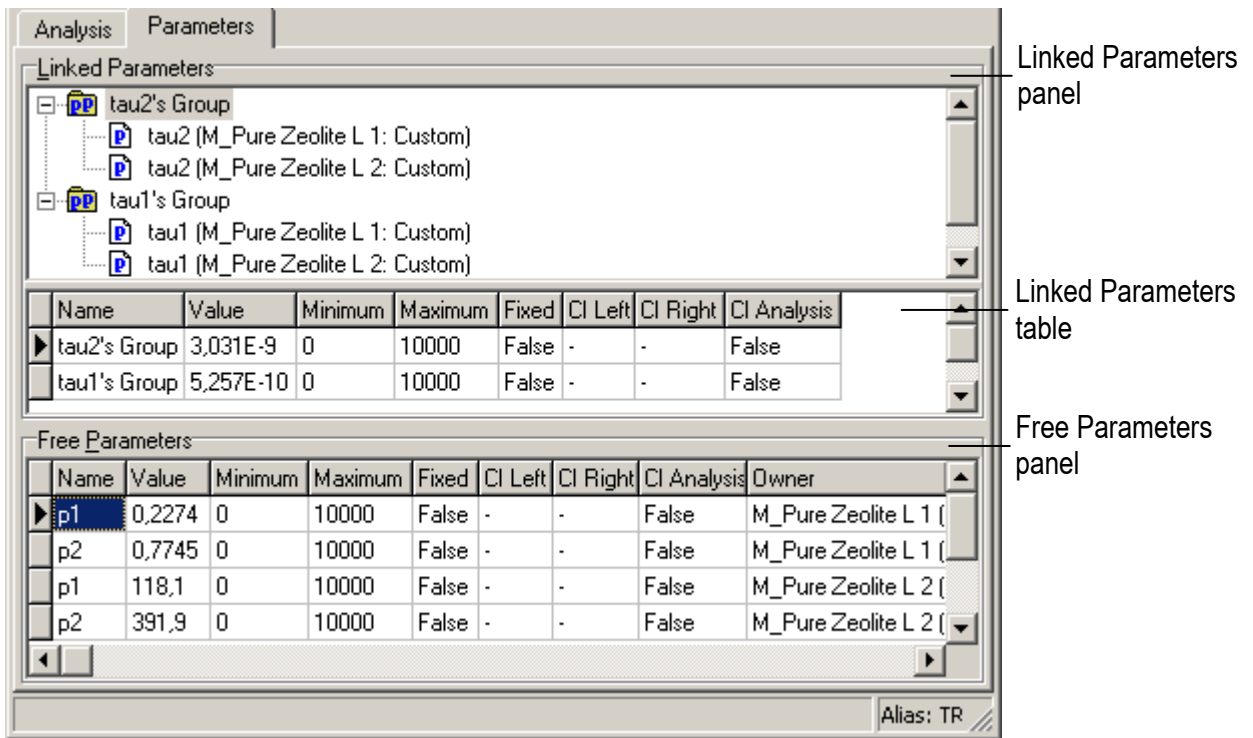
### Analysis configuration panel

On this panel you can see the structure of the Data Sets that are related to the current Experiment. It might contain the source of Data and the model type. Using Properties and Parameters tabs you can view corresponding information about selected Data Set and its components.



### Parameters page

Parameters page displays the settings of the estimated parameters, parameters groups and parameters linkage of the current Analysis. Current Analysis, its properties and configuration are displayed on the Analysis page.



Parameters page includes following components:

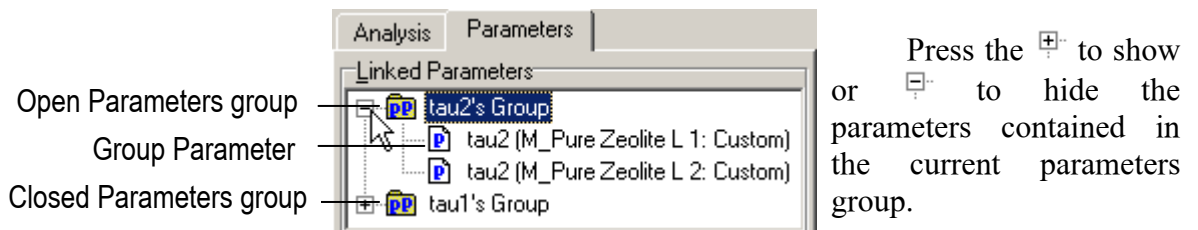
- Linked Parameters panel
- Free Parameters panel

### ***Linked Parameters panel***

Linked Parameters panel contains:

- Linked Parameters tree
- Linked Parameters table

In the Linked Parameters tree the names of the parameters groups and parameters are displayed on the right of the corresponding icons.



Linked Parameters table consists of Linked parameters related to the current Analysis and their characteristics.

### ***Free Parameters panel***

Free Parameters panel contains Free Parameters table that consists of free parameters related to the current Analysis and their characteristics.

Note, if the current Experiment does not have linked parameters than the Parameters page will take a simple form with just general Parameters table.



Analysis		Parameters							
Parameters									
Name	Value	Minimum	Maximum	Fixed	CI Left	CI Right	CI Analysis	Owner	
p1	1	0	10000	False	-	-	False	M_Real3 (Exponential)	
tau1	1,913E-9	0	10000	False	-	-	False	M_Real3 (Exponential)	
p2	1	0	10000	False	-	-	False	M_Real3 (Exponential)	
tau2	3,659E-9	0	10000	False	-	-	False	M_Real3 (Exponential)	

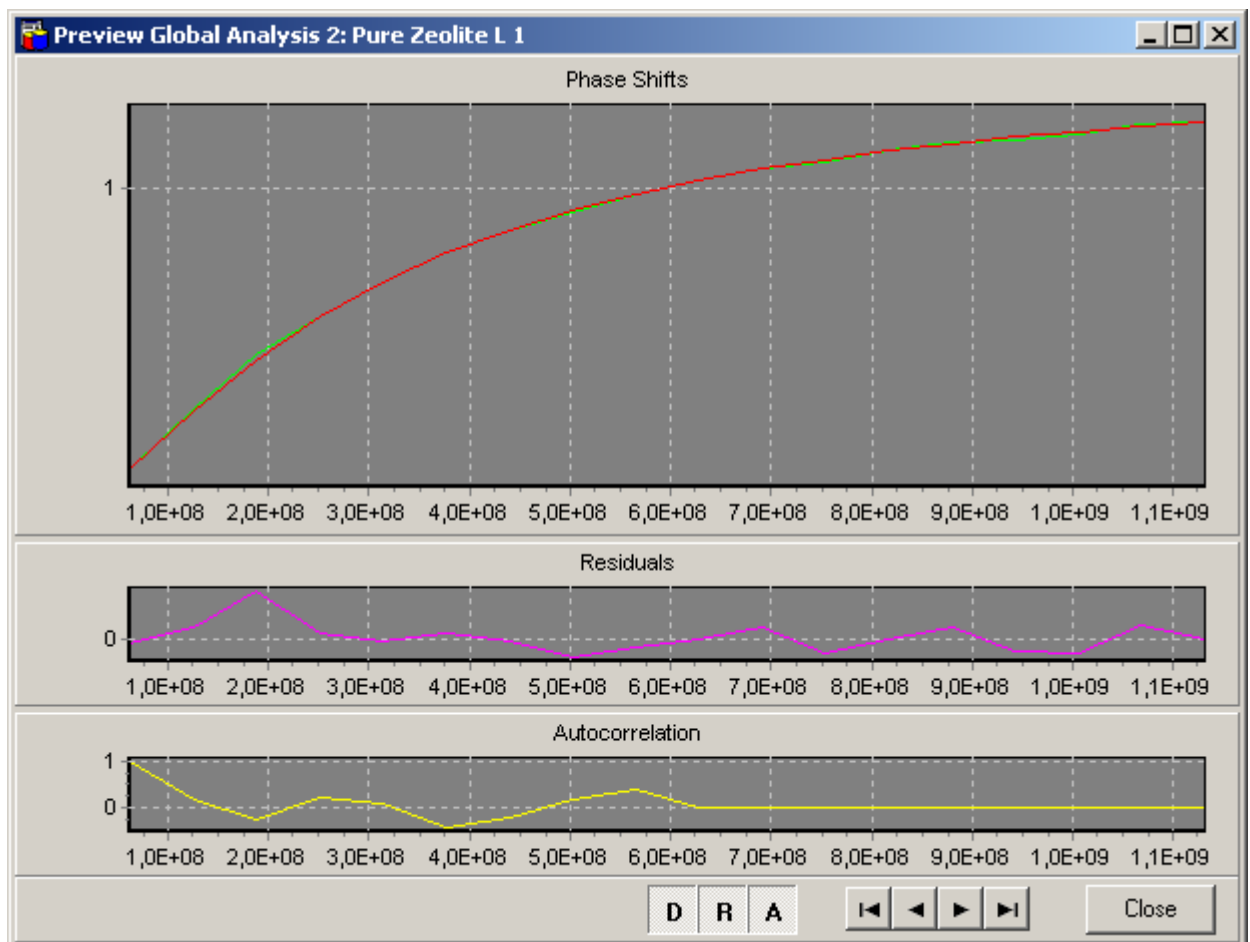
## Data Preview

Use Parameters page to view the values and linkages of the current Experiment parameters.

Use Analysis page to view the configuration and properties of the current Analysis. On this page on the Analysis configuration panel select the model to view its properties and parameters.

## Experiment Preview

You can view experimental and recovered Phase Shift Dependence, weighted residuals and autocorrelation function of residuals all together in one window or separately. Use application menu “Preview | Preview Graphs Ctrl+P” or **Preview** button on the Toolbar.

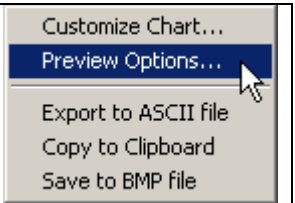



On the Chart you can:

- move the curves by keeping the right mouse button down and moving the mouse pointer;
- zoom in/out the image by keeping the left mouse button down and moving the mouse pointer diagonally across the necessary area from the left top corner to the right bottom corner;
- restore the whole view of the image by keeping the left mouse button down and moving the mouse pointer diagonally up and on the left;

- change the scale of the Y axis (linear or logarithmic) by double-clicking on the chart area and choosing appropriate box in the Options dialog.

You can right-click on the chart to open the local menu, where besides changing the scale you can customize the chart (colors, axis, titles, labels), export the data to ASCII file, copy image to the clipboard or save it to the BMP file.

