

Isodat 2.0

Operating Manual

Revision A
115 4991

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- ☐ Energy
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- ☐ Other _____

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<i>Isodat 2.0 Operating Manual</i>	<i>Revision A 115 4991</i>			
	Strongly Agree	Agree	Disagree	Strongly Disagree
The manual is well organized.	1	2	3	4
The manual is clearly written.	1	2	3	4
The manual contains all of the information I need.	1	2	3	4
The instructions are easy to follow.	1	2	3	4
The instructions are complete.	1	2	3	4
The technical information is easy to understand.	1	2	3	4
The figures are helpful.	1	2	3	4

Additional Comments: (Attach additional sheets if necessary.)

Tear this sheet from the manual, fold it closed, stamp it, and drop it in the mail.

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Read This First

This **Isodat 2.0 Operating Manual** describes the features that have been added to ISODAT NT.

The **Isodat 2.0 Operating Manual** includes the following chapters:

Survey of recent Features in Isodat 2.0 gives an overview of the new and improved features.

Chapter 1: Hardware-related Features describes the improved and added features that concern the hardware.

Chapter 2: Evaluation-related Features describes the features that concern the evaluation.

Chapter 3: Script-related Features describes the script-related features that have been integrated or improved.

Chapter 4: Reporting-related Features describes the improved and added features that concern the reporting.

Chapter 5: Miscellaneous Features describes miscellaneous features that have been added or improved.

Changes to the Manual and Online Help

To suggest changes to this manual or the online Help, please send your comments to:

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You are encouraged to report errors or omissions in the text or index.
Thank you.

Abbreviations

The following abbreviations are used in this and other manuals and in the online Help.

A	ampere
ac	alternating current
ADC	analog-to-digital converter
AP	acquisition processor
APCI	atmospheric pressure chemical ionization
API	atmospheric pressure ionization
ASCII	American Standard Code for Information Interchange
b	bit
B	byte (8 b)
baud rate	data transmission speed in events per second
°C	degrees Celsius
cfm	cubic feet per minute
CI	chemical ionization
CIP	carriage and insurance paid to
cm	centimeter
cm ³	cubic centimeter
CPU	central processing unit (of a computer)
CRC	cyclic redundancy check
CRM	consecutive reaction monitoring
<Ctrl>	control key on the terminal keyboard
<i>d</i>	depth
DAC	digital-to-analog converter
dc	direct current
DDS	direct digital synthesizer
DEP™	direct exposure probe
DS	data system
DSP	digital signal processor
EI	electron ionization
<Enter>	enter key on the terminal keyboard

ESD	electrostatic discharge
ESI	electrospray ionization
eV	electron volt
f	femto (10^{-15})
°F	degrees Fahrenheit
ft	foot
FTP	file transfer protocol
g	gram
G	Gauss; giga (10^9)
GC	gas chromatograph; gas chromatography
GC/MS	gas chromatograph / mass spectrometer
GND	electrical ground
GPIO	general-purpose interface bus
GUI	graphical user interface
h	hour
<i>h</i>	height
HPLC	high-performance liquid chromatograph
HTML	Hyper Text Markup Language
HV	high voltage
Hz	hertz (cycles per second)
ICIS™	Interactive Chemical Information System
ICL™	Instrument Control Language™
ID	inside diameter
IEC	International Electrotechnical Commission
IEEE	Institute of Electrical and Electronics Engineers
in.	inch
I/O	input/output
IS	extraction standard
ISTD	internal standard
k	kilo (10^3 , 1000)
K	kilo (2^{10} , 1024)
kg	kilogram
<i>l</i>	length

L	liter
LAN	local area network
lb	pound
LC	liquid chromatograph; liquid chromatography
LC/MS	liquid chromatograph / mass spectrometer
LED	light-emitting diode
μ	micro (10 ⁻⁶)
m	meter
mm	milli (10 ⁻³)
M	mega (10 ⁶)
M+	molecular ion
MB	Megabyte (1048576 bytes)
MH+	protonated molecular ion
MID	multiple ion detection
min	minute
ml	milliliter
mm	millimeter
MS	mass spectrometer; mass spectrometry
MS	MS ⁿ power: where n = 1
MS/MS	MS ⁿ power: where n = 2
MS ⁿ	MS ⁿ power: where n = 1 through 10
<i>m/z</i>	mass-to-charge ratio
n	nano (10 ⁻⁹)
NCBI	National Center for Biotechnology Information (USA)
NIST	National Institute of Standards and Technology (USA)
OD	outside diameter
Ω	ohm
p	pico (10 ⁻¹²)
Pa	pascal
PCB	printed circuit board
PID	proportional / integral / differential
P/N	part number

P/P	peak-to-peak voltage
ppm	parts per million
psig	pounds per square inch, gauge
RAM	random access memory
RF	response file
RMS	root mean square
ROM	read-only memory
RS-232	industry standard for serial communications
s	second
RT	retention time
SIM	selected ion monitoring
SRM	selected reaction monitoring
TCP/IP	transmission control protocol / Internet protocol
TEF	toxic equivalent factor
TEQ	toxic equivalent
TIC	total ion current
Torr	torr
u	atomic mass unit
V	volt
V ac	volts alternating current
V dc	volts direct current
vol	volume
w	width
W	watt

Note. Exponents are written as superscripts. In the corresponding online Help, exponents are sometimes written with a caret (^) or with *e* notation because of design constraints in the online Help. For example:

MSⁿ (in this manual) Msⁿ (in the online Help)

10⁵ (in this manual) 10^{^5} (in the online Help)

Typographical Conventions

Typographical conventions have been established for Thermo Electron Bremen manuals for the following:

- Data input
- Boxed information
- Topic headings

Data Input

Throughout this manual, the following conventions indicate data input and output via the computer:

- Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
- Input that you enter by keyboard is represented in **bold face letters**. (Titles of topics, chapters, and manuals also appear in bold face letters.)
- For brevity, expressions such as “choose **File > Directories**” are used rather than “pull down the File menu and choose Directories.”
- Any command enclosed in angle brackets < > represents a single keystroke. For example, “press <F1>” means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, “press <Shift> + <F1>” means press and hold the <Shift> key and then press the <F1> key.
- Any button that you click on the screen is represented in bold face letters and a different font. For example, “click on **Close**”.

Boxed Information

Information that is important, but not part of the main flow of text, is displayed in a box such as the one below.

Note. Boxes such as this are used to display information.

Boxed information can be of the following types:

- **Note** – information that can affect the quality of your data. In addition, notes often contain information that you might need if you are having trouble.
- **Caution** – information necessary to protect your instrument from damage.
- **Warning** – hazards to human beings. Each Warning is accompanied by a Warning symbol.

Topic Headings

The following headings are used to show the organization of topics within a chapter:

Chapter 1

Chapter Name

1.2 Second Level Topics

Third Level Topics

Fourth Level Topics

Fifth Level Topics

Reply Cards

Thermo Electron Bremen manuals contain one or two reply cards. All manuals contain a Customer Registration / Reader Survey card and some contain a Change of Location card. These cards are located at the front of each manual.

The Customer Registration / Reader Survey card has two functions. First, when you return the card, you are placed on the Thermo Electron Bremen mailing list. As a member of this list, you receive application reports and technical reports in your area of interest, and you are notified of events of interest, such as user meetings. Second, it allows you to tell us what you like and do not like about the manual.

The Change of Location card allows us to track the whereabouts of the instrument. Fill out and return the card if you move the instrument to another site within your company or if you sell the instrument. Occasionally, we need to notify owners of our products about safety or other issues.

Survey of recent Features in Isodat 2.0

The following features have recently been included in Isodat 2.0. They span any of the four basic topics Hardware, Evaluation, Scripts and Reporting, therefore drastically enhancing its flexibility on a broad basis:

Hardware	Evaluation	Scripts	Reporting
Device editor	Ratio editor	ISODAT Script Language (ISL)	Export editor
Control panel designer	Standard editor	Dynamic Variables Exchange (DVE)	Result workshop
Third party support	External data processing (script-controlled)	Debugging acquisition scripts and evaluation scripts	

Hardware-related Features

Device Editor

In addition to the “classical” predefined devices, users can create specific devices completely on their own. The device editor is used to

- create new devices
- modify existing devices

Panel design

After creating new own devices users can modify and graphically customize their visualization in any application. This panel design is markedly assisted by several graphical objects. The control panel designer is used to

- create new control panels
- modify existing control panels

Third party support

The third party support concerns Trace GC, AS 2000, Agilent 6890 and the CTC autosampler.

Evaluation-related Features

Ratio editor

The ratio editor allows to determine

- element/molecule ratios
(by simply selecting denominator and divisor from lists)
- intermolecular/interelement ratios
(i.e. ratios between different elements and molecules)

Standard editor

The standard editor allows to define

- element/molecule standards
- interelement/intermolecular standards

External data processing (script-controlled)

- Edit data in user-defined scripts via the ISL interface.
- Perform flexible ion corrections by changing a- and k-factors in predefined algorithms.

Script-related Features

Users can access, edit and run ISL scripts to control and facilitate data evaluation.

External Acquisition Control

- User-defined process control with multiple threads via the ISL interface
- The user can define dynamic variables via Dynamic Variables Exchange - DVE - and modify them in the method (script-dependent parameter).
- The user can define parameters for devices that are used in any script (device-related parameters).

Debugging scripts and parameter control

- Debug acquisition scripts and evaluation scripts stepwise while the processes are running. Control the variables, stacks, threads and functions involved.

Reporting-related Features

Export Editor

- To export templates, use the drag&drop functionality of the export editor.
- Define multiple templates for one export cycle. Export to the formats “Excel”, “*.wk1” and “*.csv”.

ResultWorkshop

- Any Isodat 2.0 objects and graphical objects can be placed arbitrarily on a page and tailored before being printed.

Chapter 1

Hardware-related Features

This chapter contains the following topics:

- Device Editor
- Panel Design
- Third Party Support

1.1 Device Editor

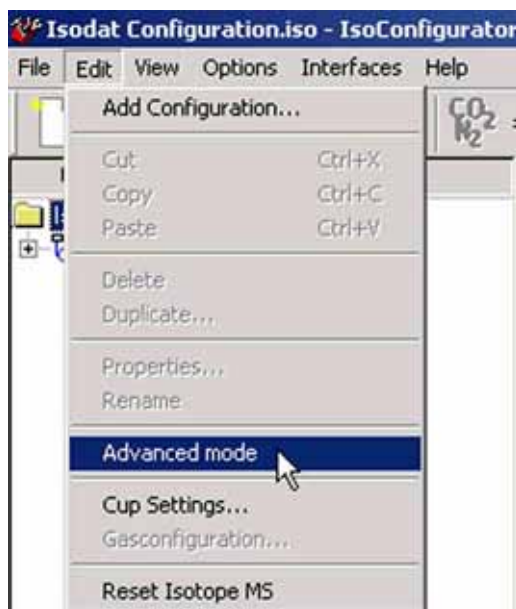
Principle: In addition to the predetermined “classical” devices, user-specific devices can personally be created. Before using them for the various applications, they can furthermore be modified, graphically customized and triggered.

Opening the Configurator

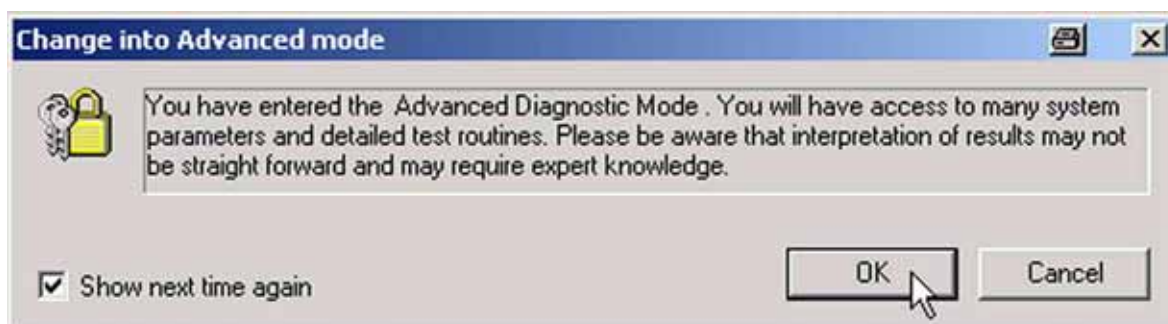
1. Start *Isodat* .



2. Open the *Configurator*.

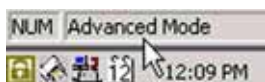


3. In the Configurator, choose **Edit > Advanced Mode**.

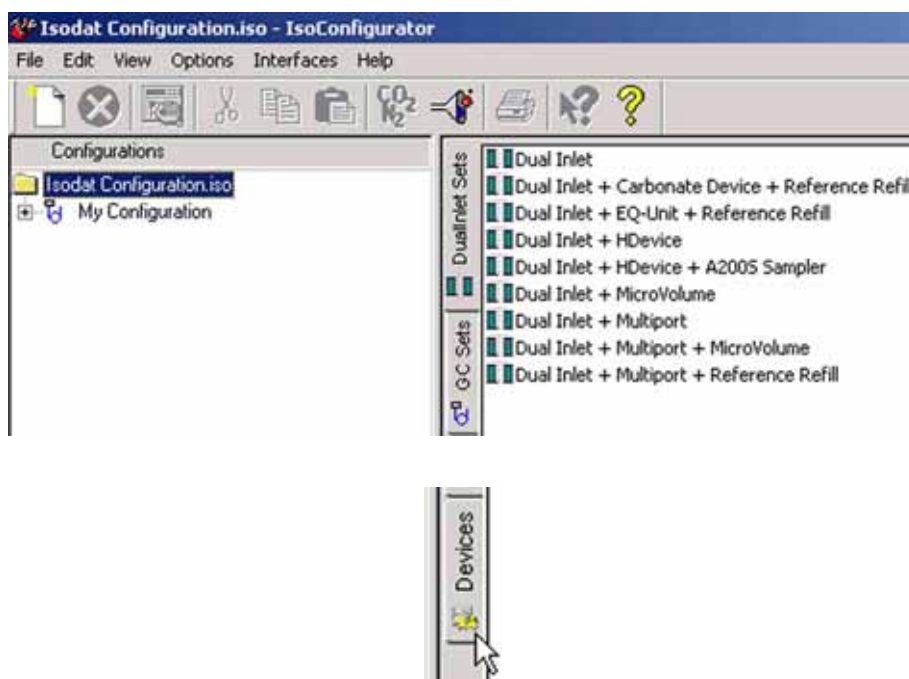


4. Press **OK** to enter Advanced Mode.

Note. Creating and editing of user devices is impossible in Normal Mode!

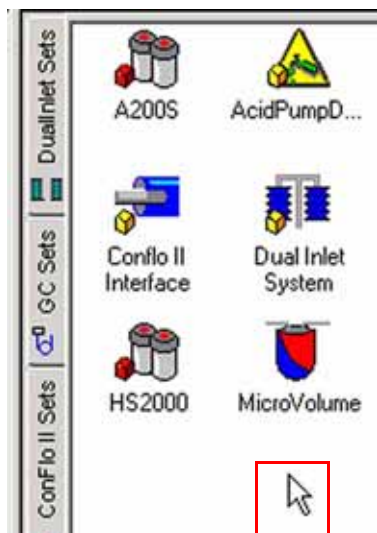


5. Note that *Advanced Mode* is displayed down right above the system tray.



6. Click the *Devices* tab.

Creating a new User Device

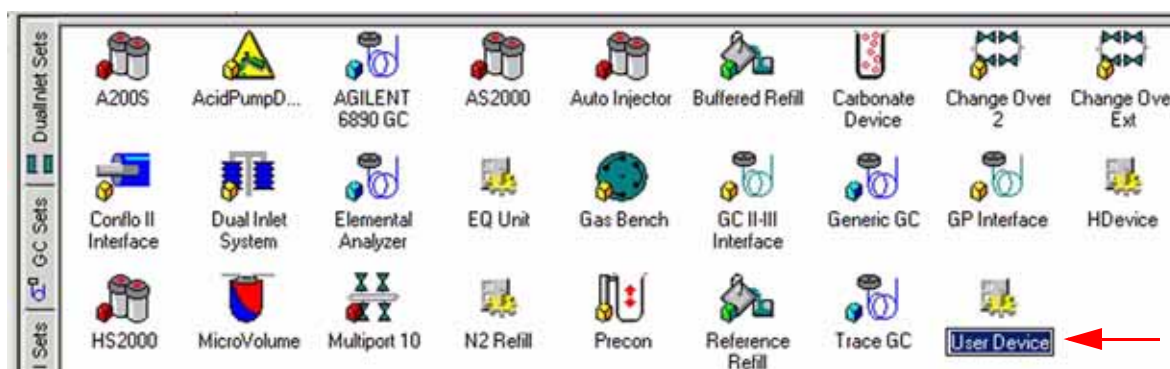


1. The window shown above is called **Configuration Editor**. The devices **predefined** by Thermo Electron are shown in its right pane.
2. To create a **new user device**, right-click somewhere in the pane.

Note. Do not click on an existing device!



3. The **Add User Device** button appears. Click on it.



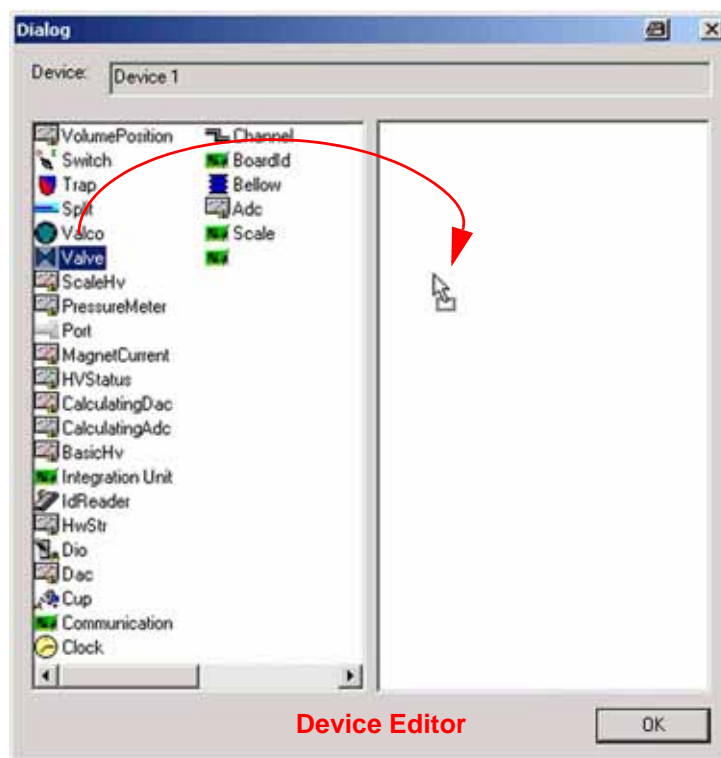
4. A new user device has been created and added to the predefined devices.
5. Give it a significant name (e.g. "Device 1").

Editing a new User Device

The new user device just created contains nothing and must now be specified. To edit it proceed as follows:

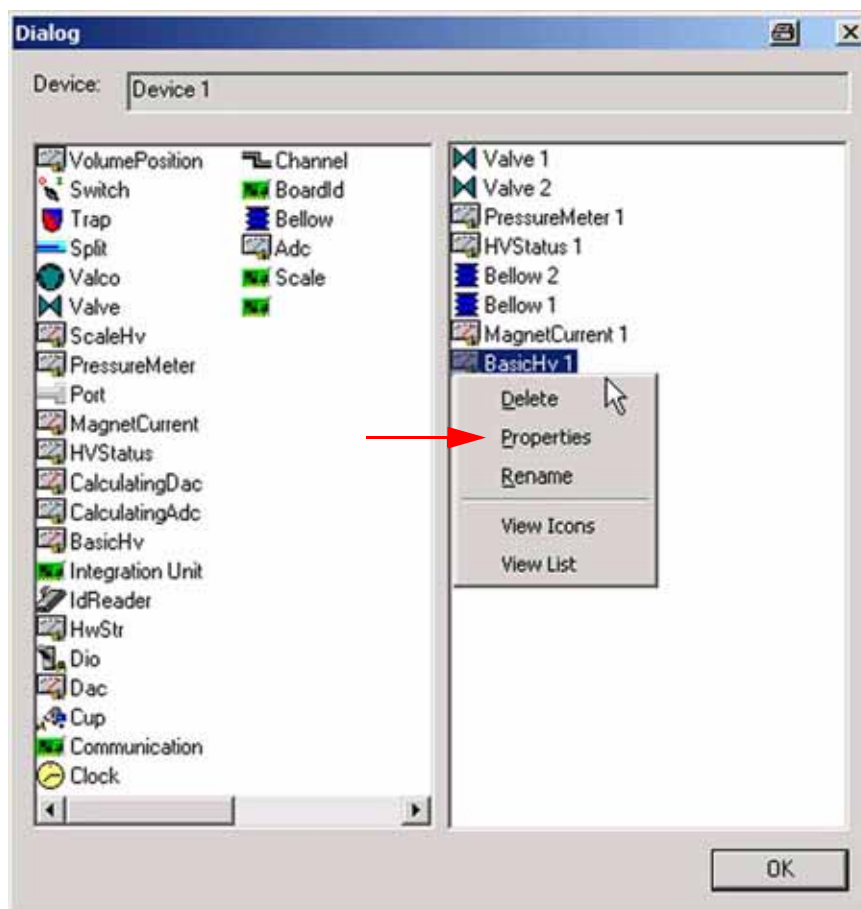


1. **Right-click** on the device:
Delete will remove the device.
Duplicate leads to another new user device.
Properties allows to specify properties of the *device* itself (e.g. IDs).
Rename assigns a new device name.
Edit allows to specify properties of the *objects* that are components of the device.
2. Select **Edit** or **double-click** the device.



3. The **Device Editor** appears.
4. Mark the first object intended (e.g. a Valve).
5. **Drag&Drop** it to the right pane.

6. Repeat this with further objects until your device is complete.



7. You can revise your decisions by a **right-click** on an object:
Delete removes the object. To delete more than one object, mark them by **<Shift>** or **<Ctrl>** before pressing **Delete**.
Properties gives detailed object information.
Rename assigns an alternative object name.
View Icons shows the objects as icons.
View List shows the objects in a list.
8. Select **Properties** to define the properties of an object (e.g. of a valve).

9. The parameters to be specified in the particular box differ between objects.

Example: The case of a valve

- **Optional:** if this checkbox is marked, you will be asked during each drag&drop whether the corresponding valve has been installed at all.
- **Standard Inlet:** this checkbox must be marked, if it is a standard inlet (e.g. Reference 1). If so, the valve will be available at “Standard Ports” in the Continuous Flow Method.
- **Installed:** Under certain conditions hardware is optional. If it is optional, you are asked during insertion, whether the valve has been installed or not.

Note. This check box is system-controlled. Always keep it marked!

- **Monitor during Acquisition:** Mark this checkbox, if you want the status of this object to be monitored during acquisition.

10. Make your decisions and finally confirm by **OK**.

1.2 Panel Design

Principle: Besides to creating and editing a new user device in the Configurator (see topics **Creating a new User Device** on page 1-4 and **Editing a new User Device** on page 1-5) you can customize its visualization in any application. This is called Panel Design.

Creating a Visualization

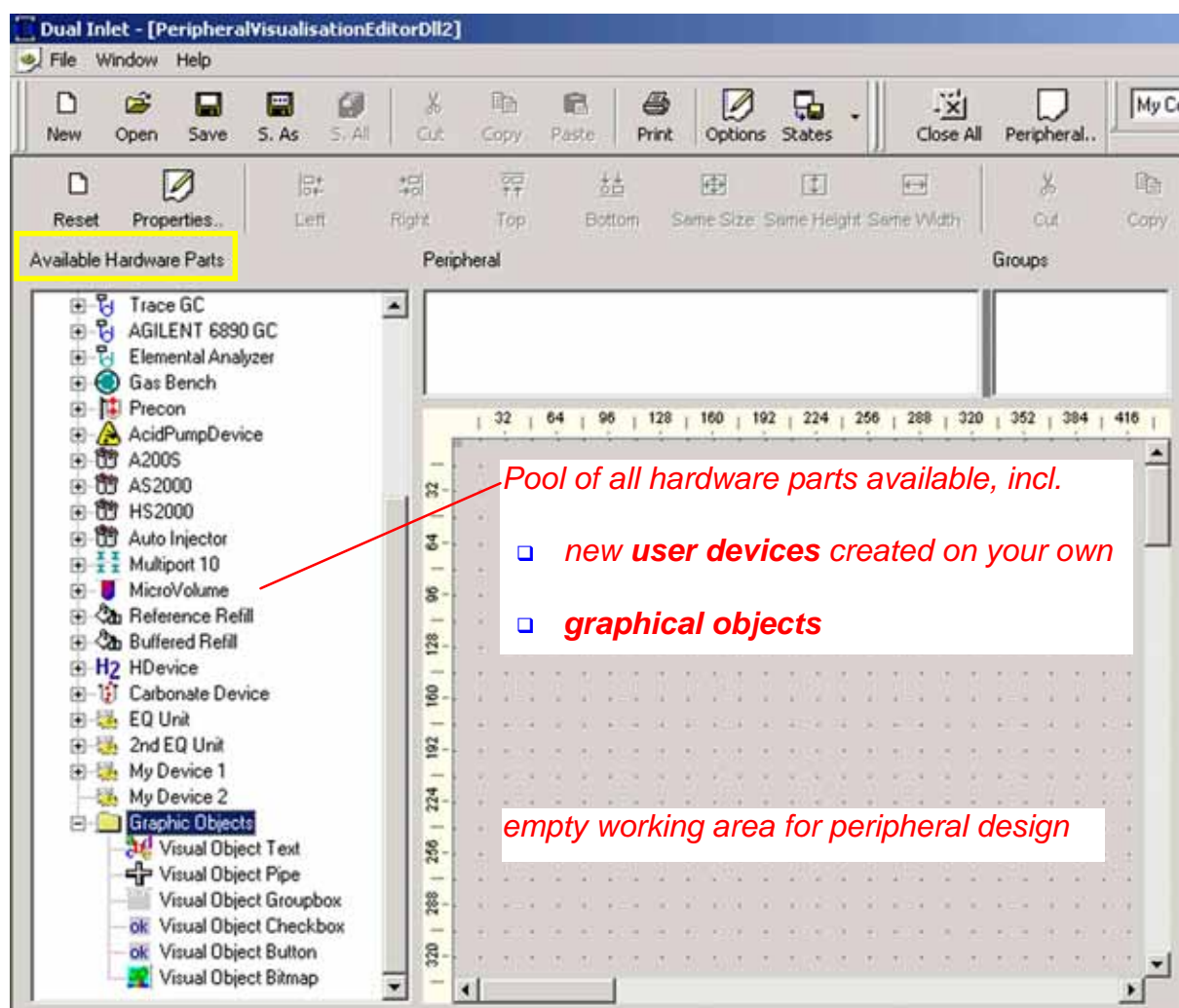


1. Start an arbitrary application, e.g. “Dual Inlet ACQ”.

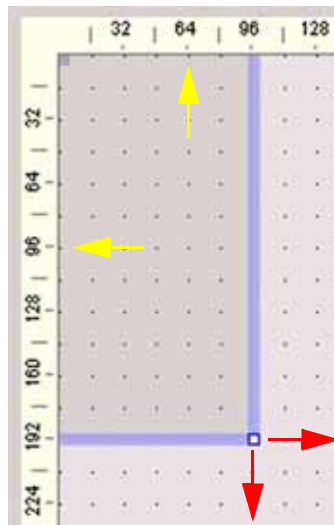
2. Press the **New** button .



3. Press **Peripheral Visualisation Editor Dll** and confirm by **OK**.
The Panel Editor will appear.



4. The entire document is called **Control Panel Designer**.
5. The empty working area on the right is utilized for panel design.



Two violet lines enclose it, one in vertical and one in horizontal direction. They serve as an orientation aid: to ensure identical sizes and appearances of the different dialogs within the working area use the vertical and horizontal rulers (e.g. always create standardized dialogs of 480 pixels * 480 pixels). Use the sizing handle at the edge to adjust the dimensions of the actual dialog.

Panel Design using Hardware Components

Principle: Thermo Electron still predefines the “classical” panels for the standard peripherals and devices. You can now change them. In addition, you can combine single hardware components or peripherals to design complete panels on your own, e.g. using your new user devices (see topic **Creating a new User Device** on page 1-4).

- Drag & drop a hardware component into the working area.

Panel Design using Graphical Objects

Principle: Graphical objects are used as an illustration aid for predefined and self-designed hardware devices (see topics **Creating a new User Device** on page 1-4 and **Editing a new User Device** on page 1-5). Graphical objects are mostly passive as they are not involved in hardware actions. The only exception, Visual Object Button, describes actions, as it actively allows scripts to be accessed and executed.

On the contrary, active hardware and hardware actions are summarized directly beneath “Available Hardware Parts” (see topic **Creating a Visualization** on page 1-8).

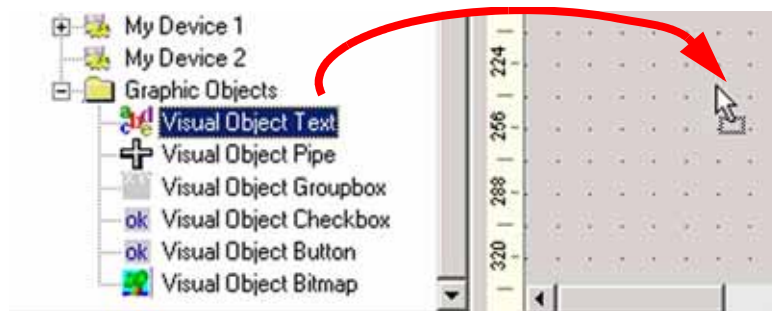
Panel design using graphical objects will be described in detail only for Visual Object Text. The properties of the other graphical objects are very similar. Therefore, only their particularities will be discussed.

The following six graphical objects are available:

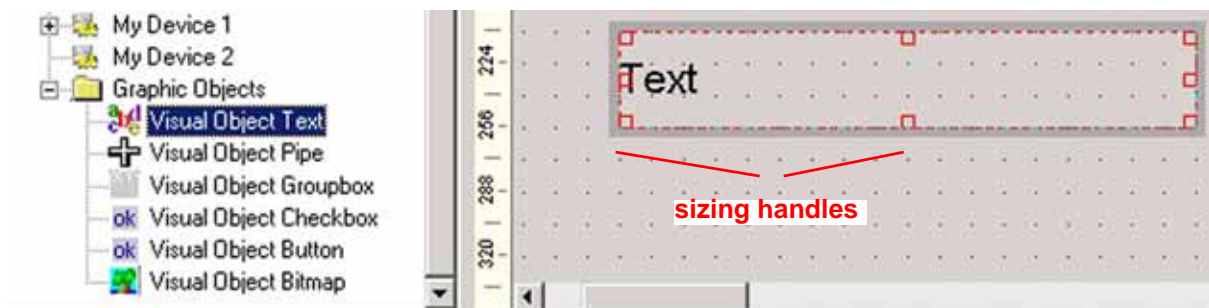
- Visual Object *Text*
- Visual Object *Groupbox*
- Visual Object *Button*
- Visual Object *Pipe*
- Visual Object *Checkbox*
- Visual Object *Bitmap*

Visual Object Text

Principle: Use text within a text box to describe the function of single hardware components, combinations of them or even complete panels.



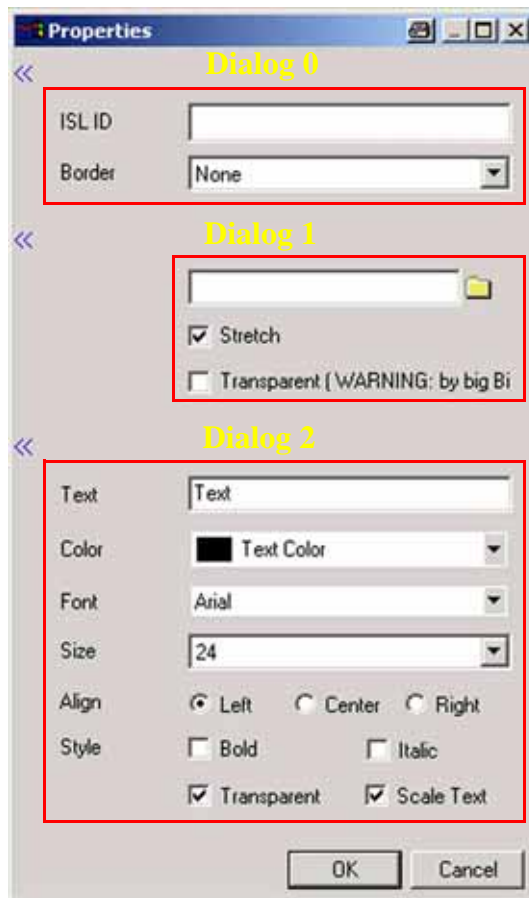
1. Click on a graphical object.
2. Drag & drop it into the working area (e.g. “Visual Object Text”).
The graphical object will be shown on the right side (e.g. a text box).
3. To change its *position*, click into the box, keep the left mouse button pressed and move your mouse.
4. To change its *dimensions*, use the sizing handles at the edges of the object.



5. Note that an entry appears in the **Peripheral** box above the working area (e.g. “Visual Object Text”).



6. The graphical object can be modified by **double-clicking** it.



ISL ID assign an ISL ID to the graphical object. Via this ID, the object can be analyzed by ISL scripts. This makes especially sense in case of text fields and checkboxes.

Border choose between four rectangular border types around the text box or, by “None”, select no border at all.

Type the name of a graphic as background picture or click the folder symbol to specify its path.

It can be stretched to span the entire text box or be transparent.

Gif-files can not be used as background pictures within text boxes.

7. **Text** type in the text to be displayed in the text box.
8. **Color** define text color and color of the background. **To display the background color, unmark the “Transparent” check box. To display a background picture, mark it.**
9. Define **Font**, **Font Size**, **Alignment** and **Style** of the text.
10. **Scale Text** The text can further be scaled: if the checkbox is marked, the text dimensions will be changed depending on the working area’s size. If it is unmarked, the text dimensions remain as originally set.

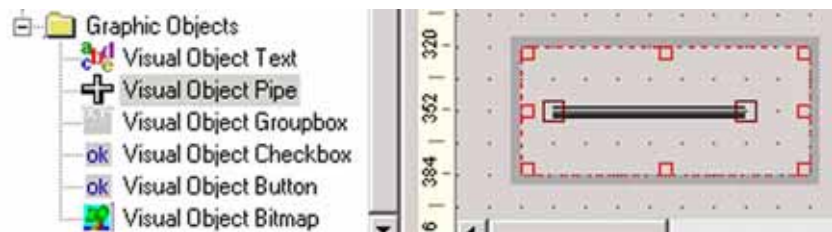
11. **Transparent** The entire object will be displayed transparent, if the checkbox is marked. Thereby, in case of several text boxes, one or more of them can be covered by other objects.

To increase clarity, use <<. Thereby, single dialogs can selectively be masked.

12. Define the properties of the graphical object. Note that most of your statements are updated immediately. Finally, confirm by **OK**.

Visual Object Pipe

Principle: This visual object serves to represent gas flows through pipes or capillaries (i.e. layout of piping systems).



1. After drag&drop, a pipe is displayed.
It is recommended to increase the surrounding box above maximum spread of the pipe using the sizing handles of the box.
The pipe can then be edited by a **double-click**.



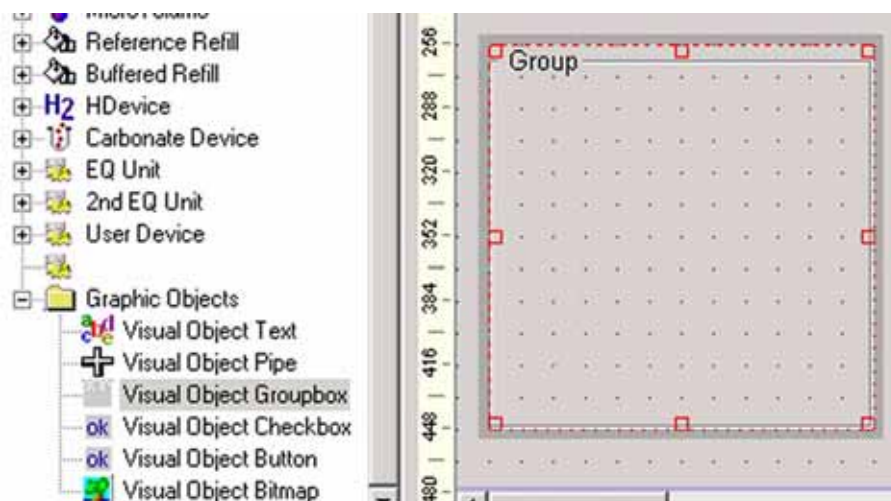
2. Assign an **ISL ID** and choose a **border** type as was shown for a text.
3. Finally, confirm by **OK**.
4. Change the **shape and orientation of the pipe** inside the box using the sizing handles at the ends of the pipe.
5. Change the **dimensions of the box** using its sizing handles (according to the dimensions of the piping system to be represented).
6. **Move the box** that contains the pipe by a click in the box and keep the left mouse button pressed while moving your mouse.



7. To represent branched gas flows, a right-click on a sizing handle allows to *insert* new points or to *delete* old ones. A left-click confirms the new point.

Visual Object Groupbox

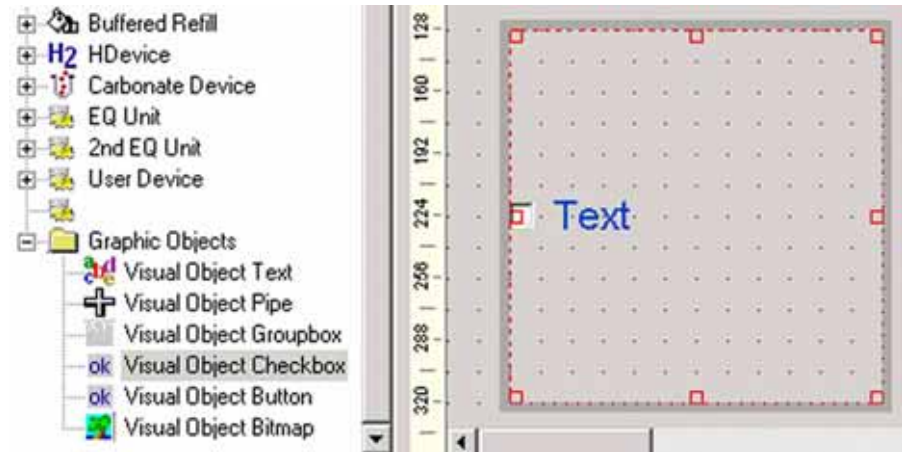
Principle: This graphical object merely serves as visualization aid as it bunches together several objects optically - not logically - within one box. The groupbox is moved as a whole, i.e. the single objects within it are moved together without changing their relative positions.



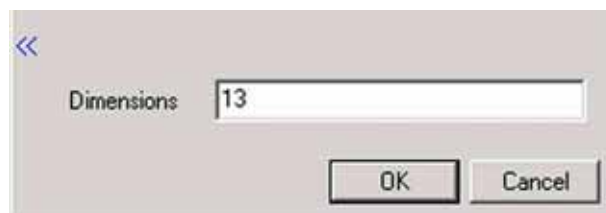
1. After drag&drop, a groupbox is displayed, which can be edited by a *double-click*.
2. To define its properties and to modify its dimensions, refer to Visual Object *Text*.

Visual Object Checkbox

Principle: This object visualizes that parameters must be checked by a script (e.g. the parameter “Text” or an ISL ID). A checkbox can be combined with a button.