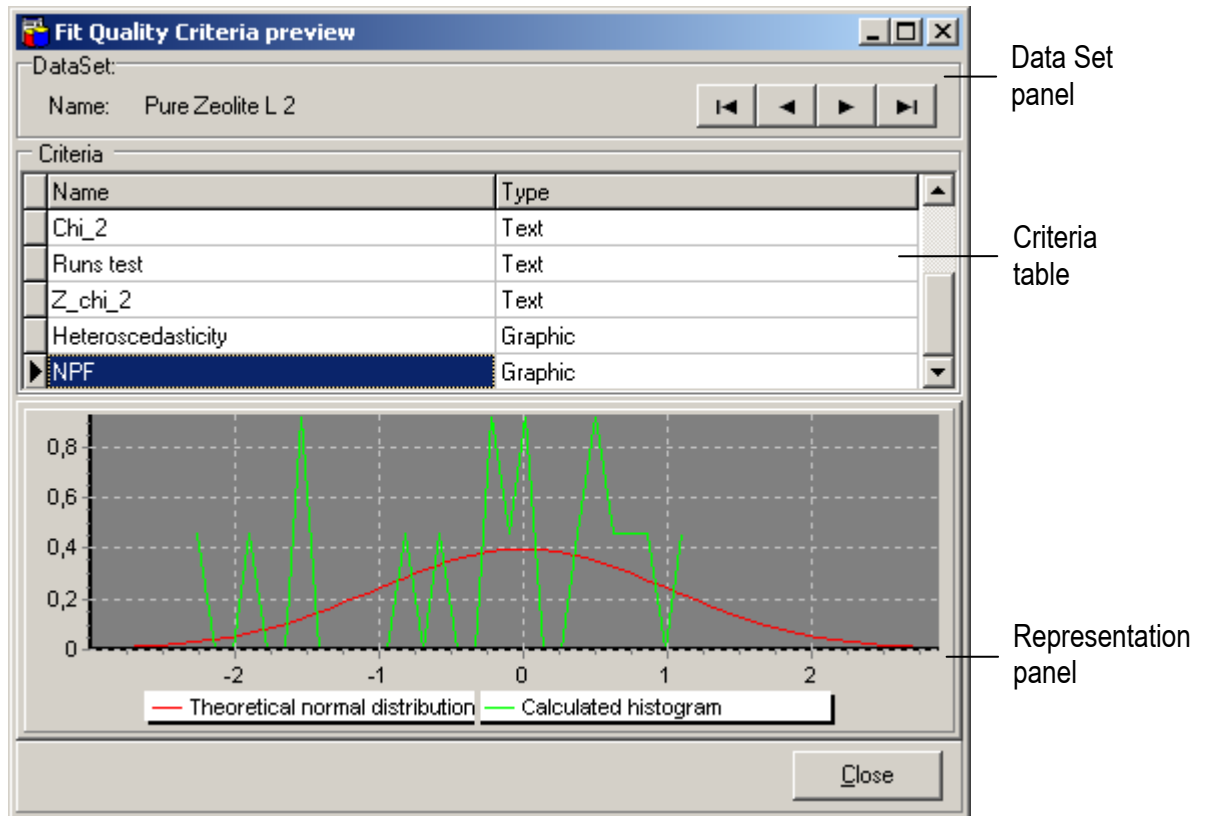




Use Navigator on the bottom of the Preview Window to move through the Data Sets of the current Analysis. Use buttons **D**, **R**, **A**, to view/hide the graphs of Phase Shift Dependence, weighted residuals and autocorrelation function correspondently. Pressing **Close** button you close this window.

## FQ Criterion Preview

Use the “*Preview | Preview FQ Criterion*” from the application menu to view the values and graphical representations of the used fit quality criteria.



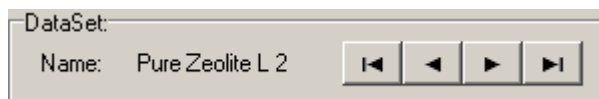
The screenshot shows the 'Fit Quality Criteria preview' window. The 'DataSet' panel displays 'Name: Pure Zeolite L 2' and navigation buttons. The 'Criteria' table lists the following criteria:

Name	Type
Chi_2	Text
Runs test	Text
Z_chi_2	Text
Heteroscedasticity	Graphic
NPF	Graphic

The 'Representation panel' shows a plot with a red curve for 'Theoretical normal distribution' and green bars for 'Calculated histogram'. The x-axis ranges from -2 to 2, and the y-axis ranges from 0 to 0.8.

FQ Criterion Preview window consists of the following panels:

- Data Set panel
- Criteria table
- Representation panel



Data Set panel displays the current Data Set. Using the Navigator you can change the current Data Set.

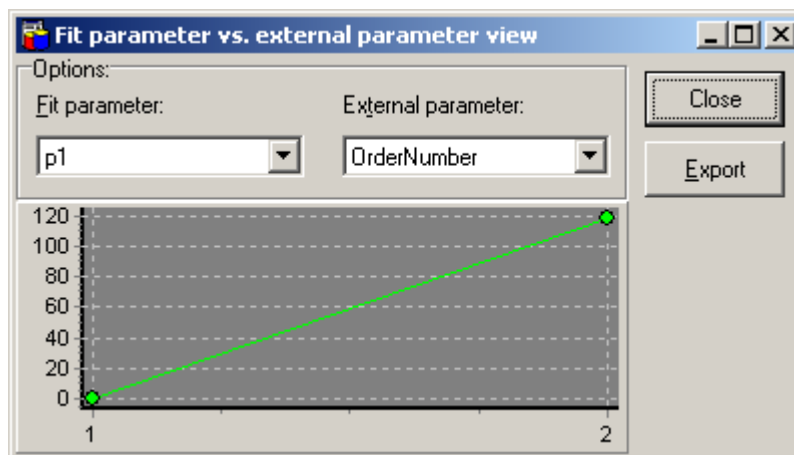
Name	Type
Runs test	Text
Z_chi_2	Text
Heteroscedasticity	Graphic
<b>NPF</b>	Graphic

Criteria table contains a list of available criteria. The table has two fields: the name of the criteria and the type of its representation.

Representation panel displays text information about selected criteria in case the criterion does not have graphical representation or the corresponding Graph otherwise. Usually curve names are on the bottom of the Graph. You can perform any standard action on the Chart: moving the image, zooming it in and out, changing the scale of the Y axis (linear or logarithmic).

## Parameters Dependence Preview

You can get “Fit parameter vs. external parameter view” window from the application menu “*Preview | Preview FQ Criterion*”.



On the graph of this preview window you can see fit parameter dependence vs. any external parameters available from the list. The values of the X axis correspond to the Fit parameter and the values of the Y axis correspond to the External parameter.

You can Fit and External parameters using corresponding combo boxes above the Graph.

On the Chart using your mouse you can perform any standard action: moving the image, zooming in and out.

Press **Export** button if you want to export visualized Data to the text file.

Pressing **Close** button you close the window.

## Analysis Report

You can create a current Analysis report that can be printed later on. The Analysis report may include different information about Experiments Analysis:

- analysis properties;
- analysis configuration;
- model configuration;
- model properties;
- analysis graphs (Phase shifts, Residuals, Autocorrelation, Fit quality criterion);
- parameters and it's linkage.

To create an Analysis report:

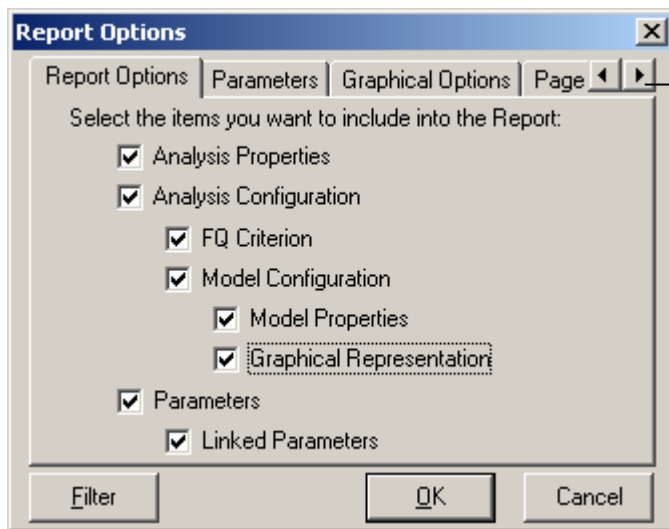
1. Choose “*Reports | Analysis Report...*” item from the application menu.
2. In the appeared Report Options dialog on the first tab using the Filter pick out wanted for report Experiments. Choose the items, information that you want to include into your Analysis report.

3. If you include graphical representations into your report “Graphical Option” tab appear on which you can choose the scale of the graphs.
4. If you choose Parameters to be represented in the report another tab with the corresponding name appears on which you can choose particular parameters to be added. To add linked parameters use the same named check box.
5. Click Page Setup tab and change Page parameters if it’s necessary.
6. Press **OK** and see the Print Preview window of the newly-created report.

You can create your report for the particular Experiment Analysis by selecting it the Analysis table and choosing “Generate report...” from the local menu.

### Report Options dialog

There could be five tabs in Report Options dialog. In that case you can move through the tabs using navigation arrows at the top right corner of the Report Options window.



Tab Navigator

This is the first tab of the Report Options dialog. Here you can choose what Analysis information you want to have in your report.

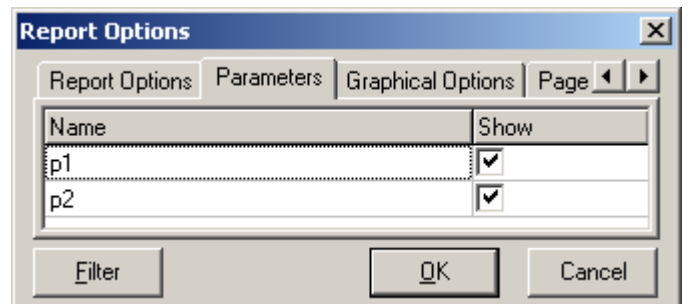
If you want the graphs and the parameters to be represented in the report corresponding tabs appear.

Use Filter to leave particular Experiments Analysis to in your report.

If you choose Parameters to be represented in the report this tab appears.

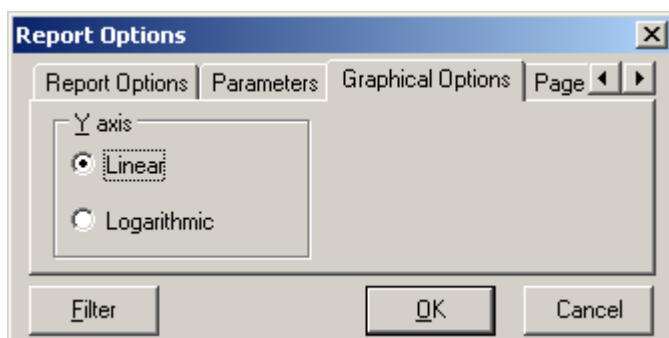
Use check boxes to add particular free parameters.

To add linked parameters use the same named check box on the Report Options tab.



If you choose Graphical Representations to be included into your report this tab appears

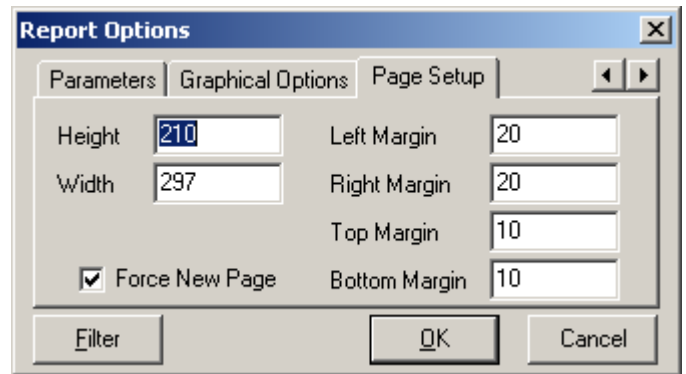
Here you can choose the scale for the graphs.



On the Page Setup tab you can change margins values and page format for further correct printing.

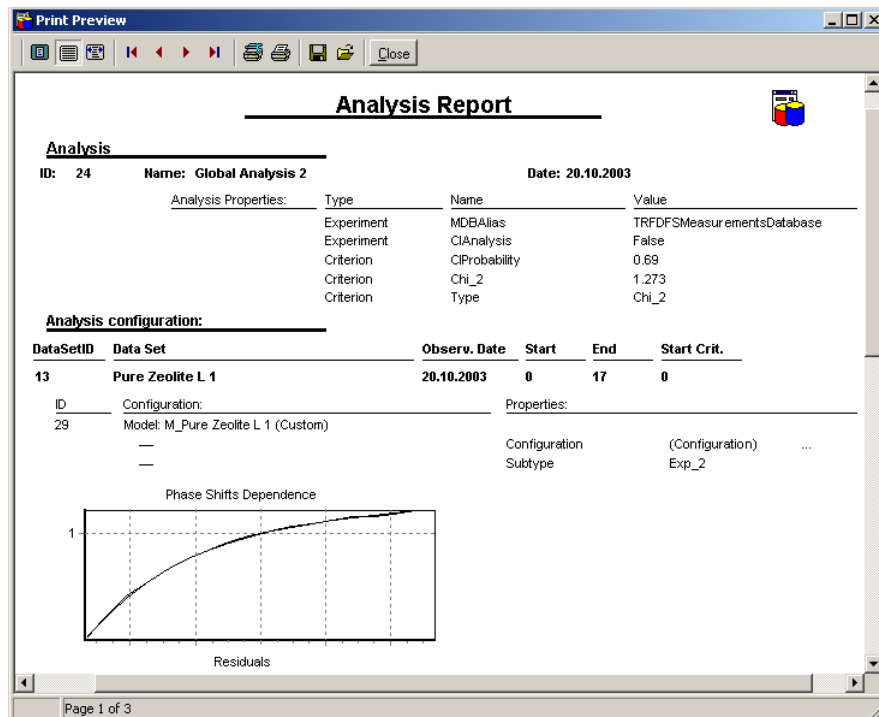
Use “Force New Page” option if necessary.

You can perform the same actions in the Page Setup window that is available from the main menu *Reports | Page Setup...*



## Print Preview window

You see this window before you send your newly-created report to print.



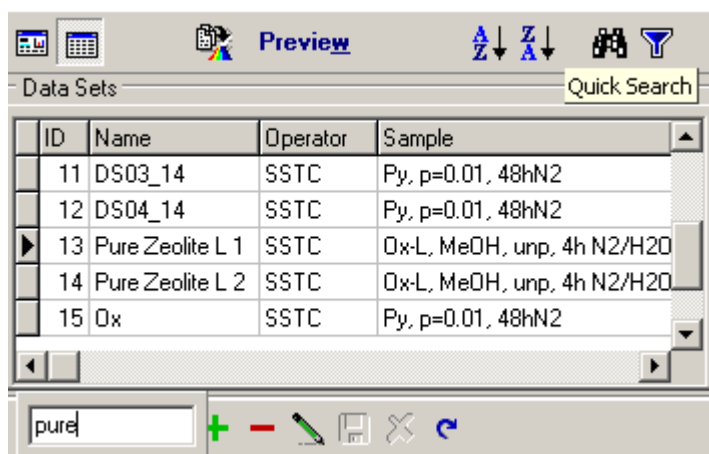
	<p>Print Preview toolbar on the top of the window lets you navigate through the print copy of the document, save and load reports; provides access to printer setup and let you print the current report.</p>
--	---

## Data Management

### Searching

You can search through any Analysis Database table by any field.

1. Select the field you want to search through.
2. Press the Quick Search button on the main Tool Bar.
3. In the appeared Search box type few characters.



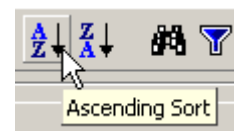
The cursor will move to the first record, which contains the characters you have entered. You can open Search box using main menu Find | Quick Search Ctrl+S.

## Sorting

To get similar records in the table together or to speed up your search you can sort Data in the current table. Ascending and Descending Sort is available through the Sort main menu item to any Database table.

1. Select the field in the table.
2. Press Sort button on the main Tool Bar.
3. You can sort any table by any field.

Ascending and Descending Sort is available in the local menu as well.



## Filtering

By using the Filter you can reduce the number of displayed records of the table. There are two options in the Filter menu

- Filter...
- Removing all filters

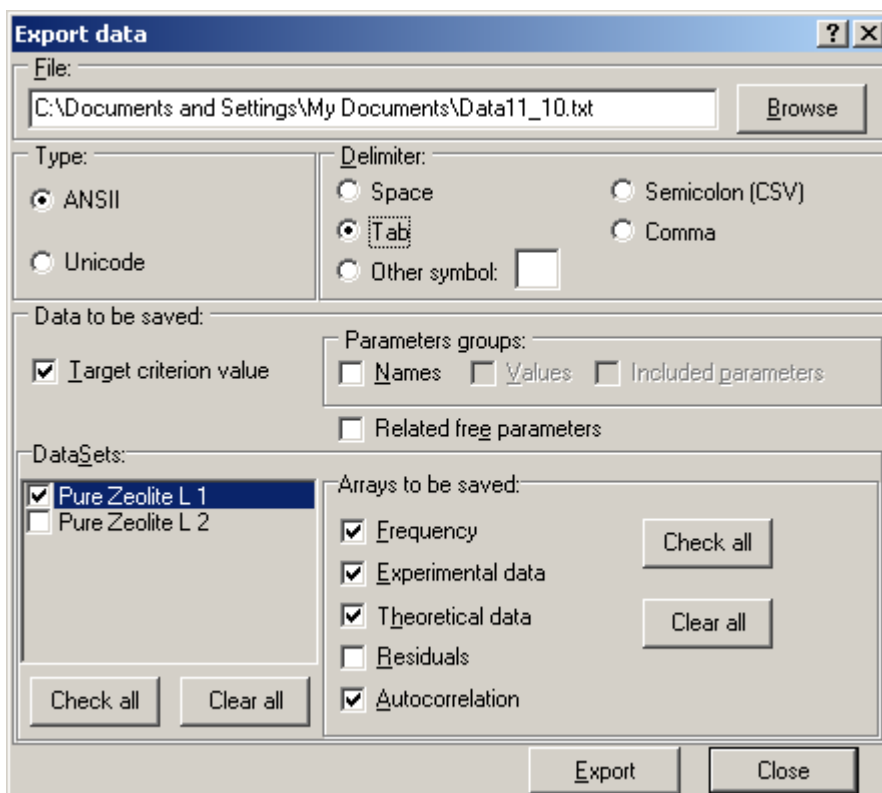
## Data Export

Use Data Export option to export the Experiment Data into text file. You can save such information as:

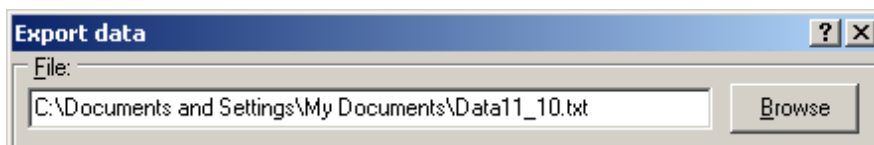
- target criterion value;
- parameters groups and free parameters;
- frequencies;
- experimental and theoretical data;
- arrays of correlation functions and residuals.

To export the Data into the file follow next steps:

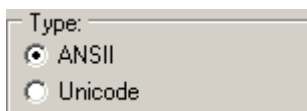
5. Select Experimental Analysis in the Analysis table.
6. Choose "Export Data" item from the local or application menu.



7. In the appeared Export Data window first of all type the name of the file that will be used to store the Data. Use Browse button to find appropriate folder.



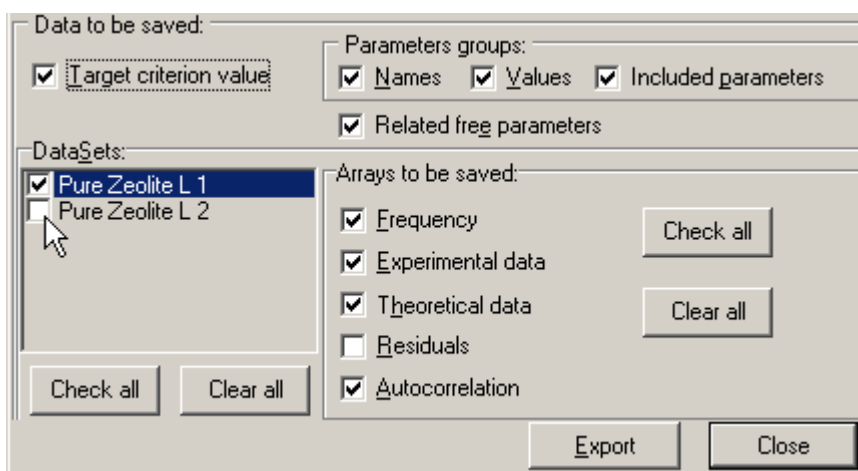
8. On the Type panel choose the coding of your text file.



9. On the Delimiter panel choose the way in which the stored Data will be separated.



10. On the “Data to be saved” panel choose the Data you want to export. You can save Target criterion value, liked and free parameters, frequencies, experimental and theoretical data, residuals and autocorrelation function.



Use **Check All** and **Clear all** buttons when you work with check boxes.

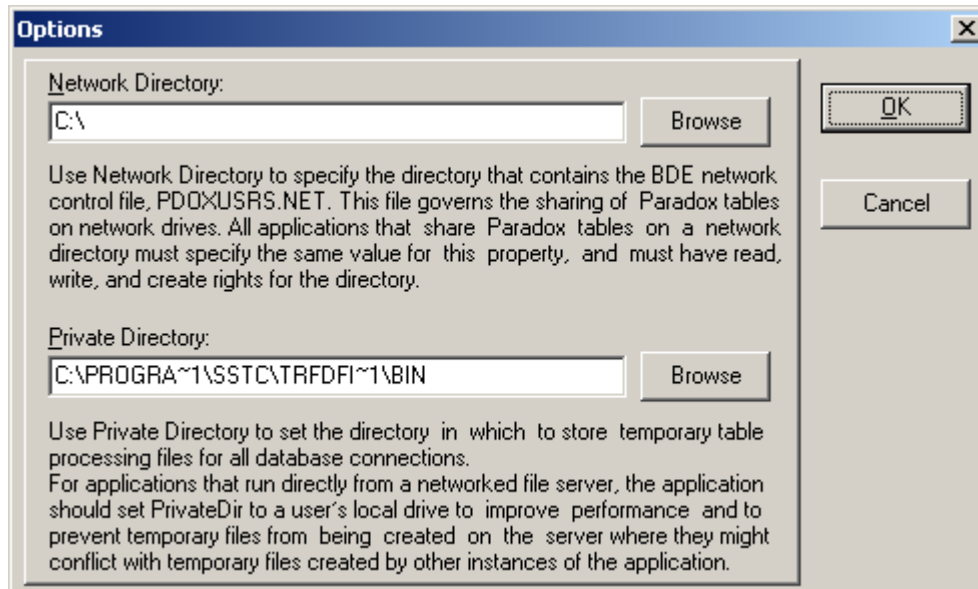
11. Press **Export** button to finish Export operation and then **Close** to close Export Data dialog.



## Database Tables Tools

### Options

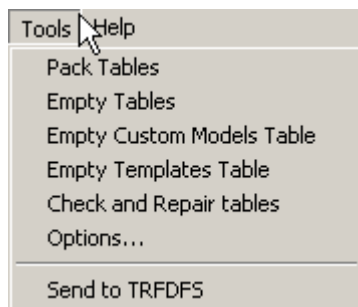
Use this Options dialog box to set internal variables of the Borland Database Engine. The window has two directory paths.



The instruction (how to use the Options dialog box) are written straight in the window above each Directory path.

### Tables Tools

Table tools are available from the application menu *Tools*.



Listed options let you manage Database tables.

### Tables Packing

Packing tables helps to save disk space that Database takes for the tables.

In the TRFD ADB application you can pack all Tables together. At the end of the operation you get a message either the action was successful or not.

### Tables Emptying

There are three destructive operations you can perform to empty data tables:

- Empty Tables
- Empty Custom Models Tables
- Empty Templates Tables

These operations could be used for the safety and economical reason to get rid of the Data: a) you don't need any more; b) you do not want to share with anybody.

After any of these operations you loose the information. That is why a confirmation message appears to confirm your intention.

## Tables Checking

There are two check operations available:

- Check Tables.
- Check all Tables.

You can check for errors either one particular table or all tables. When the tables are checked you get a result message. If any table has an error you should repair that table using “Tools | Repair Table” item from the main menu.

## Tables Check and Repairing

During the work some tables of the Database can be damages (for an example, a data management operation wasn't completed correctly because of losing electricity). From time to time you can use “Tools | Check and Repair tables” operation that checks all the tables of the current Database and repairs them I case of any error.

## TRFD Measurements Database

Basically there are two Database applications in the TRFD Fitting Software package. On the one hand them are independent programs and can be used and examined separately, each performs own function within TRFD Fitting Software package.

On the other hand both applications are connected in several ways. The main common point is that both programs deal with almost the same Data.