1. After drag&drop, a checkbox is displayed, which can be edited by a **double-click**.



Note the additional dialog **Dimensions**.

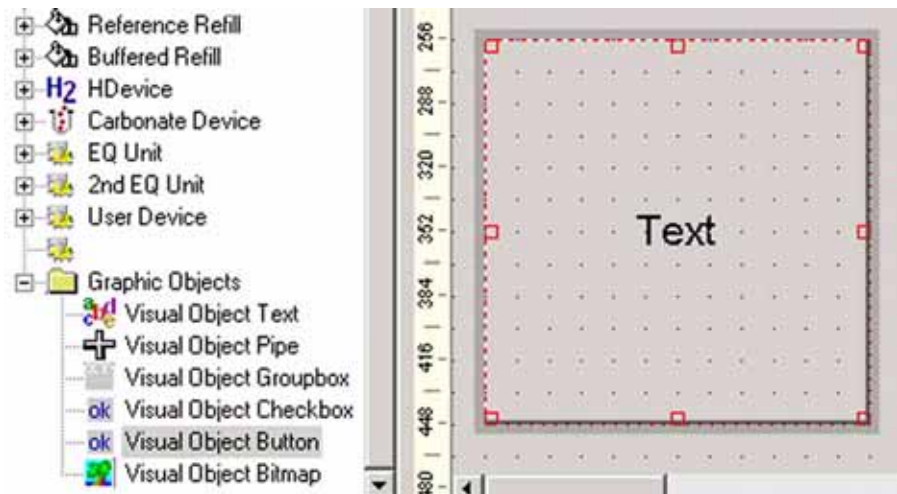
2. Type a number to define the dimensions of the checkbox (default: 13).

Note. To mark or unmark a checkbox, switch to Simulation Mode. This is impossible in Design Mode.

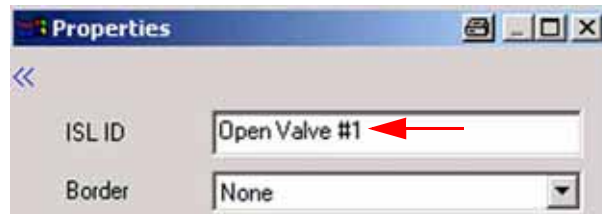
Visual Object Button and Script Editing

Principle: A button can be used to completely control various kinds of scripts externally: apply a script to a button to get it processed after the button has been pressed.

Example: Via the ISL ID, the script verifies whether a valve is open and whether the user has marked or unmarked the corresponding checkbox.



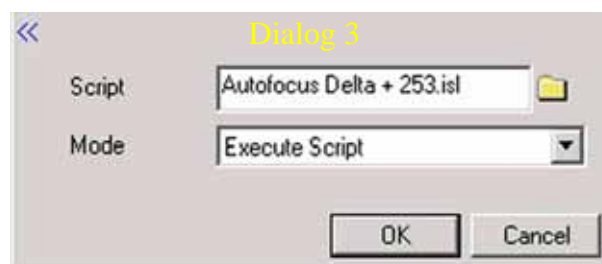
1. After drag&drop, a button is displayed in the shape of a text box, which can be edited by a **double-click**.



2. **ISL ID** Type a significant name for the ISL ID (e.g. “Open Valve #1”, if the ISL ID will be used to verify the status of valve #1).



3. **Text** Type a significant name for the button (e.g. “Open Valve #1”, if the button will be used to start a script that controls the status of valve #1).



Note the additional dialog.

Script To apply a script to the button, type the name of an ISL-script (e.g. “Autofocus Delta + 253.isl”) or click the folder symbol to specify its path.

Mode To define what is intended with the script, choose between:

Execute Script The script will simply be executed when the button is pressed.

Edit Dyn. Externals Dynamic Externals are dynamic variables within scripts that can be changed externally here.

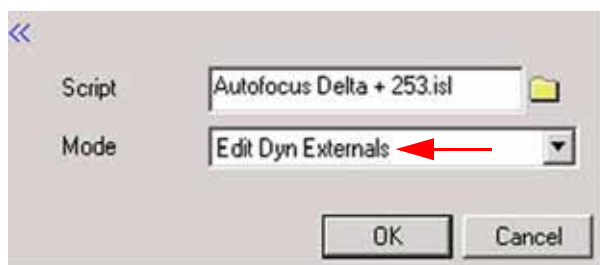
Edit Hardware Components Changes hardware parameters, a particular type of Dynamic Externals.

4. Switch to *Simulation Mode* by a right-click.

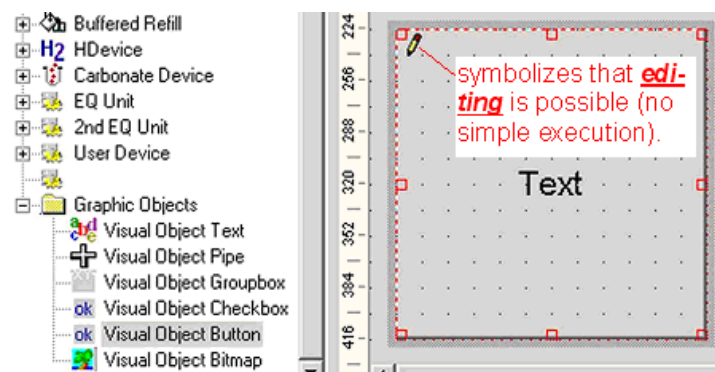
In *Design Mode*, no effects will be obtained.

5. Finally, click on the button. The process, which has been specified at Mode will run (e.g. the script is processed).

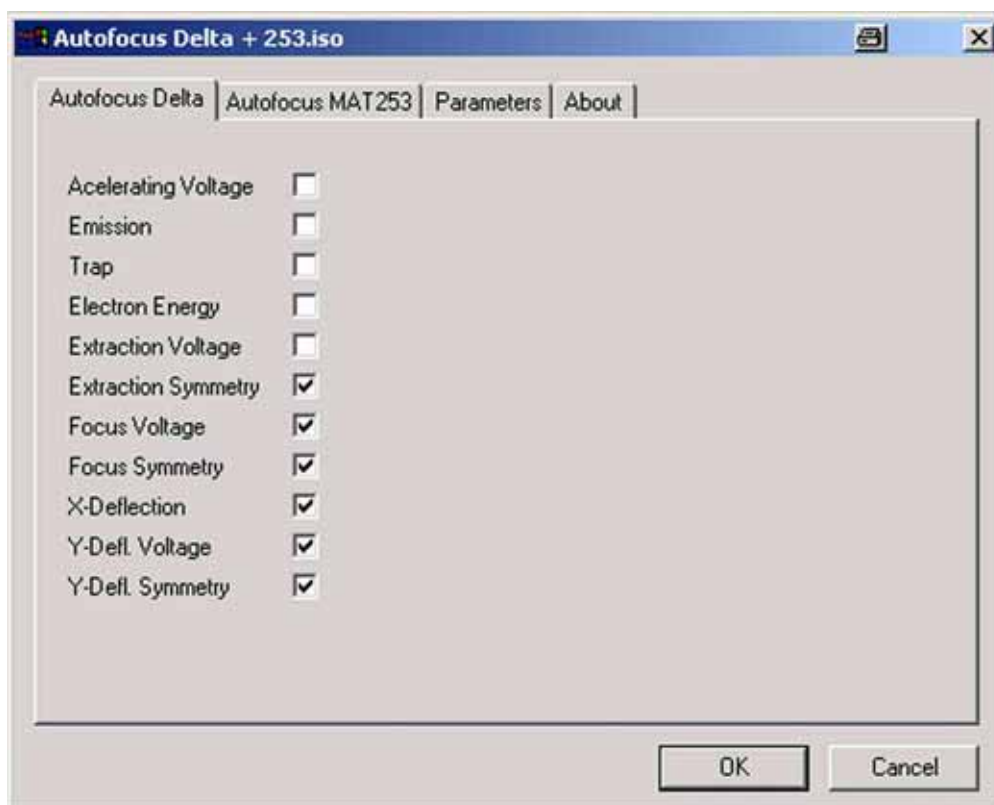
Example: Edit Dyn. Externals



1. Choose *Edit Dyn. Externals* and select a script.
2. Confirm by **OK**.



3. The symbol indicates that editing is possible (not a simple execution as usual).
4. Right-click somewhere on the working area.
5. Switch to *Simulation Mode*.
6. In Simulation Mode, click the button.

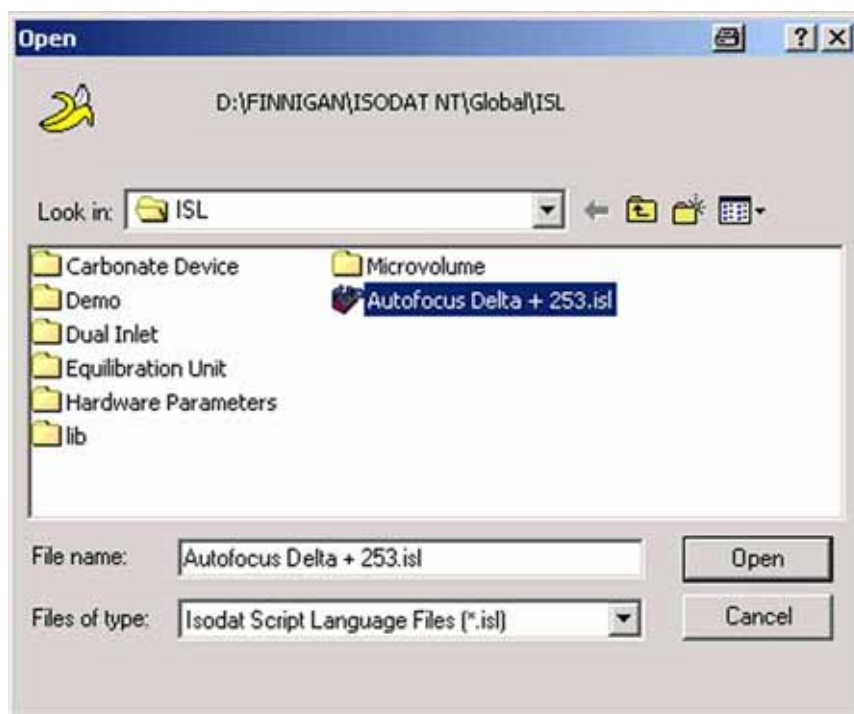


7. **Edit** the dynamic externals across the different tabs (e.g. “accelerating voltage”). The tabs and positions where the variables occur are stated together with their dialog identifiers (*.iso indicates the future parameter set of an *.isl script).
8. Finally, confirm by **OK**.

Script editing (case of dynamic externals)

1. To open a script, press the **Open** button





2. Select the script to be opened (e.g. “Autofocus Delta + 253.isl”) in the directory *[Finnigan\ISODAT NT\Global\ISL]*.
3. Confirm by **Open** and wait until the script is loaded.

```

dynexternal bool b_DeltaAcceleratingVoltage=0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=20; DIALOG_IDENTIFIER="Acelerat
dynexternal bool b_DeltaEmission =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=40; DIALOG_IDENTIFIER="Emission
dynexternal bool b_DeltaTrap =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=60; DIALOG_IDENTIFIER="Trap";
dynexternal bool b_DeltaElectronEnergy =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=80; DIALOG_IDENTIFIER="Electron
dynexternal bool b_DeltaExtractionVoltage =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=100; DIALOG_IDENTIFIER="Extraction
dynexternal bool b_DeltaExtractionSymmetry =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=120; DIALOG_IDENTIFIER="Extracti
dynexternal bool b_DeltaFocusVoltage =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=140; DIALOG_IDENTIFIER="Focus Vc
dynexternal bool b_DeltaFocusSymmetry =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=160; DIALOG_IDENTIFIER="Focus Syan
dynexternal bool b_DeltaXDefl =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=180; DIALOG_IDENTIFIER="X-Deflecti
dynexternal bool b_DeltaYDeflVoltage =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=200; DIALOG_IDENTIFIER="Y-Defl. Sy
dynexternal bool b_DeltaYDeflSymmetry =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=220; DIALOG_IDENTIFIER="Y-Defl. Sy

dynexternal bool b_253AcceleratingVoltage=0; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=10; DIALOG_IDENTIFIER="Aceleration
dynexternal bool b_253Emission =0; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=30; DIALOG_IDENTIFIER="Emission
dynexternal bool b_253Trap =0; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=50; DIALOG_IDENTIFIER="Trap";
dynexternal bool b_253ElectronEnergy =0; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=70; DIALOG_IDENTIFIER="Electron
dynexternal bool b_253Extraction =0; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=90; DIALOG_IDENTIFIER="Extracti
dynexternal bool b_253Shield =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=110; DIALOG_IDENTIFIER="Shield";
dynexternal bool b_253FocusVoltage =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=130; DIALOG_IDENTIFIER="Focus Vc
dynexternal bool b_253FocusSymmetry =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=150; DIALOG_IDENTIFIER="Focus Syan
dynexternal bool b_253RPlate =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=170; DIALOG_IDENTIFIER="R-Plate"
dynexternal bool b_253YDeflVoltage =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=190; DIALOG_IDENTIFIER="Y-Defl.
dynexternal bool b_253YDeflSymmetry =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=210; DIALOG_IDENTIFIER="Y-Defl. Sy
dynexternal bool b_253EinzelVoltage =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=230; DIALOG_IDENTIFIER="Einzel Len
dynexternal bool b_253EinzelSymmetry =1; TAB_PAGE="Autofocus MAT253"; POSX=5; POSY=250; DIALOG_IDENTIFIER="Einzel I

dynexternal channel dyn_cChannel =0; TAB_PAGE="Parameters"; POSX=5; POSY=25; DIALOG_IDENTIFIER="Measuring Channel";
dynexternal int iIntegTime =125; TAB_PAGE="Parameters"; POSX=5; POSY=50; DIALOG_IDENTIFIER="Integration time";
dynexternal int MinStepWidth =1; TAB_PAGE="Parameters"; POSX=5; POSY=75; DIALOG_IDENTIFIER="Minimum Step width";
dynexternal int MaxStepWidth=100; TAB_PAGE="Parameters"; POSX=5; POSY=100; DIALOG_IDENTIFIER="Maximum Step width";
dynexternal int MinDelayTime=50; TAB_PAGE="Parameters"; POSX=5; POSY=125; DIALOG_IDENTIFIER="Minimum Delay time";
dynexternal int MaxDelayTime=500; TAB_PAGE="Parameters"; POSX=5; POSY=150; DIALOG_IDENTIFIER="Maximum Delay time";
dynexternal int MaxIterations=3; TAB_PAGE="Parameters"; POSX=5; POSY=175; DIALOG_IDENTIFIER="Maximum Iterations";
dynexternal int PotiTurns=2; TAB_PAGE="Parameters"; POSX=5; POSY=200; DIALOG_IDENTIFIER="Simulated Poti turns"

```

Principle: The script above controls the occurrence of dynamic externals in their dialogs (i.e. where and how they appear). It is organized in “blocks”.

A “block” covers any of the dynamic externals that will occur on the *same tab page*. A single row inside the “block” defines details of *one* particular dynamic external.

Use script editing to customize the appearance of variables, dialogs and tab pages totally on your own. E.g. change a dialog identifier to modify the text representing a dynamic external. After editing it, a script can be tested in Simulation Mode.

```
script Autofocus
{
    1          2          3
    dynexternal bool b_DeltaAcceleratingVoltage=0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=20; DIALOG_IDENTIFIER="Acelerat
    dynexternal bool b_DeltaEmission =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=40; DIALOG_IDENTIFIER="Emission
    dynexternal bool b_DeltaTrap =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=60; DIALOG_IDENTIFIER="Trap";
    dynexternal bool b_DeltaElectronEnergy =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=80; DIALOG_IDENTIFIER="Electron
    dynexternal bool b_DeltaExtractionVoltage =0; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=100; DIALOG_IDENTIFIER="Extracti
    dynexternal bool b_DeltaExtractionSymmetry =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=120; DIALOG_IDENTIFIER="Extracti
    dynexternal bool b_DeltaFocusVoltage =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=140; DIALOG_IDENTIFIER="Focus Vo
    dynexternal bool b_DeltaFocusSymmetry =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=160; DIALOG_IDENTIFIER="Focus Sy
    dynexternal bool b_DeltaXDefl =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=180; DIALOG_IDENTIFIER="X-Deflec
    dynexternal bool b_DeltaYDeflVoltage =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=200; DIALOG_IDENTIFIER="Y-Defl.
    dynexternal bool b_DeltaYDeflSymmetry =1; TAB_PAGE="Autofocus Delta"; POSX=5; POSY=220; DIALOG_IDENTIFIER="Y-Defl.
```

The uppermost “block” of the script is shown above.

```
dynexternal bool b_DeltaAcceleratingVoltage=0;
dynexternal bool b_DeltaEmission =0;
dynexternal bool b_DeltaTrap =0;
dynexternal bool b_DeltaElectronEnergy =0;
dynexternal bool b_DeltaExtractionVoltage =0;
dynexternal bool b_DeltaExtractionSymmetry =1; 1
dynexternal bool b_DeltaFocusVoltage =1;
dynexternal bool b_DeltaFocusSymmetry =1;
dynexternal bool b_DeltaXDefl =1;
dynexternal bool b_DeltaYDeflVoltage =1;
dynexternal bool b_DeltaYDeflSymmetry =1;
```

dynexternal declares a *dynamic external*, i.e. a *variable* that can be shown as part of a dialog (e.g. *b_DeltaAcceleratingVoltage*, *b_DeltaEmission*, etc.).

bool is the *type of this variable* (as is integer, channel etc.). As a true/false decision, it implies a checkbox that is either marked or unmarked (E.g. *channel* would be another type of variable leading to a list of the channels which are available in the actual gas configuration).

DeltaAcceleratingVoltage, *DeltaEmission*, etc. are the declared *dynamic externals* themselves.

1 indicates that the checkbox in the dialog is *marked*, i.e. the dynamic external will be *checked*. In case of *0*, the checkbox in the dialog is *unmarked* and therefore, the dynamic external will *not* be checked.


```
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=20;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=40;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=60;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=80;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=100;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=120;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=140;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=160;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=180;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=200;
TAB_PAGE="Autofocus Delta"; POSX=5; POSY=220;
```

2

“Autofocus Delta” is the *name of the tab page* where the dynamic external will occur.

PosX describes the *horizontal position* of the dynamic external on that tab page (e.g. 5).

PosY describes the *vertical position* of the dynamic external on that tab page (e.g. 20).

```
DIALOG_IDENTIFIER="Accelerating Voltage";
DIALOG_IDENTIFIER="Emission";
DIALOG_IDENTIFIER="Trap";
DIALOG_IDENTIFIER="Electron Energy";
DIALOG_IDENTIFIER="Extraction Voltage";
DIALOG_IDENTIFIER="Extraction Symmetry";
DIALOG_IDENTIFIER="Focus Voltage";
DIALOG_IDENTIFIER="Focus Symmetry";
DIALOG_IDENTIFIER="X-Deflection";
DIALOG_IDENTIFIER="Y-Defl. Voltage";
DIALOG_IDENTIFIER="Y-Defl. Symmetry";
```

3

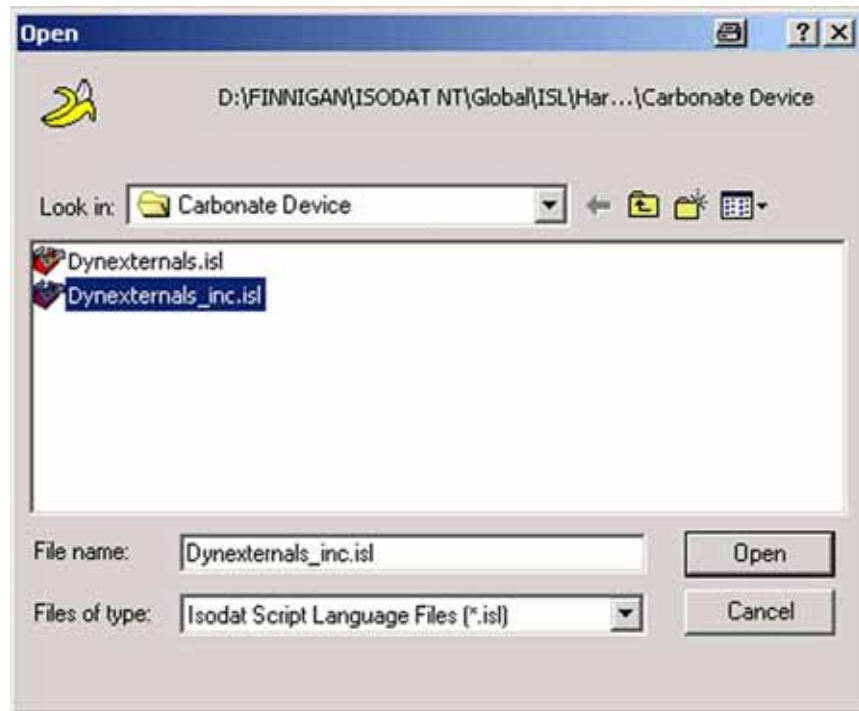
Dialog Identifier serves as *representation* to identify the dynamic external by describing the *text* that will occur next to it in the dialog (e.g. “Accelerating Voltage”, “Emission”, “Trap”, etc.).

Example: Edit Hardware Components

A hardware device is characterized by hardware-specific parameter sets of its own (e.g. the carbonate device). As these parameters are used during acquisition, they will be loaded by acquisition scripts.

1. To load these parameter sets, press the **Open** button





2. Select the script to be opened (e.g. “Dynexternals_inc.isl” in the directory *\Finnigan\ISODAT NT\Global\ISL\Hardware Parameters\Carbonate Device*). Confirm by **Open** and wait until the script is loaded.

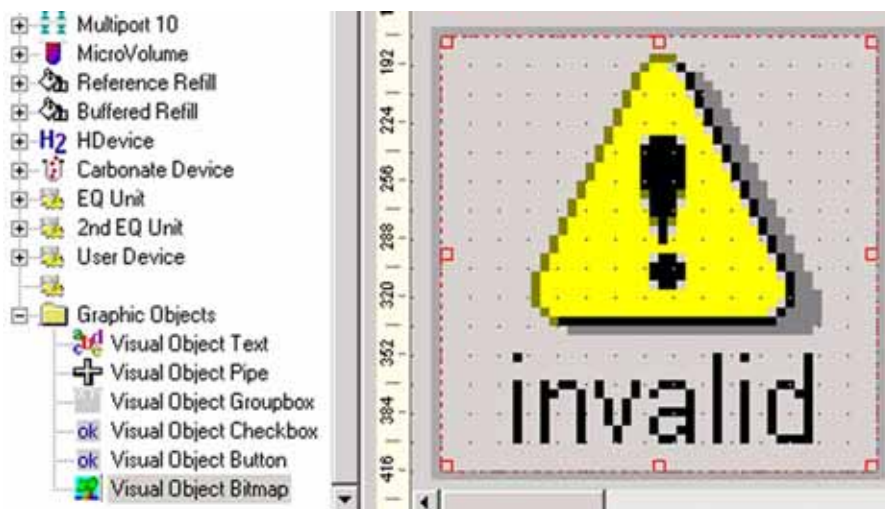
```
//carbonate definitions.....
// Page : Pressure Adjust
dynexternal number PREADJUSTPRESSURE1      =300;TAB_PAGE="@Hardware@Pressure Pre Adjust";
dynexternal number PREADJUSTSIGNAL1          =3000;TAB_PAGE="@Hardware@Pressure Pre Adjust";
dynexternal number PREADJUSTPRESSURE2       =700;TAB_PAGE="@Hardware@Pressure Pre Adjust";
dynexternal number PREADJUSTSIGNAL2         =7000;TAB_PAGE="@Hardware@Pressure Pre Adjust";
dynexternal number MIN_SIGNAL_INTENSITY     =500;TAB_PAGE="@Hardware@Pressure Pre Adjust";
dynexternal number MAX_SIGNAL_INTENSITY     =7500;TAB_PAGE="@Hardware@Pressure Pre Adjust";
```

3. At the “TAB_PAGE” entry, note the term **@Hardware@** before the name of the tab page begins (e.g. “Pressure Pre Adjust”).

Hardware parameters are a particular class of dynamic externals. The only difference is, that they are filtered when being displayed. To let a dynamic external be displayed as a hardware parameter (i.e. as a hardware parameter set of a device), it must be marked by the preceding term **@Hardware@** as is shown above. If this term is missing, it will not be displayed as hardware parameter, but as a “normal” dynamic external.

Visual Object Bitmap

Principle: This visual object illustrates relationships graphically.



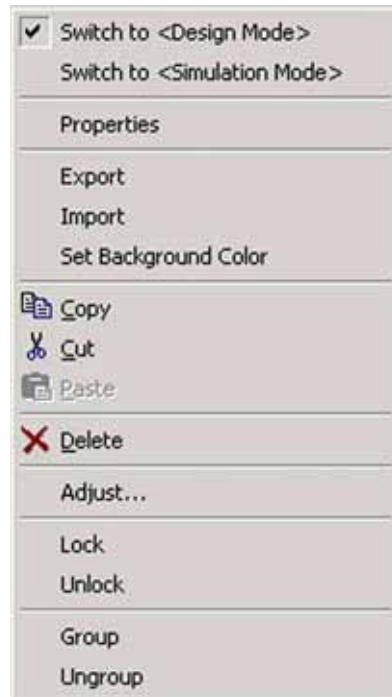
1. After drag&drop, a default bitmap is displayed, which can be edited by a *double-click*.



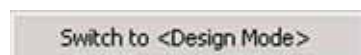
2. *ISL ID / Border*: refer to Visual Object *Text*.
3. Type the name of the picture of interest or click on the folder to specify its path. Choose between a variety of graphic formats:
In contrast to Visual Object Text, even gif-files can be used here as background pictures (animated or not).
 E.g. use an animated gif to represent pumps at work.
4. *Stretch / Transparent*: refer to Visual Object *Text*.

Context Menu

Principle: In Design Mode (default), the context menu appears upon a right-click on the working area. It offers a wide variety of commands, which will be discussed one by one in detail. The context menu is not available in Simulation Mode.



- **Design Mode** Default Mode, used to *edit* graphical objects and hardware components.
- **Simulation Mode** Used to *execute* scripts and *change* parameters after the editing phase in Design Mode. To return to Design Mode, right-click on the working area and then press **Switch to <Design Mode>**:



- **Properties**

Shows the Properties box of the object actually selected (e.g. a pipe) to edit its parameters. Therefore, this command is inactive until a graphical object has been placed onto the working area.

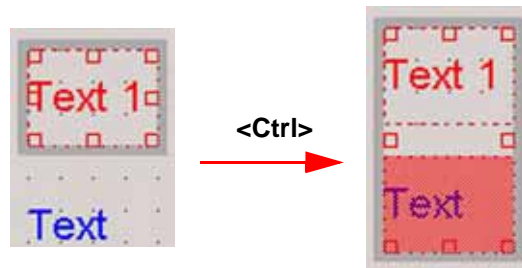


- **Set Background Color**



- a. Click on your favorite color or on **Define Custom Colors >>**.
- b. Then, confirm by **OK**.

Select more than one object



1. To handle more than one object simultaneously as a group, first select them all by keeping the **<Ctrl>** key pressed.

The object that was selected at last is active and therefore highlighted red (e.g. “Text”). As master, it determines all adjustments, i.e. the other graphical objects will be arranged relatively to it.

Special case: a single object can also be grouped (i.e. group consisting of only one element). Then, you can proceed with **Copy**, **Cut**, **Paste** or **Delete** as will be described below.

Copy / Paste:

- a. *Select* one or more objects (see above).
- b. *Right-click* and press **Copy**.
Right-click and press **Paste**.
Find the position of the copied object(s) by moving them with your mouse.
- c. After the position has been found, perform a *left click*.

Cut / Paste:

- a. *Select* one or more objects (see above).
- b. *Right-click* and press **Cut**.
Right-click and press **Paste**.
Find the position of the cut object(s) by moving them with your mouse.
- c. After the position has been found, perform a *left click*.

Delete:

- a. *Select* one or more objects (see above).
- b. *Right-click* and press **Delete**.



- c. Confirm by **Yes**.

As an alternative, use the *taskbar* above the working area:



Adjust:

Use this command to arrange objects relative to each other.

- a. Select one or more objects (see above).
b. **Right-click** and press **Adjust**.



- c. Choose **Adjust Left**, **Adjust Top**, **Adjust Right** or **Adjust Bottom** to match the relative *positions* of the selected objects.
The object that was selected at last is highlighted red.

As an alternative, use the *taskbar* above the working area:



- d. Choose **Same Size**, **Same Height** or **Same Width** to match the dimensions of the selected objects.

The object that was selected at last is highlighted red and forces its dimensions on the other selected objects.

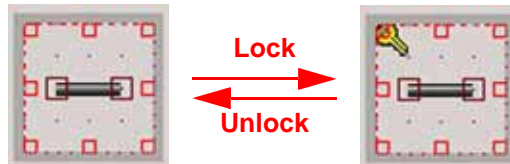
As an alternative, use the taskbar above the working area:



Lock:

Protects position and dimensions of an object from being changed.

- a. **Click** on the object to be locked.
- b. **Right-click** and press **Lock**. A key symbol appears.



Unlock:

Allows changing position and dimensions of an object again.

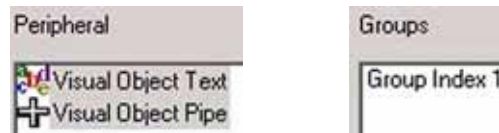
- a. **Click** on the locked object.
- b. **Right-click** and press **Unlock**. The key symbol disappears.

To create an *optical* group, group boxes are used (see above).

Contrary to that, use the **Group** command to obtain a *logical* group. **Ungroup** breaks up the group leading to independent graphical objects again.

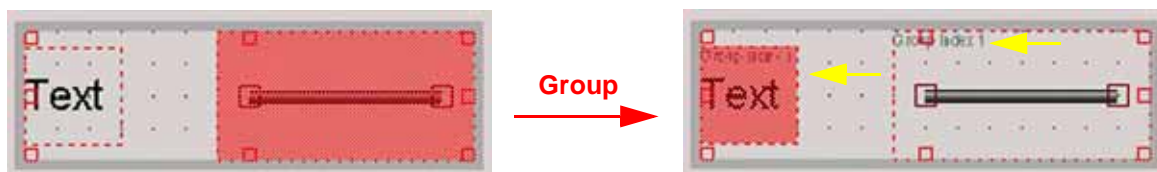
Group:

Notice that a new entry appears in the Groups box above the working area (e.g. "Group Index 1"). It denotes that the objects shaded gray in the Peripheral box now form a group.



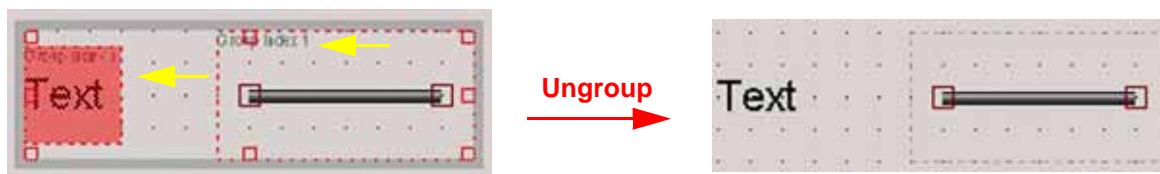
Click somewhere on the working area.

Notice that each object of the group is labeled as in the Groups box.



Ungroup:

- a. Click on a group to mark it.
- a. Right-click and press **Ungroup**.
- b. Click somewhere on the working area. The group no longer exists, but individual objects do.



You can **combine** the commands of the context menu, e.g. group objects that have previously been locked.

“Reset” button

Principle: Use it to clear your actual working area with or without saving it - e.g. to create a new visualization. The fields “Peripheral” and “Groups” above the working area will be cleared as well.

1. On the **taskbar** above the working area press the **Reset** button



2. If the actual visualization has never been saved before, you are asked to decide it now.
3. To save it, press **Yes** and refer to topic **Saving a Visualization** on page 1-30.
To discard your visualization without saving it, press **No**.
The working area will be cleared.

“Properties” button

1. On the **taskbar** above the working area, press the **Properties** button



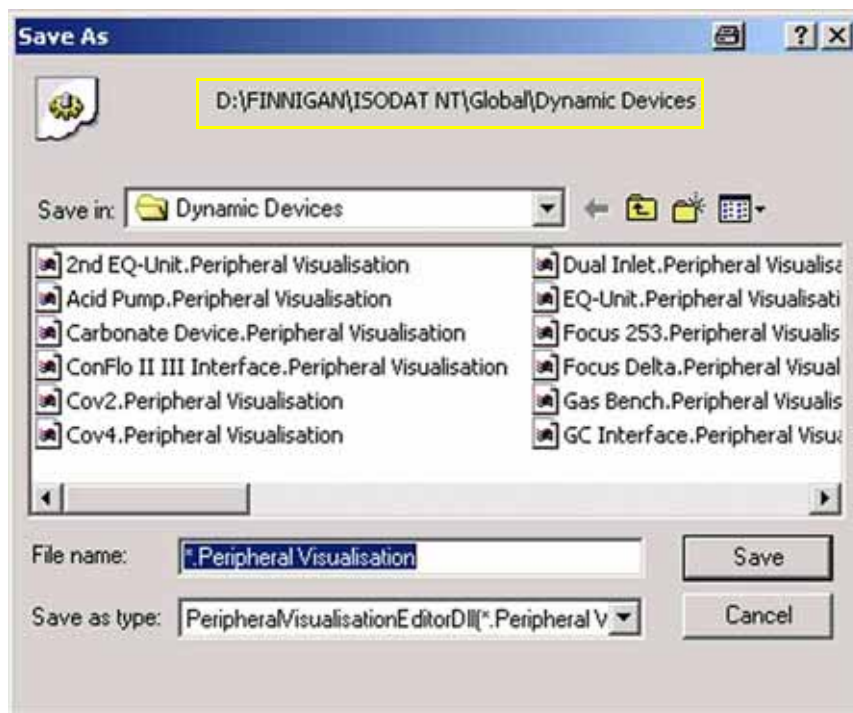
Combination of several graphical objects

Several graphical objects can be combined within one visualization.

Saving a Visualization

1. After designing one or more graphical objects, the entire visualization

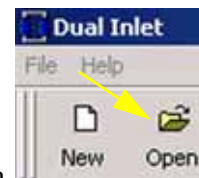
can be saved: press the **Save** or **Save As** button



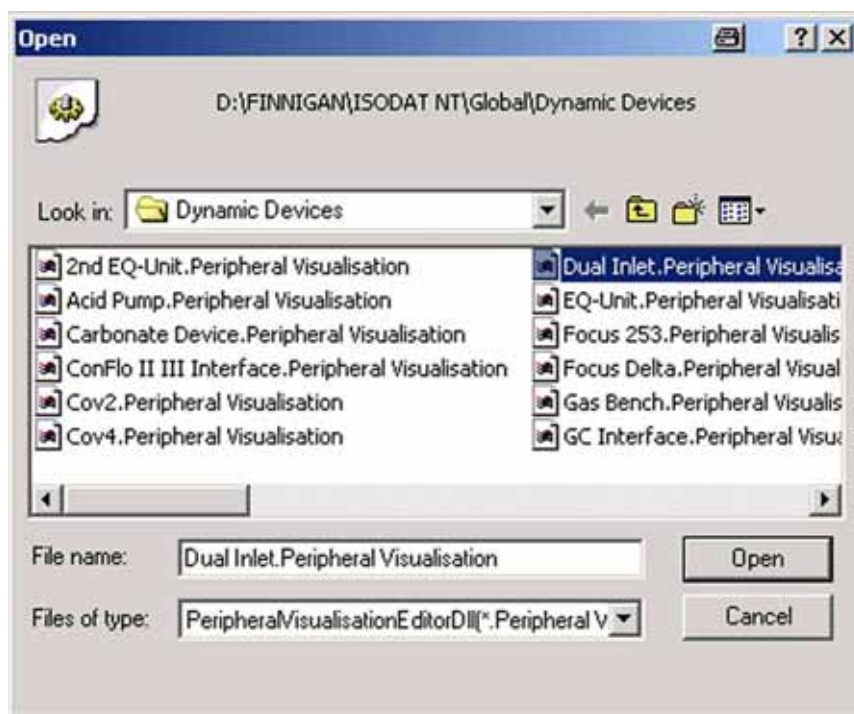
2. By default, the visualization will be stored in the folder *Dynamic Devices*. Accept it or choose another folder.
3. Type a significant file name and accept the extension *Peripheral Visualization*.
4. Press **Save**.

Loading a Visualization

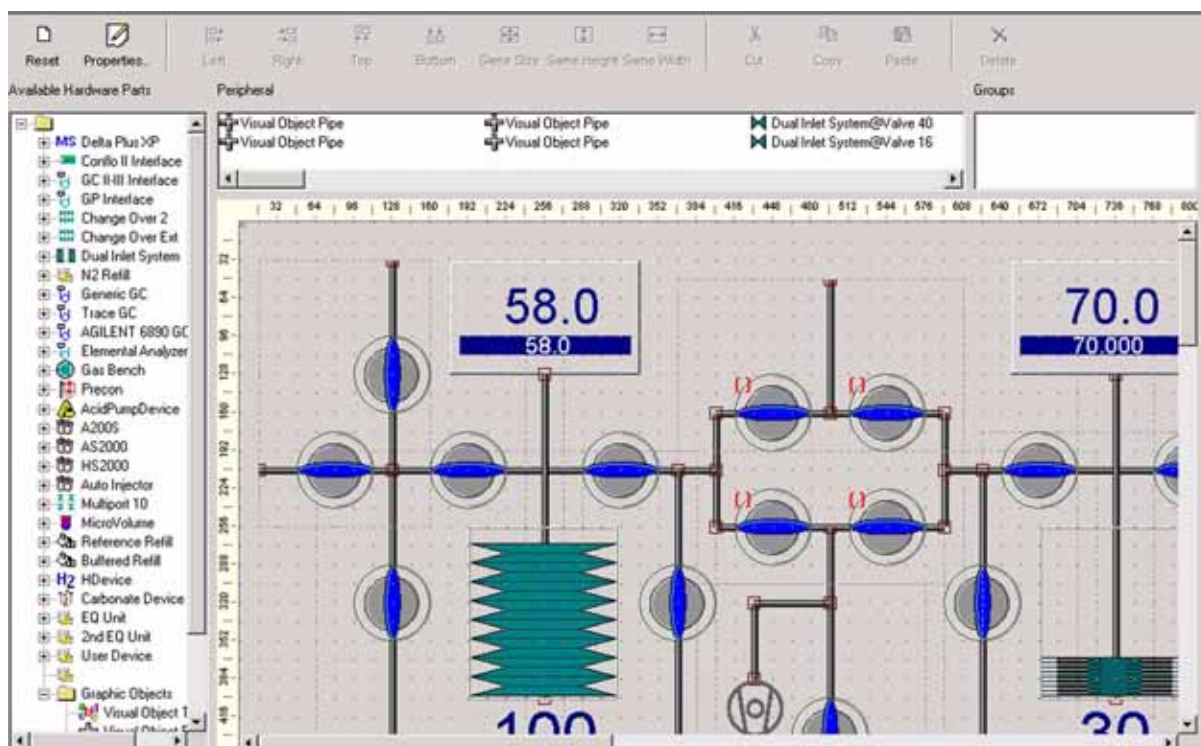
Thermo Electron delivered some predefined peripheral visualizations. Load one of them or one you created on your own as follows.



1. In the Application Mode, press the **Open** button



2. Search the folder that contains the visualizations (e.g. *Dynamic Devices*).
3. Choose the visualization to be loaded. Press **Open**.



4. The visualization can be used directly or edited.

1.3 Third Party Support

Principle: Thermo Electron offers configurations and methods to operate the following devices offered by external manufacturers (i.e. for “external devices”):

- A200S
- Agilent GC 6890
- PAL autosamplers
(GC PAL and Combi PAL)
- AS2000
- Trace GC

PAL autosamplers, e.g. GC PAL - as the direct successor of A200S - and Combi PAL, are to be run in A200S mode. Therefore later on, select A200S. The extension is A200S as well.

Adjusting the Properties of an external Device

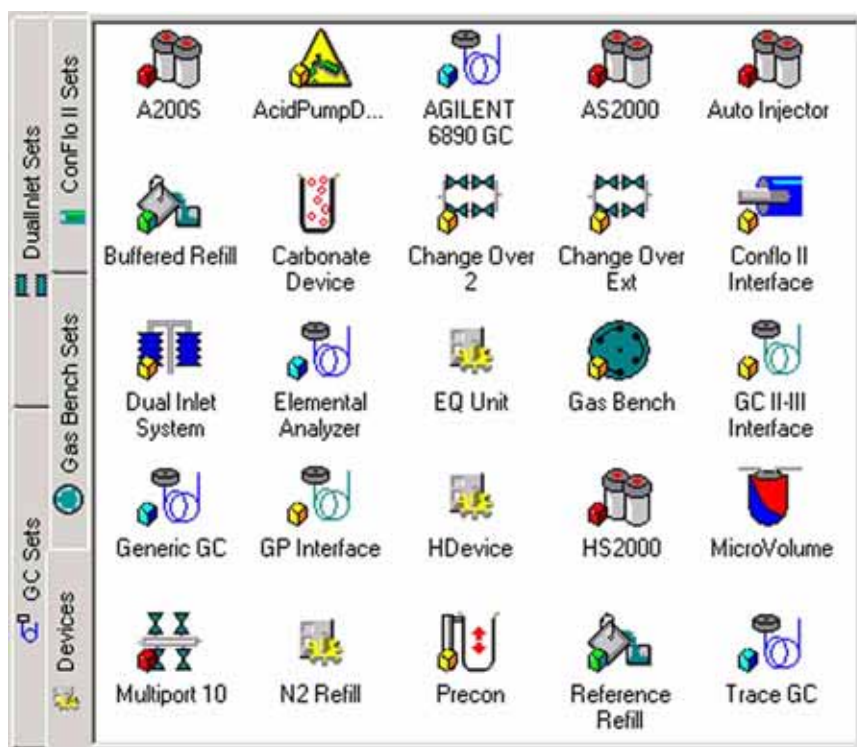
Principle: Many properties of the external manufacturer's device can be adjusted in the *Configurator*.



1. Open the Configurator .



2. Press the *Devices* tab .



3. Right-click or double-click on the external device whose properties you want to adjust (e.g. "A200S").

Note. If you have a PAL autosampler, i.e. a GC PAL or a Combi PAL, select A200S!



4. Click the **Properties** button.
5. The Configuration box appears. It allows individually adjusting the properties of the external device that has been selected. The adjustment of properties will now be shown for each of the various external devices.

Trace GC

Note. For further details about injectors and detectors, refer to the manual of the Trace GC.

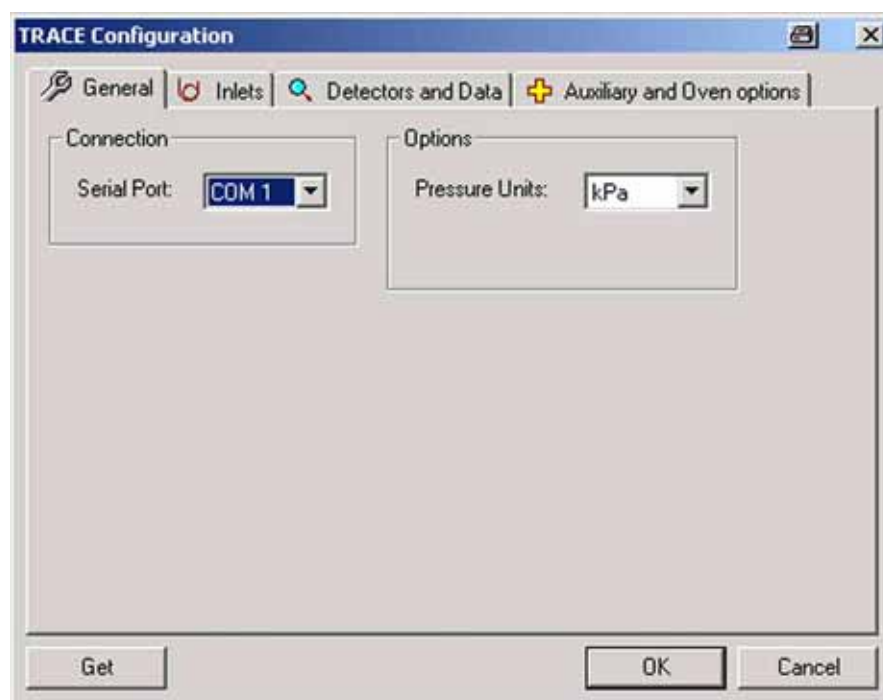
Configure your Trace GC as follows:



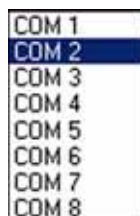
Trace GC

1. Double-click or right-click the **Trace GC** button

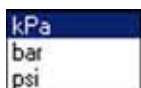
General tab



2. At **Serial Port**, specify **COM 2** as serial port your Trace GC is connected to.



3. At *Options*, choose between several pressure units (e.g. kPa).

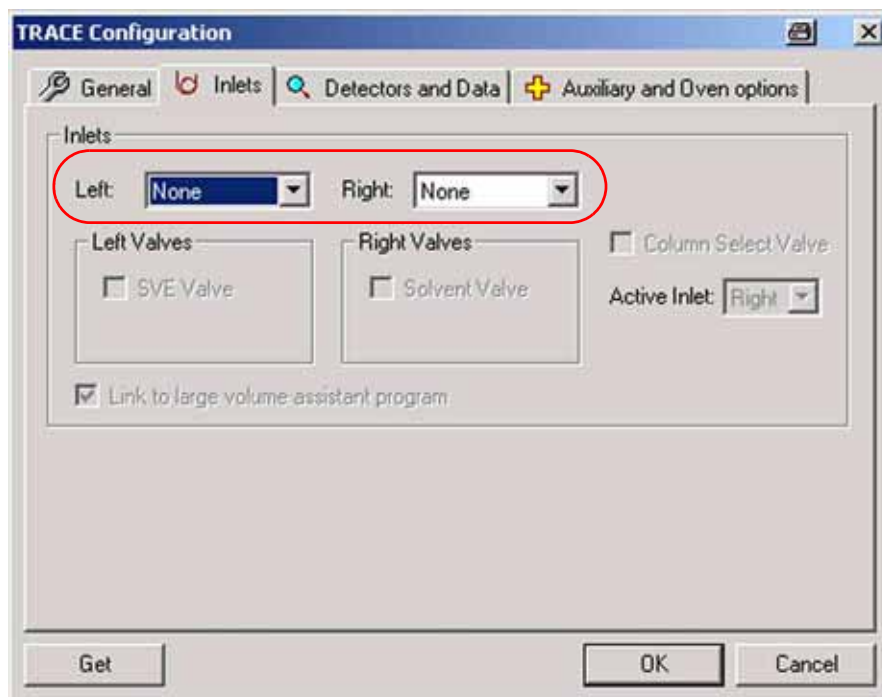


Setup via Trace GC (using the Get button)

Principle: You can edit a method not only via the Isodat software, but also at the Trace GC itself (i.e. at the hardware side). The method provided by the Trace GC can then be loaded into Isodat and will be used instead of the statements you declared in Isodat.

Note. The Get button always enables upload of GC parameters. Then, all inlets - i.e. injectors - and detectors are selected (in this case, it is unnecessary to specify these parameters via Isodat).

In case of Agilent 6890 GC and A200S, the editing options via the Isodat software are much more restricted. Therefore, many parameters must be adjusted externally, i.e. at the hardware.



Setup via Isodat 2.0 (i.e. manual setup)**Inlets tab**

- At Inlets tab, specify both the left and right injectors.

Note. In this version, Thermo Electron supports SSL and OCI as injector types, but not PTV.

Example: Left: SSL and Right: OCI

SSL split/splitless injector

OCI on-column injector

HOTOC high oven temperature cold on-column injector

LVOCI large volume on-column injector

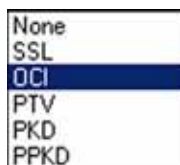
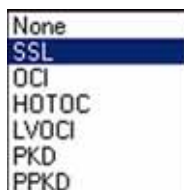
PTV programmable temperature vaporizing injector

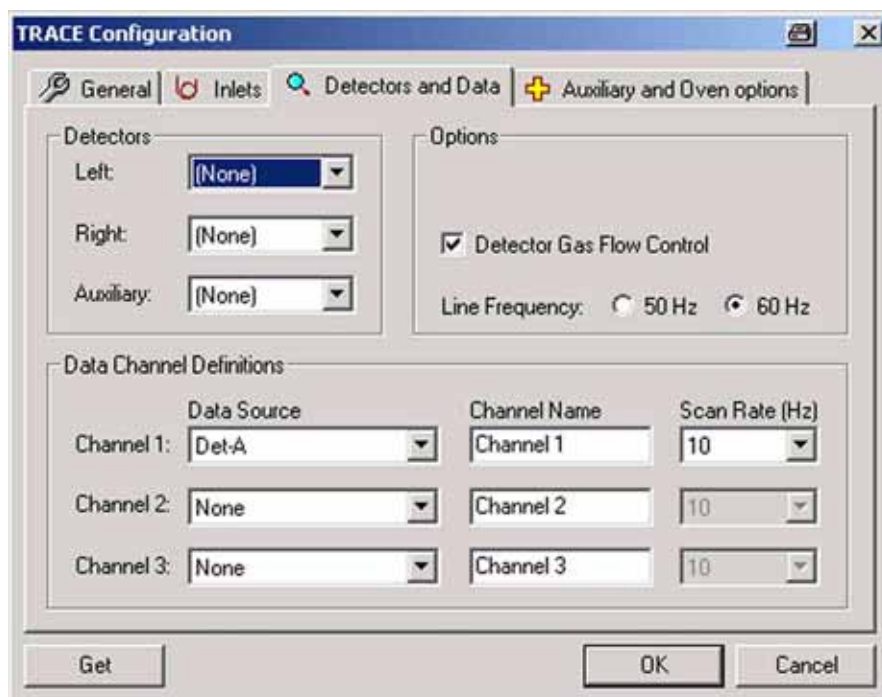
Not used for GC-IRMS:

PKD packed column injector

PPKD purged packed column injector

Note. If you select “None”, the respective tabs will not occur in the method later on!

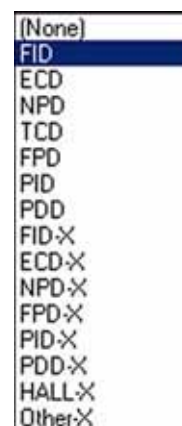


Detectors and Data tab

1. Specify the detectors available (left, right and auxiliary detector). In many cases, None will be selected (default), especially at Auxiliary. Mostly, only one detector will be present, i.e. left or right, whereas usage of two detectors (i.e. left and right) is rare.
2. The **Get** button will automatically upload the correct hardware position (i.e. whether a detector is located left or right).

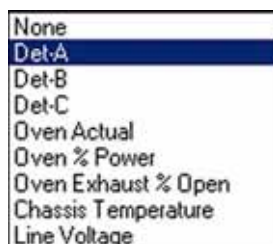
Used detectors are:

FID	Flame Ionization Detector
ECD	Electron Capture Detector
NPD	Nitrogen Phosphorus Detector
TCD	Thermal Conductivity Detector



Example: As left detector you might have a FID, and an ECD as the right one.

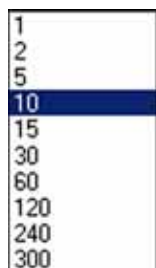
3. Select the data sources (i.e. channel sources) to be read out from Trace GC via different channels. Three channels - 1, 2, and 3 - can simultaneously be read out and will be displayed in the Acquisition module.

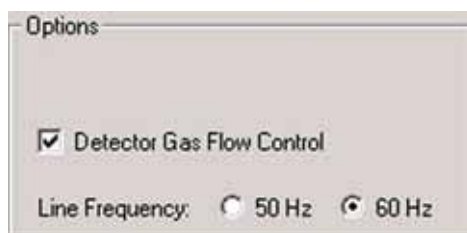


Example: At Data Source, assign “Det-A” to Channel 1, “Det-B” to channel 2 and “Oven actual” to Channel 3. (see above.)

At Channel Name, type a significant name for each channel (e.g. “FID” for Channel 1, “ECD” for Channel 2, “Oven actual” for Channel 3, see above).

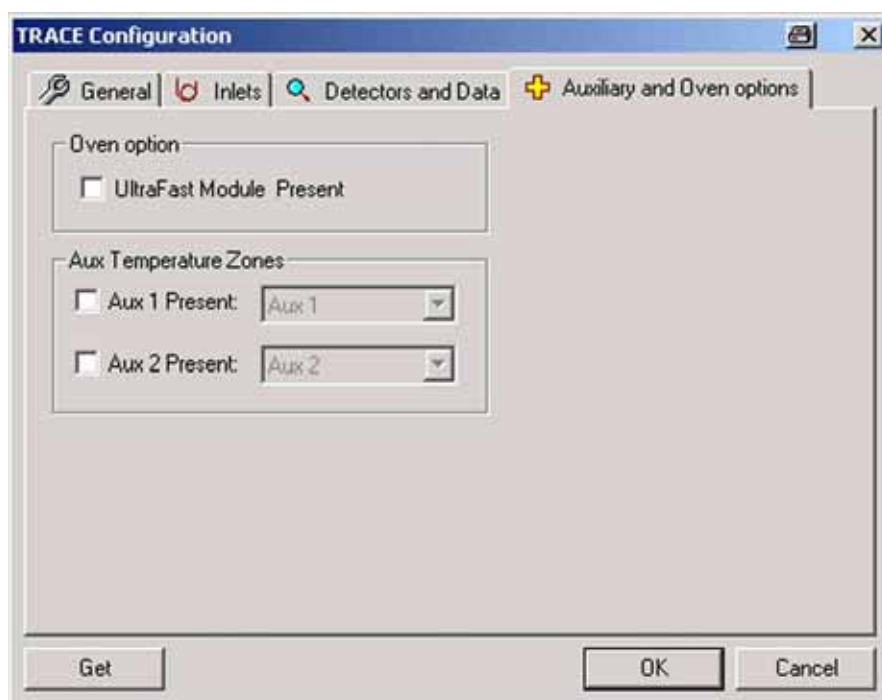
4. At Scan Rate (Hz), select the sampling rate for the respective channel between 1 Hz and 300 Hz (default: for each channel: 10 Hz). It is possible to scan one channel in a given period of time, only.





5. Choose between pressure mode and flow mode via the checkbox (default: checkbox is marked, i.e. flow mode).
6. Select either 50 Hz or 60 Hz (default) for the line frequency.

Auxiliary and Oven options tab



- If an ultrafast module exists, you can activate it by marking the checkbox.

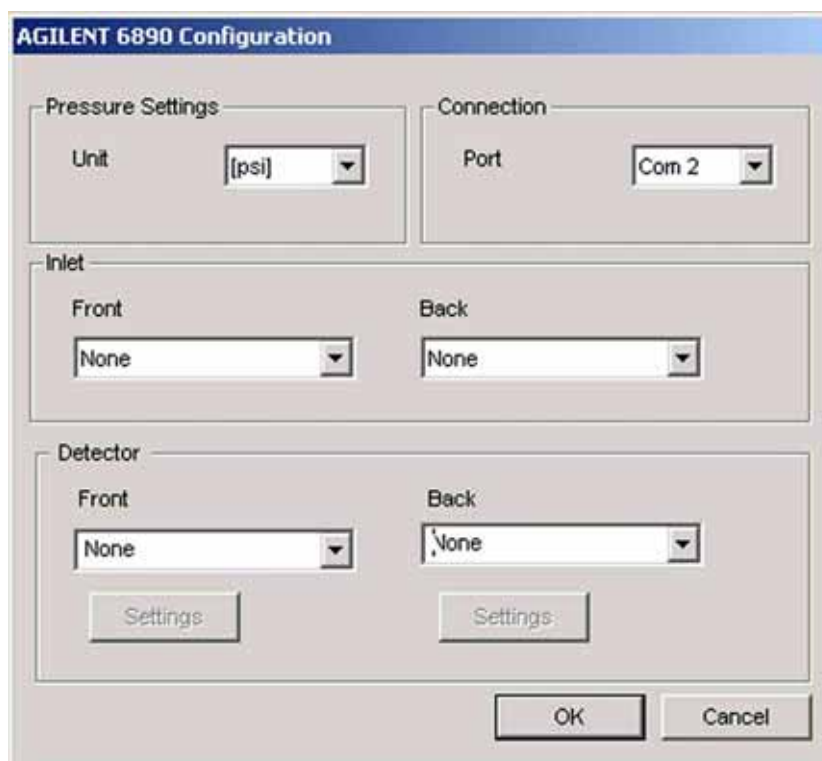
Agilent 6890 GC

Note. For further details about injectors and detectors, refer to the manual of the Agilent 6890 GC.

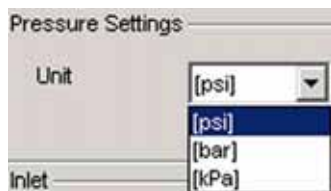
Configure your Agilent 6890 GC as follows:



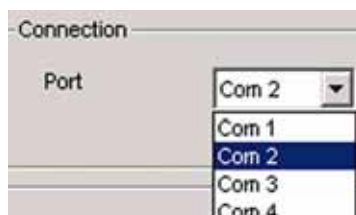
1. Double-click or right-click the **Agilent 6890 GC** button



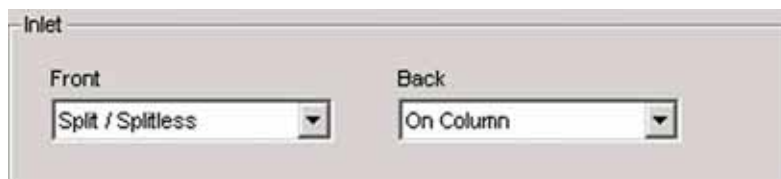
2. At **Pressure Settings**, choose the unit of pressure between psi, bar and kPa.



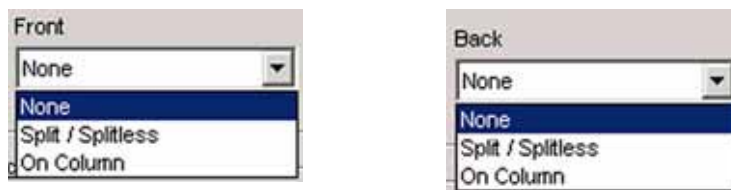
3. At **Connection**, specify COM2 as the computer's COM Port your Agilent 6890 GC is connected to.



4. At **Inlet**, specify both front and back inlet system, i.e. the injectors.



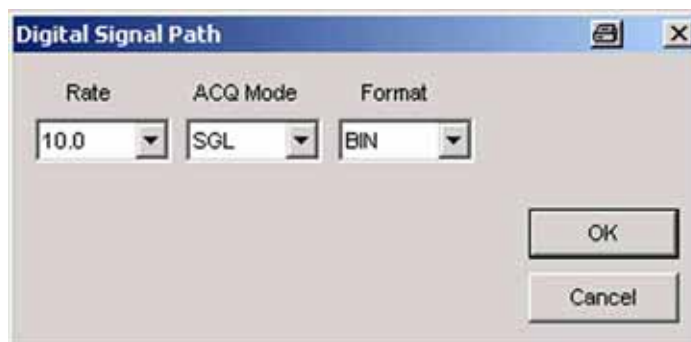
5. In both cases, choose between *None*, *Split/Splitless* and *On Column*:



6. At **Signals**, indicate which detectors will be monitored on Signal Path 1 and 2, respectively. In both cases, choose between *None*, **Front Detector**, and **Back Detector**.
7. Additionally, a broad variety of parameters can be adjusted, e.g. temperature- or flow-related data:



8. If you did not choose “None”, the **Settings** buttons will both be active. Press them in order to adjust Rate, Acquisition Mode and Format.



9. The sampling Rate can be adjusted between 0.1 Hz and 200 Hz (default: 10 Hz).

10. For Acquisition Mode, accept the default, SGL.
RUN: data acquisition only while the GC is in Run mode.
CON: GC will permanently be inquired (i.e. Continuous Mode).
SGL: Single run mode
11. At Format accept the default, BIN (other formats are DEC, HEX or CMP).
12. Finally, confirm by **OK** twice.

A200S

Note. For further details about injectors and detectors refer to the manual of the A200S autosampler.

Configure your A200S autosampler as follows:



1. Double-click or right-click the **A200S** button



2. Usually, the A200S autosampler is connected via COM 2.
3. Confirm by **OK**.

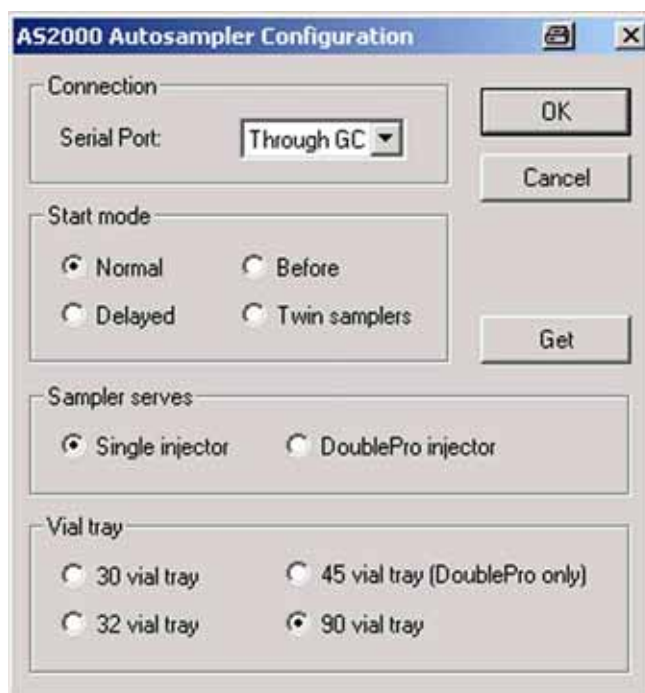
AS2000

Note. For further details about injectors and detectors refer to the manual of the AS2000 autosampler.

Configure your AS2000 autosampler as follows:



1. Double-click or right-click the **AS2000** button




2. Define how the AS2000 autosampler is connected (usually “through GC”, but it may also have a COM Port of its own).
3. Define the Start Mode (default: “Normal”).
4. At Sampler serves, choose between “Single injector” (default) and “DoublePro injector”.
5. Select the type of vial tray (default: 90 vial tray).
6. Again use the **Get** button, if you prefer to upload parameters from the AS2000 (i.e. from the hardware rather than from the Isodat 2.0 software).
7. Finally, confirm by **OK**.

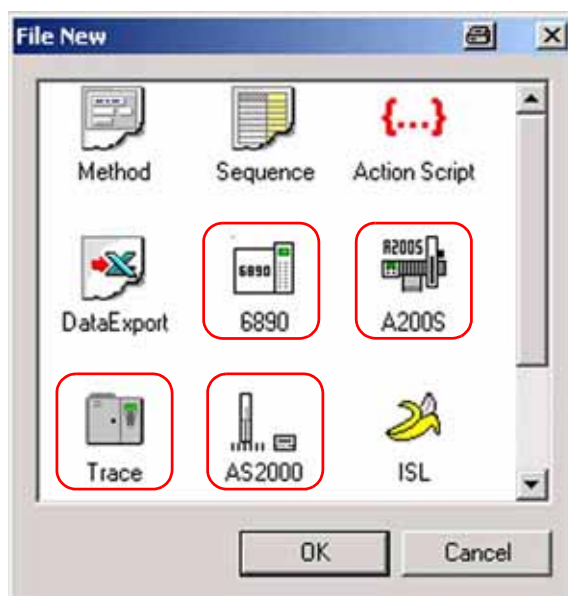
Creating a new Method for an external Device

1. Ensure that a Configuration containing the complete external device (e.g. a GC II-III Interface + Trace GC + AS2000) has been established in the Configurator before. This guarantees that the functionality will be available in the measurement mode, i.e. in Acquisition mode.



2. Open the Acquisition module .


3. Press the **New** button  in the appearing Acquisition window.

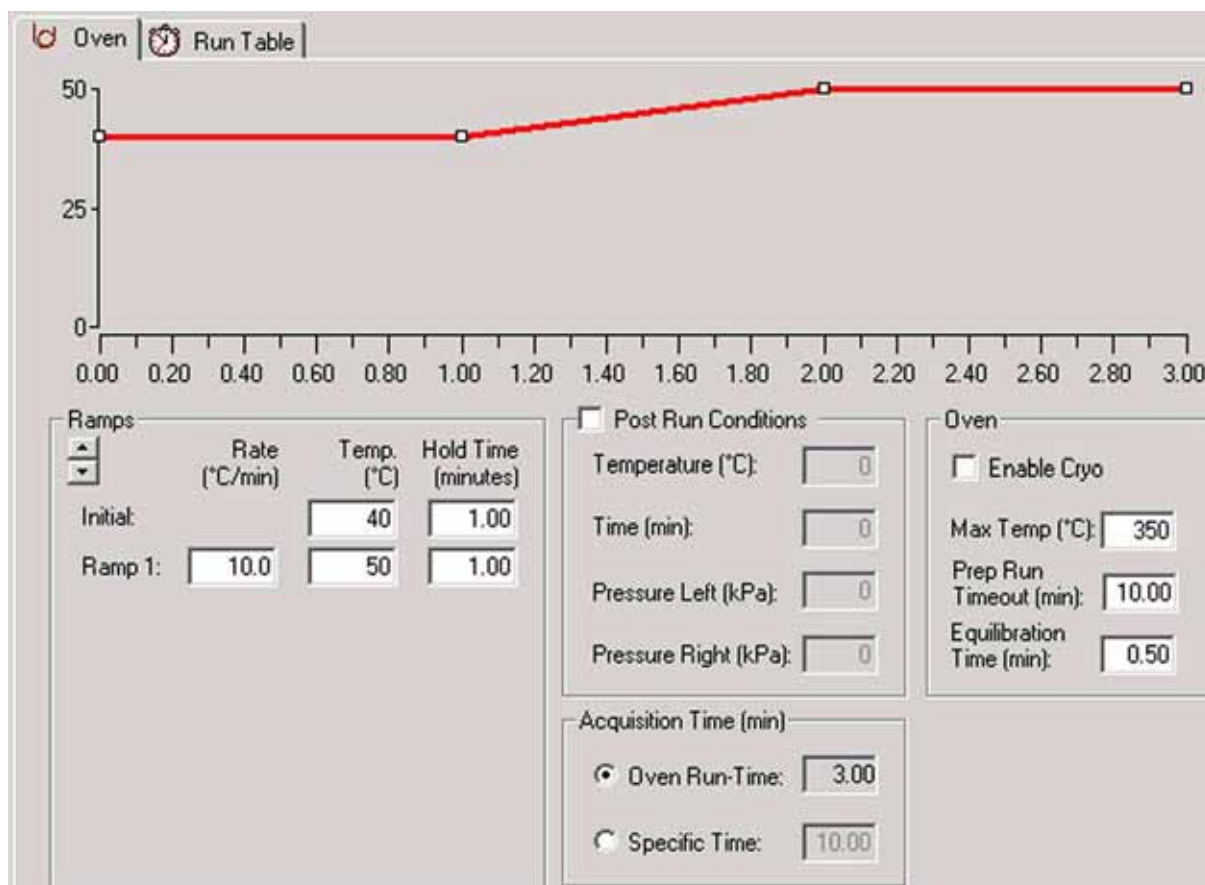


4. Mark the icon designed for your external manufacturer device: “6890”, “A200S”, “Trace” or “AS2000”.
5. Confirm by **OK**.

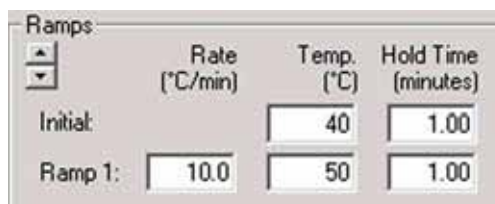
Method Structure of external Devices

Structure of a Trace GC Method

1. Double-click on the **Trace** icon . The Trace GC method opens. It is organized in tab pages.

Oven tab

1. On the **Oven** tab, temperature ramps can be defined and added.



2. The initial temperature is displayed, e.g. 40 °C, together with its duration, e.g. 1.00 min. When the ramp, e.g. Ramp 1 starts, a heating rate, e.g. 10.0 °C/min, will be prevalent until the end temperature of this ramp is reached, e.g. 50 °C. This end temperature will be kept for e.g. 1.00 min.

3. Marking the Post Run Conditions checkbox assures that the parameters above will be applied after the run to condition the system or to switch it into the standby mode.

Temperature (°C) prevailing temperature after the run

Time (min) duration of the post run parameters

Pressure Left (kPa) left pressure after the run

Pressure Right (kPa) right pressure after the run

4. Specify an oven run time or a specific time.

5. Marking the **Enable Cryo** checkbox allows the cryogenic equipment to turn on at a setpoint temperature.
6. **Max Temp (°C)** limits the oven temperature to the setpoint.
7. **Prep Run Timeout (min)** returns the GC to standby mode, if injection does not occur within the time set.
8. **Equilibration Time (min)** allows the oven temperature to stabilize after cooling for the duration of time set (injector and detector temperature as well).

Run Table tab

The Run Table tab is used only for special applications, e.g. control of external valves, switching of valves. During usual applications, however, it remains empty.



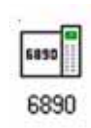
- At the Run Table tab, you can program events to happen during a run. If no run events have been programmed, the list will be empty. To create a run time event, press the **Add** button.

Example: A valve could be switched (opened/closed) or an external event from another device can be programmed.



Eight external events are available, but each extra valve (i.e. other valves than inlet valves) takes up two external events: one to open the valve, the other one to close it. If you have one valve configured, only six external events will appear. The run table events occur on a decimal-minute clock, that begins counting when the run starts.

Structure of an Agilent 6890 GC Method



1. Double-click on the 6890 icon .

Oven Method | Front : Split / Splitless | Back : On Column | Detector

☒ Temperature Program Enable

Oven

☐ Cryo on

☐ Quick Cryo Cooling on

Ambiente Temp [°C]

Max Temp [°C]

Prep Run Timeout [min]

Equilibration Time [min]

☒ Post Run Conditions

Temperature [°C]

Time [min]

Pressure Front [psi]

Pressure Back [psi]

Rate [°C] / min | Temp [°C] | Time [min]

Oven Run Time [min] : 0.0

Oven Run Time [sec] : 0

Temp [°C]

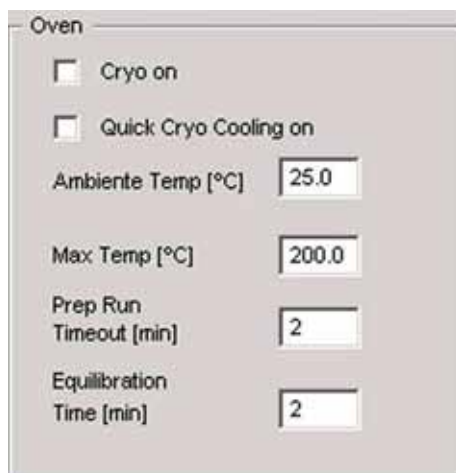
Time [min]

The Agilent 6890 GC method opens. As with other methods, it is organized in tab pages.

Note. You must have specified injector(s) and detector(s) to let the three tabs “Front”, “Back” and “Detector” appear. If you specified “None”, the respective tab will not appear.

2. **Temperature Program Enable:** Enable the checkbox to load a temperature program. It is possible however by clearing the checkbox, to specify parameter values on the “Oven Method” tab without loading the temperature program.

Oven Method tab



The screenshot shows a dialog box titled "Oven" with the following settings:

- ☐ Cryo on
- ☐ Quick Cryo Cooling on
- Ambiente Temp [°C]: 25.0
- Max Temp [°C]: 200.0
- Prep Run Timeout [min]: 2
- Equilibration Time [min]: 2

Cryo on enables cryogenic cooling, if a cryogenic valve is installed and if the coolant is available.

The cryogenic valve allows you to operate the oven below ambient temperature. The minimum attainable oven temperature depends on the type of valve installed.

Quick Cryo Cooling on is different from “Cryo on”: it makes the oven cool faster after a run than it would without assistance. This feature is useful when maximum sample throughput is necessary, however it uses more coolant. “Quick Cryo Cooling” turns off soon after the oven reaches its setpoint and “Cryo” takes over, if needed.

Ambient Temp denotes the temperature in the laboratory. This setpoint determines the temperature at which cryogenic cooling is enabled.

Set “Ambient Temp” to + 25 °C for regular cryo operation.

Set “Ambient Temp” to + 45 °C for quick cryo cool.

Max Temp denotes the maximum allowable oven temperature setpoint. Some accessories, such as columns and valves, have specific temperature limits.

Prep Run Timeout: The Prep Run function is activated to prepare a run. If all setpoints are reached, the instrument is waiting for injection (timeout).

The Prep Run function is used for the following functions:

Gas saver - cancels gas saver flow and brings inlet flow to its setpoint value.

Splitless injection - closes the purge valve.

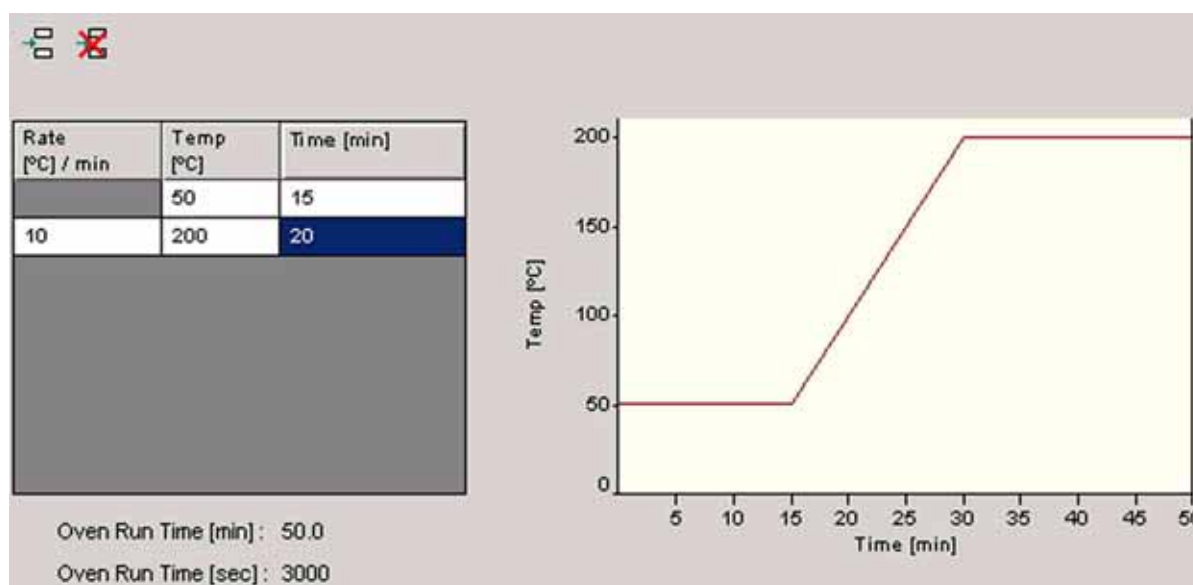
Pulsed split or splitless injection - increases the inlet pressure to the pulse setpoint.

Solvent vent injection - changes the inlet pressure to the vent pressure setpoint and the split vent flow to the vent flow setpoint.

Equilibration Time: This time is required for the oven temperature to equilibrate after the temperature has been modified. Equilibration time begins when the actual oven temperature comes within 1 °C of the oven temperature setting. The equilibration time setpoint can be 0 to 999.99 min.



Making a temperature-programmed run

You can program the oven temperature from an initial temperature to a final temperature using up to six ramps during a run. Multiple ramps can also be programmed for temperature decreases as well as for increases.

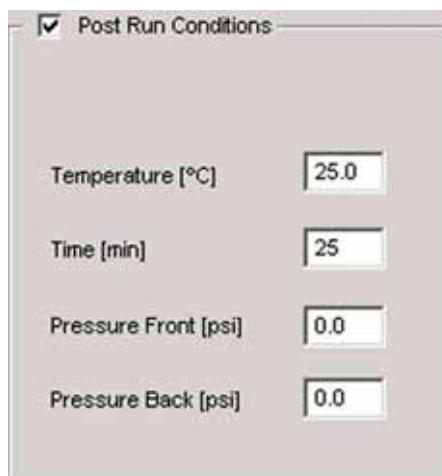


1. Establish a temperature program, i.e. specify the temperature characteristics over time:

Example:

- a. Insert lines by pressing  and delete lines by pressing .
- b. Type a start value for the temperature into the Temp column (e.g. 50 °C).
- c. Type a time value into the Time column (e.g. 15 min). Thus, the temperature will be kept at its start value for this period of time.
- d. Type a temperature rate value into the Rate column (e.g. 10 °C/min).
- e. Type a temperature value into the Temp column (e.g. 200 °C). The temperature will be changed according to this rate until the temperature is reached.

- f. Type a time value into the Time column (e.g. 20 min). Thus, the reached temperature value will be kept constant for this period of time.




2. Marking the Post Run Conditions checkbox assures that the parameters above will be applied after the run to condition the system or to switch it into the standby mode.

Temperature (°C) Temperature after the run (see Trace GC at **Structure of a Trace GC Method** on page 1-44).

Time (min) Duration of this temperature after the run (see Trace GC at **Structure of a Trace GC Method** on page 1-44).

Pressure Front (psi) Pressure at Front injector after the run

Pressure Back (psi) Pressure at Back injector after the run

3. Pressing the **Upload Method** button  enables the manual upload of a method just in time. However, the usual way is to fill out the **Oven tab** page and save it, before you call up this method in the sequence. When the sequence is started, the method will be loaded line after line.

Front tab

Note. The Front tab only appears, if you did not select None above at “Front Injectors”. Usually, “Split/Splitless” has been chosen.

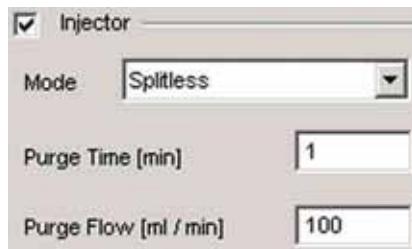
1. **Injector** Mark the checkbox to set an injector.

Note. If you unmark the checkbox, the parameters within the surrounding frame will not be loaded.

2. **Mode** Select the injection mode. Choose between *Split*, *Splitless*, *Pulsed Split* and *Pulsed Splitless*.

3. **Temperature (°C)** Temperature of the injector you selected (e.g. 220 °C). The value depends on the actual application.

Injection Mode “Splitless”

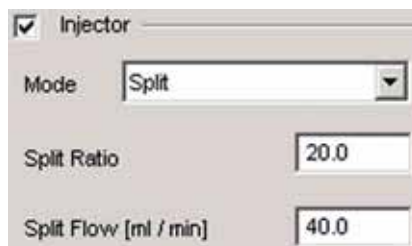


The screenshot shows the 'Injector' settings window. The 'Mode' dropdown is set to 'Splitless'. Below it, the 'Purge Time [min]' is set to 1, and the 'Purge Flow [ml / min]' is set to 100.