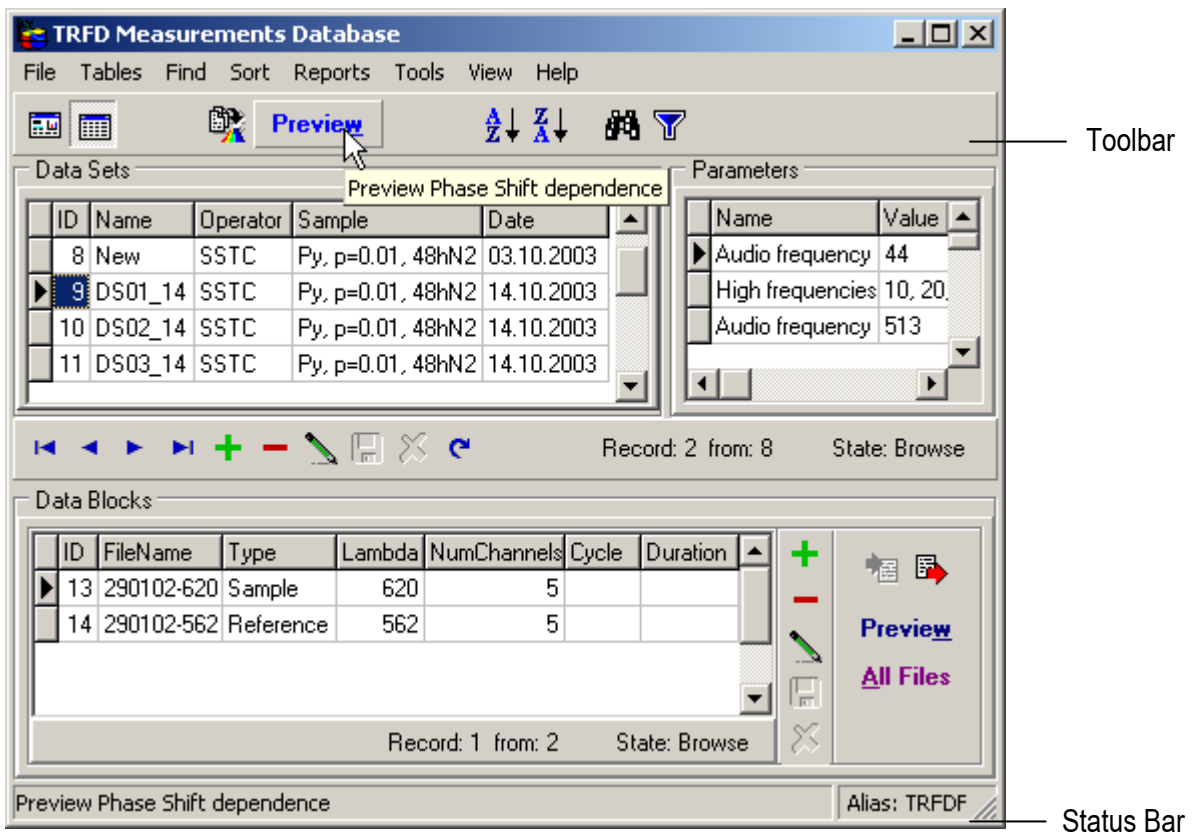
## *A tour of the environment*

### Starting Measurements Database

You can start TRFD MDB in several ways:

- From the main TRFD Fitting Software program (F3 or clicking Toolbar button)
- Choose Programs | TRFD Fitting Software | Measurements Database 2.0 from the Windows Start menu.
- Choose Run from the Windows Start menu, and then enter TRFDMDB.exe.
- Double-click \Program Files\SSTC\TRFD Fitting Software\Bin\TRFDMDB.exe.

Once you are in TRFD MDB, you see the major tools of the program environment.



Main Window consists of the following components:

- Menu
- Toolbar
- Data Sets panel
- Data Blocks panel
- Parameters panel
- Status Bar

Menu and Toolbar provide quick way to invoke the commands of the application. Status bar provides information about the current state of the application.

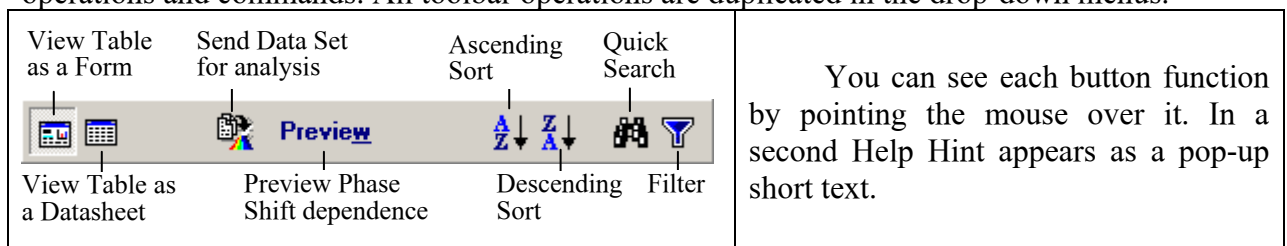
## Menu

All features of the program are available from the main menu. Through the menu you get full control of Database tables and contained information. You can run Import Data Wizard, search through the Database, create Database reports and get Data preview.

## Using toolbars, menus, and keyboard shortcuts

Many operations have keyboard shortcuts and toolbar buttons. When a keyboard shortcut is available, it is always shown next to the command on the drop-down menu.

TRFD MDB toolbar, located in the main window, provides quick access to frequently used operations and commands. All toolbar operations are duplicated in the drop-down menus.



It should be noted that not only the main window but all other application windows have similar Toolbars as well as Navigator and Status Bar to work with Database tables.

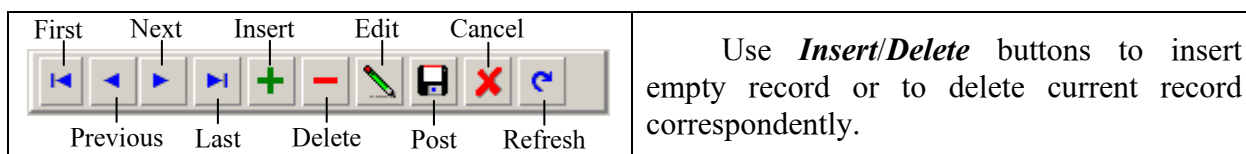
## Data Sets panel

Data Sets panel represents information stored in the Data Sets table.

Briefly about the fields on the Data Sets panel:

Field	Explanation
Name	Data Set name
Guest	Information about a person, who requests the measurement
Sample	Sample information
Date	Date of measurement
Description	Short description of the measurement

Convenient Database Navigator which is situated on the bottom of the panel will help you to navigate through Data Sets. Use the buttons *First*, *Previous*, *Next*, *Last* to find appropriate Data Set.



Once you press *Edit* button you can edit Data Set fields. Press *Post* button to save Data Set changes or *Cancel* to return previous information back. Press *Refresh* button to refresh data in Data Set fields.

Record: 1 from: 8 State: Edit

There is a Status Bar in the right corner on the bottom of the Data Sets panel where you can see the number of the current record, all records number and the current state (mode) of the table.

To add a new Guest press green arrow button. This button is available only in Edit or Insert mode. New Sample information can be entered in the same way.

Data Sets table can be viewed as a form view or datasheet view. To change the view mode use Toolbar buttons or proper items in the menu.

Name	Operator	Sample
DS03_14	SSTC	Py, p=0.01, 48hN2
DS04_14	SSTC	Py, p=0.01, 48hN2
Pure Zeolite L 1	SSTC	Ox-L, MeOH, unp, 4h N2/H2O
Pure Zeolite L 2	SSTC	Ox-L, MeOH, unp, 4h N2/H2O

Record: 7 from: 8 State: Edit

All actions that you can perform with the Data Sets table and contained information are available in the local and main menu. To open the local menu, right-click on the Data Sets panel.

## Data Block panel







Data Block panel represents all information about the measured data (Observant table) related to the current record in Data Sets table (displayed in Data Sets panel).

ID	FileName	Type	Lambda	NumChannels	Cycle	Duration
23	Example2-620	Sample	620	18		
24	Example2-562	Reference	562	18		


Record: 1 from: 2 State: Browse

Local Tool Bar: Preview, All Files  
Navigator  
Status Bar

Each record of the table describes particular measurement and contains such experimental parameters as Sample Type, Wave Length Lambda, Number of Analyzer Channels, etc. Several records from the Observant table are related to one record in the Data Sets table (relationship "many-to-one"). This relationship reflects the experimental configuration when measurements of the same sample are being performed under the same external conditions serially. In this case, certain number of particular measurements should be collected into one global group corresponding to the investigated object.

<ul style="list-style-type: none"> <li> Insert</li> <li> Delete</li> <li> Edit</li> <li> Post</li> <li> Cancel</li> <li> Refresh</li> </ul>	<p>You can manipulate records of the Observant table using Database Navigator which is placed on the right of the table. Use <b>Insert/Delete</b> buttons to insert empty record or to delete current record correspondently.</p> <p>Once you press <b>Edit</b> button you can edit the current record. Press <b>Post</b> button to save record changes or <b>Cancel</b> to return previous state. Press <b>Refresh</b> button to refresh data in the table.</p>
---	--

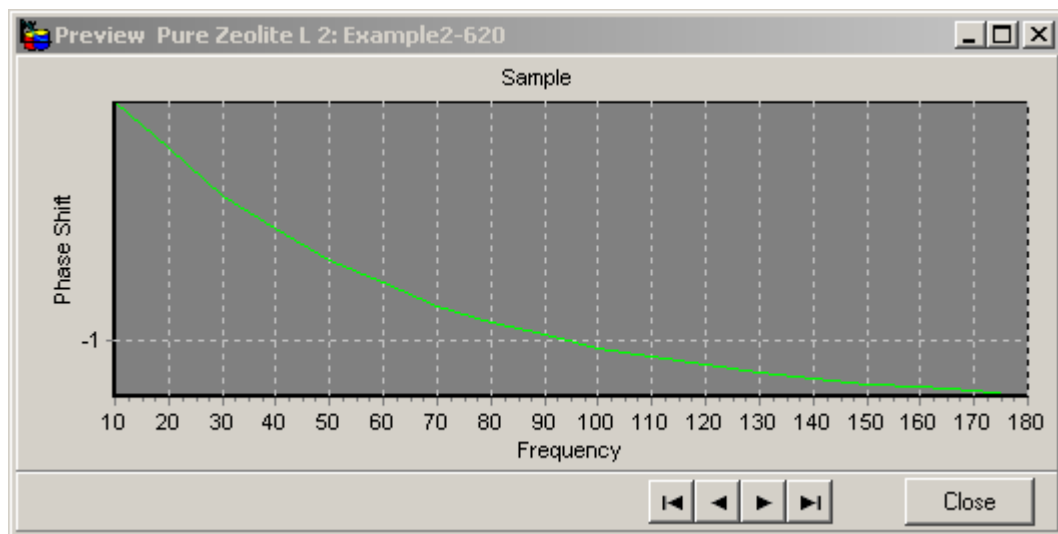
Record: 1 from: 2 State: Browse	There is a Status Bar under the table, which displays the number of the current record, all records number and the current state (mode) of the table.
---------------------------------	---

 <p><b>Preview</b> <b>All Files</b></p>	<p>Data Blocks toolbar provides quick access to frequently used operations. You can import data from the file (this operation is available in Edit mode), export data to ASCII file, perform a preview of the measured data and view all Data Blocks. To find out about the functionality of any button, point the mouse over it and get a Help.</p>
--	--

All actions that you can perform with the Observant table and contained information are available in the local and main menu. To open the local menu, right-click on the Data Blocks panel.

### Preview window

Preview window is used to display measured data stored in the current file of the Data Blocks panel in two-dimensional space.

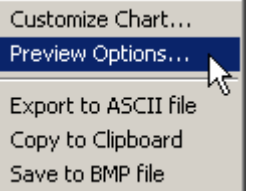


You can get Preview Windows from the local menu or by clicking **Preview** button on the Data Blocks toolbar. The name of the considered file and the name of the Data Set as well as type of stored data are displayed in the title of this window.