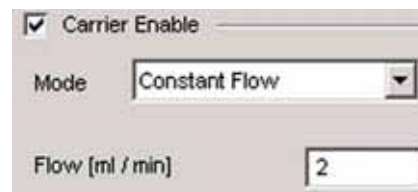
If you selected *Splitless* at *Mode*:

- **Purge Time (min)** time, during which the split - i.e. the purge line - is closed, after injection (typically 1 min).
- **Purge Flow (ml/min)** flow used to purge the injector after the purge time has elapsed and the purge line has been opened again (considerably high, typically 100 ml/min).

Injection Mode “Split”



The screenshot shows the 'Injector' settings window. The 'Mode' dropdown is set to 'Split'. Below it, the 'Split Ratio' is set to 20.0, and the 'Split Flow [ml / min]' is set to 40.0.



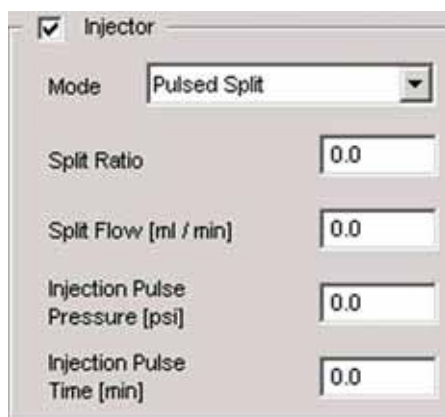
The screenshot shows the 'Carrier Enable' settings window. The 'Mode' dropdown is set to 'Constant Flow'. Below it, the 'Flow [ml / min]' is set to 2.

If you selected *Split* at *Mode*:

- **Split Ratio** is defined as Split Flow/Flow along the column.
- **Split Flow (ml/min)** depends on the Split Ratio. If you define a Split Ratio, a Split Flow will automatically be calculated and vice versa.

Example: A Split Ratio of 20 is calculated from a Split Flow of 40 ml/min and a flow along the column of 2 ml/min.

Injection Mode “Pulsed Split”



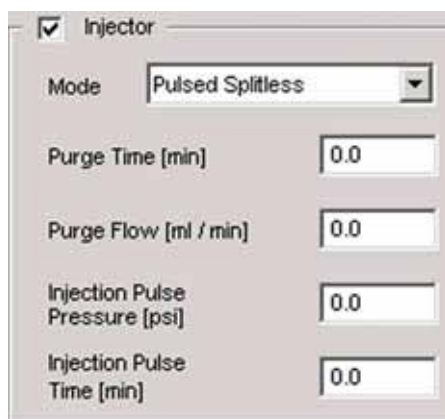
The screenshot shows a dialog box titled "Injector" with a checked checkbox. The "Mode" dropdown menu is set to "Pulsed Split". Below this, there are four input fields, all of which are currently set to "0.0": "Split Ratio", "Split Flow [ml / min]", "Injection Pulse Pressure [psi]", and "Injection Pulse Time [min]".

Principle of the two Pulsed Modes: the transfer time along the injector is increased.

If you selected **Pulsed Split** at **Mode** (i.e. a modified split mode), the pressure will be increased for a definite period of time.

- **Split Ratio:** see above.
- **Split Flow (ml/min):** see above.
- **Injection Pulse Pressure (psi):** the pressure to be applied
- **Injection Pulse Time (min):** the duration of applying the pressure

Injection Mode “Pulsed Splitless”



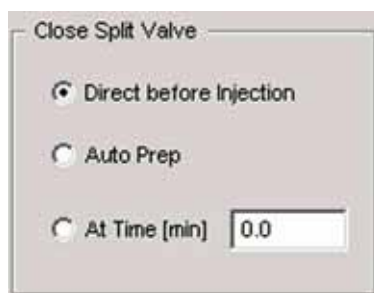
The screenshot shows a dialog box titled "Injector" with a checked checkbox. The "Mode" dropdown menu is set to "Pulsed Splitless". Below this, there are four input fields, all of which are currently set to "0.0": "Purge Time [min]", "Purge Flow [ml / min]", "Injection Pulse Pressure [psi]", and "Injection Pulse Time [min]".

Principle of the two Pulsed Modes: the transfer time along the injector is increased.

If you selected **Pulsed Splitless** at **Mode** (i.e. a modified splitless mode):

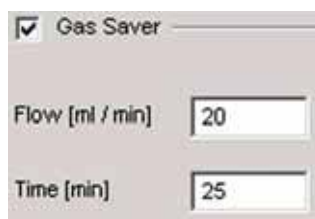
- **Purge Time (min):** see above.
- **Purge Flow (ml/min):** see above.

- **Injection Pulse Pressure (psi)**: see above.
- **Injection Pulse Time (min)**: see above.



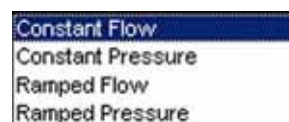
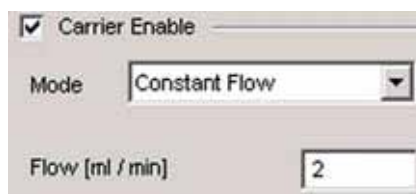
This box is only available, when you either selected **Splitless** or **Pulsed Splitless** at **Mode**. It defines the time at which the split line is closed:

- **Direct before injection**: the split line is closed immediately before injection.
- **Auto Prep**: enable or disable the Auto Prep functionality.
- **At Time (min)**: define a time after which the split valve will be closed.



- **Gas Saver**: can be enabled by marking the checkbox. The Gas Saver Mode is typical for the Splitless Modes (i.e. Splitless and Pulsed Splitless).
- **Flow (ml/min)**: defines the flow value under gas saving conditions.
- **Time (min)**: period, after which the Gas Saver Mode will start.

Example: To save gas, the Gas Saver Mode will start after 25 min. The split flow (e.g. 100 ml/min) will then be reduced to the value specified at flow (e.g. 20 ml/min).

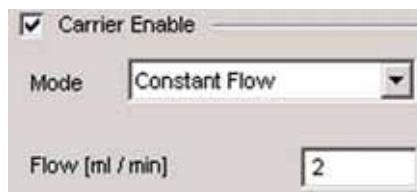


Carrier Enable: enable or disable a carrier gas.

Note. If you unmark the checkbox, the parameters within the surrounding frame will not be loaded.

Specify the mode in which you want to set the carrier gas. Thermo Electron recommends **Constant Flow** Mode, i.e. to work using a constant flow on the column. Other modes are **Constant Pressure** Mode, **Ramped Flow** Mode and **Ramped Pressure** Mode.

Constant Flow Mode



Carrier Enable ☒

Mode Constant Flow

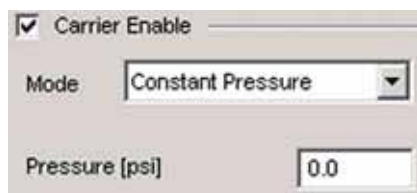
Flow [ml / min] 2

Flow (ml/min): flow of the carrier gas to be kept constant. It depends on the inner diameter of the column in use. Typical values may be:

for a column of 0.25 mm inner diameter: 0.8 ml/min - 1.2 ml/min

for a column of 0.35 mm inner diameter: 1.6 ml/min - 2.2 ml/min

Constant Pressure Mode

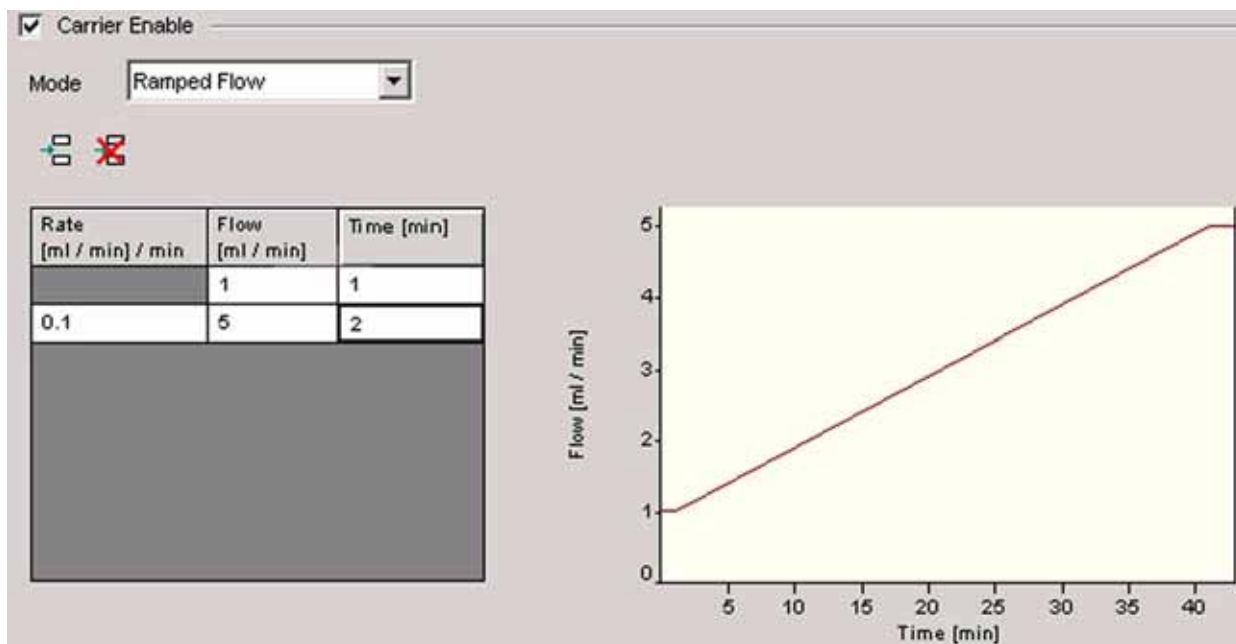


Carrier Enable ☒

Mode Constant Pressure



Pressure [psi] 0.0

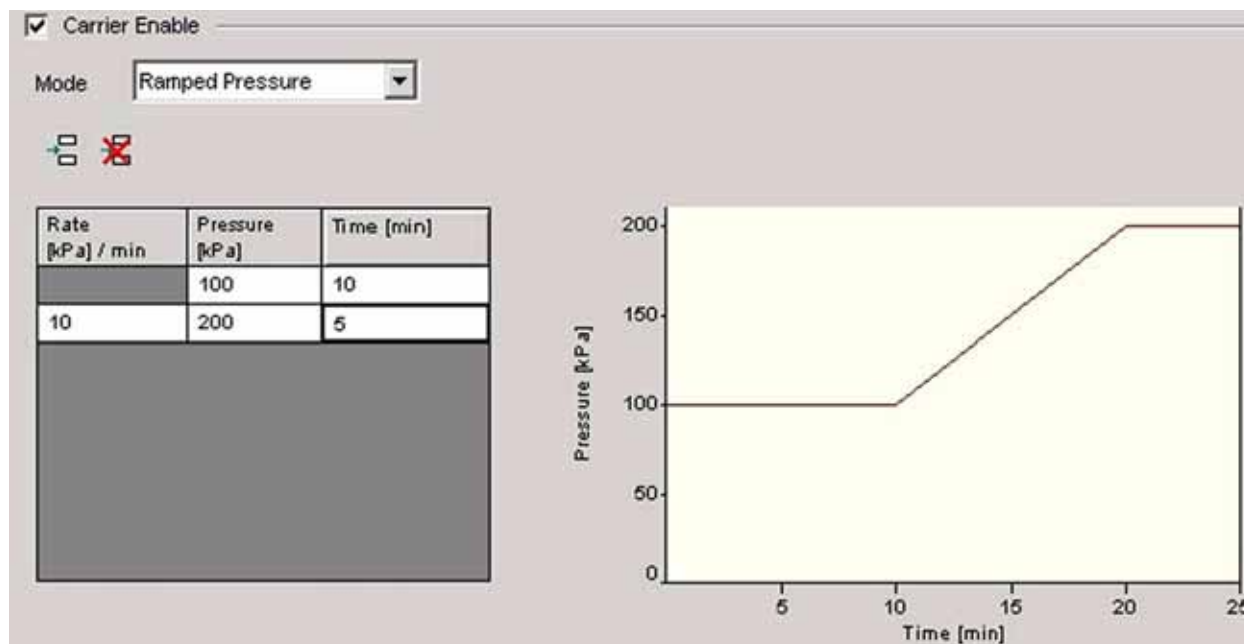
Pressure (psi): specify the pressure to be kept constant.

Ramped Flow Mode

- Establish a flow program, i.e. specify the flow characteristics over time:



Example:

- Insert lines by pressing  and delete lines by pressing .
- Type a start value for the flow into the **Flow** column (e.g. 1 ml/min).
- Type a time value into the **Time** column (e.g. 1 min). Thus, the flow will be kept at its start value for this period of time.
- Type a flow rate value into the **Rate** column (e.g. 0.1 [ml/min]/min).
- Type a flow value into the **Flow** column (e.g. 5 ml/min). Thus, the flow will be changed according to this rate until the flow value is reached.
- Type a time value into the **Time** column (e.g. 2 min). Thus, the reached flow value will be kept constant for this period of time.

Ramped Pressure Mode

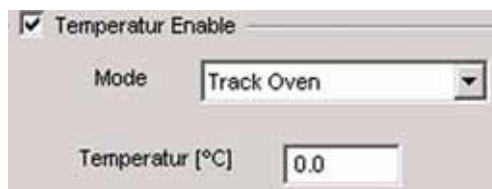
- Establish a pressure program, i.e. the pressure characteristics over time.

Example:

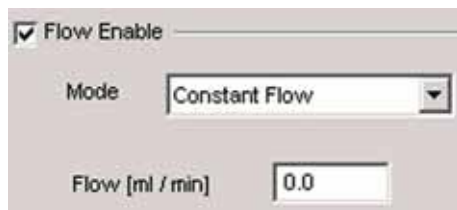
- Insert lines by pressing  and delete lines by pressing .
- Type a start value for the pressure into the **Pressure** column (e.g. 100 kPa).
- Type a time value into the **Time** column (e.g. 10 min). Thus, the pressure will be kept at its start value for this period of time.
- Type a pressure rate value into the **Rate** column (e.g. 10 kPa/min).
- Type a pressure value into the **Pressure** column (e.g. 200 kPa). The pressure will be changed according to this rate until the value is reached.
- Type a time value into the **Time** column (e.g. 5 min). Thus, the reached pressure value will be kept constant for this period of time.

Back tab

Note. The Back tab only appears, if you did not select None above at “Back Injectors”. Usually, “On column” has been chosen.



1. Mark the **Temperature Enable** checkbox to load the parameters within the surrounding frame.
2. At **Mode**, choose between **Track Oven** and **Ramped Temperature**. In case of Track Oven, the oven temperature will follow the injector temperature.
3. At **Temperature**, define the temperature value. In case of **Ramped Temperature**, establish a temperature program for the injector. This is analogous to establishing a flow program or a pressure program (see above).



1. Again, at **Mode**, choose between **Constant Flow**, **Constant Pressure**, **Ramped Flow** and **Ramped Pressure**.
2. Define either the working flow/flow program or the working pressure/pressure program as has been shown above.

Detector tab

Note. The Detector tab only appears, if you did not select “None” above at one of the “Detectors”. E.g. “FID” and “TCD” have been chosen.

1. Typically, choose the **Front** detector (e.g. at “Signal Path 1”) and the **Back** detector (e.g. at “Signal Path 2”).
2. Define the Temperatures for both detectors (e.g. 250 °C and 150 °C).

3. In addition to Front Detector and Back Detector, there is a wide variety of other parameters available as well.

Structure of an A200S Method

PAL Setup

Note. The PAL autosamplers (i.e. Combi PAL and GC PAL) are momentarily run via A200S mode!

There are nine different methods available, which are maintained even if the power to the A200S is switched off: A200-1 to A200-9 (cf. the internal file names “Internal No. 1” to “Internal No. 9” at the “AS Method” column in topic **Creating a new Sequence for an external Device** on page 1-68).

Note. If you create a new file name however, the method is uploaded to the method A200S-1 in the control panel, and this method is overwritten!



1. Double-click on the A200S icon .The A200S method is divided into four sections.

Before Injection

Wash Solvent: Home

Solvent Wash Cycles: 0

Clean Cycles with Sample: 0

Air Volume before Sample [ul]: 0.0

Syringe Filling Cycles: 0

Syringe Filling Volume [ul]: 0.0

Syringe Pullup Delay [sec]: 0.0

Sample

Sample Volume [ul]: 0.1

Air Volume after Sample [ul]: 0.0

Filling Speed [ul / sec]: 1.0

Injection Speed [ul / sec]: 1.0

Pre Injection Delay [sec]: 0.0

Post Injection Delay [sec]: 0.0

After Injection

Solvent Wash Cycles: 0

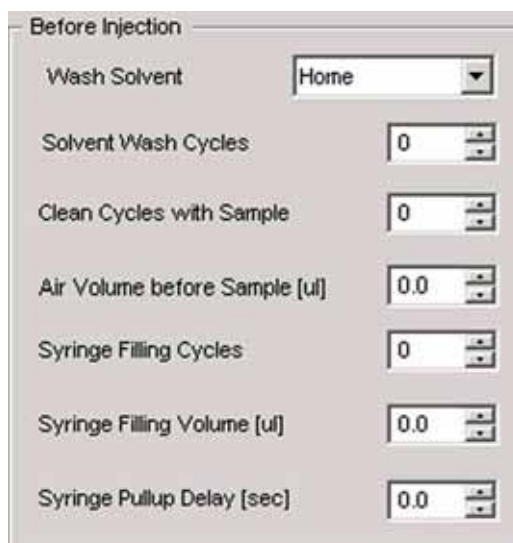
Wash Solvent: Home

Syringe

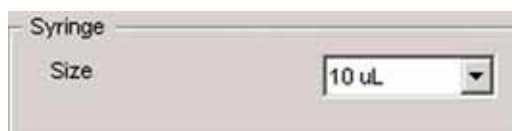
Syringe Size: 10 uL

Buttons: Upload, Dump Method, Send Command

Actions, which are taken before injection

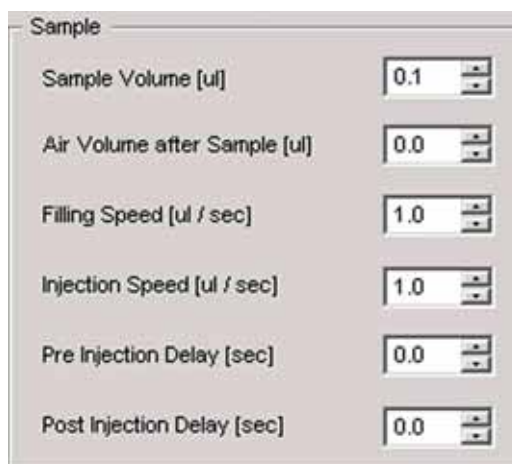


- ***Solvent Wash Cycles:*** To avoid contamination of the syringe and needle, they may be washed with solvent before the sample is picked up. This helps also to avoid air bubbles below the plunger because the syringe is wet afterwards and is more gastight.
Pre-injection is also a possibility to have a solvent plug with the volume of the syringe needle above the sample.
- ***Clean Cycle with Sample:*** This option is utilized when the solvent used in a post injection clean cycle is not compatible with the analysis, or when no pre-injection solvent clean cycle is used.
Set to zero when pre-injection solvent wash is used and you want a solvent plug on top of the sample to compensate for needle dead volume.
- ***Air Volume before Sample:*** Specifies the air volume that is pulled up after the needle is moved in the sample vial.
An air plug is set between sample liquid and the solvent plug by setting of solvent wash cycles. For this option, clean cycles with sample are not used. This option is not available for the PAL-Autosamplers (Combi-PAL, GC-PAL).
- ***Syringe Filling Cycles:*** This parameter serves to control the filling of the syringe. It may happen that some air bubbles remain below the plunger after the first pull up. If the plunger is moved up and down several times, these air bubbles are worked out.
- ***Syringe Filling Volume:*** All filling cycles, except for the last one, use the selected minimum filling volume.
- ***Syringe Pullup Delay:*** In this display, a delay between sample pullup and ejection while filling the syringe is selected. The same delay is used after the last plunger pullup until the syringe needle is moved out of the vial. This feature is especially useful for handling viscous fluids.



- **Syringe:** Volume of the syringe in use

Actions, which are directly related to sample injection




- **Sample Volume (μl):** The sample volume to fill the syringe.
- **Air Volume after Sample (μl):** The air volume, that is pulled up after the needle is moved out of the vial. By pulling up some air after taking the sample, evaporation from the needle is reduced.
- **Filling Speed ($\mu\text{l/s}$):** The speed of the plunger movement can be selected for the filling cycles.
- **Injection Speed ($\mu\text{l/s}$):** The speed for sample injection
- **Pre Injection Delay (s):** After the needle of the syringe is moved down into the injector, it may be desirable to wait a certain time so that the needle warms up before the sample is injected, i.e. the plunger goes down (hot needle injection).
- **Post Injection Delay (s):** After the injection it is possible to wait for evaporation of the needle content before the needle is pulled out of the injection block.

Actions, which are taken after sample injection

- **Solvent Wash Cycles:** After the sample has been injected, the syringe is cleaned by repeatedly filling it with solvent.

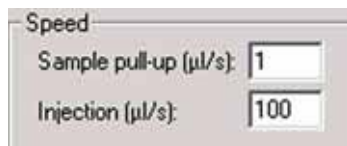
Structure of an AS2000 Method

- Double-click on the AS2000 icon . The AS2000 method opens.

General tab

- **Sample (µl):** the sample volume that will be injected (0–500 µl).
- **Filling (µl):** the sample volume used when flushing the syringe with the sample before finally taking it up (0–500 µl).

- **Air (μl):** the air volume that will be injected after the sample (0–500 μl). Air is injected to perceive clearly the sample amount within the syringe. Further, it facilitates positioning the sample to prevent it from instantaneous evaporation.

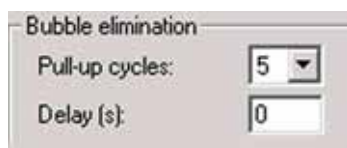


Speed

Sample pull-up ($\mu\text{l/s}$): 1

Injection ($\mu\text{l/s}$): 100

- **Sample pull-up ($\mu\text{l/s}$):** the velocity of lifting the plunger after the syringe has been immersed into the vial (1–100 $\mu\text{l/s}$).
- **Injection ($\mu\text{l/s}$):** the velocity of injection, i.e. velocity of pressing down the plunger after being introduced into the injector (1–100 $\mu\text{l/s}$). Note that the sample-pull-up is performed very slowly compared to the rapid injection.



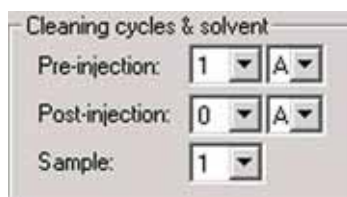
Bubble elimination

Pull-up cycles: 5

Delay (s): 0

The syringe is flushed with the sample by repeatedly moving up- and downwards the plunger: Thus, before finally taking up the sample, it is pulled up into the syringe and flushed back into the vial (pull-up cycle) several times. Pull-up cycles are performed to cover the surfaces inside the syringe with the sample and to press out air bubbles (e.g. out of the needle volume).

- **Pull-up cycles:** Specify the number of pull-up cycles between 0 and 15. The default value is 5, whereas 0 means no pull-up cycle but instantaneously taking up the sample.
- **Delay (s):** the time between two subsequent pull-up cycles (0–15 s). The default is 0, i.e. the pull-up cycles follow directly one after the other (usual value). As rather viscous solvents need more time to flow along, it is advisable in such cases to use a delay (e.g. 1 s or 2 s). Note the **sample pull-up speed** value above.



Cleaning cycles & solvent

Pre-injection: 1 A

Post-injection: 0 A

Sample: 1

- **Pre-injection:** number of cleaning cycles using solvent before injection (0–15). Choose the solvent (A, B, C or D) for purging.
- **Post-injection:** number of cleaning cycles using solvent after injection (0–15). Choose the solvent (A, B, C or D) for purging.

- **Sample:** number of cleaning cycles using the sample (0–15, default: 1).
The sample volume in μl is specified at **Filling**, see above.

Cleaning cycle volume

Pre-inj. (μl):	4
Post-inj. (μl):	0

- **Pre-inj. (μl):** solvent volume for cleaning cycles before injection (0–500 μl)
- **Post-inj. (μl):** solvent volume for cleaning cycles after injection (0–500 μl)


Delay time

Pre-inj. (s):	3
Post-inj. (s):	0

- **Pre-inj. (s):** delay between pulling down the needle and injection (0–63 s)
- **Post-inj. (s):** delay between injection and pulling up the needle (0–63 s)

Internal Standard tab

General Internal Standard



Internal standard

☐ Use internal standard

Internal standard volume (μl): 2

Air gap mode: Post

Air gap volume (μl): 1

Internal standard vial: 90

Enable/disable the use of Internal standard method



In addition to the sample, an internal standard can be filled into the syringe. The internal standard is located in an external vial.

- **Use internal standard:** mark the checkbox to use an internal standard method. Thus, the following parameters become available:
- **Internal standard volume (µl):** the volume of the internal standard to be filled into the syringe (0–500 µl, default is 2 µl)
- **Air gap mode:** use an air gap (i.e. an air plug) to prevent the two liquid films of standard and sample from flowing into each other. Select **Post**



(default) or **Double** to define the position of the air plug relative to sample plug, solvent plug and internal standard plug (e.g. before or behind sample).

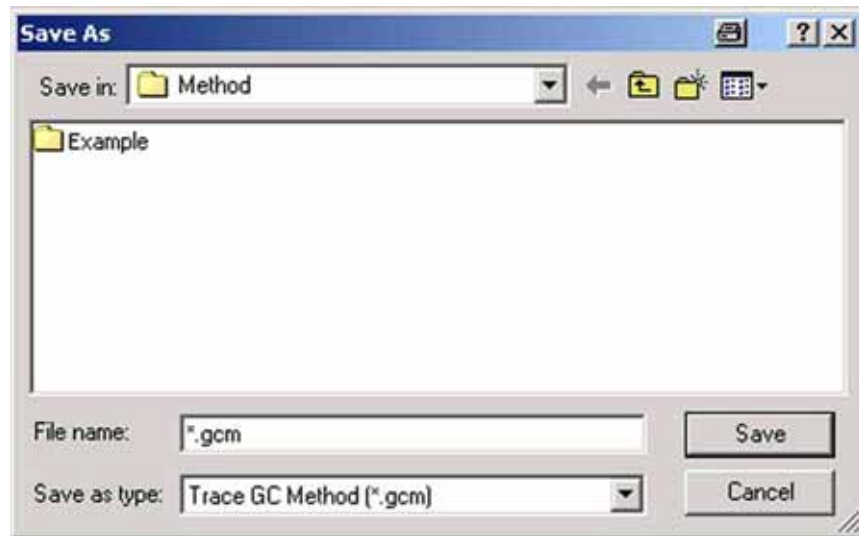
- **Air gap volume (µl):** the volume of the air gap (0–500 µl, default: 1 µl)
- **Internal standard vial:** the number of the vial that contains the internal standard. Choose between A, B, C, D and 1 to 90 (default: 90).

Saving a Method for an external Device

1. After you made your decisions throughout the tab pages of your method,



save it by pressing the **Save** button. This will make the method available in later applications.




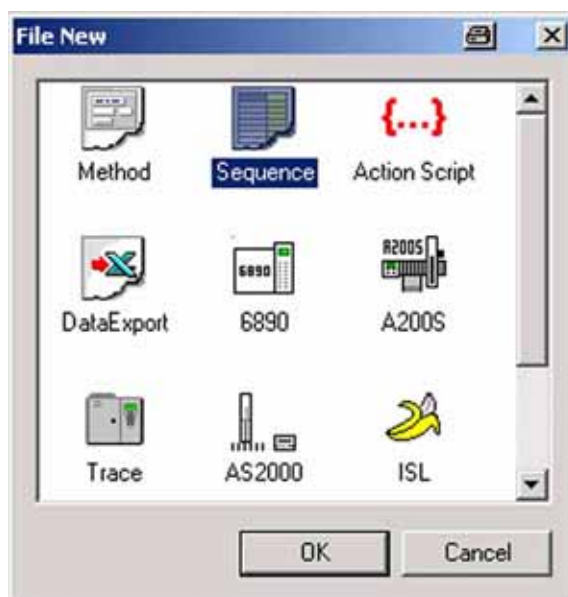
2. Specify the folder for the method and type a significant name.
3. Accept the method-specific extension:
.gcm for Trace GC methods,
.6890 for Agilent 6890 GC methods,
.asm for AS2000 or HS2000 methods,
.A200S for A200S methods (cf. PAL autosamplers).
4. Confirm by **Save**.

Creating a new Sequence for an external Device



1. First of all, choose the correct Configuration (e.g. “Trace GC”).
2. After having created a method (see topic **Creating a new Method for an**

external Device on page 1-43), press the **New** button  to create an associated sequence.



3. Mark the *Sequence* button and confirm by **OK**.

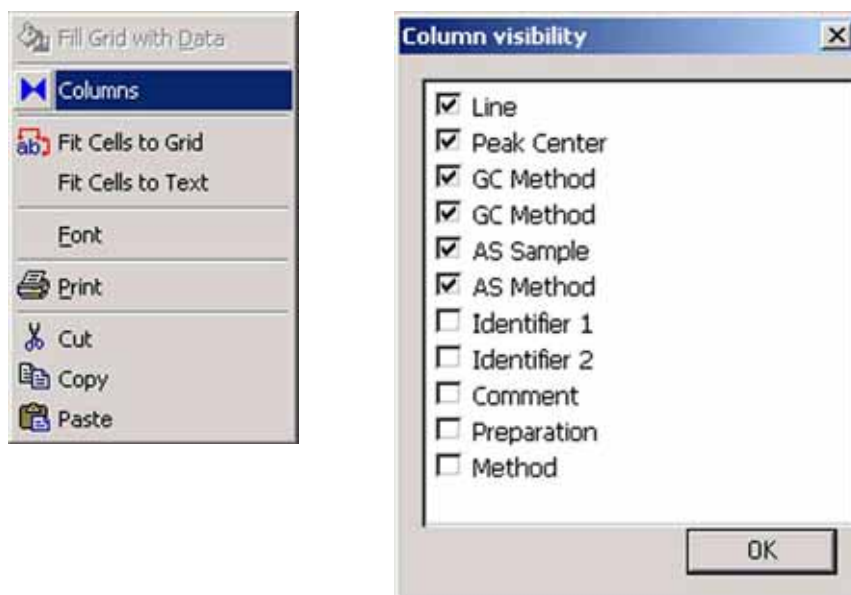


4. Type your number of samples (e.g. 3) and confirm by **OK**.

Line		GC Method	AS Sample	AS Method
1	✓	Disabled		Disabled
2	✓	Disabled		Disabled
3	✓	Disabled		Disabled

5. The sequence is shown (e.g. a Trace GC sequence).


Note. Two methods occur, a GC method and an AS method!




6. To make more or less columns visible, perform a **right mouse click**.
7. From the pull-down menu, select **Columns**.
8. To see a particular column, mark its checkbox. If you unmark a checkbox, the respective column will not be visible in the sequence.

Line		GC Method	AS Sample	AS Method
1	✓	Disabled		Disabled
2	✓	Disabled		Disabled
3	✓	Trace 1.gcm		Disabled
		Trace 2.gcm		

9. Look at the GC method by a click upon . The actual line will be activated and occurs in bold style (e.g. **1**, i.e. Sample 1). The column “**GC Method**” will be activated and occurs in bold style.
10. Choose between **all GC methods** you created before for the **actual Configuration** (e.g. “Trace GC”).
 Example: The extension gcm denotes all **Trace GC** methods.
 (e.g. “Trace 1.gcm” or “Trace 2.gcm” are available here).
 The extension 6890 denotes all **Agilent 6890 GC** methods.
 The extension asm denotes all **Autosampler** methods.
11. Choose **Disabled**, if you do not want to load any GC method.

Line		GC Method	AS Sample	AS Method
1	✓	Disabled		Disabled
2	✓	Disabled		>Internal No 3
3	✓	Disabled		>Internal No 4
				>Internal No 5
				>Internal No 6
				>Internal No 7
				>Internal No 8
				>Internal No 9
				AS2000_1.asm
				AS2000_2.asm
				Disabled

12. Look at the AS method by a click upon . The actual line will be activated and occurs in bold style (e.g. 1, i.e. Sample 1).

The column “**AS Method**” will be activated and occurs in bold style.

13. Choose between *all autosampler methods* you created before *for the autosampler defined in your actual Configuration* (e.g. “AS2000_1.asm” or “AS2000_2.asm” are available).
14. Choose **Disabled**, if you do not want to load any autosampler method.
15. Choose between **Internal No 1** to **Internal No 9** (i.e. internal method positions).

Identifier 1	Preparation	Method
		Method 1.met
		Method 2.met



16. At **Method**, choose between all *mass spectrometer methods* you created before via **New > Method** button (e.g. “Method 1.met” or “Method 2.met” are available).

Different locations of different methods

During Isodat 2.0 installation, different folders for storage of Isodat 2.0 methods and GC/AS methods are created:

Name	Size	Type
AS_Method		File Folder
Example		File Folder
GC_Method		File Folder
CH3_Flavor_Comp.met	92 KB	Finnigan Method File
CO_Conditioning.met	93 KB	Finnigan Method File
CO_Flavor_Comp.met	94 KB	Finnigan Method File
CO_Std on-off.met	98 KB	Finnigan Method File
CO_Tyramine.met	94 KB	Finnigan Method File
CO_Tyramine_2dim.met	94 KB	Finnigan Method File
CO2_Flavor_Comp.met	96 KB	Finnigan Method File
CO2_Flavor_Comp_DI.met	105 KB	Finnigan Method File
CO2_Std on-off.met	95 KB	Finnigan Method File
Flavor_Comp_CPSil_8.cmp	1 KB	CMP File
H2_Flavor_Comp.met	91 KB	Finnigan Method File
H2_Flavor_Comp_DI.met	100 KB	Finnigan Method File
H2_Std on-off.met	148 KB	Finnigan Method File

Isodat 2.0 methods are usually stored at a folder of their own, e.g. ... \ FINNIGAN \ ISODAT NT \ Global \ User \ **GC II-III Interface \ Method**. **Autosampler** methods are e.g. stored in a **subfolder** (e.g. “AS_Method”).

Name	Size	Type	Mo
Pump_Inj_1-0ul.A2005	5 KB	A2005	20
Pump_Inj_3-0ul.A2005	5 KB	A2005	20
Solvent_Inj_1-0ul.A2005	5 KB	A2005	20
tyramine.A2005	5 KB	A2005	20

GC methods are e.g. stored in another **subfolder** (e.g. “GC_Method”).

Name	Size	Type	Mo
Flavor_Comp.gcm	3 KB	Trace	20
Flavor_Comp_0-8ml_flow.gcm	3 KB	Trace	20
Std.gcm	3 KB	Trace	20
Tyramine.gcm	3 KB	Trace	20
Tyramine_2dim.gcm	3 KB	Trace	20

Chapter 2

Evaluation-related Features

This chapter contains the following topics:

- Standard Editor
- Ratio Editor

2.1 Standard Editor

This section contains the following topics:

- Principle of the Standard Editor
- Opening the Standard Editor
- Creating a new Standard
- Choosing Standards during Method Creation

Principle of the Standard Editor

The Standard editor manages all working standards. It provides the system with information about the standards in use.

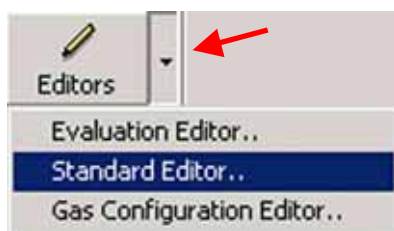
Choose among a lot of different molecules that can be used for standardization. Molecular standards can be managed and edited as well.


Note. When creating a method, at the Evaluation tab, a standard will be chosen from the Standard Editor's list.

Opening the Standard Editor



1. Open the *Acquisition* mode



2. Press  right to the Editors icon.

3. Select **Standard Editor**.

The screenshot shows the 'Standard Editor' window with a toolbar containing 'New', 'Add', and 'Delete' icons. Below the toolbar is a tab labeled 'Working Standards'. The main area contains a table with the following data:

Name	Gas	Delta	Value	Primary Standards
Haus2	CO2			
		δ 18O/16O	-25.540	VSMOW
		δ 13C/12C	-39.260	VPDB
O2	O2			
		δ 18O/16O	0.000	VSMOW
		δ 17O/16O	-12.000	VSMOW
IAEA CO2	CO2			
		δ 17O/16O	0.000	VPDB
		δ 18O/16O	0.000	VPDB
		δ 13C/12C	0.000	VPDB
N2O	N2O			
		δ 15N/14N	0.000	Air-N2
		δ 18O/16O	0.000	VSMOW
CO-Lab.Tank	CO			
		δ 18O/16O	9.050	VSMOW
		δ 13C/12C	0.000	VPDB

At the bottom right of the window are two buttons: 'Save & Close' and 'Cancel'.

The Standard editor will be loaded.

Creating a new Standard



1. Press the **New** button.

2. At **Name**, type a significant name for the standard, e.g. “Haus 4”.
3. At **Gas Name**, type the formula of the gas the standard will be created for. Alternatively, select the name from the pull-down menu.
4. Confirm by **OK**.

		d 29N2/28N2	0.000	None
Haus 3	CO2			
		d 18O/16O	5.000	VSMOW
		d 13C/12C	2.000	VPDB
Haus 4	CO2			
		d 18O/16O	0.000	VSMOW
		d 13C/12C	0.000	VPDB

The new Standard will be included at the bottom of the list of standards defined. Its name, e.g. “Haus 4”, appears in the **Name** column.

The **Gas** column shows the gas to which it has been assigned (e.g. “CO2”).

In the **Delta** column, the respective deltas are displayed (e.g. “d 18O/16O” and “d 13C/12C”).

The **Value** column shows the value of the respective delta (default: 0.000).

The **Primary Standards** column allows to select a primary standard from the pull-down list (e.g. “VSMOW” or “VPDB”).

Choosing Standards during Method Creation

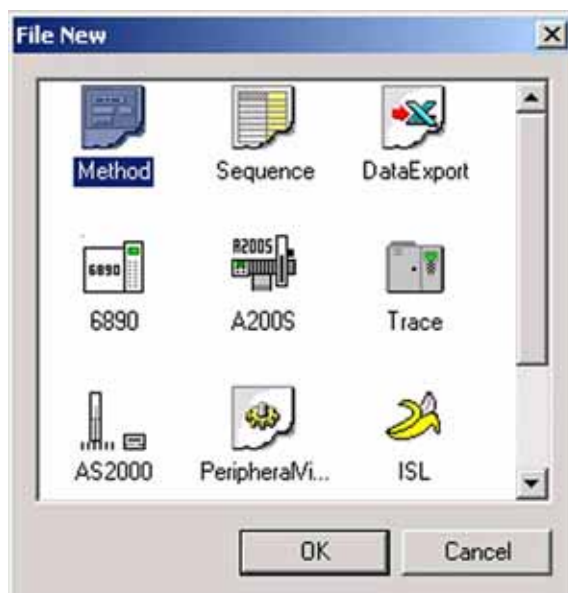
Note. When creating a method, at the Evaluation tab, a standard will be chosen from the Standard Editor's list!