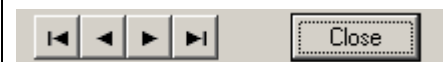
On the Chart you can:

- move the curve by keeping the right mouse button down and moving the mouse pointer;
- zoom in/out the image by keeping the left mouse button down and moving the mouse pointer diagonally across the necessary area from the left top corner to the right bottom corner;
- restore the whole view of the image by keeping the left mouse button down and moving the mouse pointer diagonally up and on the left;
- change the scale of the Y axis (linear or logarithmic) by double-clicking on the chart area and choosing appropriate box in the Options dialog.

You can right-click on the chart to open the local menu, where besides changing the scale you can customize the chart (colors, axis, titles, labels), export the data to ASCII file, copy image to the clipboard or save it to the BMP file.

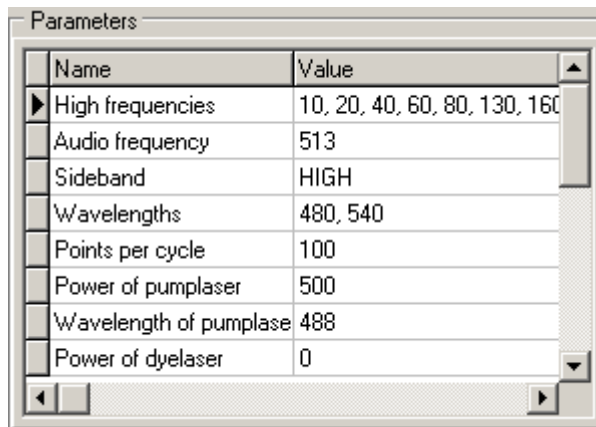


Use Navigator on the bottom of the Preview Window to move **through the files of the current Data Set**. **Close** button closes this window.



## Parameters panel

All parameters of the current Data are collected in the Parameters panel.



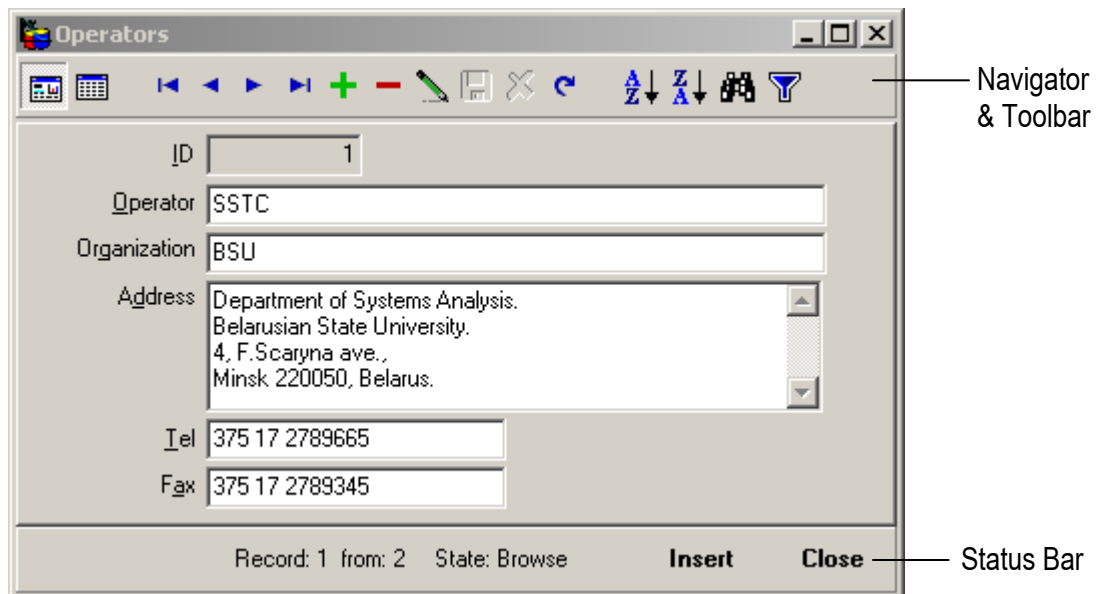
Name	Value
High frequencies	10, 20, 40, 60, 80, 130, 160
Audio frequency	513
Sideband	HIGH
Wavelengths	480, 540
Points per cycle	100
Power of pumplaser	500
Wavelength of pumplase	488
Power of dyelaser	0

In the parameter table you can see a value of any parameter of the current Data Set

## Application Windows

### *Operators window*

This window is used to work with Operators table. It displays all information about a person or organization that orders measurements. The window appears when you add new Operator at Data Import Wizard or when you edit the current Data Set (“Add new Guest” item from the local menu on the Data Set panel or green arrow button).



Operators

ID: 1

Operator: SSTC

Organization: BSU

Address: Department of Systems Analysis,  
Belarusian State University,  
4, F. Scaryna ave.,  
Minsk 220050, Belarus.

Tel: 375 17 2789665

Fax: 375 17 2789345

Record: 1 from: 2 State: Browse Insert Close

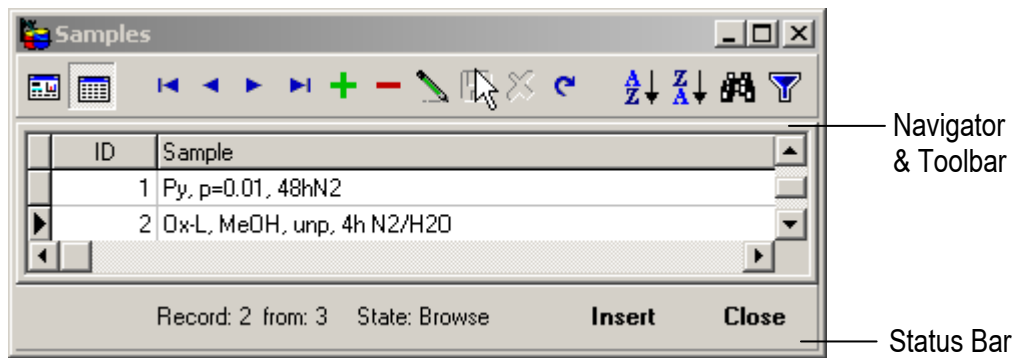
Navigator & Toolbar

Status Bar

Window Toolbar, Navigator and Status Bar is very similar to those which were described previously. Also most actions that you can perform in this window are duplicated in the local menu. Also you can run this window from the main menu Tables | Operators Ctrl+G.

### *Samples window*

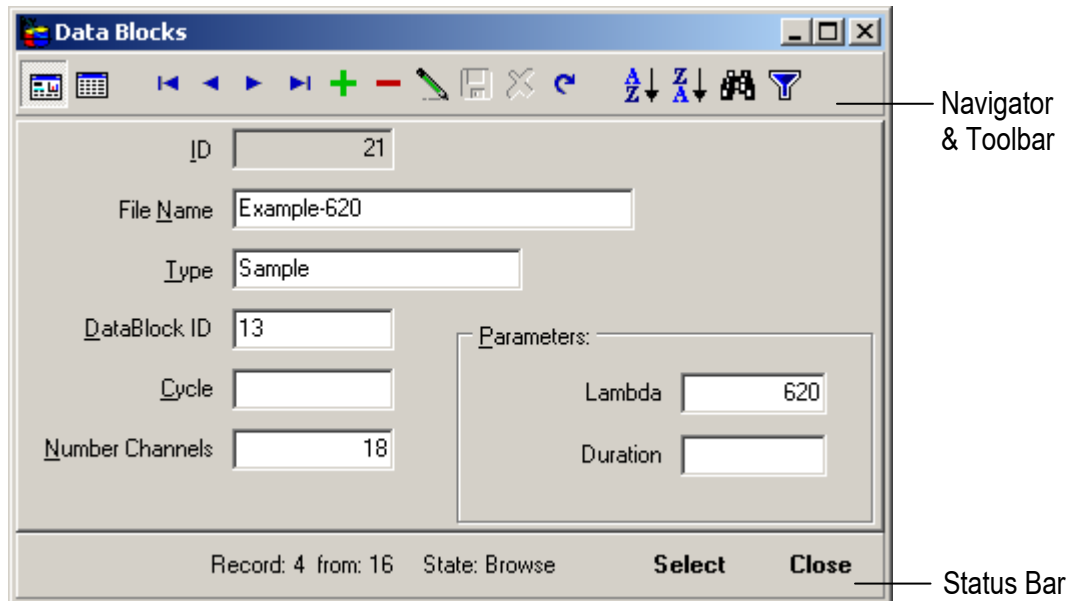
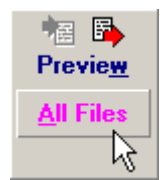
This window is used to work with Samples table. Samples table contain all information about samples which were used in measurements. The window appears when you add a new Sample at Data Import Wizard or when you edit the current Data Set (“Add new Sample” item from the local menu on the Data Set panel or green arrow button).



Window Toolbar, Navigator and Status Bar is the same as in Operator window and very similar to those which were described previously. Also most actions that you can perform in this window are duplicated in the local menu. Also you can run this window from the main menu Tables | Operators Ctrl+M.

### Data Blocks window

This window is used to work with Observant table. It displays all information about a person or organization that orders measurements. The window appears when you press “All Files” button on the Data Blocks panel Toolbar. Using this window you can select and edit any record of the file table. Also you can perform all the standard operation that you can normally do with the table in the application.



Window Toolbar, Navigator and Status Bar is very similar to those which were described previously. Also most actions that you can perform in this window are duplicated in the local menu. Also you can run this window from the main menu Tables | Operators Ctrl+O.

All other windows are described below where the corresponding actions are examined:

- Preview Phase Shift dependence – Preview window;
- Filter – Filter (Data Set, Data Blocks, Operators, Samples) window;

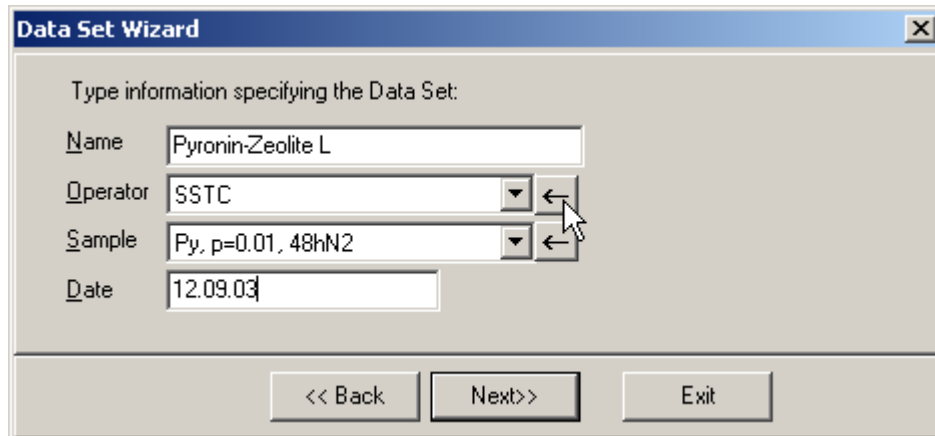
### Data Import

To import TRFD data and to create a new Data Set start choose File | “Import Data Wizard...” from the main menu and follow the instructions of the Data Set Wizard. Press Next or Back buttons to move through the Wizard’s pages.