1. Open the *Acquisition Mode*.

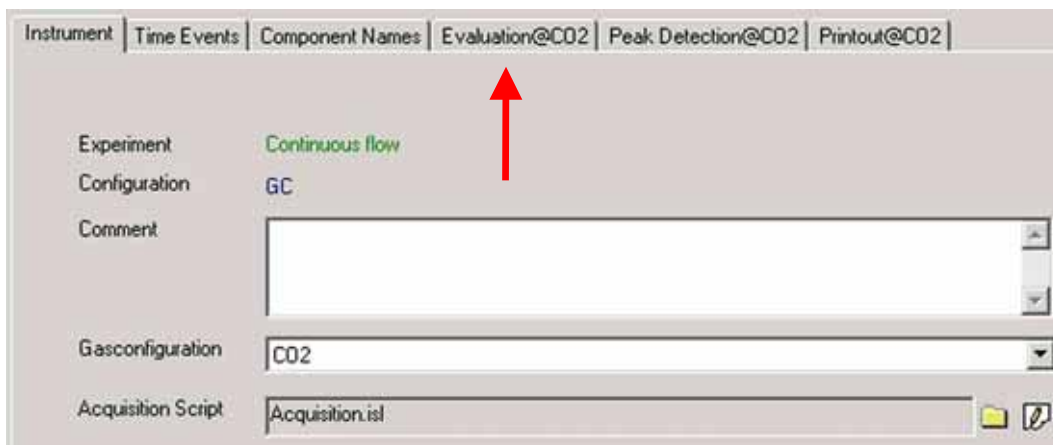


2. Press the **New** button.



3. Mark the *Method* icon.

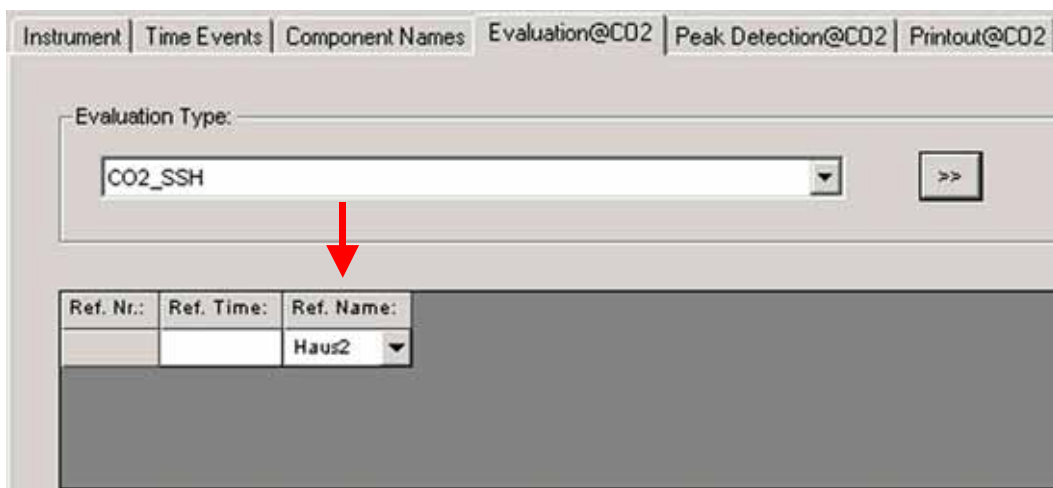
4. Confirm by **OK** and wait until the method is loaded.



The screenshot shows the 'Standard Editor' window with the 'Evaluation@CO2' tab selected. The 'Evaluation' tab is highlighted with a red arrow. The window displays the following information:

- Instrument: Instrument
- Time Events: Time Events
- Component Names: Component Names
- Evaluation@CO2: Evaluation@CO2 (selected)
- Peak Detection@CO2: Peak Detection@CO2
- Printout@CO2: Printout@CO2
- Experiment: Continuous flow
- Configuration: GC
- Comment: [Empty text box]
- Gasconfiguration: CO2
- Acquisition Script: Acquisition.isl

5. Choose the *Evaluation* tab.



The screenshot shows the 'Standard Editor' window with the 'Evaluation' tab selected. The 'Evaluation' tab is highlighted with a red arrow. The window displays the following information:

- Instrument: Instrument
- Time Events: Time Events
- Component Names: Component Names
- Evaluation@CO2: Evaluation@CO2 (selected)
- Peak Detection@CO2: Peak Detection@CO2
- Printout@CO2: Printout@CO2
- Evaluation Type: CO2_SSH
- Ref. Nr.: [Empty]
- Ref. Time: [Empty]
- Ref. Name: Haus2

6. Click on  in the *Ref. Name* column.



The screenshot shows the 'Standard Editor' window with the 'Ref. Name' column dropdown menu open. The menu lists the following options:

- Haus2
- IAEA CO2
- CO2 Lab. Ta
- CO2_zero
- Haus 3

Depending on the actual Gas Configuration, the pull-down menu offers the working standards that have previously been defined in the Standard Editor.

7. Choose the working standard you want to use, e.g. "Haus2".

Ref. Nr.:	Ref. Time:	Ref. Name:	d 13C/12C	vs.	d 18O/16O	vs.
1	0.00	Haus2 ▼	-39.260	VPDB	-25.540	VSMOW

The row will automatically be filled with the standard-related values from the Standard Editor. Thus, additional columns appear (if you type a reference time value into the **Ref. Time** column, this will happen as well).

Ref. Nr.:	Ref. Time:	Ref. Name:	d 13C/12C	vs.	d 18O/16O	vs.
1	0.00	User Defined ▼	-39.000	VPDB	-25.540	VSMOW

8. If you manually change one of these values inserted from the Standard Editor (e.g. the d 13C/12C value from - 39.260 of the Standard Editor to - 39.000), the Standard Name changes to **User Defined**. Other values in the row remain untouched.

2.2 Ratio Editor

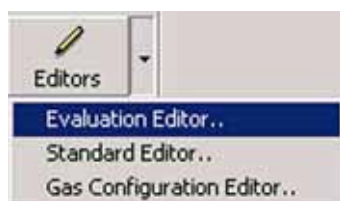
This section contains the following topics:


- Opening the Ratio Editor
- Adding an Evaluation to the Evaluations List
- Adding a Gas to the Filter List
- Information about Gases in the Filter List
- Incorporating a first Group of Ratios into the active Evaluation
- Incorporating a second Group of Ratios into the active Evaluation
- Incorporating an intermolecular Ratio into the active Evaluation
- Accessing Ratios in the Gas Configuration

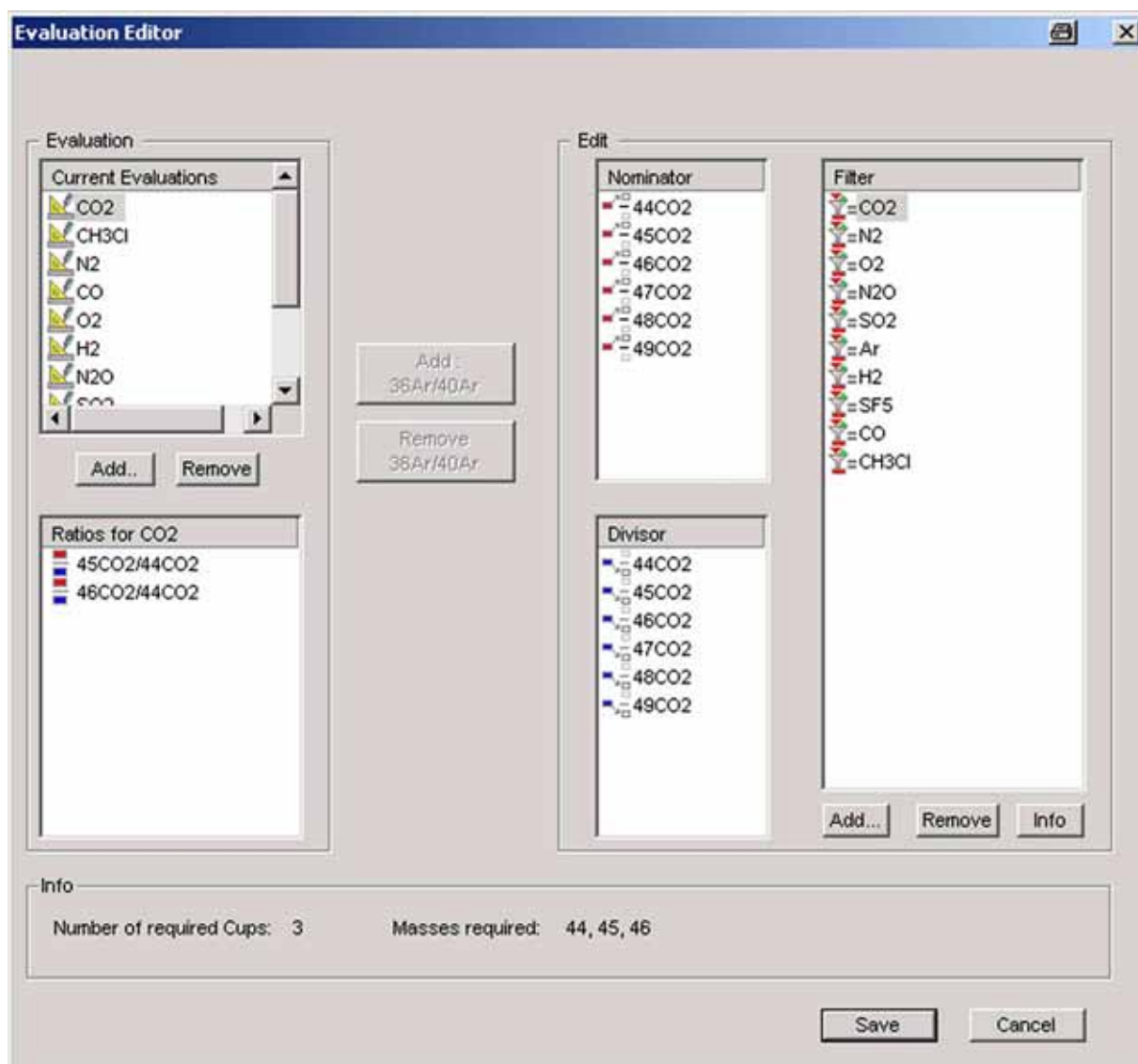
Opening the Ratio Editor



1. Open the *Acquisition* mode .

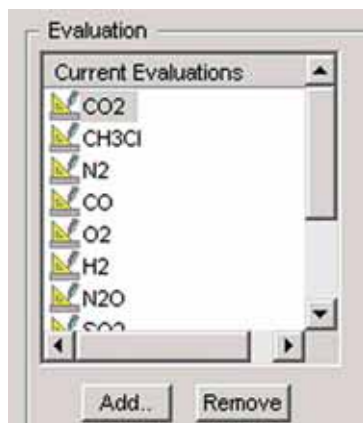


2. Press  right to the *Editors* icon.
3. Select **Evaluation Editor**.



The Ratio editor opens.

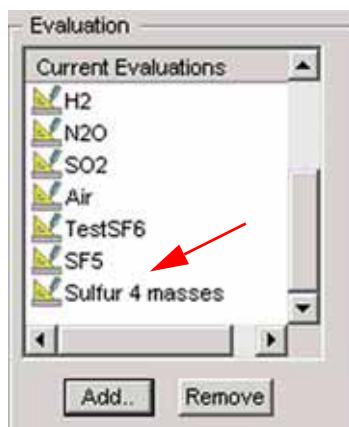
Adding an Evaluation to the Evaluations List



1. At **Current Evaluations**, the predefined evaluations to be used for filtering are listed.
2. Via **Add**, add a new evaluation to the list.



3. Type the Name of the evaluation to be added (e.g. “Sulfur 4 masses”).
4. Confirm by **OK**.



The new evaluation appears at the bottom of the list.

5. Via **Remove**, remove evaluations from the list.

Adding a Gas to the Filter List



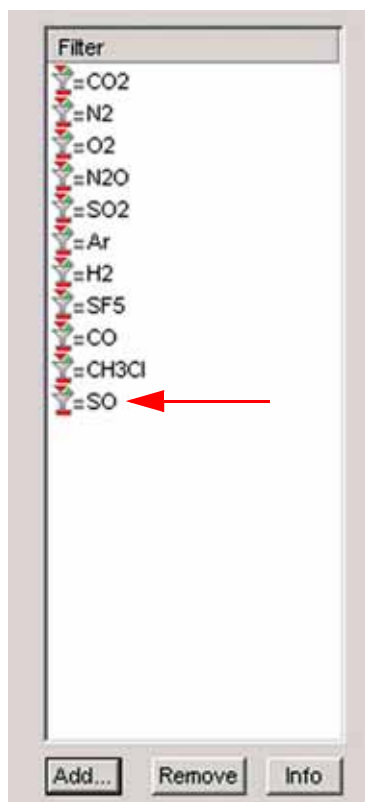
Take a look at the **Filter** list on the right:

If the gas to be used for ratio determination (e.g. “SO”) is missing there, it must be added to it as follows:

1. Press the **Add** button.



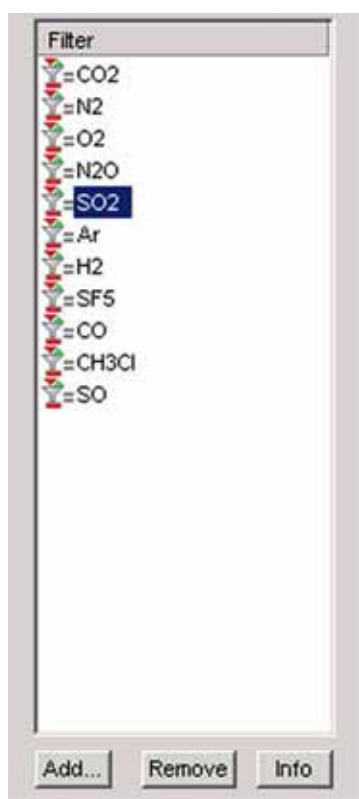
2. Type the gas name (e.g. “SO”) and confirm by **OK**.
If you type a non-existing element, an error message will occur.
The stoichiometry of the molecule will not be verified.



3. The gas (e.g. SO) has been added to the *Filter* list.

Information about Gases in the Filter List

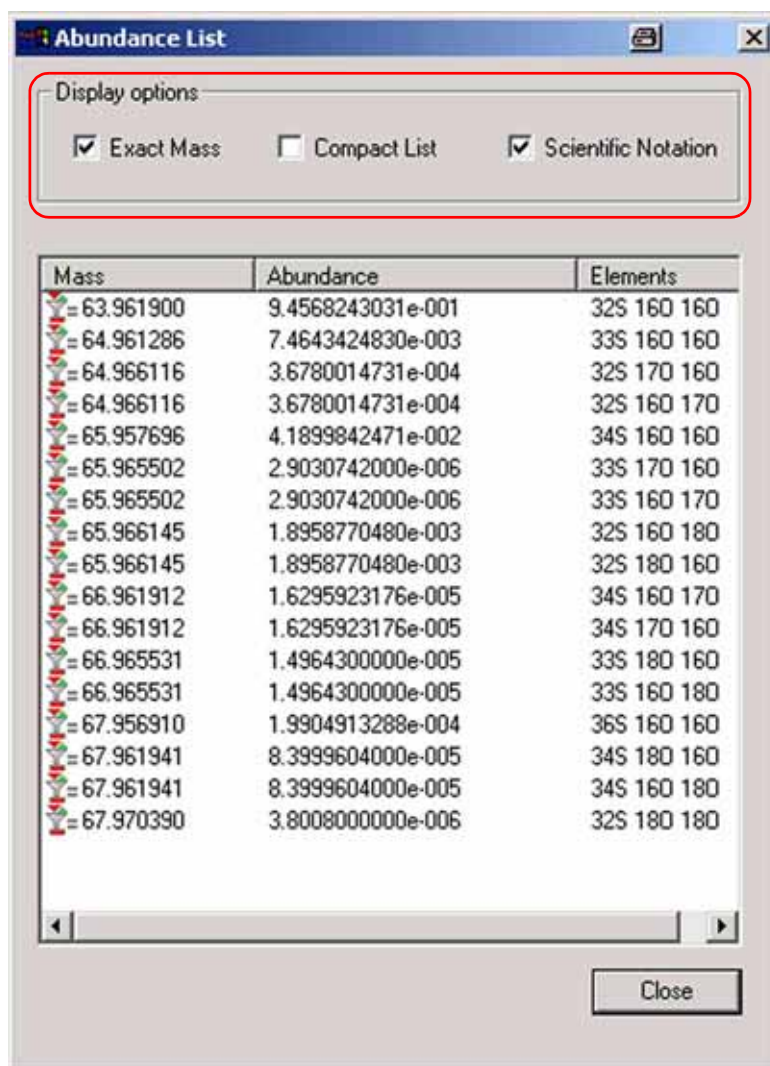
Principle: To facilitate the choice of masses and ratios and to control its reasonability, Isodat 2.0 provides mass-, element- and abundance-related data of a wide variety of gases. Especially calculating quotients of abundance values may be helpful to avoid measurement difficulties e.g. to select suitable amplifiers.



1. In the **Filter** list, mark the gas of interest (e.g. “SO₂”).
2. Press the **Info** button.

Mass	Abundance	Elements
= 64	0.94568243031288	32S 16O 16O
= 65	0.00819994277762	32S 16O 17O ; 32S 17O 16O ; 33S 16O 16O
= 66	0.04569740271564	32S 16O 18O ; 32S 18O 16O ; 33S 16O 17O ; 33S 17O 16O
= 67	0.00006252044635	33S 16O 18O ; 33S 18O 16O ; 34S 16O 17O ; 34S 17O 16O
= 68	0.00037084914088	32S 18O 18O ; 34S 16O 18O ; 34S 18O 16O ; 36S 16O 16O

3. The individual masses are displayed together with their abundances. In addition, possible isotopic combinations leading to a particular mass are shown.
4. You can sort the columns “Mass” and “Abundance” in ascending or descending order by clicking on them (see the arrows above).



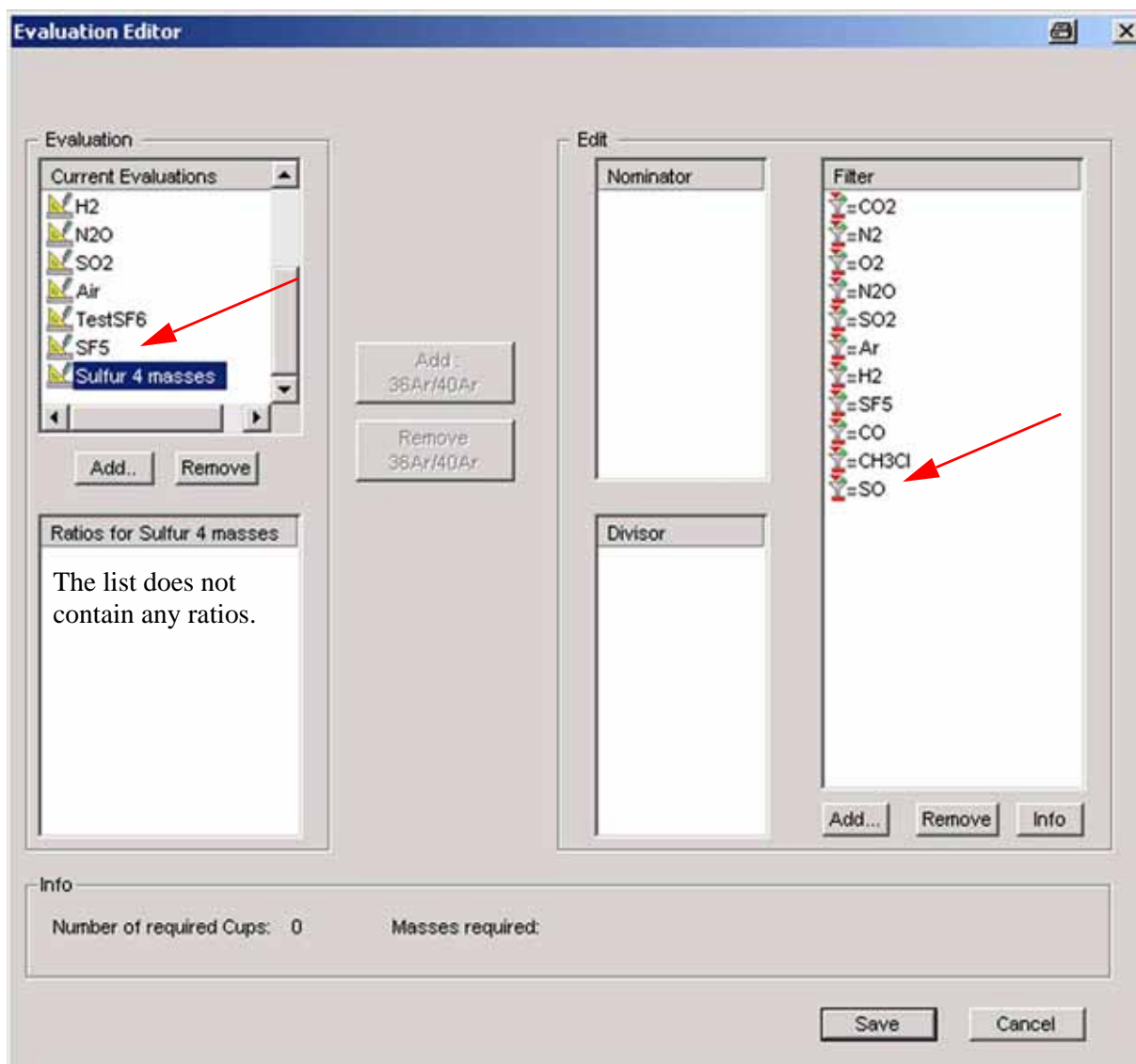
Choose among three *display options*:

- **Exact Mass**: a mass will not be displayed as a rough mass, but “exactly”, i.e. showing six decimal places (e.g. 63.961900 instead of 64).
- **Compact List**: if a bundle of species having the same mass occurs, only one of them will be displayed (e.g. 34S 18O 16O and 34S 16O 18O, see above).
To activate this checkbox, the “Exact Mass” checkbox must be marked.
- **Scientific Notation**: an abundance will not be shown as a decimal number but using scientific notation.

Incorporating a first Group of Ratios into the active Evaluation

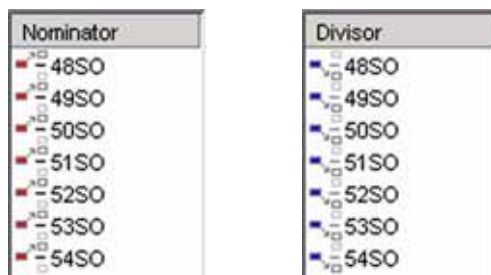
Ratios from the different lists on the right can now be incorporated into the active evaluation.

Example: Incorporation of the SO ratios 50SO/48SO, 49SO/48SO into the evaluation “Sulfur 4 masses”

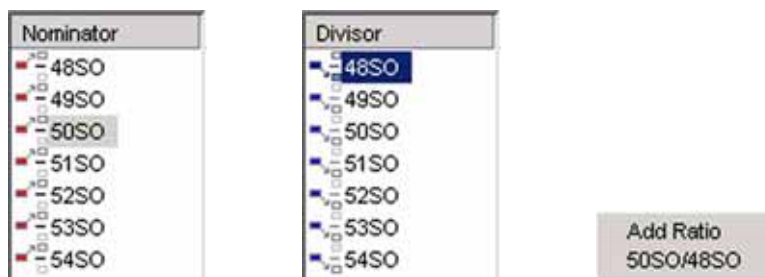


1. Note that the list “**Ratios for** Sulfur 4 masses” is empty, because no ratios have been incorporated yet.
2. Activate **one particular evaluation** by clicking on it (e.g. “Sulfur 4 masses”).

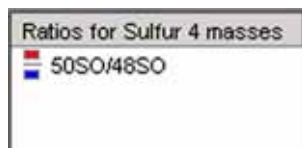
3. In the **Filter** list, click on the **gas** of interest (e.g. “SO”).
Note that “Sulfur 4 masses” turns into gray, i.e. it remains the active evaluation all the time.



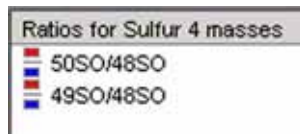
4. The isotopical combinations available are now displayed in the **Nominator** and **Divisor** lists, respectively.
5. To determine a ratio made up by a nominator and a divisor, choose one at a time from both lists. Begin with e.g. 50SO/48SO as follows:



6. Mark the **Nominator** (e.g. 50SO).
7. Mark the **Divisor** (e.g. 48SO). The Nominator turns into gray, i.e. it remains active.
8. Press the **Add Ratio** button (e.g. 50SO/48SO).



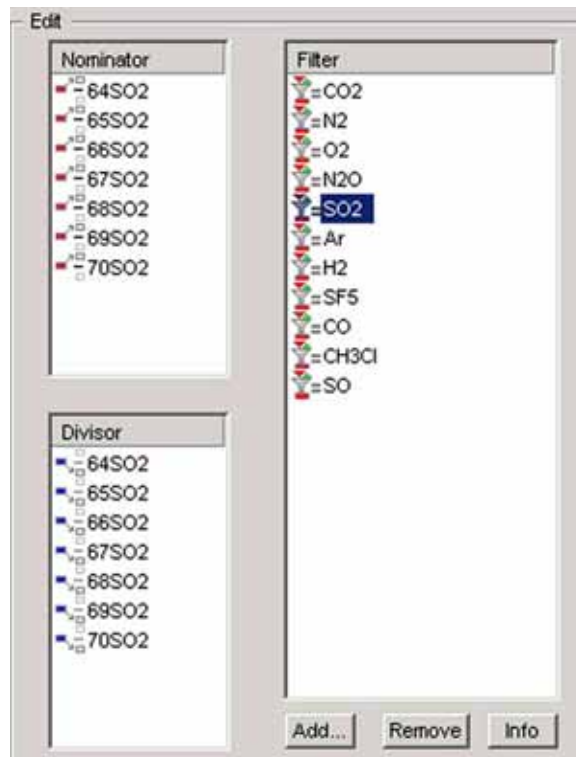
9. The ratio (e.g. 50SO/48SO) appears in the **Ratios** list.
It is now part of the evaluation “Sulfur 4 masses”.
10. Repeat the last steps for the second SO ratio (49SO/48SO).



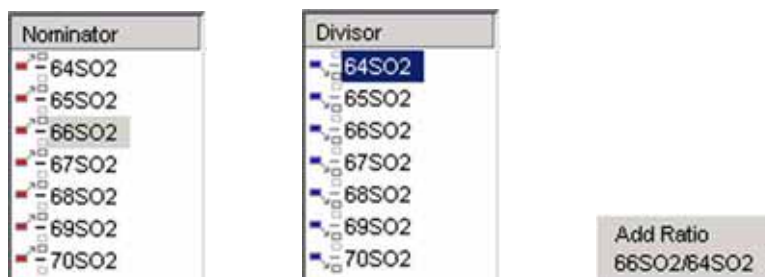
11. Both SO ratios appear in the **Ratios** list.
Both are now part of the evaluation “Sulfur 4 masses”.

Incorporating a second Group of Ratios into the active Evaluation

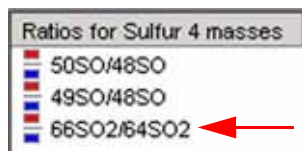
To measure SO₂ ratios (e.g. 66SO₂/64SO₂) in parallel within the same evaluation “Sulfur 4 masses”, they must be added to the evaluation as follows:



1. In the **Filter** list, mark **SO₂**.
The associated molecular masses available will appear in the **Nominator** list and **Divisor** list, respectively.



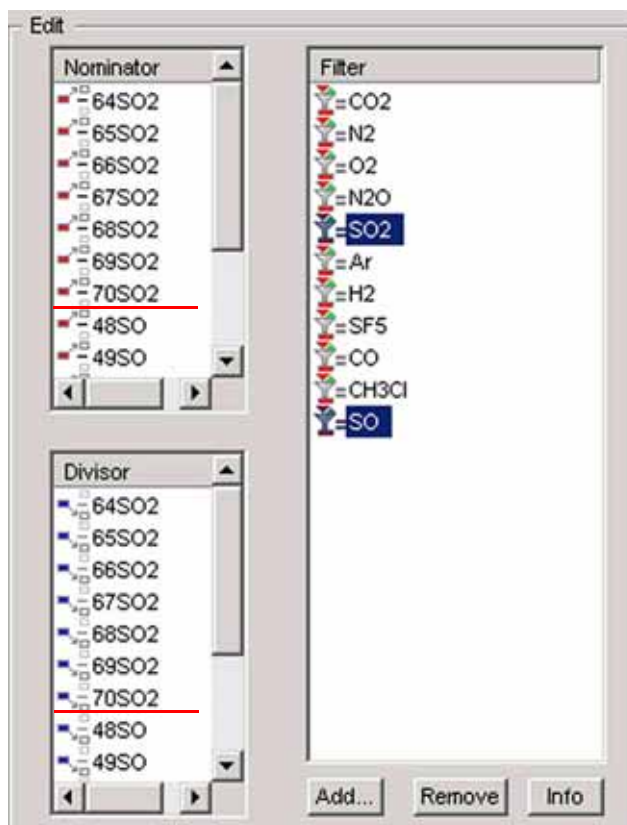
2. Mark the **Nominator** (e.g. 66SO₂).
3. Mark the **Divisor** (e.g. 64SO₂). The Nominator turns into gray, i.e. it remains active.
4. Press the **Add Ratio** button (e.g. 66SO₂/64SO₂).



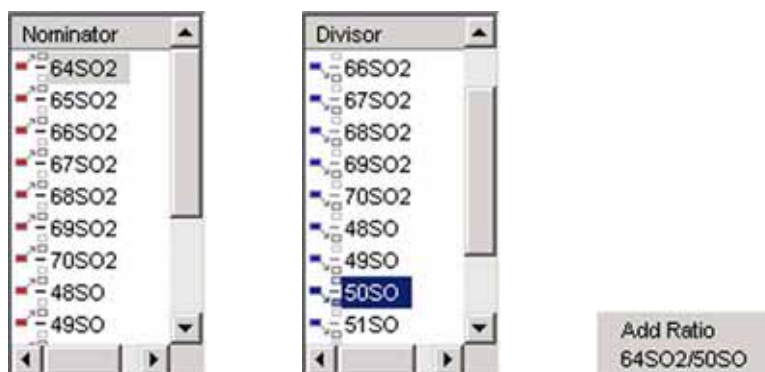
The ratio (e.g. 66SO₂/64SO₂) appears in the **Ratios** list.
It is now part of the evaluation “Sulfur 4 masses” as well.

Incorporating an intermolecular Ratio into the active Evaluation

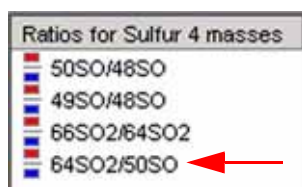
To measure intermolecular ratios (e.g. $64\text{SO}_2/50\text{SO}$) in parallel within the same evaluation “Sulfur 4 masses”, they must be added to the evaluation as follows:



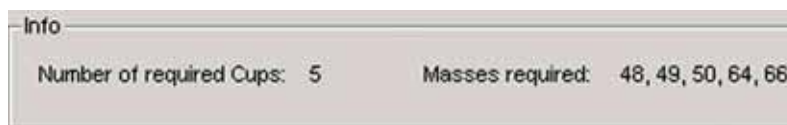
1. In the **Filter** list, mark **SO₂**.
2. Press the **<Ctrl>** key and mark **SO** simultaneously. Thereby, both gases will be marked. All associated molecular masses of **both** gases will appear in the **Nominator** list and the **Divisor** list, respectively.



3. Mark the *Nominator* (e.g. 64SO₂).
4. Mark the *Divisor* (e.g. 50SO). The Nominator turns into gray, i.e. it remains active.
5. Press the **Add Ratio** button (e.g. 64SO₂/50SO).



6. The intermolecular ratio (e.g. 64SO₂/50SO) appears in the *Ratios* list. It is now part of the evaluation “Sulfur 4 masses” as well.



During the entire incorporation of ratios into an evaluation, the *number of cups required* is displayed together with the corresponding *masses* to be measured.

7. After all different ratios have been incorporated into the active evaluation, finally press the **Save** button.
The Ratio editor will be closed. Your statements will be saved in the ratio database.
When the Ratio editor is opened again later, the evaluation “Sulfur 4 masses” contains all ratios that have been incorporated previously (see topic **Opening the Ratio Editor** on page 2-8).
The **Save** command will overwrite older definitions of the evaluation.

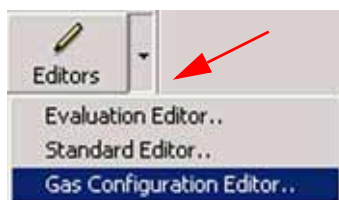
Accessing Ratios in the Gas Configuration


Principle: Evaluations must be anchored in a particular Gas Configuration. During measurement using the Gas Configuration, these evaluations will be executed.

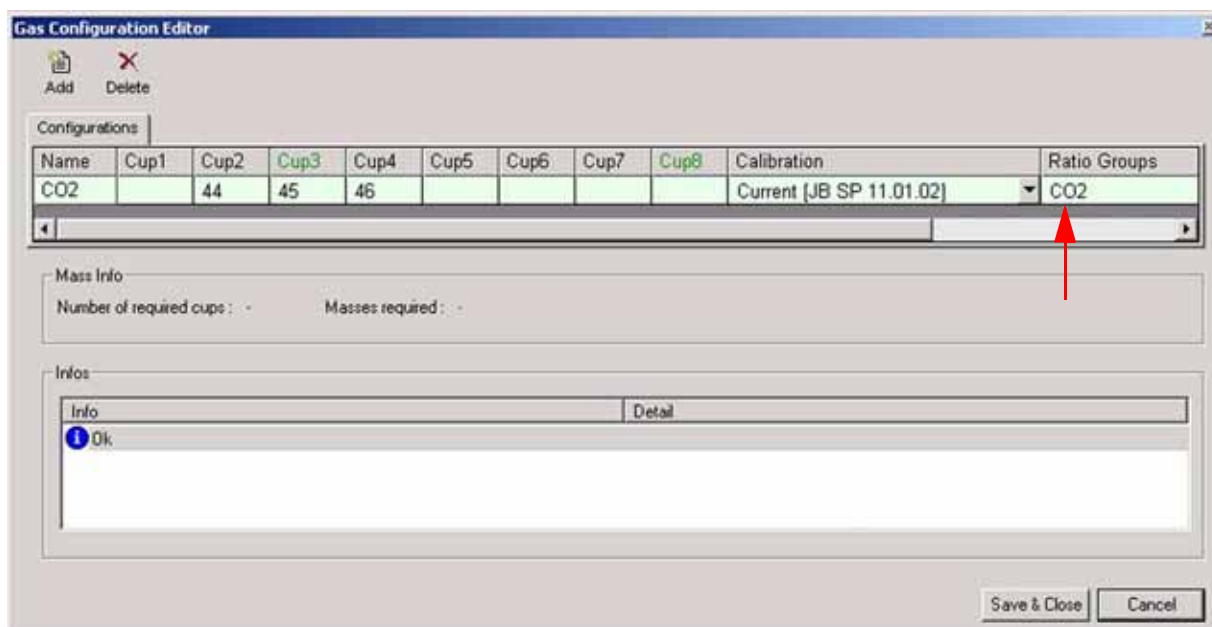
The ratios that have been incorporated into an evaluation (see topics **Incorporating a first Group of Ratios into the active Evaluation** on page 2-16 to **Incorporating an intermolecular Ratio into the active Evaluation** on page 2-20) can now be accessed via the Gas Configuration editor as follows:



1. Open the *Acquisition* mode



2. Press  right to the *Editors* icon.
3. Select **Gas Configuration Editor**.



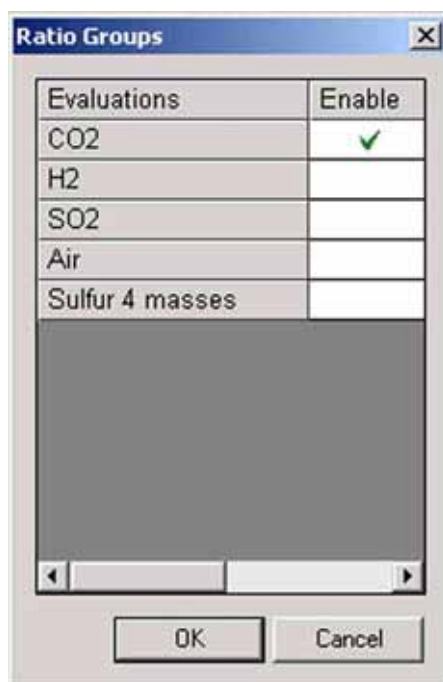
The Gas Configuration Editor opens.

In the **Ratio Groups** column, the **ratio groups** currently enabled for the actual Configuration are listed (e.g. ratio group “CO2” for the Configuration “CO2”). The **ratio group database** contains all ratio groups previously defined.

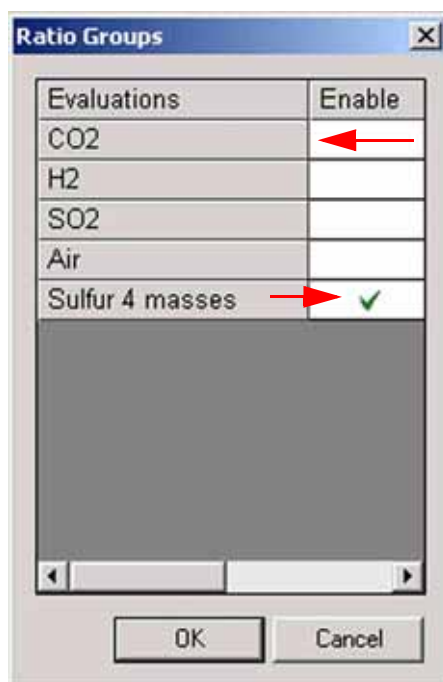
Ratio Groups
CO2

Ratio Groups
CO2

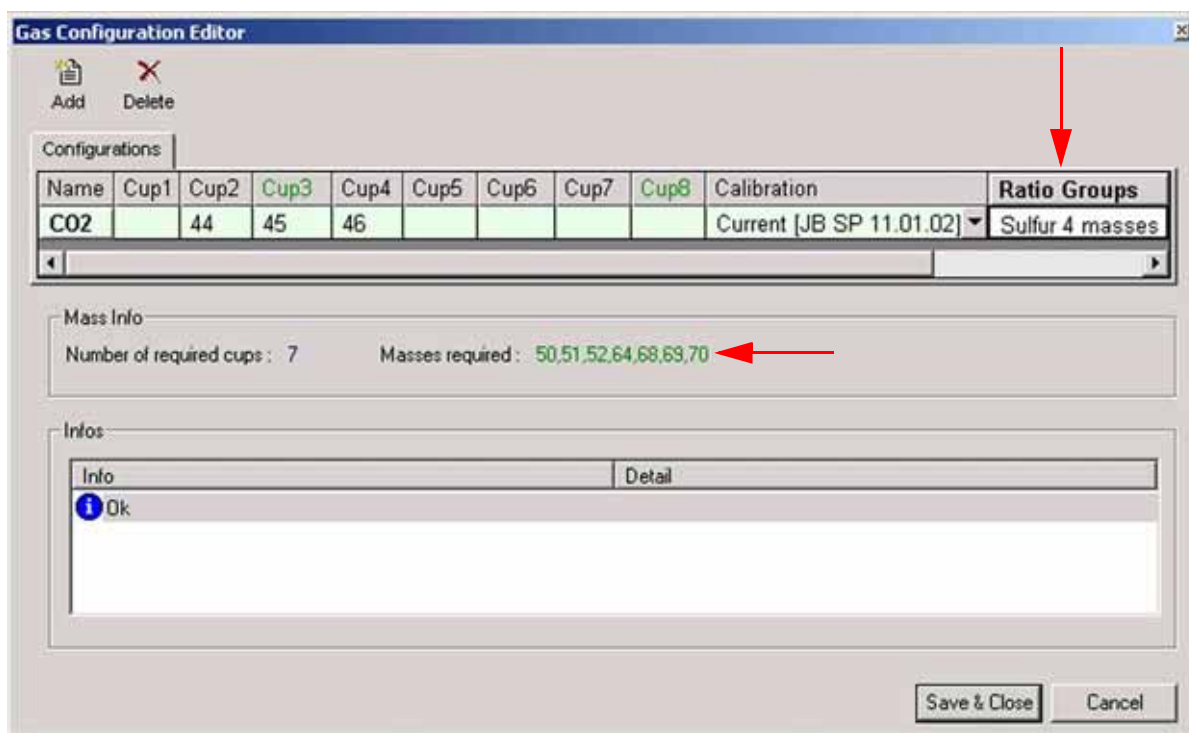
4. **Click** on the entry within the “Ratio Groups” cell of interest (e.g. on “CO2”).
The column header “Ratio Groups” thereby appears in bold style.
The color of the ratio group (i.e. CO2) changes from light green to white.
5. Again **click** on the entry.



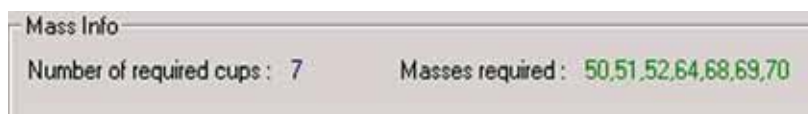
6. The different evaluations that have previously been defined are listed (see topic **Adding an Evaluation to the Evaluations List** on page 2-10). As the evaluation “CO2” is currently enabled, it appeared in the “Ratio Groups” column above.



7. To disable the evaluation “CO2”, **click** into the cell with the green hook. The hook disappears and the cell is empty.
8. The evaluation “Sulfur 4 masses” is currently disabled. To enable it, **click** into the empty cell. A hook appears and “Sulfur 4 masses” is displayed in bold style.
9. Confirm by **OK**.



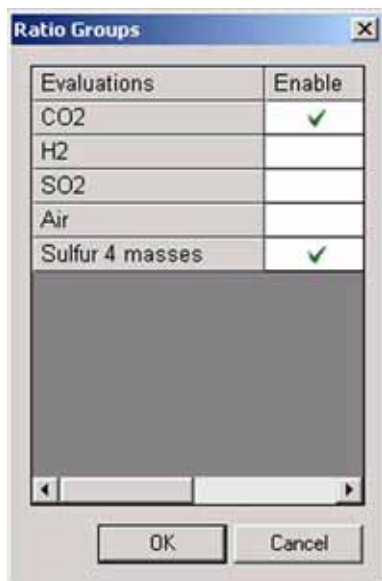
10. As “Sulfur 4 masses” is the evaluation currently enabled, it will be shown in the “Ratio Groups” column.



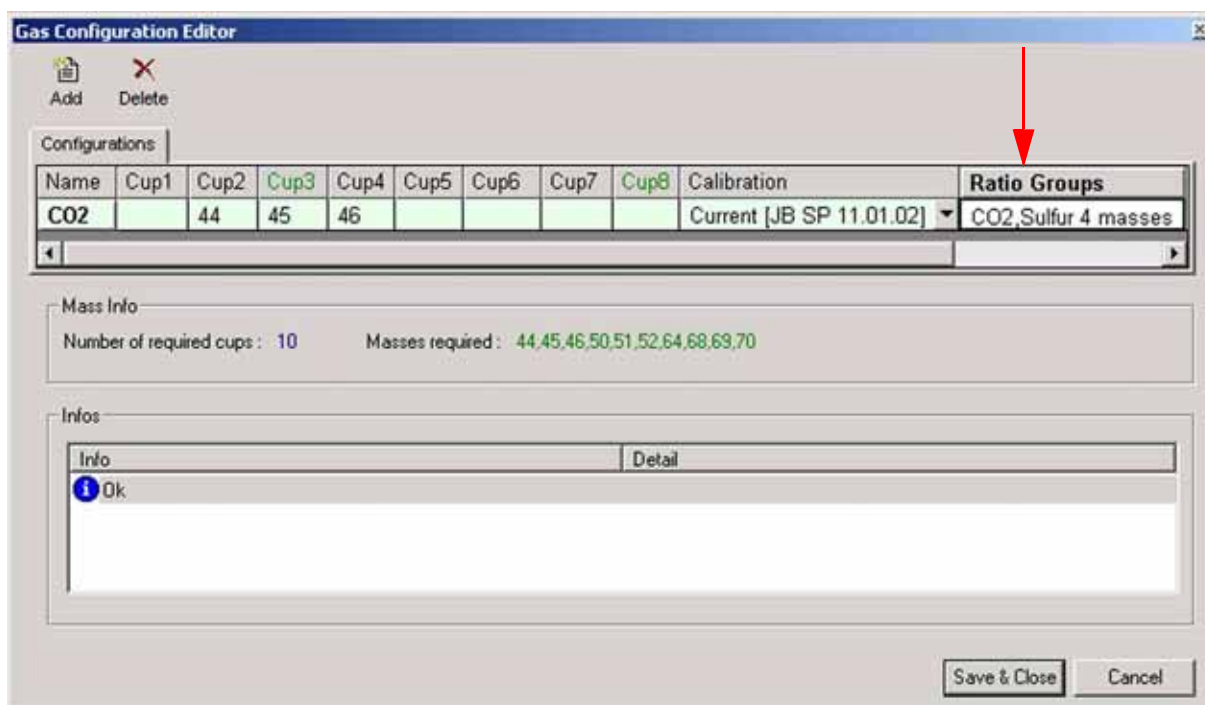
As in the Evaluation Editor, the number of cups required is again displayed together with the masses to be measured. Isodat 2.0 compares these cup- and mass-related requirements to the statements you gave in the early beginning while configuring your mass spectrometer.

11. Type the masses being displayed into the appropriate cup columns (i.e. assignment of the masses to the cups).
12. Finally, press **Save & Close**.

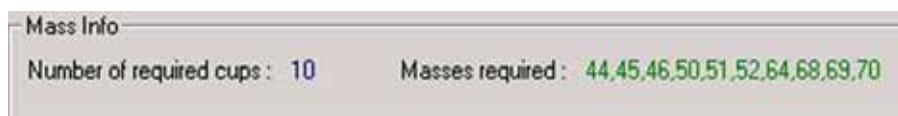
It is possible to enable two or more evaluations in one and the same Gas Configuration simultaneously (e.g. evaluation “CO2” and evaluation “Sulfur 4 masses”):



1. Enable both evaluations by clicking into the respective cells.
2. Confirm by **OK**.



Both evaluations appear in the “Ratio Groups” column.



Again, the number of cups required is displayed together with the masses to be measured.

Note that the number of cups required may exceed the number of available ones (e.g. only 8 cups available whereas 10 are required).

Measurement will be impossible then, because Isodat 2.0 again compares these requirements to your statements during mass spectrometer configuration.

3. Type the masses being displayed into the appropriate cup columns (i.e. assignment of the masses to the cups).

During an evaluation, the ratio group will be analyzed according to the masses required. If masses cannot be found and thus not be measured, they will not be part of an evaluation. Ratios and all subsequent parameters will not be calculated.

4. Finally, press **Save & Close**.

Chapter 3

Script-related Features

The three script-related features recently integrated or improved:

- ISODAT Script Language (ISL) and the ISL Editor
- Dynamic Variables Exchange (DVE)
- A powerful debugger

are closely interrelated and conceived as a package. Therefore, their separate description below might seem somehow artificial.

3.1 ISL Editor

The script language *ISL* (ISODAT Script *L*anguage) itself and its commands have already been described in detail in the ISL-Online-Help. In this section, only the functions within the ISL Editor will be explained: emphasis is placed on how to edit ISL-Scripts and how to navigate through ISL.

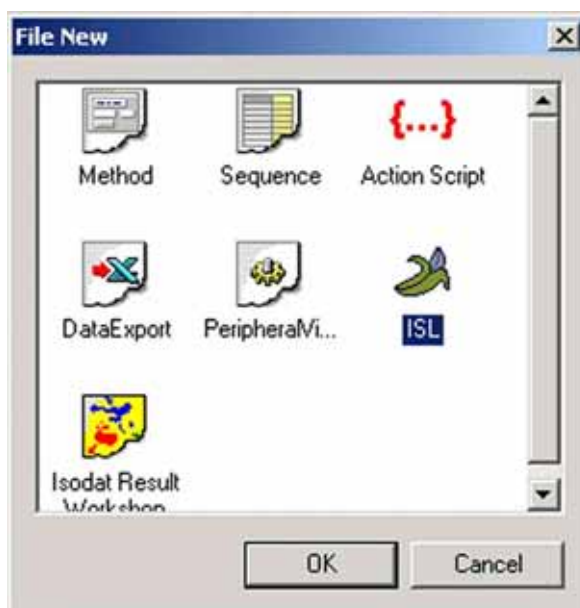
Opening different Types of ISL Scripts



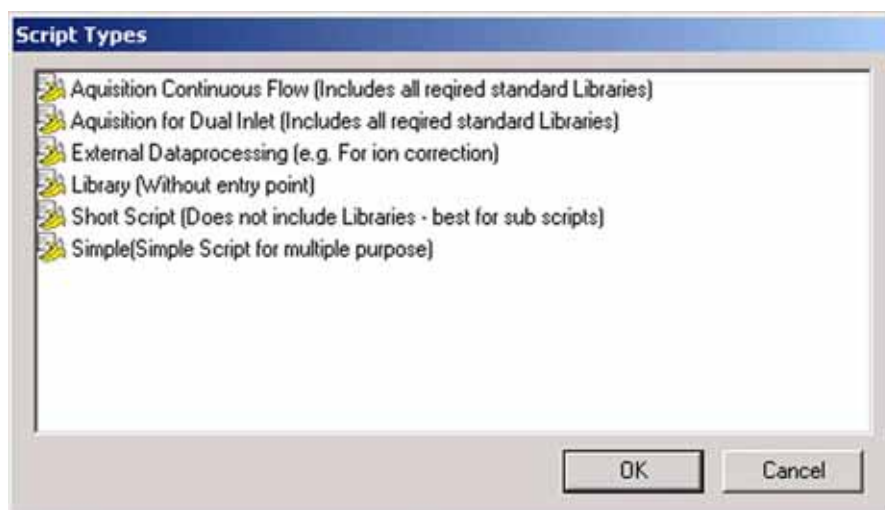
1. Open the Application Mode .
The “Application Mode” window opens.



2. Press the **New** button .



3. Mark *ISL* and confirm by **OK**.



4. Choose a template for a script among the following six script types. They are different only with respect to the libraries to be included.
 - Script for **Continuous Flow** acquisition
All standard libraries required are included.
 - Script for **Dual Inlet** acquisition
All standard libraries required are included.
 - Script for **external data processing**
This type may be used for e.g. an ion correction.
 - **Library** (without entry point)
This script type is used to create a library.
 - **Short script**
Use this type to create short scripts that e.g. will run as subscripts.
Furthermore, scripts can be assigned to e.g. valves to induce a valve switch or to buttons (see Panel Design).
 - **Simple** script
These scripts are used for different purposes.
5. Mark the script type of your choice (e.g. “Acquisition for Dual Inlet”).
6. Confirm by **OK**.

A script of the chosen type is opened. The ISL Editor appears. Its functions will now be described in detail.

General Remarks concerning ISL Scripts

Variables and functions in ISL

In ISL, **variables** denote objects that can assume certain values. **Functions** are active components working with variables.

For detailed information about the difference between variables and functions and about particular ones, use context-sensitive ISL Help via <F1> as follows: position your cursor on an arbitrary string and press <F1>. The actual variable or function will be accessed and the corresponding help topic be opened.

Colors of keywords

Internal functions, i.e. **ISL** functions are highlighted by colors automatically:

```
//-----  
//place your includes here  
//-----  
include "lib\stdisl.isl"  
include "lib\instrument.isl"  
include "lib\Acquisition_lib.isl"  
//-----
```

- a **blue** function is an internal one denoting a control structure (e.g. a for-next loop).
- a **lavender** function also denotes an internal one (e.g. “set”).
- a **green** function has been commented out and has thus lost its meaning.
- a black function is part of the library and will be called up by “call”.

This is helpful for finding typing errors: if the text stays black, no internal function has been called, and the typo can easily be corrected. Afterwards, the corrected text is colored again.

Commenting out lines or blocks

`function CleanUp()` → `//function CleanUp()`

- To comment out a single line, insert a double slash // where it begins. The line turns into green and loses its function.

`include "lib\stdisl.isl"`
`include "lib\instrument.isl"`
`include "lib\Acquisition_lib.isl"` → `/*include "lib\stdisl.isl"`
`include "lib\instrument.isl"`
`include "lib\Acquisition_lib.isl"*/`

- To comment out an entire block, insert /* where it begins. Do not miss to insert */ where it ends, because otherwise, the complete remainder of the script will turn into green and lose its function.

Only the block turns into green and loses its function.

Finding out the content of variables

- Right-click somewhere into the script.



The context menu appears. It will be discussed in detail below.

Context Menu within the ISL Editor


The ISL Editor is an ordinary text editor. E.g. cut or paste content, drag & drop content, select a line or a block or indent a marked block via **<Shift>** key. Data will even be saved in *.txt-format.

Open File Command

To be able to take a look at a file that is mentioned in a script, position the cursor somewhere in the file name.

Example: To take a look at the file “Acquisition_lib.isl” position the cursor somewhere in this name. “Acquisition_lib.isl” is a typical library used to perform Dual Inlet Acquisitions. “Include” is a control structure to include a library.

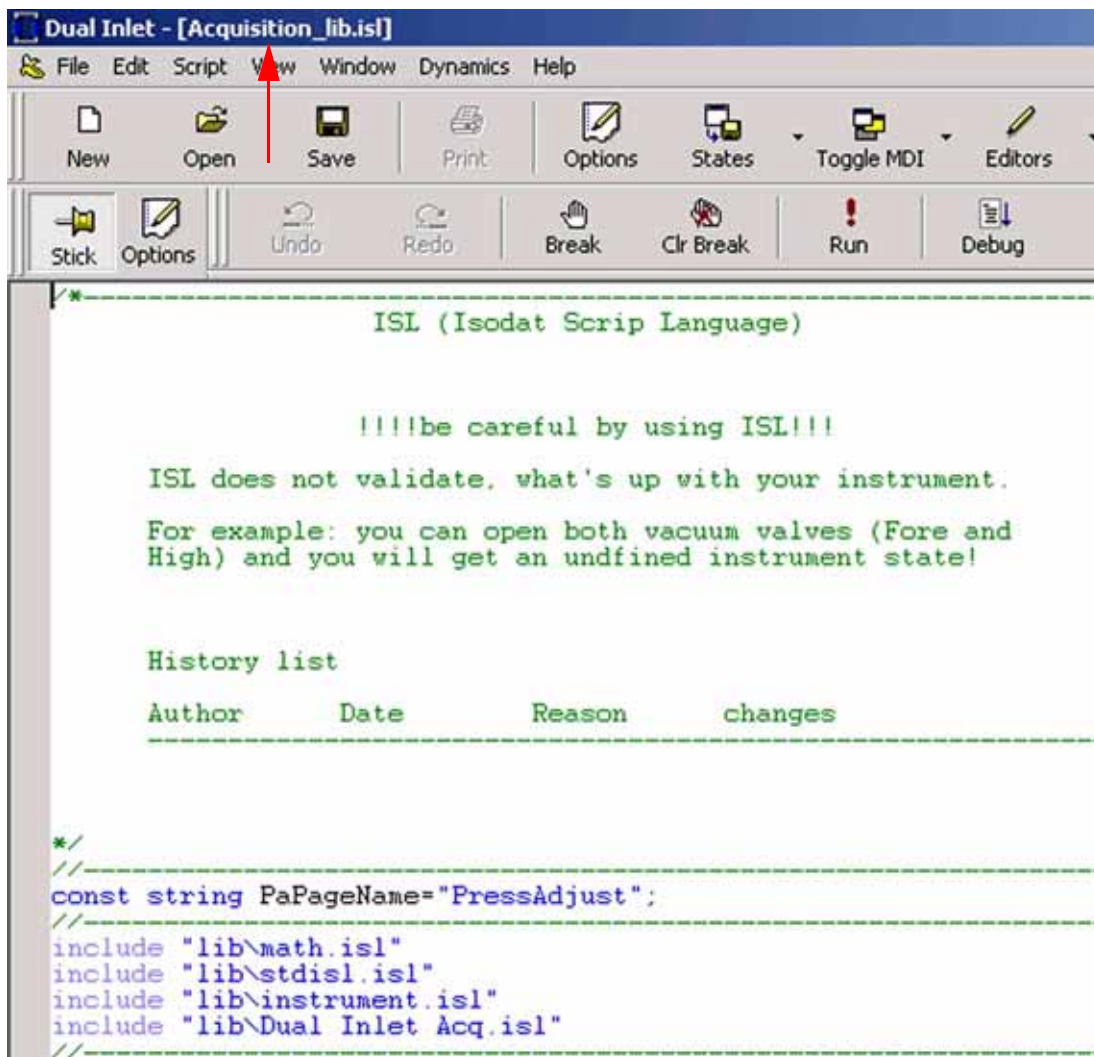
```
//-----  
//place your includes here  
//-----  
include "lib\stdisl.isl"  
include "lib\instrument.isl"  
include "lib\Acquisition_lib.isl"  
//-----
```



1. Right-click on the file name (e.g. “Acquisition_lib.isl”).



2. Choose **Open File**.



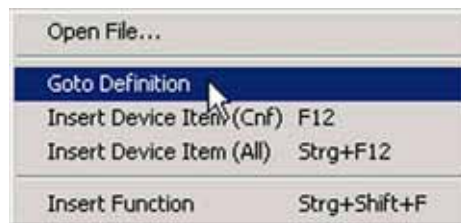
3. The file will be loaded in a window of its own (e.g. "Acquisition_lib.isl").

Goto Definition Command

This command is meaningful, if you do not know the location where a particular function has been defined (not an internal function but a library function, e.g. "InitScript"). To call up such a function, position the cursor somewhere in the function name.

```
//-----
function InitScript()
{
    OnBreak CleanUp;
}
```

1. Right-click on the function (e.g. "InitScript").



2. Choose **Goto Definition** or press **Edit > Goto Definition** or **<F11>**.

```
//-----  
script ScriptName//TO DO: Replace with your script name  
{  
}  
//-----  
//place your includes here  
//-----  
include "lib\stdisl.isl"  
include "lib\instrument.isl"  
include "lib\Acquisition_lib.isl"  
//-----  
function CleanUp()  
{  
}  
//-----  
function InitScript() ←  
{  
    OnBreak CleanUp;  
}  
//-----  
//this is the main point entry - this function is essential  
//-----  
main()  
{  
    call InitScript();  
}  
//-----
```

The file is loaded. The function will be accessed and marked (e.g. "InitScript"). This is the definition of the library function.

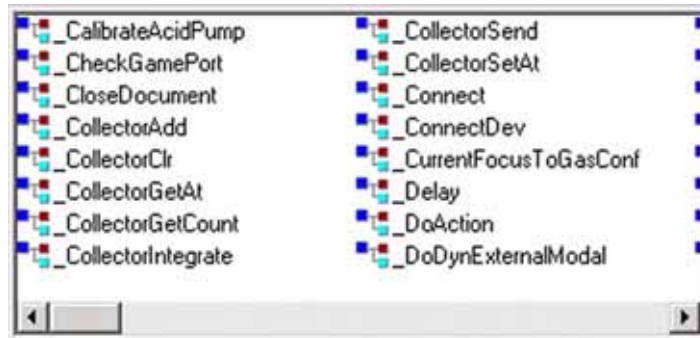
Insert Function Command

Maybe, you do not know exactly the name of a particular internal function.

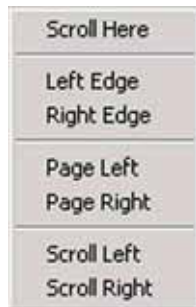


1. Position your cursor where you want to insert the internal function.

2. Right-click on this position and choose **Internal Function**.
Alternative: Press **<Shift> + <Ctrl> + <F>** simultaneously.



3. A survey of the names of all internal functions is shown.
4. Increase or decrease the box by dragging its edges.
5. Find your internal function of interest by a right-click on the scroll-bar:



6. Mark the internal function you are looking for (e.g. “_CalibrateAcidPump”).
7. Press **Enter**.
It will be inserted into the ISL Script at cursor position.
The box is closed (also by a double-click).

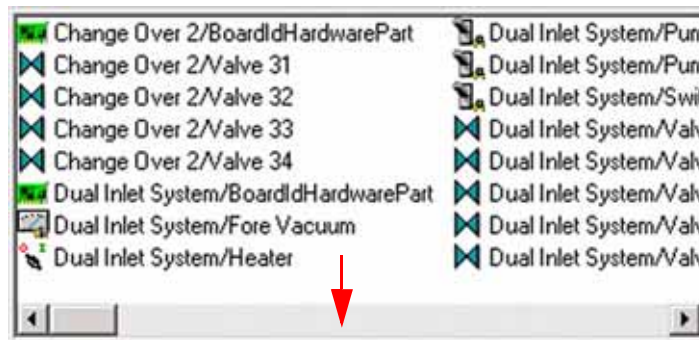
Insert Device Item (Cnf) Command

After you have thereby found the internal function, maybe you do not know the exact name of the peripheral it should act upon.



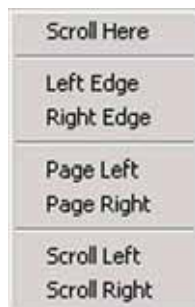
1. Set your cursor at the correct position.

2. Upon a right-click select **Insert Device Item (Cnf)**.
Alternative: Press **<F6>**.



A box opens that contains all peripherals of the actual configuration.

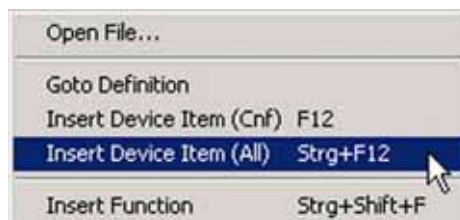
3. Increase or decrease the box by dragging its edges.
4. Find your peripheral of interest easily by a right-click on the scrollbar



5. Mark the peripheral you are looking for (e.g. "Change Over 2/Valve 34").
6. Press **Enter**. It will be inserted into the ISL Script at cursor position. The box is closed (also by a double-click).

Insert Device Item (All) Command

This command is meaningful when writing scripts for a configuration that is not the actual one at the moment.



- Upon a right-click select **Insert Device Item (All)**.
Alternative: Press **<Ctrl> + <F6>** simultaneously (instead of **<F6>**). A box opens that contains all peripherals known in Isodat 2.0 (i.e. not filtered according to the actual configuration).

Basic Functions - The ISL Toolbar

After you opened an ISL script (see topic **Opening different Types of ISL Scripts** on page 3-2), the ISL toolbar shown above offers a wide variety of commands.

They are helpful for handling ISL scripts and facilitate orientation within them. These commands will be discussed one by one below.

Undo and Redo Commands



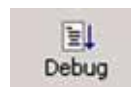
- The **Undo** command reverses the last action or deletes the last entry you typed.
- The **Redo** command reverses the action of the **Undo** command (i.e. the **Undo** command must have been used immediately before).

Break and Control Break Commands

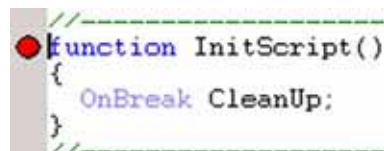
Breakpoints are used to check programs section by section with respect to bugs: if you know that a program works properly down to an unstable position, set a break point there to verify it.



1. Press **Break** to set a breakpoint at the line of your cursor. Alternative: Press **Edit > Toggle Breakpoint** or **<F9>**. A red point appears at the left edge of the ISL Script.



2. Then, press the **Debug** button to start the script in Debug Mode (used for stepwise execution of a script in order to debug it). As always, debugging starts at the entry address of the program ("main") and stops at the break point that just now has been set.

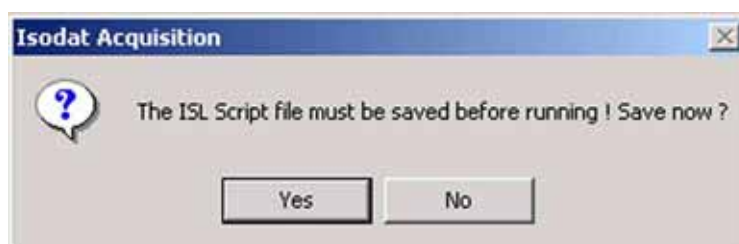


- Break is a toggle command: press it twice to remove the break point again.
Alternatives: Press **Edit > Toggle Breakpoint** twice or **<F9>** twice.



- Press **Clr Break** to eliminate all break points. Remember that pressing **Break** twice will only remove the single break point of the actual line.
Alternative: Press **Edit > Remove all Breakpoints** to eliminate all break points.

Run and Debug Commands



- You are reminded to save the ISL Script prior to choose either **Run** or **Debug**. Confirm by **Yes**.




- Select an appropriate folder.
- Type a significant file name (e.g. "Execution.isl").
- Confirm by **Save**.


Note the difference between **Run** and **Debug**:

Run Breakpoints *will not be* considered (i.e. the execution of the script overrides break points without stopping).


Debug Breakpoints *will be* considered (i.e. the execution of the script stops at break points).

5. Press **Run**  to simply start a script from the beginning until it reaches its end without debugging it. In contrast to Debug, breakpoints will not be considered. This is used to check whether a script is working properly or not.

Alternatives: Press **Script > Go** or **<Ctrl> + <F5>**.

6. Press **Debug**  to start a script in Debug Mode i.e. breakpoints will be considered. Debugging without breakpoints is meaningless.

Alternatives: Press **Script > Debug** or **<F5>**.


Press the **Options**  button. Then mark **Debug**.




```
//-----
script ScriptName//TO DO: Replace
{
}
//-----
//place your includes here
//-----
include "lib\stdisl.isl"
include "lib\instrument.isl"
include "lib\Acquisition_lib.isl"
//-----
```

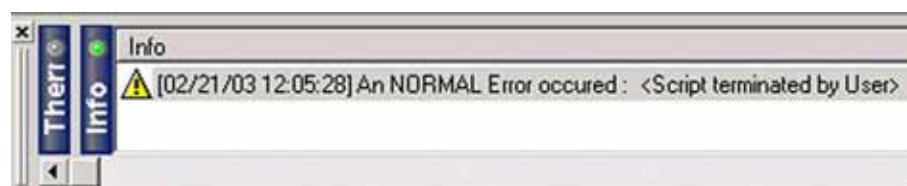
Note that Debug Mode is indicated by a yellow background whereas the ISL Editor's background is white.

Stop and Break Commands

- Press **Stop**  to stop a script that is being executed (i.e. it is running or being debugged).
Alternatives: Press **Script > Stop** or **<Alt> + <F5>**.

```
//-----
function InitScript()
{
    OnBreak CleanUp;
}
//-----
//this is the main point
X //-----
main()
{
    call InitScript();
}
```

A red **X** appears at the left edge of the script.



The last error message that occurred at **X** is displayed at Info (e.g. "A normal error occurred: Script terminated by user").



The error message is also displayed at the Status bar at the bottom right.



- Press **Break** to pause a running script at its current position (e.g. long-lasting processes or unintended endless loops are being executed).

```
//this is the main point entry
//
main()
{
    call InitScript();
}
```

- The yellow program counter together with a yellow line reveal the position (e.g. an unintended endless loop or a deadlock, i.e. two processes waiting for each other. These bugs can be corrected in this way).

Step in, Step over and Step out Commands

Note the difference between **Step over** and **Step in**:

Step over: Select a new function or execute it without leaving the actual context. Other contexts are irrelevant at the moment.

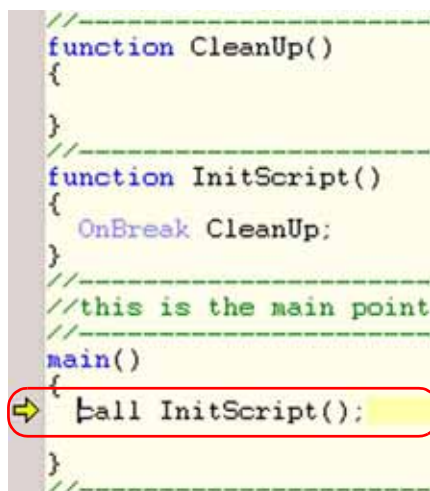
Step in: Select a new function or execute it and leave the actual context. The context of this new function one level deeper is entered in order to take a look at it.

Example: Consider the two functions “InitScript ()” and “CleanUp ()” in an arbitrary ISL Script. Below, they are both marked red.

```
function CleanUp()
{
}
//
function InitScript()
{
    OnBreak CleanUp;
}
//this is the main point
//
main()
{
    call InitScript();
}
```

- Position your cursor in the line “call InitScript ()” (within main() context).
- Press **Break** in order to set a breakpoint there. The breakpoint appears at the left edge.

3. Press **Debug**. Thereby, one changes to the Debug Mode (yellow).



```
//-----  
function CleanUp()  
{  
}  
//-----  
function InitScript()  
{  
    OnBreak CleanUp;  
}  
//-----  
//this is the main point  
//-----  
main()  
{  
    call InitScript();  
}  
//-----
```

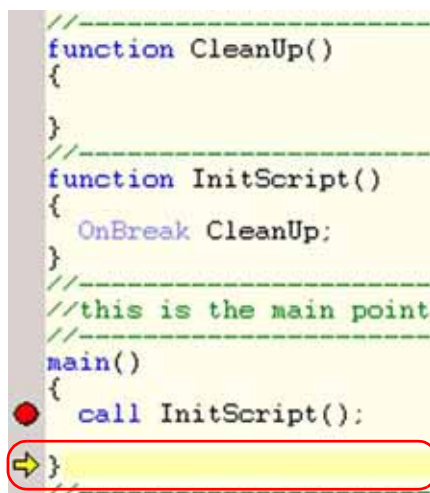
Note that debugging stops at the break point (within the main context). The yellow program counter now points to the line and has replaced the break point.

Case I: “Step over” command

- a. Press **Step over**



Alternatives: Press **Script > Step over** or **<F10>**.



```
//-----  
function CleanUp()  
{  
}  
//-----  
function InitScript()  
{  
    OnBreak CleanUp;  
}  
//-----  
//this is the main point  
//-----  
main()  
{  
    call InitScript();  
}  
//-----
```

The program counter has executed the function “InitScript ()” and stepped over it. It is now positioned in the line below the function.

Note that the *context is still the same* (i.e. context “main ()”). Therefore, contents of any other context (e.g. context “InitScript ()”) are unimportant. The break point is visible again.

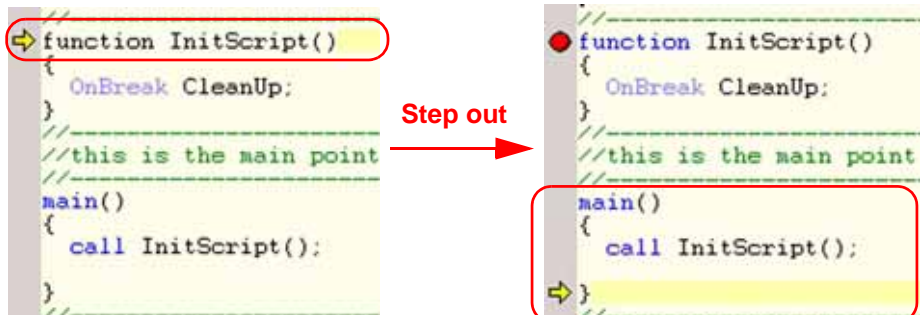
Case II: “Step in” command



- a. Press **Step in**.
Alternatives: Press **Script > Step into** or **<F8>**.

```
//
function CleanUp()
{
}
//
function InitScript()
{
    OnBreak CleanUp;
}
//this is the main point
//
main()
{
    call InitScript();
}
//
```

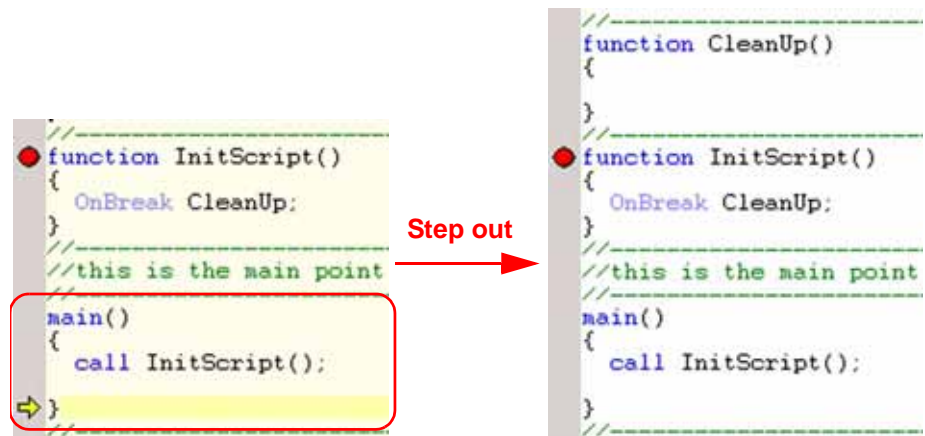
Note that the program counter has *left the original context* and is now positioned on another function (“CleanUp”) *within another context*. This new context can thus be examined. The break point is visible again.



Step out is used to terminate all processes within the actual context and to leave it (e.g. after debugging has been successful in “CleanUp” context). One moves to the next higher context (e.g. to “main” context).


Alternatives: Press **Script > Step out** or **<Shift> + <F7>**.

This command is advantageous, if in an old context a lot of functionality is active that is no longer important: simply press **Step out** to terminate this.



Pressing **Step out** repeatedly will finally lead back to the ISL Editor. The break point is visible again. **Step out** is only available in Debug Mode.

Prg Ptr Command

The program pointer indicates the position of the program within the script. The **Prg Ptr** command is useful when scrolling through long scripts: if you do not know the actual position of the program pointer  anymore, press



the **Prg Ptr** button. The cursor will instantaneously move to the program pointer. This command is only active in Debug Mode i.e. not in the ISL Editor itself.

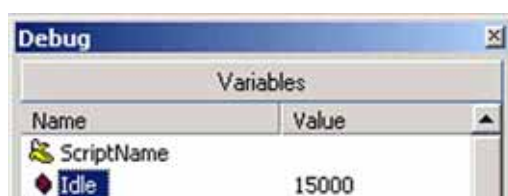
Watch Command and Debug Bar



The **Watch** command can be toggled and serves to switch on and off the **Debug** bar. Switch it off occasionally in case of long lines. The Debug bar is organized by four tabs: **Variables**, **Functions**, **Call Stack**, and **Threads**. Drag&drop it to move it around. The Debug bar is activated automatically when entering debug mode (by pressing “Debug” or “Step in”). In ISL Editor, the **Variables** tab leads to an empty list.



At **Variables** tab, the names and actual values of the variables that occur in the script are listed. A small colored block left to the name denotes the type of the variable. E.g. a blue block denotes a string variable whereas a red block symbolizes a pointer variable.

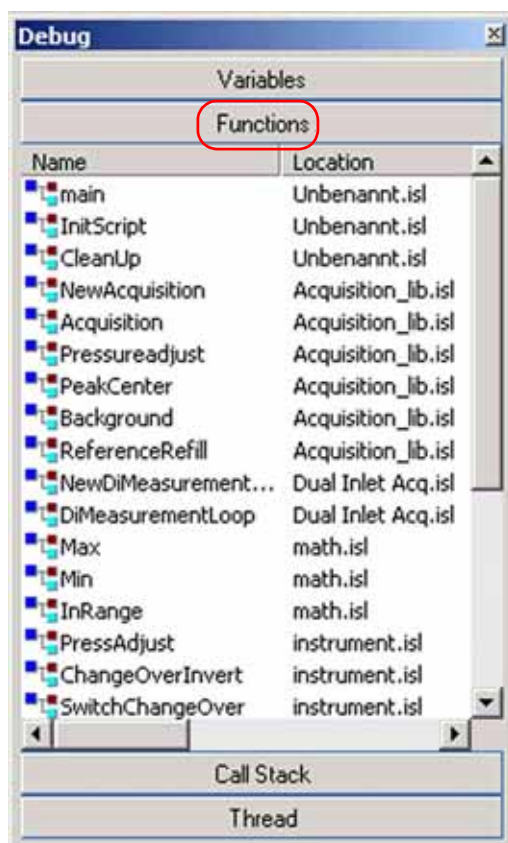



Example: The variable named “Idle” is a pointer variable (red block). Its actual value is 15000.

Various types of variables are represented differently. E.g. a boolean variable may be represented by the value 0, i.e. false, whereas a string variable may be represented by the numeric value 15.

If you define new variables in the script and enter debug mode, they will occur in the list at Variables tab. If a variable changes its value, the new one will be displayed there.

At “Script Name”, the name of the script always occurs.



At **Functions** tab, the names of the functions defined in the *different* scripts are listed in the **Name** column. At the **Location** column, find the particular ISL Script, where it is defined. E.g. The function “Pressureadjust” occurs in the script “Acquisition_lib.isl”. All functions have the same symbol  shown left to the **Name** column.

At **Call Stack** tab, the order of functions that have been called up recently is displayed. The function called up at last lies on top of the stack (i.e. the actual context). It is possible to represent even complex branchings of functions involved. This serves as a map showing the stages covered on your way when springing between different functions.

Example: If you started at context “main”, stepped over to function “InitScript” and finally stepped over to function “CleanUp”, the stack shown above results.

ISL allows you to start several processes. After starting the main process you can start another one. Threads are processes that run “independently” of the main process performing tasks asynchronously. The “independence” is not an absolute one, because usually the main process controls its subordinate processes terminating them in due time.

Stick Command



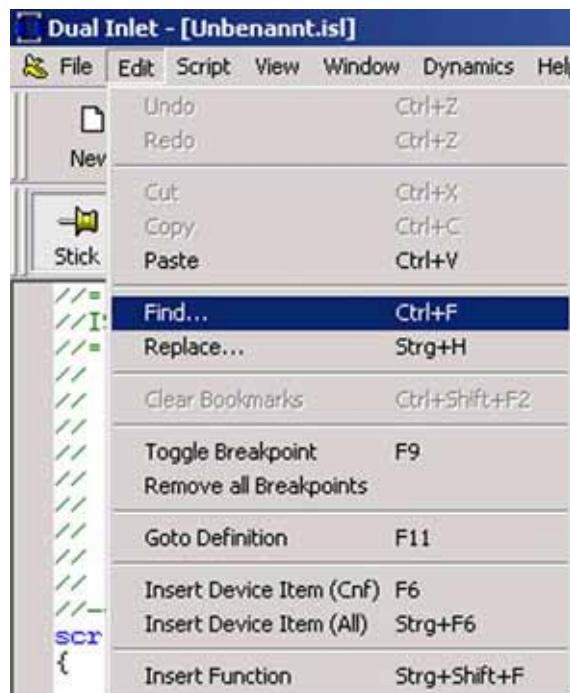
The **Stick** button is available in any Isodat 2.0 document, not only in ISL documents. It can be toggled.

- If you have opened a file - e.g. an ISL Script - and press the **Stick** button, it will be “pinned” there staying opened even if you open further ones (e.g. via File Browser).
- However, if you have opened a file - e.g. an ISL Script - with **Stick** being deactivated and you open another ISL Script of the same type, the former will be closed.

Additional Commands - The Menu Bar

The Menu Bar refers to the document that is currently open.