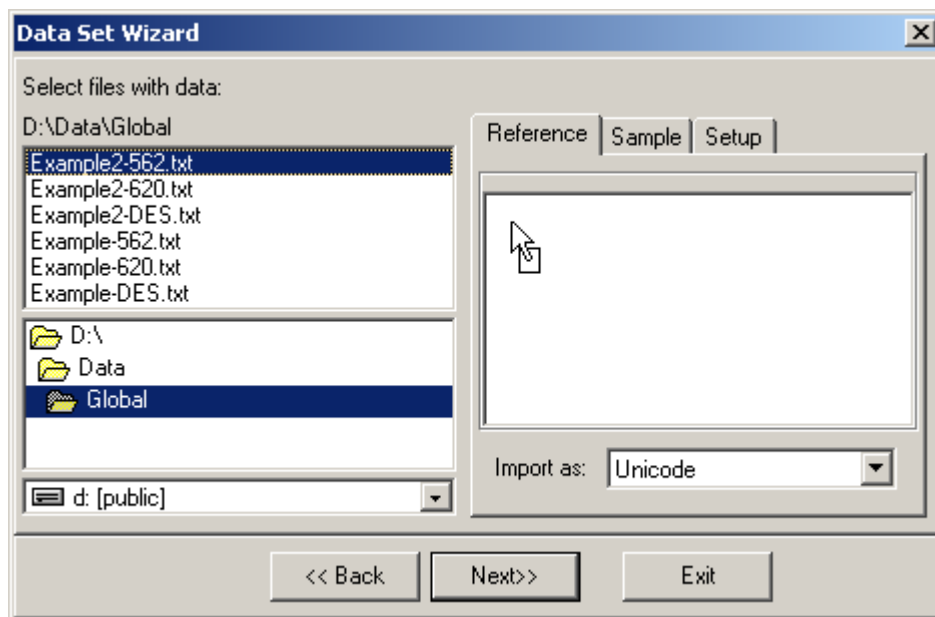
1. Click *Next* to begin creating your new Data Set.



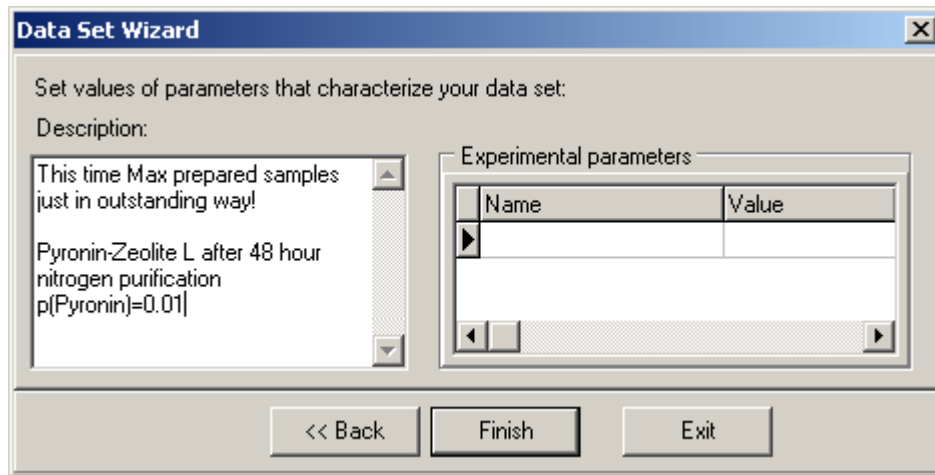
- In the appeared window specify the name of the Data Set, name of the Operator, title of the Sample and the date of the measurements. To add a new Guest press green arrow button. New Sample information can be entered in the same way. Click *Next* to go to the next window.



- In the File Selection dialog select one after another the files and drag them to appropriate tabs on the right side of the Wizard. Use the File Tree to find Data folder and “Import as:” combo box to change the encoding of the data files. When you finish click *Next*.



- Before you click *Finish* you can add experimental parameters and write additional description.



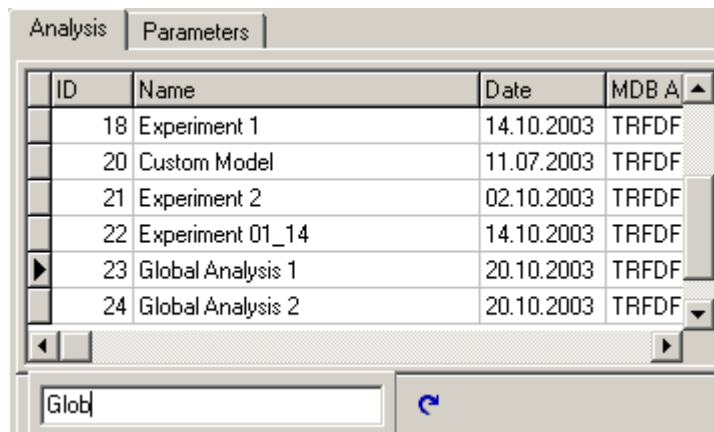
Use the “Send Data Set for analysis” button on the menu bar to send the newly-created Data Set to TRFD Data Processor. Main Application will start up and an Experiment configuration wizard will appear. Press **Ok** button to load the data from the Database.

## Data Management

### Searching

You can search through any Database table by any field.

1. Select the field you want to search through.
2. Press the **Quick Search** button on the main Tool Bar.
3. Type few characters in the appeared Search box.



The cursor will move to the first record, which contains the characters you have entered. You can open Search box using main menu “Find | Quick Search Ctrl+S”.

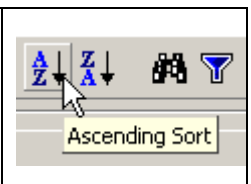
### Sorting

To get similar records in the table together or to speed up your search you can sort Data in the current table. Ascending and Descending Sort is available through the Sort main menu item to any Database table.

1. Select the field in the table.
2. Press **Sort** button on the main Tool Bar.

You can sort any table by any field.

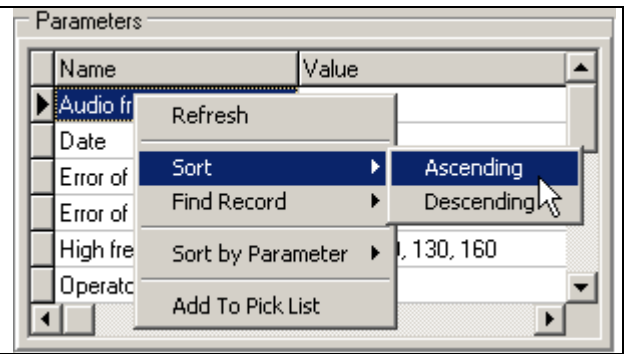
Ascending and Descending Sort operations are available in the local menu as well.



You can also sort the Data Sets table by any Experimental parameter.

1. Choose the appropriate parameter on the Parameter panel.
2. Open the local menu.
3. Click the Sort type.

Note, that those Data Sets which do not contain selected parameter will be removed from the list.



## Filtering

By using the Filter you can reduce the number of displayed records of the table.

There are two options in the Filter menu

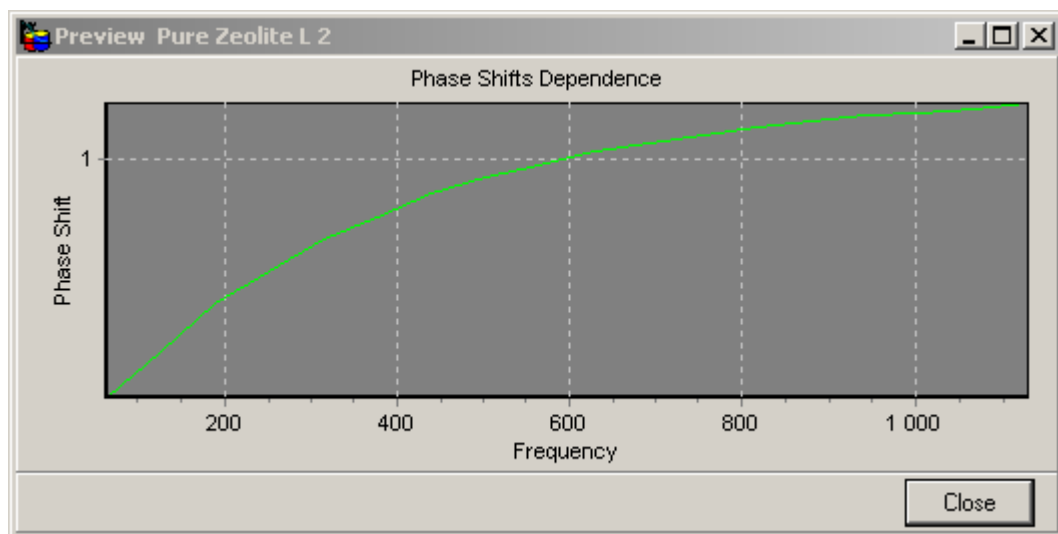
- Filter...
- Removing all filters

## Data Preview and Data Report

### Data Preview

It is described already how to **preview** measured data stored in the current file of the Data Blocks panel in two-dimensional space (see Data Blocks panel chapter). To display the Graph press **Preview** button on the Data Blocks toolbar.

Note, if you want to see Phase Shift Dependence of the current Data Set you must use the **Preview** button on the main Toolbar or “Tools | Preview Graphs Ctrl+P” from the main menu.



The name of the current Data Set is displayed in the title of this window. You can perform all the same actions with this Chart as with the measured data Chart. ([put the link](#))

## Reports

You can create a report about certain Data Sets for further printing. The report includes full information about Data Sets:

- Data Set Name, ID, Operator, Date, Sample information.
- Experimental parameters.
- Related Data Blocks.

To create your report:

1. Choose “*Reports | Data Sets Report...*” item from the application menu.
2. In the appeared Report Option dialog using Filter and Range of date options pick out wanted for report Data Sets.
3. In the Report Options dialog click Page Setup tab and change Page parameters if it’s necessary.
4. Press **OK** and see the Print Preview window of the newly-created report.

You can start creating your report through the local menu “*Generate report...*” on the Data Set panel.

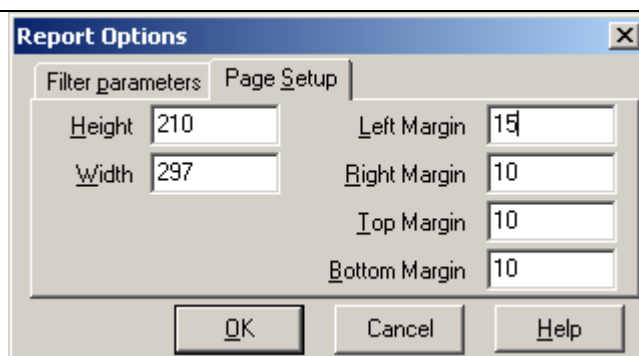
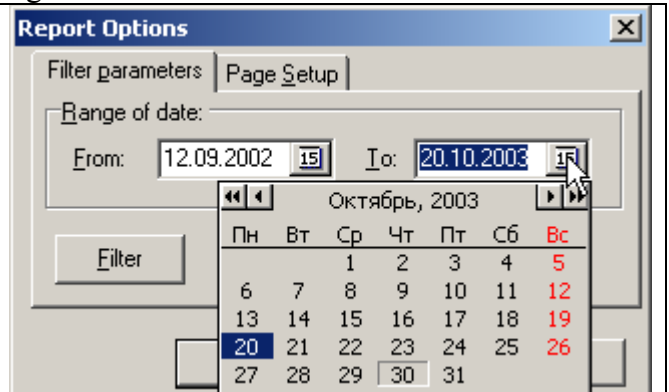
### Report Options dialog

There are two tabs in Report Options dialog.

On the Filter parameters tab you can pick out those records that you want to include into the report.

Use “Range of date” option to select Data Sets by date. You can enter the date from the keyboard or choose it from the calendar.

Use Filter to add conditions to constrain number of Data Sets in the report.