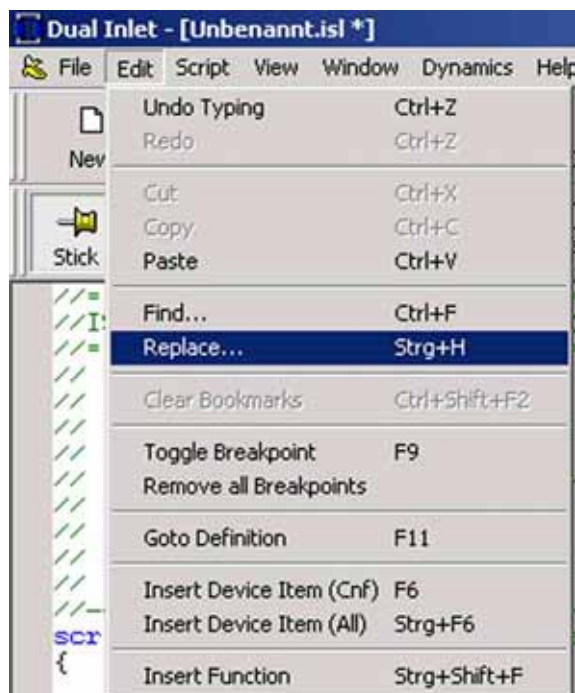
Find and Replace Commands



1. To find particular content within the script currently active, press **Edit > Find...** or **<Ctrl> + <F>**.



- a. Type the content you are looking for (e.g. “script”). If your cursor is positioned at a string, the string will appear in the **Find what** field.
 - b. Mark **Match case** to distinguish between upper case and lower case letters (e.g. find “script” but not “Script”).
 - c. Mark **Match whole word only** to find only the exact term but no composite forms (e.g. “Author” but not “Authoring”).
 - d. Specify the search **direction** (i.e. “up” or “down”).
 - e. Finally, confirm by **Find Next**.
If found, the term will be highlighted. If the term does not occur in the script, an error box appears.
2. To continue your search, press **Edit > Find...** or **<Ctrl> + <F>** again.



1. To replace particular content within the script currently active, press **Edit > Replace...** or **<Ctrl> + <H>**.



- a. Type the string to be found (e.g. “Author”) and the one that will replace it(e.g. “Writer”). If your cursor is positioned at a string, the string will appear in the *Find what* field.
 - b. Mark *Selection* to replace within selected text or *Whole file* to replace within the entire file (default).
2. Press **Find Next** to find the next match without replacement.
 3. Press **Replace** to replace only the first match.
 4. Press **Replace All** to replace all matches.

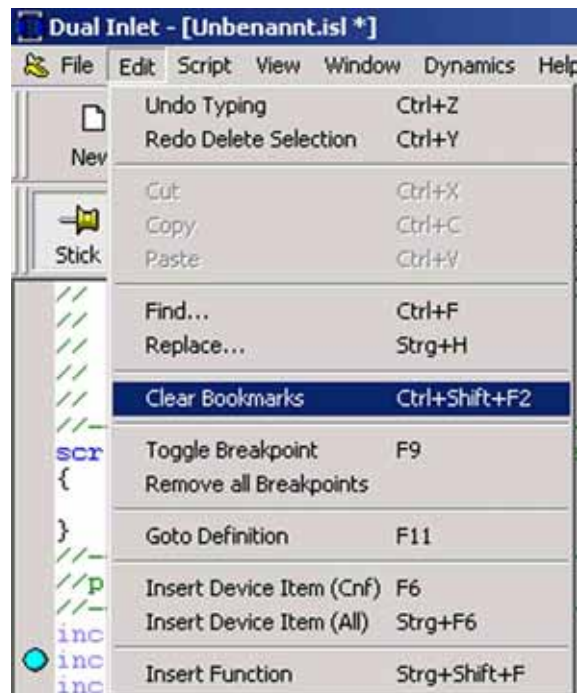
Set Bookmark and Clear Bookmark Commands

```
include "lib\stdisl.isl"  
include "lib\instrument.isl"
```

Bookmarks are especially useful in case of long scripts. They facilitate orientation and allow to move quickly within a script. Set as many bookmarks as you like. E.g. set a bookmark at a particular line. Then move to another position where you want to read something. After reading, press **<F2>** to return to the bookmark.

In case of several bookmarks, **<F2>** will lead to the next one. After the last bookmark has been found in a script, **<F2>** will lead to the first one in the script.

1. To set a bookmark at a particular line within the active script, press **<Ctrl> + <F2>**. A turquoise point appears at the left edge of the line.
2. Another **<Ctrl> + <F2>**, clears the *single* bookmark. The turquoise point disappears.

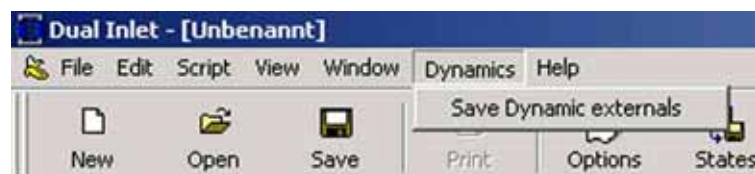


3. To clear **all** bookmarks press **Edit > Clear Bookmarks** or **<Ctrl> + <Shift> + <F2>**. All turquoise points disappear.

Save Dynamic Externals Command

Principle: An external parameter set for the dynamic externals is written into a file (*.iso file) and saved together with a script. The external parameter set can thus be used beyond the script. E.g. a hardware can access it later on.

Remember that dynamic externals can be created also for hardware parameters. When the corresponding hardware is loaded, the information will not be loaded from the script itself but from the external parameter set.



- Click **Dynamics > Save Dynamic Externals**.

Information Bar in an ISL Script

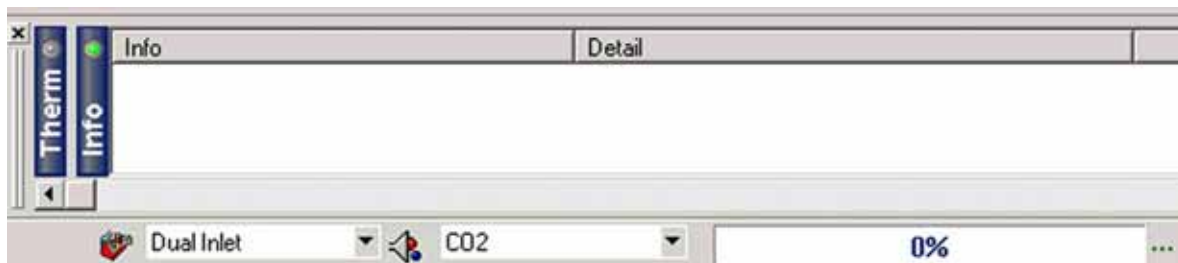
Principle: The Information bar shows detailed information on the various types of errors that might have occurred. If an error has been detected during debugging a script, the corresponding error message reveals the line, which additionally is marked by a red **X** in the script (see topic **Run and Debug Commands** on page 3-11).

```
//
//place your includes here
//
Xinclude "lib\sstdisl.isl"
include "lib\instrument.isl"
include "lib\Acquisition_lib.isl"
//
```

Moving the bar and changing its dimensions

As with every application of Isodat 2.0, the Information bar is also present at any ISL Script. Although usually located at the bottom, it can be easily moved to other places within the “Dual Inlet” window by clicking at its *left* edge and dragging your mouse.

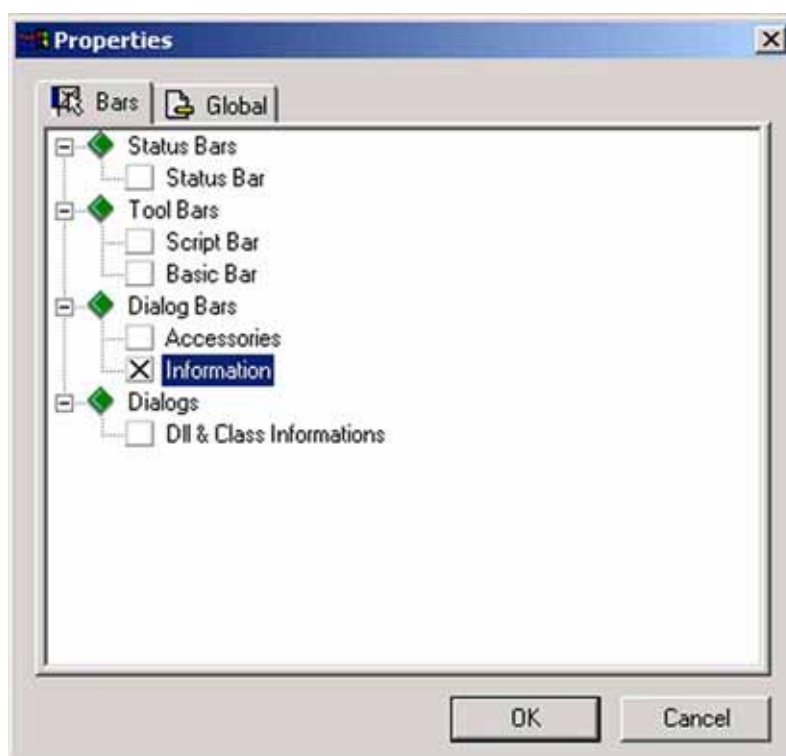
You can change its vertical dimension by clicking at its *upper* edge and dragging your mouse. After you moved it to another place, you can also modify its horizontal dimension.



Showing and hiding the bar

1. To show or hide the Information bar, press the **Options**





2. Mark or clear the *Information* checkbox.
3. Confirm by **OK**.

3.2 Dynamic Variables Exchange (DVE)

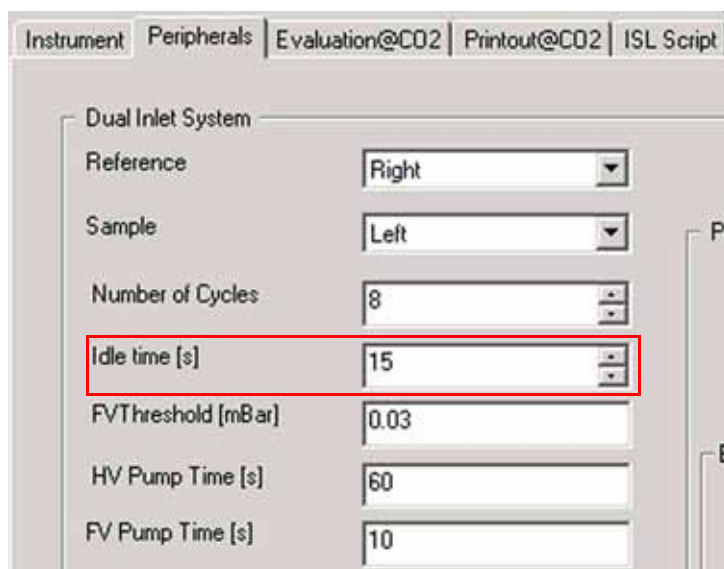
Principle: DVE allows to perform dynamic data exchange between methods and a script.

Dynamic variables can easily be generated in a method.

Write tailored scripts totally on your own and parameterize them via a method.

External variables are fixed variables that are sought and exchanged by a method. They have a distinct name beginning with “external”.

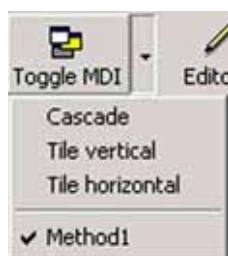
Example: The external variable “Dual Inlet Idle” is an idle time between two measuring points. It is controlled by a method.



1. Open a Dual Inlet method. At **Peripherals** tab page, the parameter “Idle time” occurs. Its actual value is 15 s. The appearance, position, and value on this particular tab page is defined in an ISL script.



Note that the **ISL Script** tab page is still empty.



2. Use the **Toggle MDI** button to switch between a method and an ISL script.

Chapter 4

Reporting-related Features

This chapter contains the following topics:

- ResultWorkshop

4.1 ResultWorkshop

This section contains the following topics:

- Principle of the ResultWorkshop
- Multidimensionality
- Opening the ResultWorkshop
- Printout Templates
- Toolbars
- Inserting Objects into the Working Grid
- Changing the Properties of Objects

Principle of the ResultWorkshop

The ResultWorkshop allows to arrange objects to display a variety of data on a printout, e.g. ratio traces, GC traces. It is possible to print components of any file that has once been generated by Isodat 2.0, e.g. method files, sequence files, result files. A broad diversity of objects can be tailored before they are printed. The approach of the ResultWorkshop is a generic one, i.e. the objects bring along their own print routines.

A result file that contains the data for the objects to be filled with during editing must be available. The result files (e.g. *.cf, *.caf) available for selection are listed in the result file browser.

Two primary features of Isodat 2.0's ResultWorkshop are

- Multidimensionality (see topic **Multidimensionality** on page 4-2)
- Self-Actualization (see topic **Opening a predefined Printout Template** on page 4-5)


Multidimensionality

One of Isodat 2.0's outstanding properties is multidimensionality: One single ResultWorkshop template can store layout information for all gas types, i.e. for all ratio groups. For each gas, a specific layout of its own will be saved (no matter how many gases are to be measured).

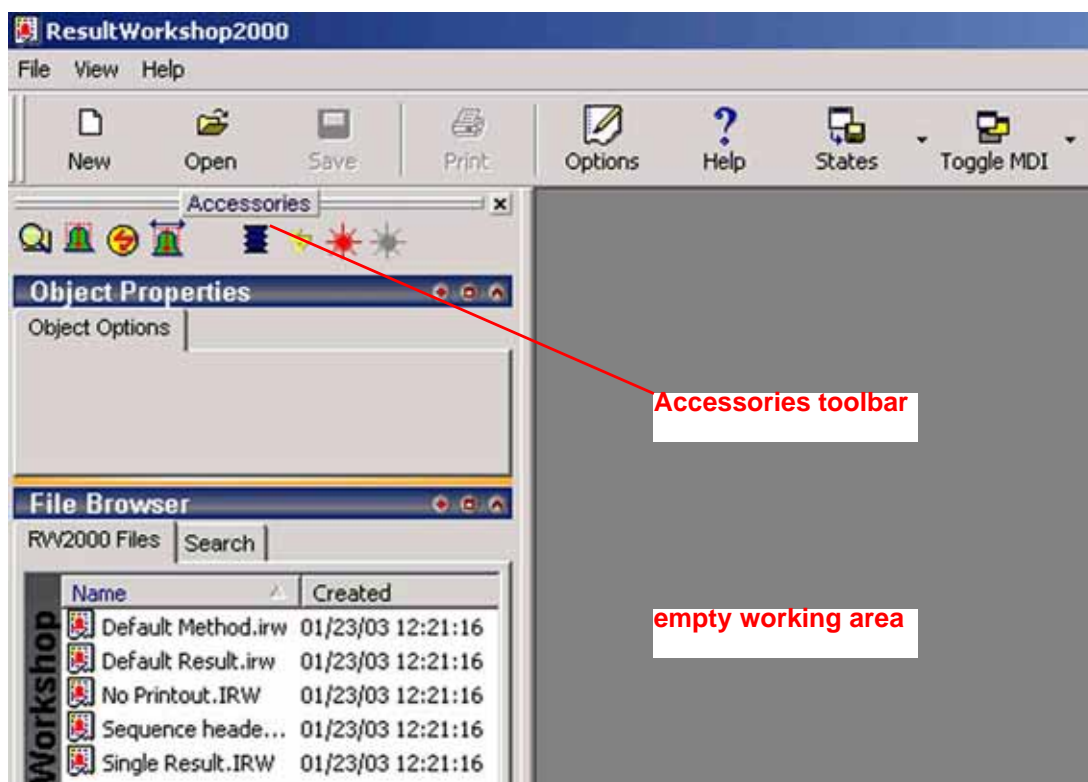
To setup this template also for another gas type, select a corresponding Acquisition file (e.g. *.cf, *.caf) from the File Browser. Modify objects according to your needs, save and use the same ResultWorkshop template filename in all of your methods.

Example: After measuring CO₂ and recording of CO₂-specific data, you may want to measure N₂. Thus, if you select a N₂-result file, it is possible to adjust completely new parameters, which are N₂-specific, using the same ResultWorkshop template. This can be generalized, i.e. extended to an arbitrary number of gases.

Opening the ResultWorkshop

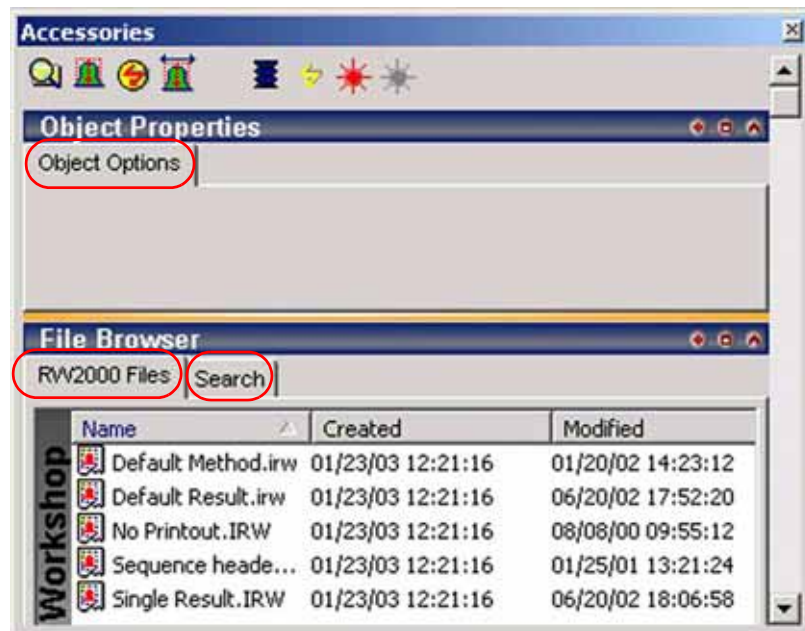
1. Start Isodat 2.0 by a double-click on the  icon.

2. Double-click the ResultWorkshop icon  .



The ResultWorkshop opens, showing the empty working area on the right. On the left, see the *Accessories* Toolbar.

Accessories Toolbar



The *Accessories* toolbar shown above contains the *Object Properties* box and the *File Browser*. Note that the *Object Options* tab at the *Object Properties* box is currently empty and the *File Browser* currently offers only two tabs, “RW2000 Files” and “Search”.

Switching between objects

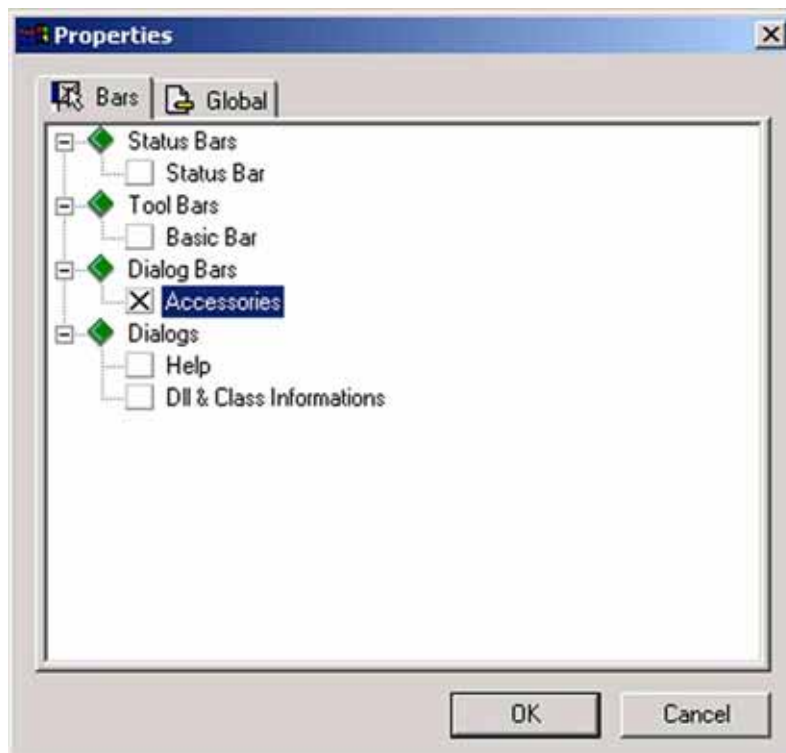
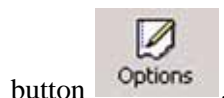


The *Object Properties* box reveals various properties of the object that is currently selected. If another object is selected, its properties will be displayed instead. If no object is selected at all, the “Object Properties” box contains no properties.

- To deselect an object, click somewhere onto the working grid but outside of any objects.

Showing / Hiding the “Accessories” toolbar

- To show/hide the “Accessories” toolbar, press the **Options**



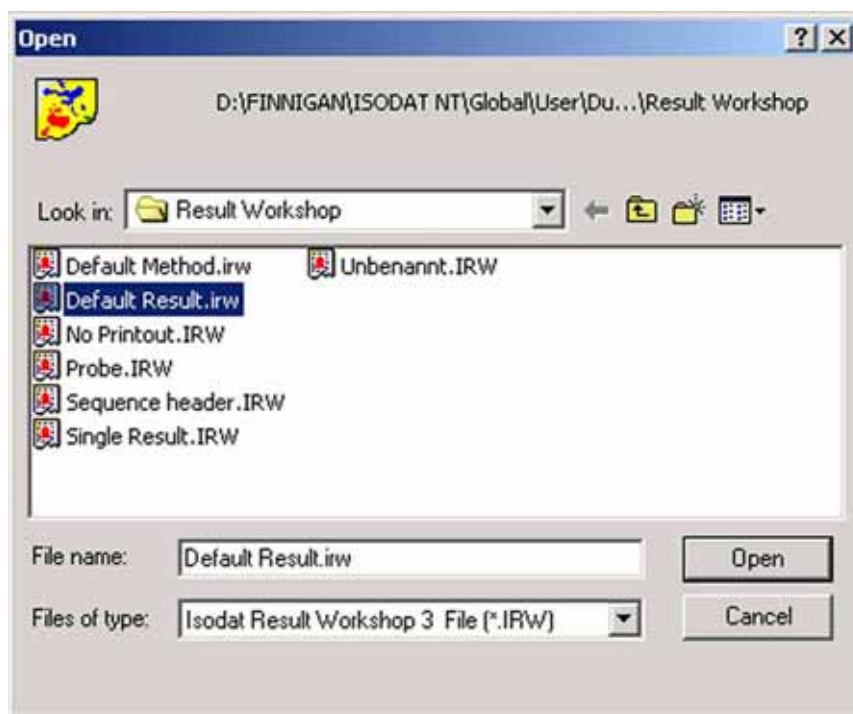
- To show the “Accessories” toolbar, mark the *Accessories* checkbox.
- To hide it, unmark the *Accessories* checkbox.

Printout Templates

Opening a predefined Printout Template

In addition to create and edit new printout templates (see topics **Creating a new Printout Template** on page 4-10 and **Creating more than one new Printout Template** on page 4-11), the ResultWorkshop allows to access a variety of predefined printout templates, i.e. working grids filled with measurement-related data.

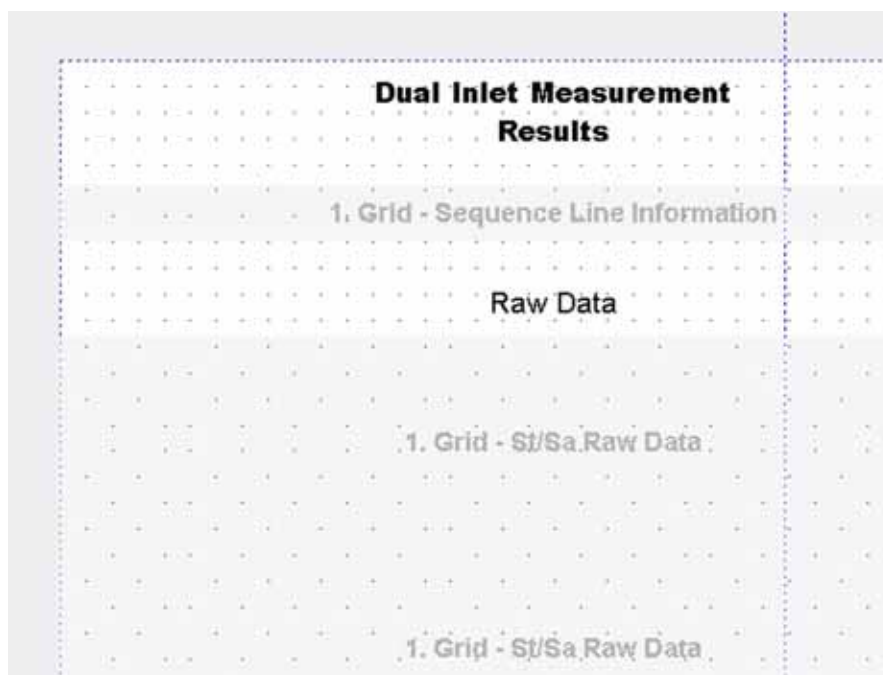
- Press the **Open** button  .



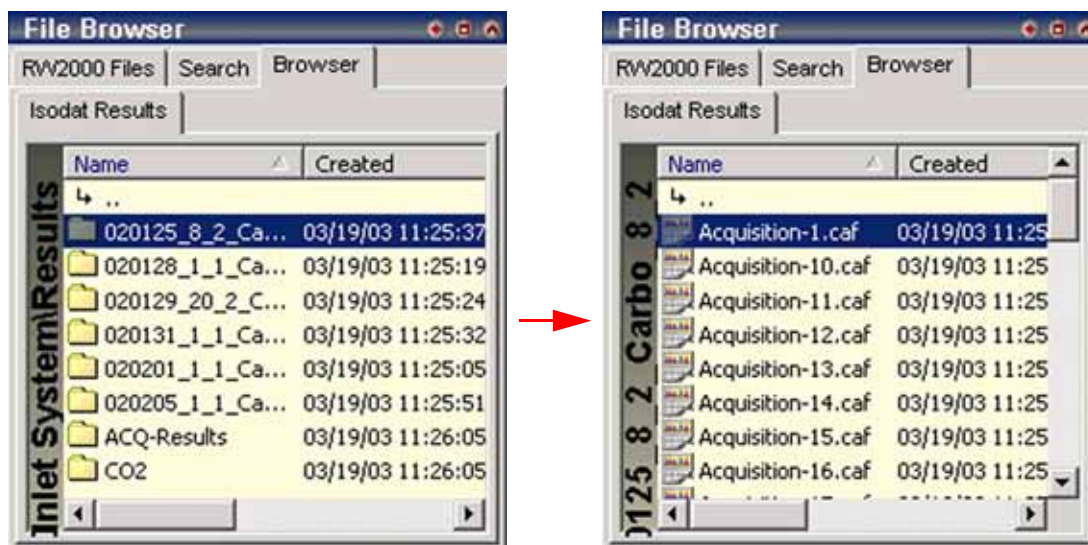
2. Select your ResultWorkshop printout template (*.irw).



Alternative: Select the *printout template* (*.irw), e.g. “Default Result.irw”, from the **File Browser's** *RW2000 Files* tab.
Double-click or drag&drop it onto the working area.



The printout template will be shown as working grid in the ResultWorkshop's main window. *It has not been filled with measurement-related data yet.*



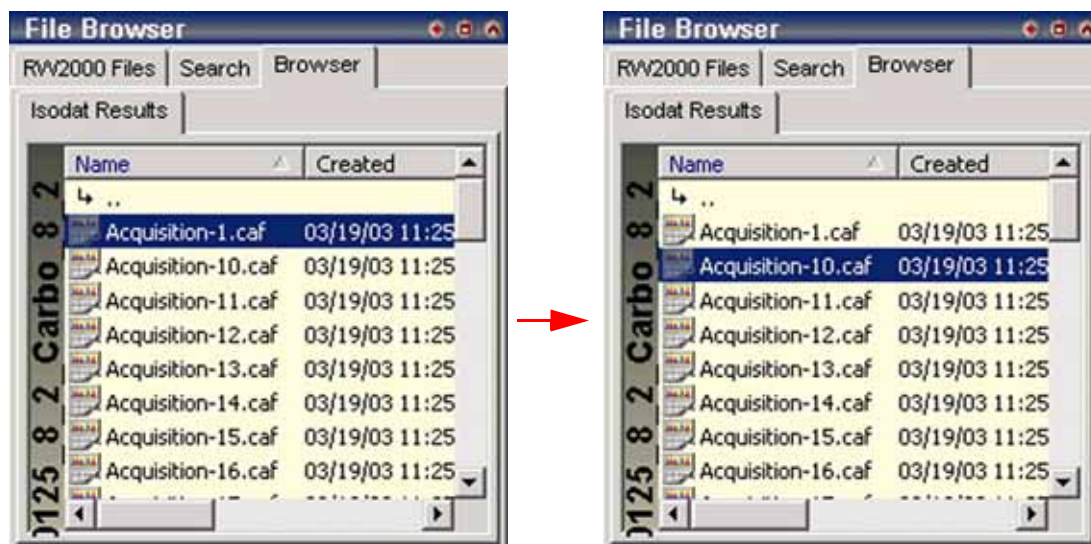
The browser displays folders that contain result files for the active configuration.

3. Click through the folders to find your result file (*.cf, *.caf).
4. Finally, just mark the result file.

Dual Inlet Measurement Results									
D:\FINNIGAN\ISODAT NT\Global\Users\Dual Inlet System\Results\020125_8_2_Carbo_8_2\Acquisition-									
Line	Weight	Sample	Line	Peak Center	Pressadjust	Reference Ref	Comment	Post Script	
9	0.06	6	1	X	X	-			
Raw Data									
	Ampl.44 Sample [mV]	Ampl.45 Sample [mV]	Ampl.46 Sample [mV]	Ampl.44 Standard [mV]	Ampl.45 Standard [mV]	Ampl.46 Standard [mV]	rR 45CO2/44CO	rR 46CO2/44CO	rR 45CO2/46CO
Pre				5985.348	6693.465	7934.136			
1	5662.019	6561.262	7672.226	5833.682	6524.003	7733.322	1.1588202	1.3550335	31
2	5451.131	6316.937	7386.506	5685.249	6358.225	7536.886	1.1588304	1.3550410	31
3	5236.515	6068.454	7095.968	5533.467	6188.429	7335.294	1.1588725	1.3550935	31
4	5027.785	5826.690	6813.062	5380.058	6016.946	7132.271	1.1588980	1.3550824	31
5	4826.034	5592.846	6539.509	5232.276	5851.687	6936.557	1.1588908	1.3550483	31
6	4646.509	5384.752	6296.552	5107.397	5712.104	6770.921	1.1588813	1.3551146	31
7	4479.684	5191.619	6070.251	4973.706	5562.623	6593.629	1.1589251	1.3550623	31
8	4303.619	4987.529	5831.865	4843.488	5416.966	6421.117	1.1589150	1.3551071	31
	Ampl.44 Sample [mV]	Ampl.45 Sample [mV]	Ampl.46 Sample [mV]	Ampl.44 Standard [mV]	Ampl.45 Standard [mV]	Ampl.46 Standard [mV]	rR 45CO2 [%] vs. H2O2	rR 46CO2 [%] vs. H2O2	rR 45CO2 [%] vs. H2O2

The result file is used as a data source: its measurement-related data fill the objects of the printout template immediately.

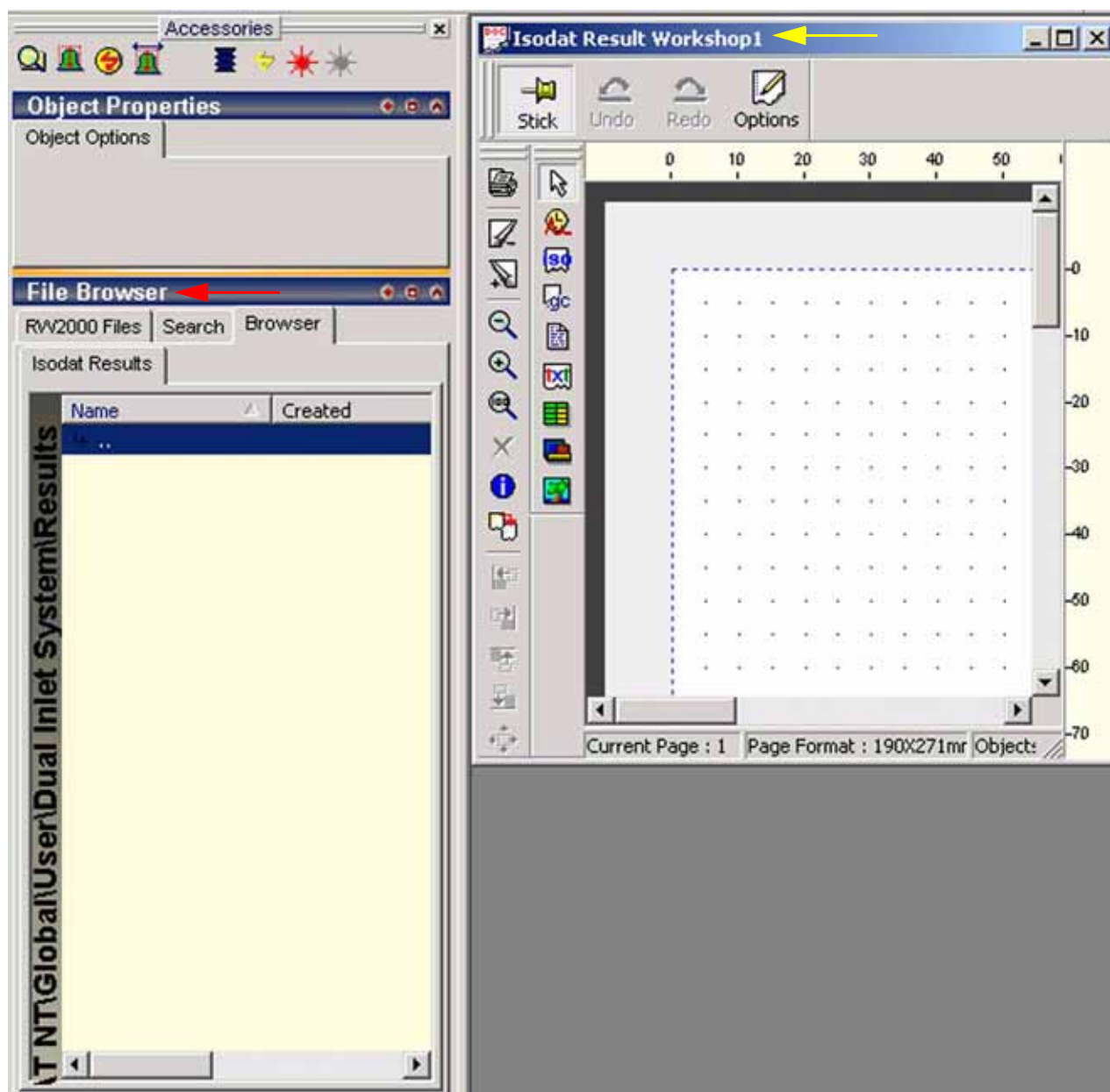
Self-actualization of data throughout different templates



1. Move to another result file. E.g. move from “Acquisition-1.caf” to “Acquisition-10.caf” as is shown above.

Creating a new Printout Template

- Press the **New** button



Note that the File Browser now offers four tabs: “*RW2000 Files*”, “*Search*”, “*Browser*” and “*Isodat Results*”. Its color has turned into yellow.

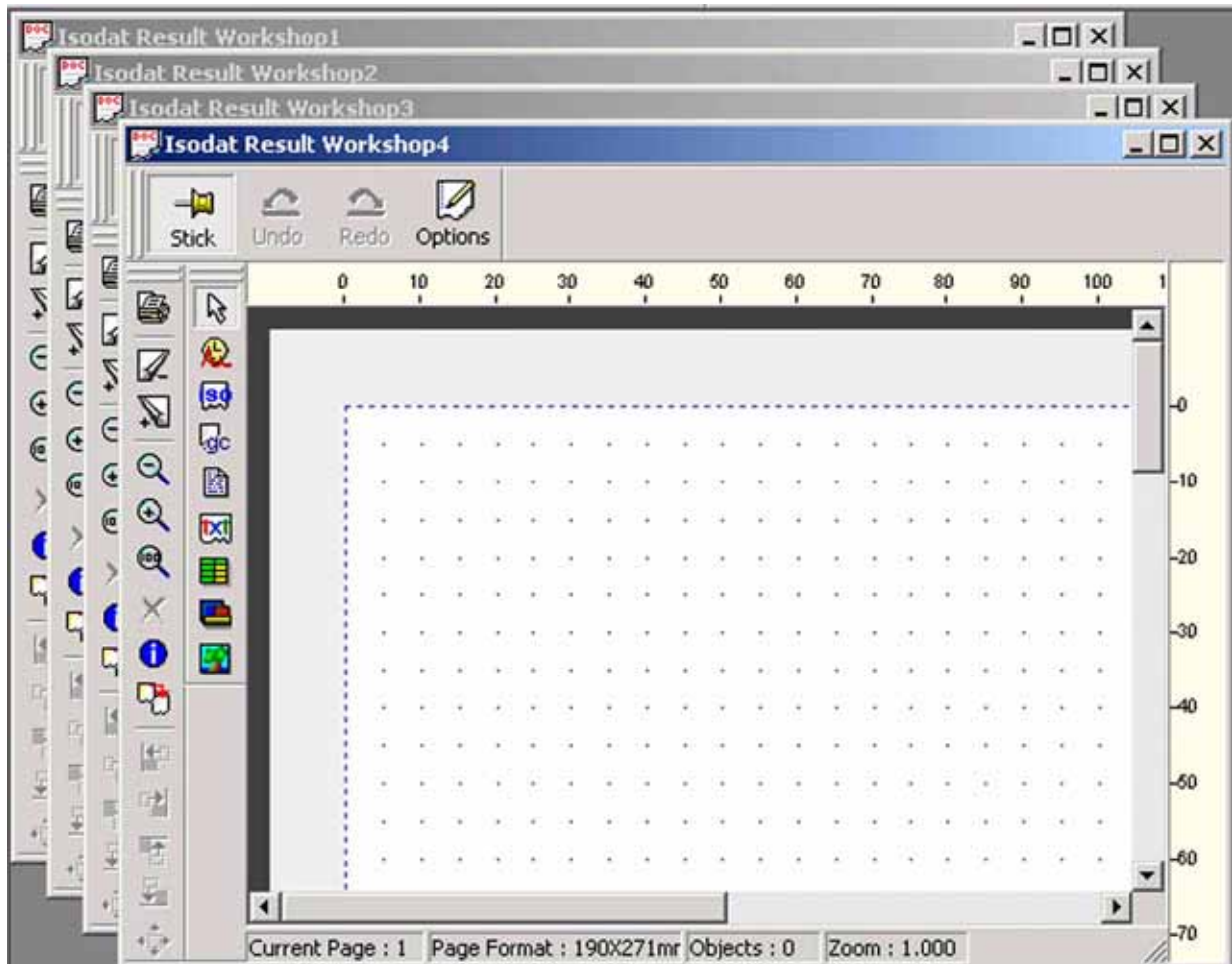
An empty working grid appears and fills the working area. Its default name is Isodat Result Workshop1.

Creating more than one new Printout Template

It is possible to open several working grids or printout templates in parallel. You can easily work with them side by side and switch between them.


1. After opening your first working grid (see topic **Opening a predefined**

Printout Template on page 4-5), press the **New** button repeatedly.