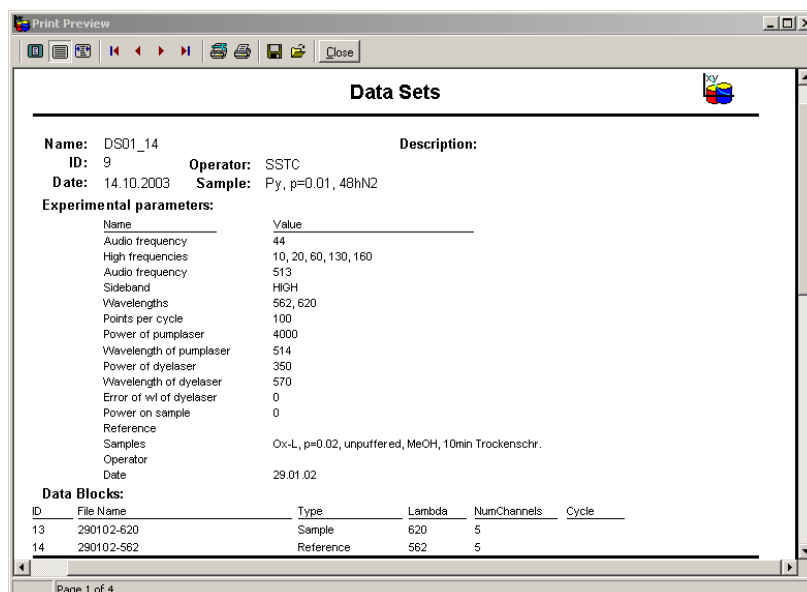


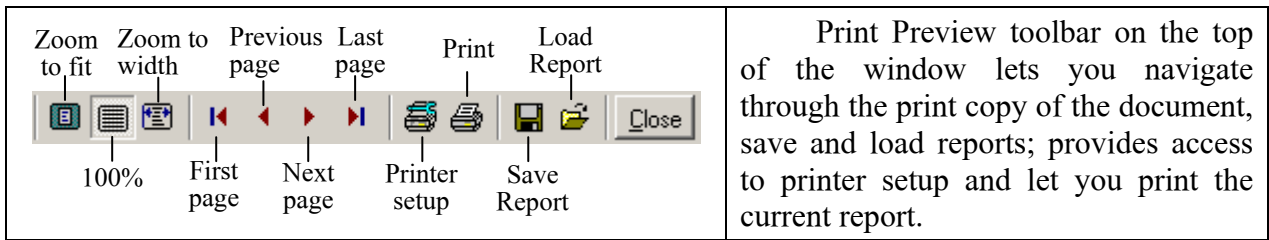
On the Page Setup tab you can change margins values and page format for further correct printing.

You can perform the same actions in the Page Setup window that is available from the main menu *Reports | Page Setup...*

### Print Preview window

You see this window before you send your newly-created report to print.





## Database Tables Management

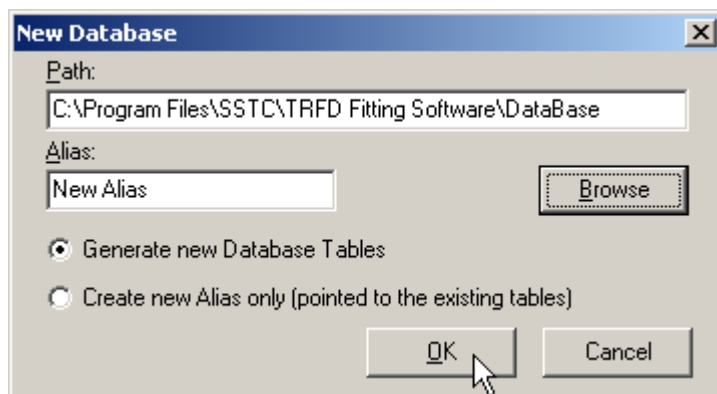
In this chapter you can find out how to

- Create new sets of tables.
- Link tables.
- Import database.
- Export database.

These features are available from the main menu *File*.

### Creating new set of tables

You can create a new set of tables (empty Database) and link with it at run time. It gives the benefit to keep Data in different folders and different computers within local network.



To create a new set of tables:

1. Choose “*File | New Tables...*” from the main menu.
2. Select the directory where you want to store the Data. Use Browse button to find the proper folder.
3. Enter a new Database Alias name.
4. Check the radio button if necessary.
5. Press **OK**.

If the “Generate new Database Tables” radio button is checked, a new empty database will be created in the specified path. The Alias that is points out to the Database will be created as well. If you have the database tables already (for example, the database tables were copied to another folder), you can create just Alias that will point out to these tables. To do this check “Create new Alias only” radio button.

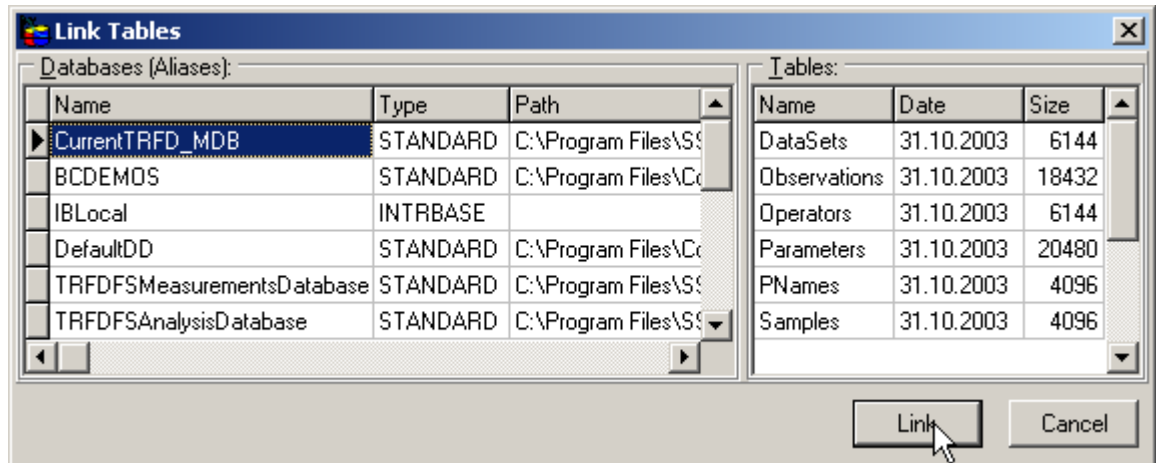
An Alias is a name and a set of parameters that describe a Database resource. BDE applications use aliases to connect with databases. Alias is a special Database object that points out to the particular tables.

If you want to use remote access (within local network) to the Database you must set the Network Directory (“*Tools | Options...*” from the main menu).

### Link tables

You can switch between Databases at run time:

1. Choose “*File | Link Tables...*” from the main menu.
2. Select wanted Database Alias and click “**Link**”



Link Tables window consists of two panels:

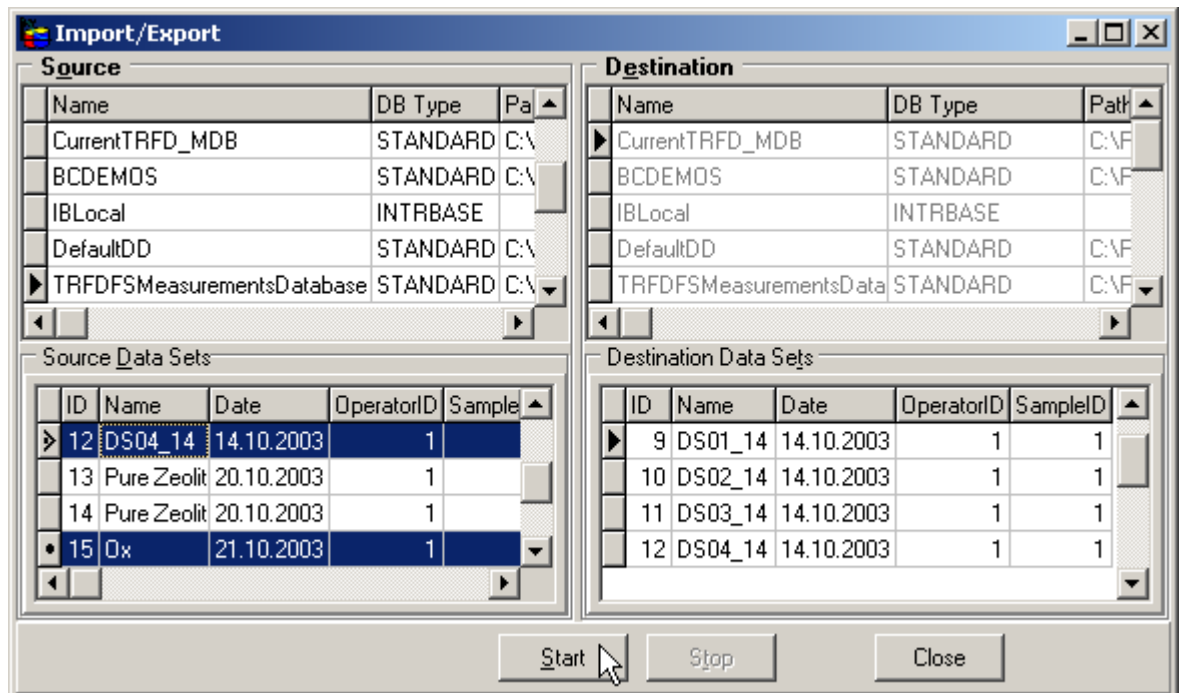
- Databases (Aliases) panel displays alias names, type and the path of all registered databases at the local machine.
- Tables panel shows names, dates and sizes of the tables in the database.

## Import/Export Database

Use “Import...” main menu item to import Data Sets with all supplemental information (Operator, Sample, external parameters and etc.) to the current Database from another Database. Use “Export...” menu item to export Data Sets from the current Database to another Database.

### Export/Import window

Export/Import window consists of four panels. Two upper panels contain the list of Database Aliases. Each of two panels on the bottom contains table of the Data Sets that corresponds to the chosen Alias.



Chosen Alias is marked with the black pointer on the left of the record. Using **Ctrl** button you can choose few Data Sets together.

Two left panels are related to the Source of Data, other two panels on the right correspond to the Destination of the Data.

### **Import**

The records in the Destination Aliases table have light grey color and the pointer is on the CurrentTRFD\_MDB Alias. To perform Data Import operation:

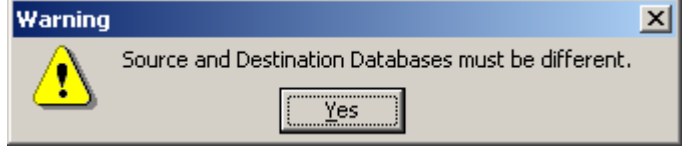
1. From the Source Alias table choose Alias of the Database that contains Data Sets you want to import.
2. In the Source Data Sets table select wanted Data Sets (use **Ctrl** button to select few records).
3. Press button "Start".

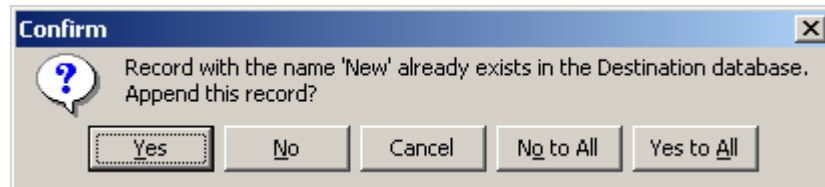
### **Export**

Now, the records in the Source Aliases table have light grey color and the pointer is on the CurrentTRFD\_MDB Alias. To perform Data Export operation:

1. From the Destination Alias table choose Alias of the Database that contains Data Sets you want to export.
2. In the Destination Data Sets table select wanted Data Sets (use **Ctrl** button to select few records).
3. Press button "Start".

### **Messages**

<p>Note, Source and Destination Databases must be different; otherwise you'll get Warning message.</p>	 <p>A warning dialog box with a yellow triangle icon. The text reads: "Warning Source and Destination Databases must be different." There is a "Yes" button at the bottom right.</p>
--	---

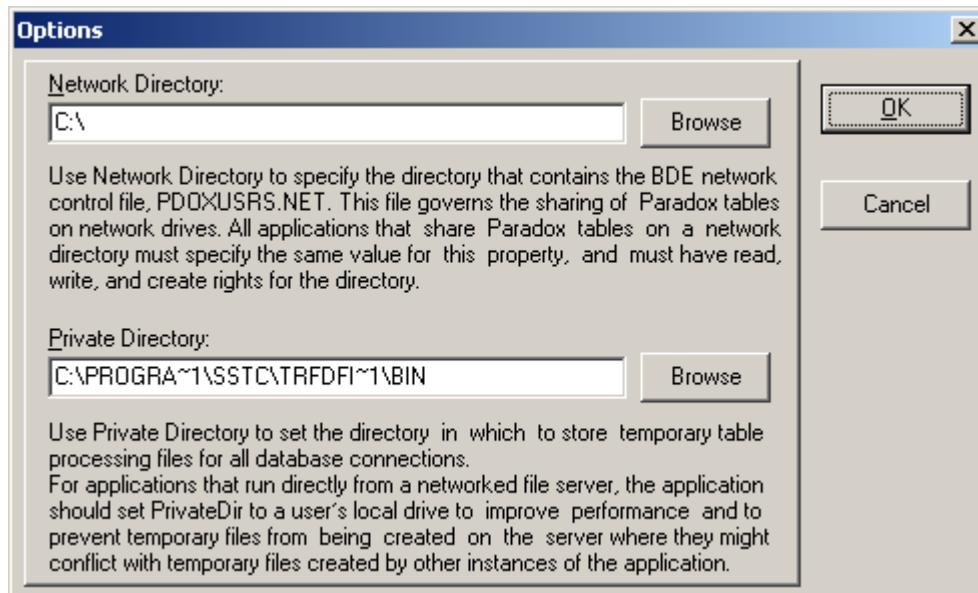


You can get Confirm message if Source and Destination Databases have the same Data Sets, for example, when Source and Destination Databases Aliases correspond to the same Database.

## **Database Tables Tools**

### **Options**

Use this Options dialog box to set internal variables of the Borland Database Engine. The window has two directory paths.

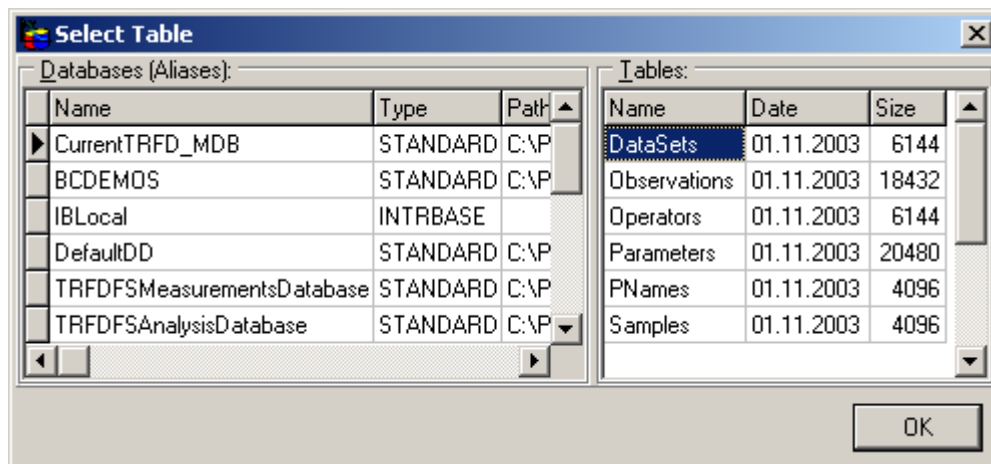


The instruction (how to use the Options dialog box) are written straight in the window above each Directory path.

## Select Table Window

This window appears when you choose one of these operations:

- Pack Tables.
- Empty Tables.
- Check Tables.
- Repair Tables.



Left panel of the window contains a table of Database Aliases. Right panel displays tables that correspond to the chosen Alias.

To perform any table operations in the *Tools* main menu:

1. Choose an operation.
2. Choose Database that contain necessary table.
3. Select wanted table.
4. Press **OK**.

## Tables Packing

There are two pack operations available:

- Pack Tables.
- Pack all Tables.



You can select and pack particular table or pack all tables together. Packing tables helps to save disk space that Database takes for the tables.

### **Tables Emptying**

There are two ways to get rid of the records stored in the Database tables:

- Empty Tables.
- Empty all Tables.

You can select and empty particular table or empty all tables. After this operation you lose all records in the selected tables.

### **Tables Checking**

There are two check operations available:

- Check Tables.
- Check all Tables.

You can check for errors either one particular table or all tables. When the tables are checked you get a result message. If any table has an error you should repair that table using “Tools | Repair Table” item from the main menu.

### **Tables Repairing**

If after checking any table of the Database you get a message about an error you can repair it using Repair Table operation. Also you can use “Tools | Check and Repair Tables” operation that checks all the tables of the current Database and repairs any error.

## TRFD Shared Tools

### Filter

Filter is a very convenient tool that can be used in work with Database tables. It let you constrain the number of viewed records of the current table. Filter tool can be used both in TRFD Analysis Database and TRFD Measurements Database applications. Use Filter when you

- Create Reports.
- View Examining Data in the Database tables.

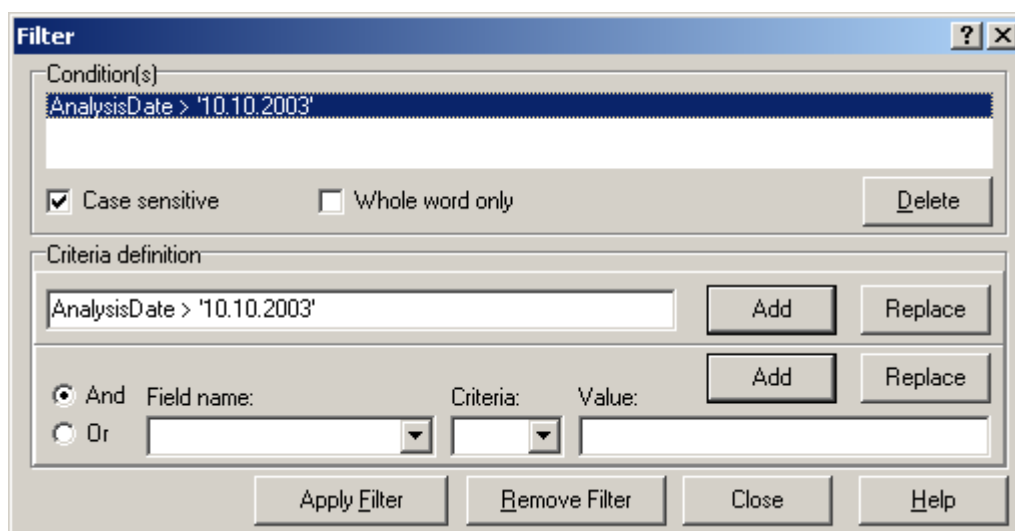
When you create a report you will want to include not the whole Data Table but only those records that you need. Use Filter to choose the proper records (e.g. Analyzed Experiments in TRFD AD or Data Sets in TRFD MD)

When you examine the information in the tables of the Database it would be probably a good idea to view just those records which could be marked out by some criterion. Use the Filter tool to constrain records in the current table.

### Filter dialog box

You can get Filter tool in several ways:

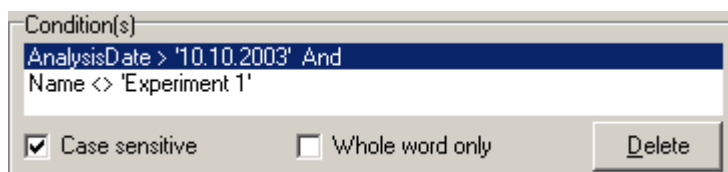
- From the Database application menu “*Find | Filter... Ctrl+F*”.
- Using **Filter** button on the application Toolbar.
- From the local menu “*Find Record | Filter...*”.
- Using **Filter** button on the Report Options dialog.



Use this dialog box to create a filter for the current table. If the filter is applied, only those table records that correspond to the filter criteria will be displayed. Filter window consists of two sections and control buttons.

### Condition(s) panel

Condition(s) panel displays the filter conditions.



Each condition line in the list represents one particular condition. “Case sensitive” and “Whole word only” check boxes are used to define the search options in the string fields. Tick “Case sensitive” check box to let your filter differ lower case and upper case characters.

Lines can be combined in a complex expression by the logical operations “And” and “Or”. Use “Criteria definition” panel controls to edit selected line. You can delete any line using **Delete** button.

### Criteria definition panel

Use the controls of "Criteria definition" panel to create a complex filter expression.

This panel consists of two sections. The top section allows you;

- To edit any condition line from the condition list (upper **Replace** button).
- To add a new condition just by typing (upper **Add** button).

The bottom section allows:

- To add a new condition using “Fields name” and “Criteria” combo boxes, “And” and “Or” logical operations and “Value” edit line (lower **Add** button).
- To replace selected condition with the created one (lower **Replace** button).

To create a new condition:

1. Choose the field of the filtered table from the “Field name” combo box.
2. Choose an appropriate criterion from the “Criteria” combo box
3. Enter the value in the “Value” edit line.
4. Use “And” and “Or” radio buttons for changing the logical operation that is used for complex condition.

### Condition example

Filter contains a string that describes the filter condition. For example, the following filter condition displays only those records that have State field 'CA' or 'MA':

*State = 'CA' or State = 'MA'*

If the field name contains spaces, you must enclose the field name in brackets:

*[Home State] = 'CA' or [Home State] = 'MA'*

Note that the Date/Time format and the Decimal separator that are used in the Date/Time and Numeric values depend on your current Regional Settings:

*ObservDate >= '10.10.2003'* when some systems might have *'01/01/98'*

Also when you make changes in the selected condition or create a new condition don't forget to press **Add** or **Replace** button to finish the operation.

### Applying the Filter

Use top section of the “Criteria definition” panel to write Filter conditions.

If you are not sure how to spell the names of the table fields correctly and how to write filter expressions use the bottom section of the “Criteria definition” panel and its controls.

Once you have completed filter conditions, you can:

- Apply the filter using Apply Filter button.
- Remove current Filter by pressing Remove Filter button.
- Cancel Filter operation by pressing Close and closing the window.

You can remove all filters in two ways:

- From the Database application menu “*Find | Remove All Filter*”.
- From the local menu “*Find Record | Remove All Filter*”.

## Appendix

### Global Analysis

The software package TRFD Fitting Software performs the analysis of single measured modulation phase shifts, noted as a trace, and a Global Analysis of a group of such traces. During Global Analysis, a number of experimental data traces measured under—different conditions, e.g. temperature, concentration/loading, excitation/detection wavelength, is combined in frame of a procedure of simultaneous fitting. Certain physical parameters related to the combined data traces can be linked, what makes these parameters equal for all data traces in the set. Each parameter can be fixed and predefined by a user. For each parameter the range of admissible values can be established by inputting the minimum and maximum constraints.

### Fitting Procedure

The Nonlinear Least-Squares (NLS) method [ ] is used in the program to compare measured trace and calculated data. The Marquard-Levenberg algorithm [ ] is used as a standard minimization algorithm for NLS.

### Data Analysis Models

### Fit quality criteria

## Tips and Frequently Asked Questions

### 1. 3D Graphics tab in the TRFD Main Application does not view Graphs correctly e.g. the window stays just black and displays just nothing. How can I see the graphs?

The problem with graphic visualization is caused by the Video Card. O view the 3D graphs in the TRFD Fitting Software we used OpenGL. If the Video Card is old and so have weak parameters you might have such problems. Try to minimize either the current Experiment or the whole Fitting Software application and then click on the graphs randomly.

### 2. I installed one software package (Borland C++ Builder) on my computer and from that time TRFD Fitting Software tells me that there is some error with the Database. Do I have to reinstall TRFD Fitting Software?

The problem appears when after installing TRFD Fitting Software you install another software that deals with Databases. During the installation of this software TRFD Aliases might be deleted. You can fix this problem either in BDE Administrator “*C:\Program Files \ Common Files \ Borland Shared \ BDE \ BDEADMIN.EXE*” or in the TRFD Measurement Database application “*File | New Tables...*”.

## Glossary

Data Set  
Filter

## Index

Filter  
Sort  
Search  
Import  
Export

**Sources**

J.N. Demas (1983) Excited State Lifetime Measurements Academic Press, New York.  
A. Grinvald, I. Steinberg, Anal. Biochem., 59 (1979) 583.

***To be completed:***

- Introduction
- Configuration and t-view windows
- Glossary, Index if necessary
- Appendix and literature if necessary
- Database structure