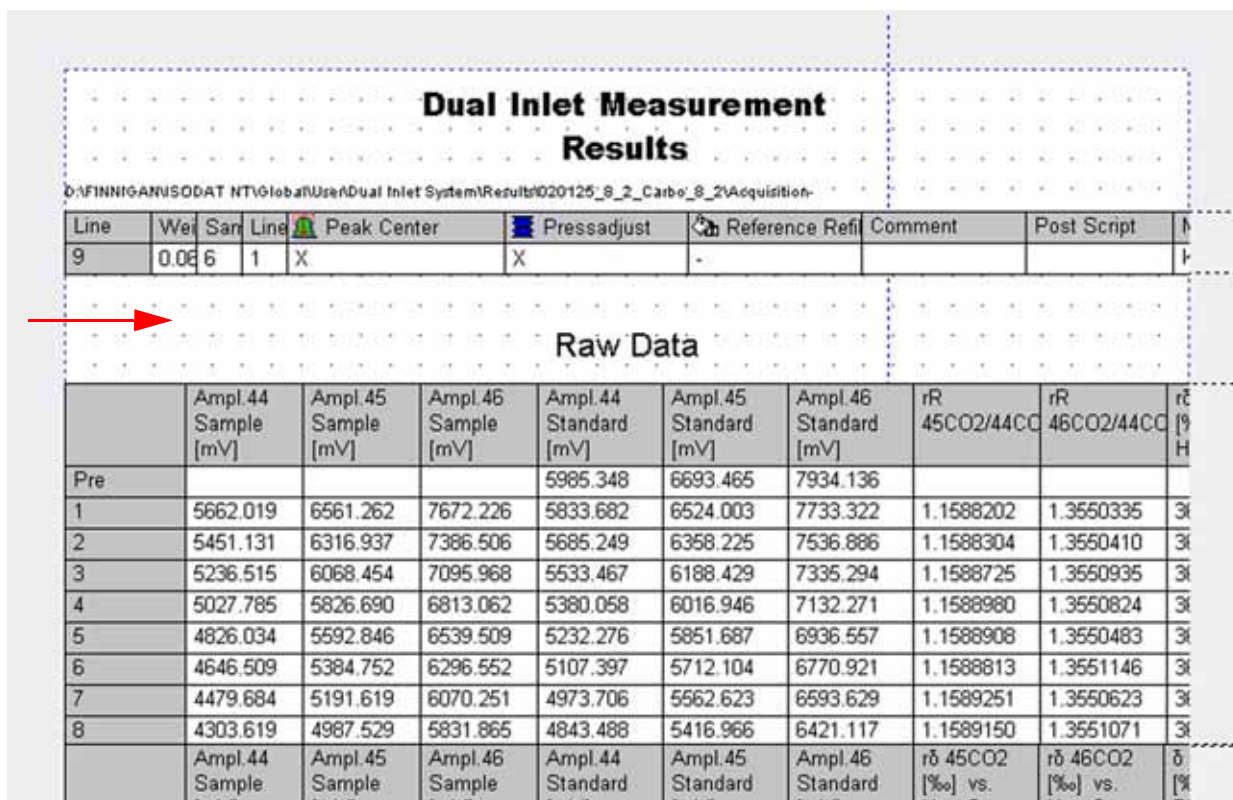
Additional working grids are opening having the same dimensions. Their default names are *Isodat Result Workshop2*, *Isodat Result Workshop3*, *Isodat Result Workshop4* etc. Each time, the number behind "Isodat Result Workshop" is augmented by one. Clicking on a particular working grid will move it into the foreground. You can selectively close one or more grids.



2. Press the  arrow next to the **Toggle MDI** button.
3. Choose between three modes of grid arrangement (**Cascade**, **Tile vertical**, **Tile horizontal**) or close all grids by **Close all**.
4. In order to move a particular grid to the foreground, click on its name (e.g. "Isodat Result Workshop 1"). It will be marked in the pull-down menu.

Editing a Printout Template

After opening a predefined printout template (see **Opening a predefined Printout Template** on page 4-5) or creating a new one (see **Creating a new Printout Template** on page 4-10 and **Creating more than one new Printout Template** on page 4-11), they can be edited, i.e. modified as:




Dual Inlet Measurement Results

D:\FINNIGANNISODAT\NTV\Global\Users\Dual Inlet System\Results\020125_8_2_Carbo_8_2\Acquisition-

Line	Weight	Sample	Line	Peak Center	Pressadjust	Reference Ref	Comment	Post Script
9	0.066	6	1	X	X	-		

Raw Data

	Ampl.44 Sample [mV]	Ampl.45 Sample [mV]	Ampl.46 Sample [mV]	Ampl.44 Standard [mV]	Ampl.45 Standard [mV]	Ampl.46 Standard [mV]	rR 45CO2/44CO2	rR 46CO2/44CO2	rR [% H
Pre				5985.348	6693.465	7934.136			
1	5662.019	6561.262	7672.226	5833.682	6524.003	7733.322	1.1588202	1.3550335	3%
2	5451.131	6316.937	7386.506	5685.249	6358.225	7536.886	1.1588304	1.3550410	3%
3	5236.515	6068.454	7095.968	5533.467	6188.429	7335.294	1.1588725	1.3550935	3%
4	5027.785	5826.690	6813.062	5380.058	6016.946	7132.271	1.1588980	1.3550824	3%
5	4826.034	5592.846	6539.509	5232.276	5851.687	6936.557	1.1588908	1.3550483	3%
6	4646.509	5384.752	6296.552	5107.397	5712.104	6770.921	1.1588813	1.3551146	3%
7	4479.684	5191.619	6070.251	4973.706	5562.623	6593.629	1.1589251	1.3550623	3%
8	4303.619	4987.529	5831.865	4843.488	5416.966	6421.117	1.1589150	1.3551071	3%
	Ampl.44 Sample [mV]	Ampl.45 Sample [mV]	Ampl.46 Sample [mV]	Ampl.44 Standard [mV]	Ampl.45 Standard [mV]	Ampl.46 Standard [mV]	rR 45CO2 [%] vs. Hanc2	rR 46CO2 [%] vs. Hanc2	rR [% H

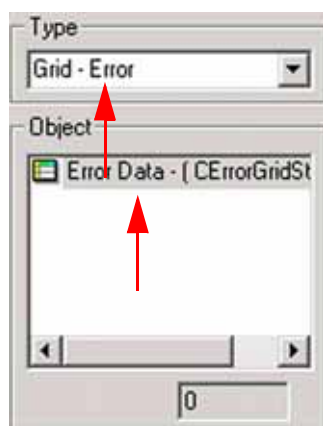
1. Open the printout template to be edited (i.e. modified, see topic **Opening a predefined Printout Template** on page 4-5).
2. Click the  icon to select a new object.
3. Define its dimensions and position on the working grid by dragging your mouse.

Dual Inlet Measurement Results									
D:\FINNIGAN\ISODAT NT\Global\User\Dual Inlet System\Results\020125_8_2_Carbo_8_2\Acquisition-									
Line	Wei	San	Line	Peak Center	Pressadjust	Reference Refl	Comment	Post Script	
9	0.06	6	1	X	X	-			
Number	Status	Object	Information	Script	Raw Data				
	Ampl.44 Sample [mV]	Ampl.45 Sample [mV]	Ampl.46 Sample [mV]	Ampl.44 Standard [mV]	Ampl.45 Standard [mV]	Ampl.46 Standard [mV]	rR 45C02/44CC	rR 46C02/44CC	rR [%] H
Pre				5985.348	6693.465	7934.136			
1	5662.019	6561.262	7672.226	5833.682	6524.003	7733.322	1.1588202	1.3550335	3i
2	5451.131	6316.937	7386.506	5685.249	6358.225	7536.886	1.1588304	1.3550410	3i
3	5236.515	6068.454	7095.968	5533.467	6188.429	7335.294	1.1588725	1.3550935	3i
4	5027.785	5826.690	6813.062	5380.058	6016.946	7132.271	1.1588980	1.3550824	3i
5	4826.034	5592.846	6539.509	5232.276	5851.687	6936.557	1.1588908	1.3550483	3i
6	4646.509	5384.752	6296.552	5107.397	5712.104	6770.921	1.1588813	1.3551146	3i
7	4479.684	5191.619	6070.251	4973.706	5562.623	6593.629	1.1589251	1.3550623	3i
8	4303.619	4987.529	5831.865	4843.488	5416.966	6421.117	1.1589150	1.3551071	3i
	Ampl.44 Sample [mV]	Ampl.45 Sample [mV]	Ampl.46 Sample [mV]	Ampl.44 Standard [mV]	Ampl.45 Standard [mV]	Ampl.46 Standard [mV]	rR 45C02 [%] vs. Haus2	rR 46C02 [%] vs. Haus2	rR [%] P

The new object has been inserted.

Changing the object type

After an object has been inserted, its type can be changed via the **Accessories** toolbar (see **Accessories Toolbar** on page 4-4).



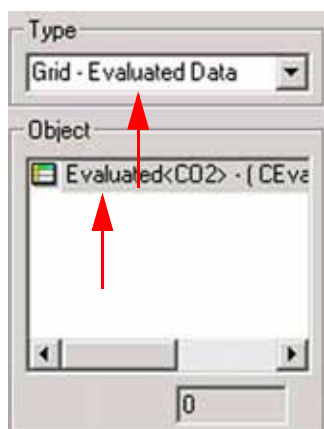
D:\FINNIGAN\ISODAT NT\Global\User\Dual Inlet System\Results\02									
Line	Wei	San	Line	Peak Center					
9	0.06	6	1	X					X
Number	Status	Object							
	Ampl.44 Sample [mV]	Ampl.45 Sample [mV]	Ampl.46 Sample [mV]						

The object on the working grid is shown above on the right. See its description on the left:

Object: Error Data

Type: Grid - Error

- Select another type from the **Type** pull-down menu (e.g. “Grid - Evaluated Data”).



D:\FINNIGAN\ISODAT NT\Global\User\Dual Inlet System\Results\

Line	Wei	San	Line	Peak Center	
9	0.06	6	1	X	X
				δ Mean	δ Std. Dev.
				δ 13C/12C	-2.7089
				δ 18O/16O	-3.9849
				Ampl. 44	Ampl. 45
				Sample	Sample
				[mV]	[mV]
				Ampl. 46	
				Sample	
				[mV]	

A new object appears at the same position replacing the old one.

Object: Evaluated <CO2>

Type: Grid - Evaluated Data

Edit Mode

Line	Wei	San	Line	Peak Center
9	0.06	6	1	X

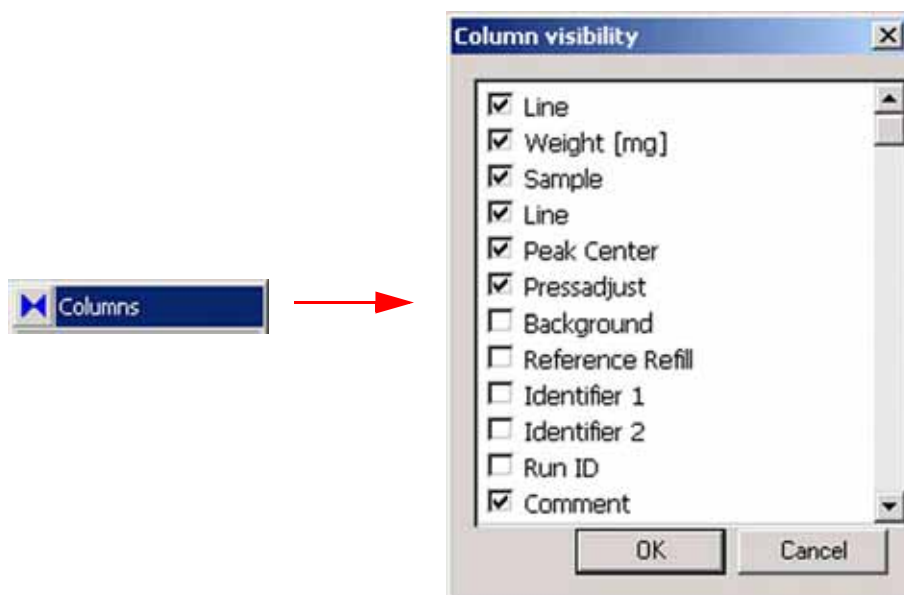
→

Line	Wei	San	Line	Peak Center
9	0.06	6	1	X

- A double-click on an object switches it to the **Edit Mode**:



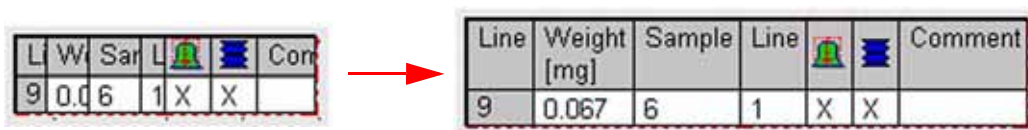
- Content** and **layout** properties can now be changed by a **right-click**. The popup menu shown above appears.




3. Use **Columns** to add or remove columns that contain object information.
4. Activate the checkboxes, if you want to see them as columns of the grid object. If a checkbox is deactivated, the column will not be visible in the grid object.



5. Use **Fit Cells to Grid**  to let the columns optimally span the available grid space.



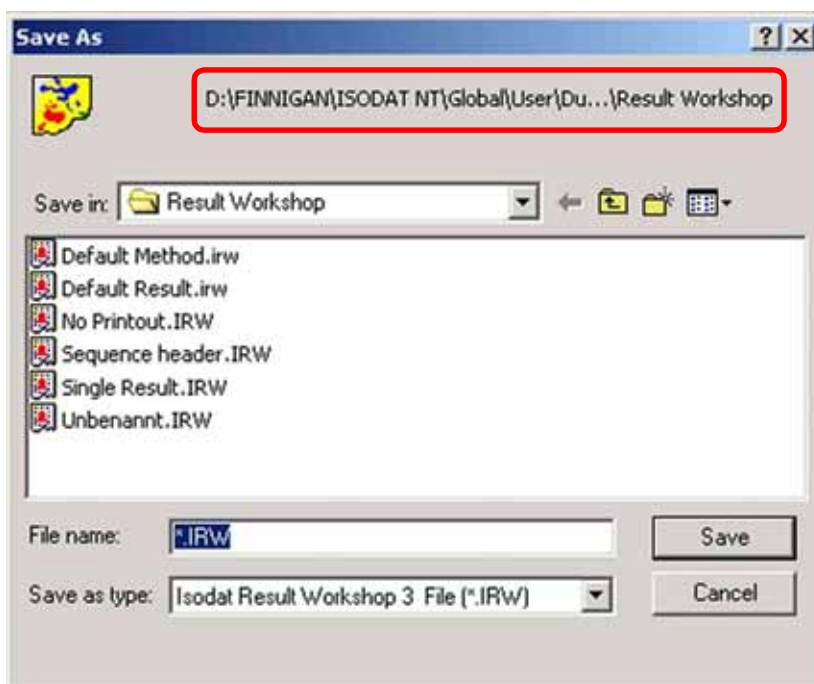
6. Use **Fit Cells to Text**  to adjust all column widths to the required space of text or numbers they contain.

Saving a Printout Template

After having finished the design of the printout template, it can be saved as follows:



1. Press **File > Save As...**

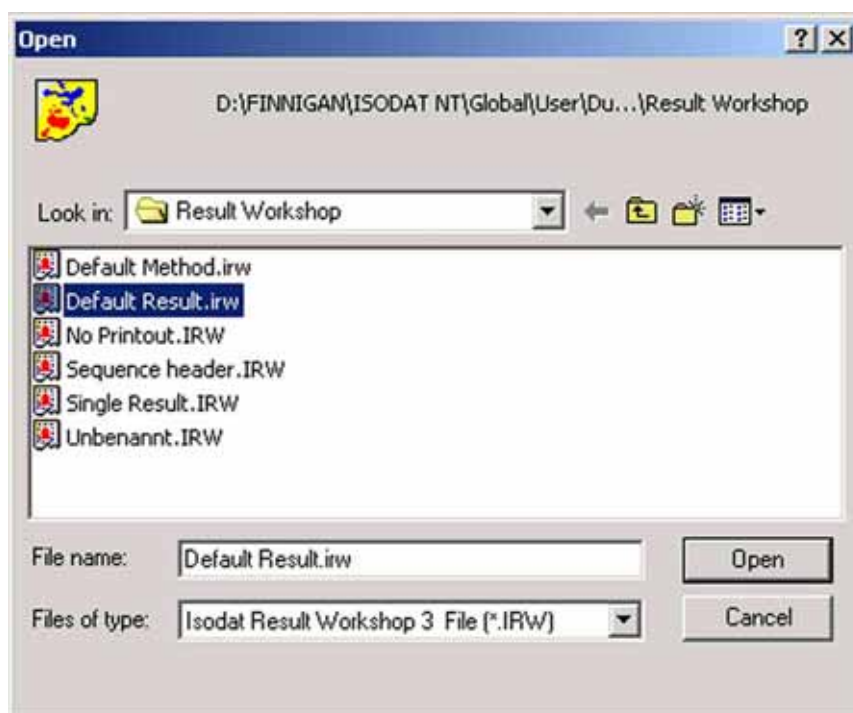


2. The ResultWorkshop file will be saved in a ResultWorkshop folder displayed on top of the box. Accept it or choose another one.
3. Type a significant name and accept the extension .irw (i.e. ISODAT NT Result Workshop Version 3 file).
4. Confirm by **Save**.

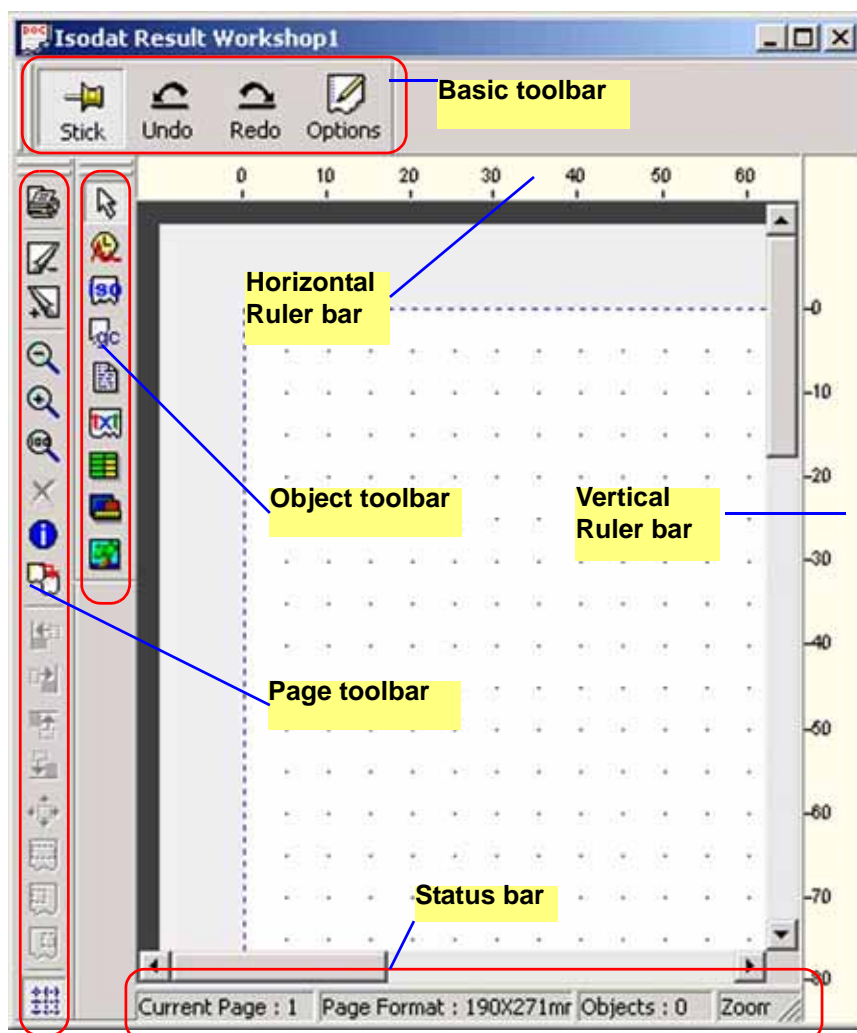
Loading a Printout Template

Load a predefined or self-made printout template as follows:

1. Press the **Open** button .



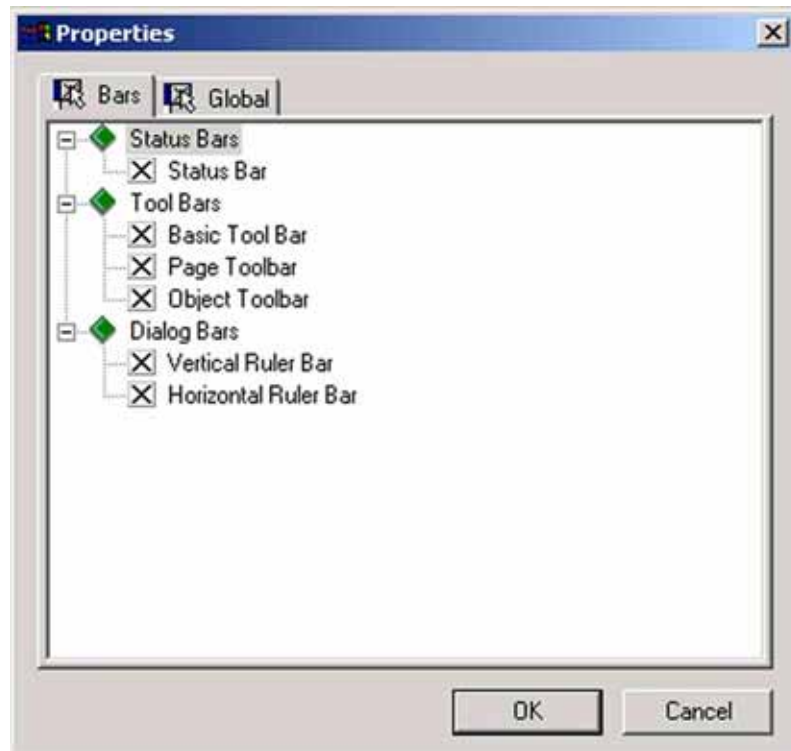
2. Select a file and confirm by **Open**. The working grid appears.



Toolbars

Several toolbars surround the working grid. Show or hide them selectively:

1. Press the **Options** button  at the **Basic** toolbar.



2. Mark or unmark the checkboxes to selectively show or hide individual bars.

Basic Toolbar



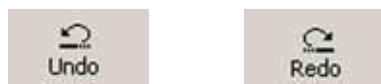
Stick command



The **Stick** button is available in *any* Isodat 2.0 document, not only in ResultWorkshop printout templates. It can be toggled.

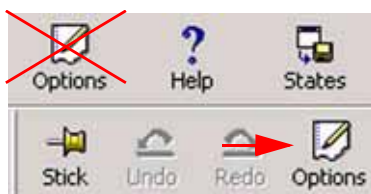
- If you have opened a printout template and press the **Stick** button, it will be “pinned” there staying opened even if you open further ones.
- However, if you have opened a printout template with **Stick** being deactivated and you open another one, the former will be closed.

Undo and Redo commands

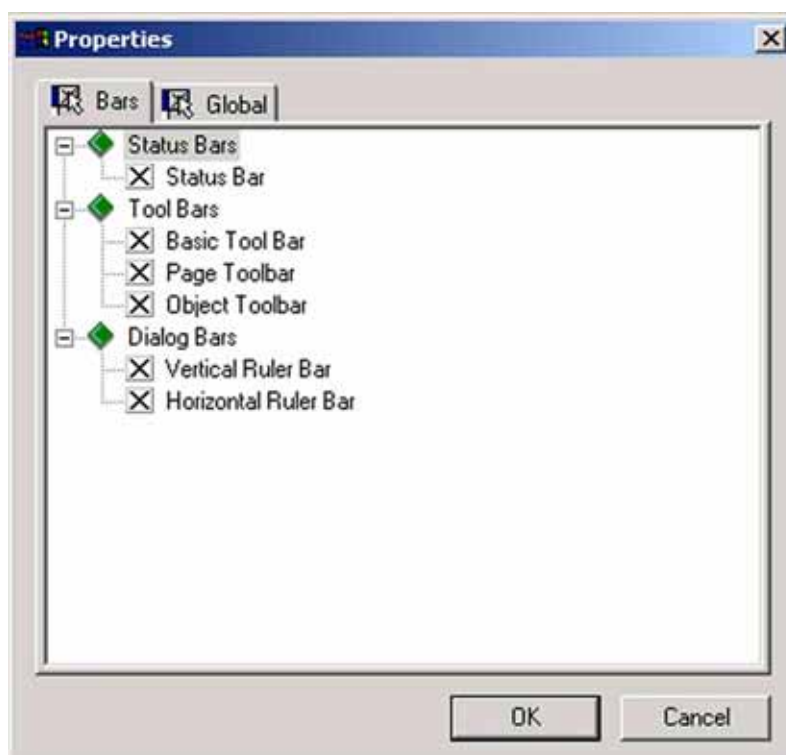


- The **Undo** command reverses the last action or deletes the last entry you typed.
- The **Redo** command reverses the action of the **Undo** command (i.e. the **Undo** command must have been used immediately before).

Options command



- On the **Basic** toolbar (i.e. right to the **Redo** button), press the **Options** button. *Do not mix it up with the **Options** button on the “Basic” bar!*

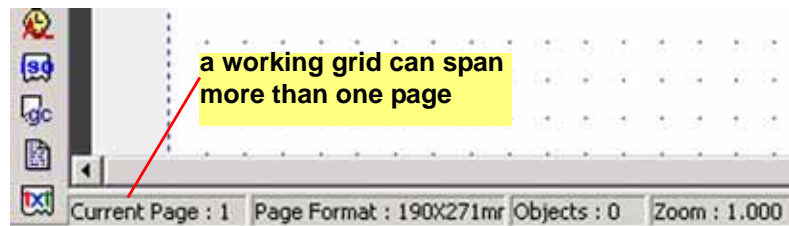


The Bars and Global tabs have been described in the topic **Page Toolbar** on page 4-22.

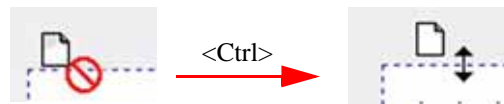
Status Bar

The *Status bar* beneath the grid reveals information about: the page you are currently working on:

- the format of the actual page.
- the number of objects located on the working grid.
- the magnification of the current page (Zoom, default = 1.0, i.e. original size).



A grid may stretch across several pages. The number of the current page is indicated at the *Status bar* (default: current page: 1).




The default format of the working grid is 190 mm × 271 mm.

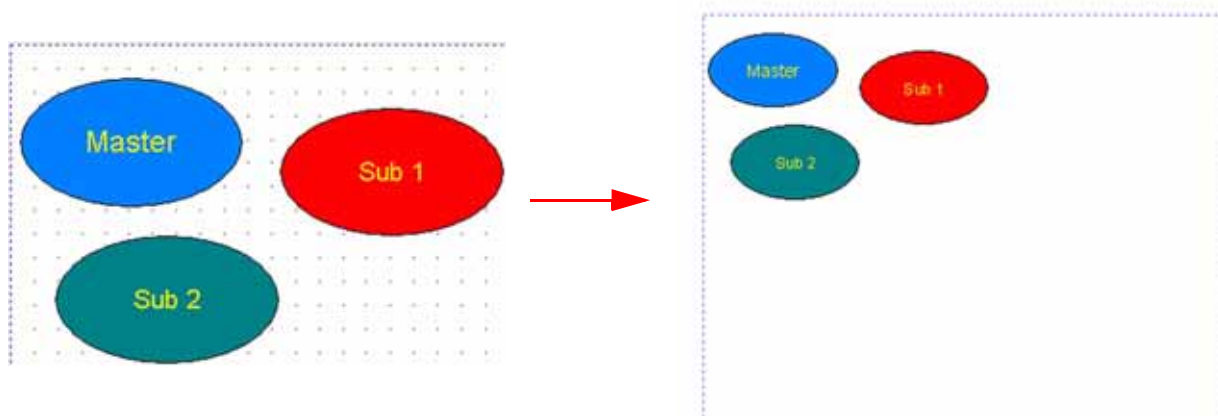
1. In order to change its dimensions move to the margin of interest. The image shown on the left appears.
2. Keep the **<Ctrl>** key pressed. The image changes to the one shown right.
3. Drag the margin to its intended new place. The grid's new dimensions will be shown at the *Status bar*.

Page Toolbar





Print Preview

- Press the **Print Preview** icon  to display the entire page as it looks if it were printed.






It is possible to zoom in or out the entire page.


Navigating through the working grid

- Use the **Previous Page**  and **Next Page**  buttons to navigate across a grid that spans more than one page. Even in case of a grid that is empty or that spans only one page, both buttons are active: **Next Page** will show empty grid pages then.

Zoom commands

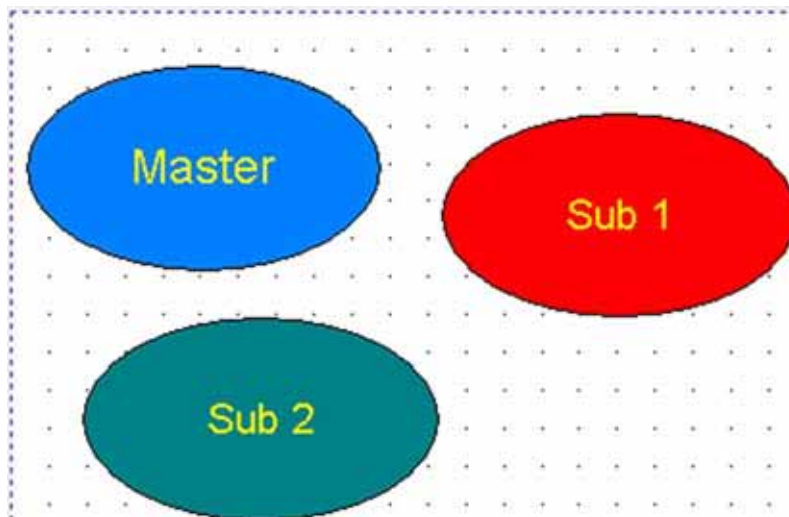
- Use the **Zoom in**  and **Zoom out**  buttons to gradually change the magnification of the grid ($\pm 10\%$ per click). The actual zoom factor is displayed beneath it.
- The **Zoom 100%**  button restores the original zoom factor (i.e. 1.0).

Deleting objects

1. Select the object(s) to be deleted.
2. Press the **Delete** icon . The object(s) will disappear from the working grid.
Alternative: Use the **Delete** command on the context menu (see **Context Menu** on page 4-47).

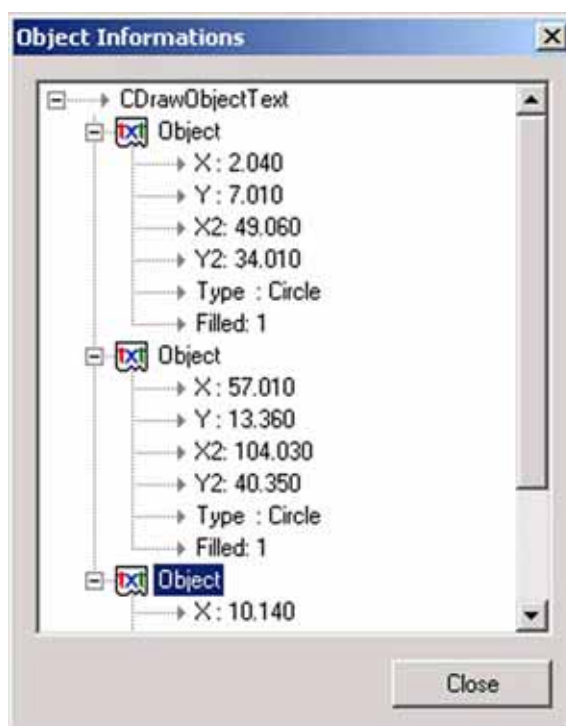
View object info tree

The object info tree quickly provides information about the various objects on the working grid.



1. Select one or more objects (e.g. above).

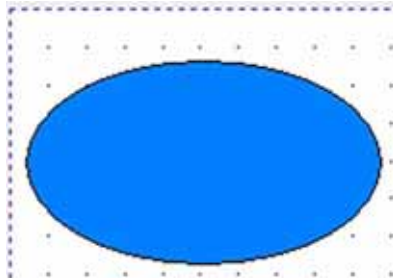
2. Press the **View Object Info Tree** button



The objects on the working grid are listed together with their individual properties (e.g. three text objects, their coordinates, shapes and filling types).

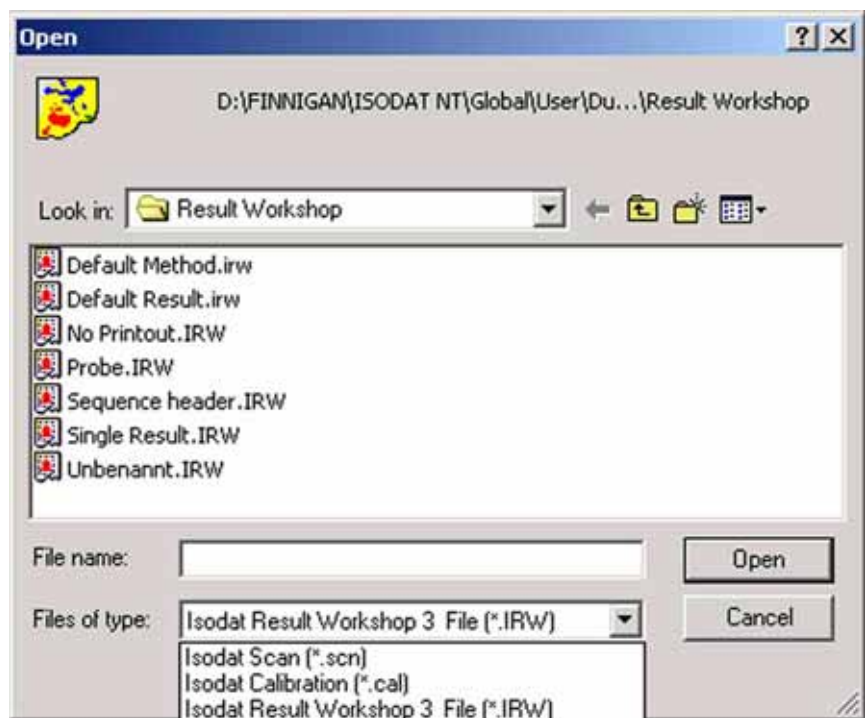
Merge and append objects from file

It is not necessary to generate objects anew after you once created them. Rather, a broad variety of objects can be imported into the actual ResultWorkshop document (.irw) from other files.



1. Click on the position within your actual grid where you want the objects of another file to be appended.

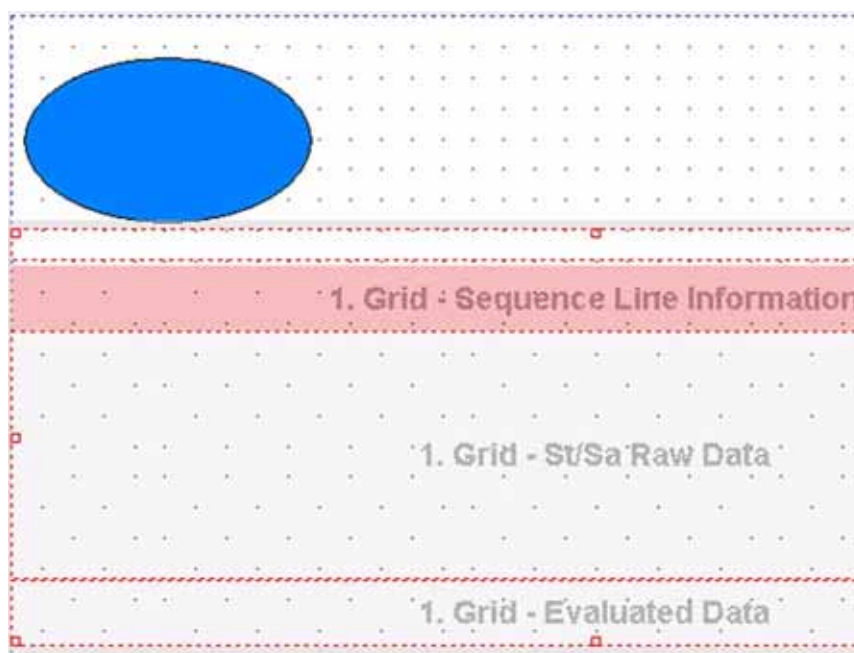
2. Press the **Merge and append objects from file** button .



3. From the **Files of type** pull-down menu, select the file type to be appended.

Note. Not only Isodat Result Workshop files (*.irw) can be appended, but also Isodat Scans (*.scn) and Isodat Calibrations (*.cal).

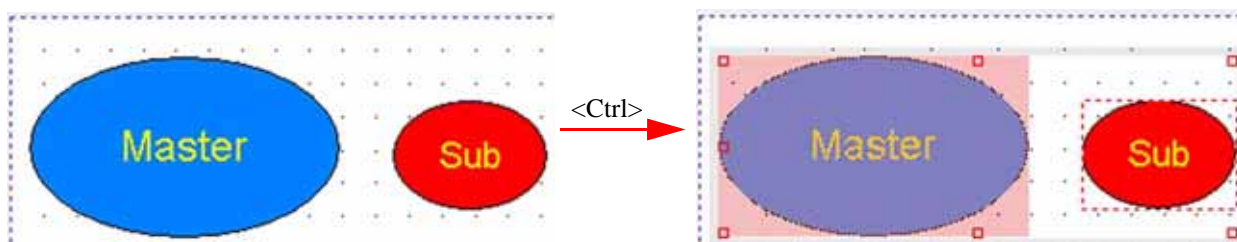
4. Select the file to be appended and confirm by **Open**.



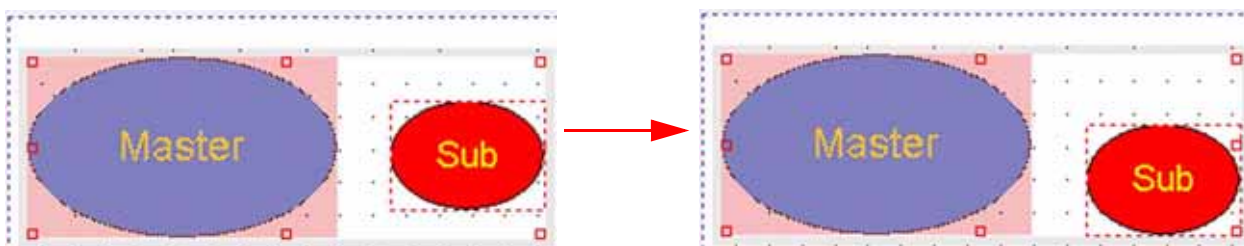
- The new file that contains objects of its own, has been appended to the active working grid. Therefore, the **Status bar** reveals the total number of objects (see **Status Bar** on page 4-22).


Adjust objects relative to the selected object

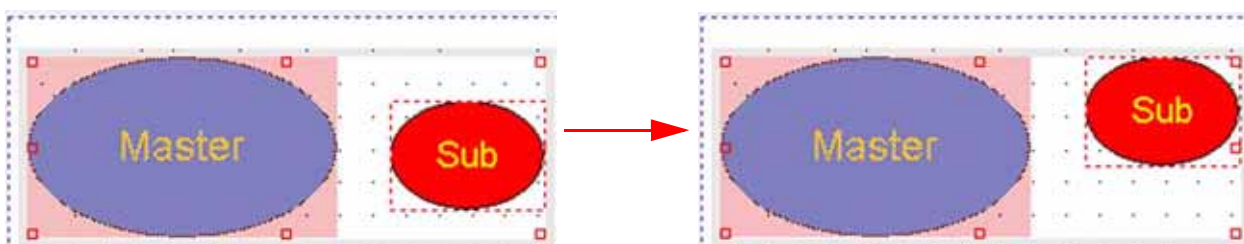
The ResultWorkshop offers five commands to adjust other objects **relative to a selected object**. Usage of these commands requires at least two objects on a working grid, one of them being currently selected (“Main”) and the other one (“Sub”) to be adjusted relative to the “Main”. The object(s) to be adjusted may not be locked, see topic **Context Menu** on page 4-47.




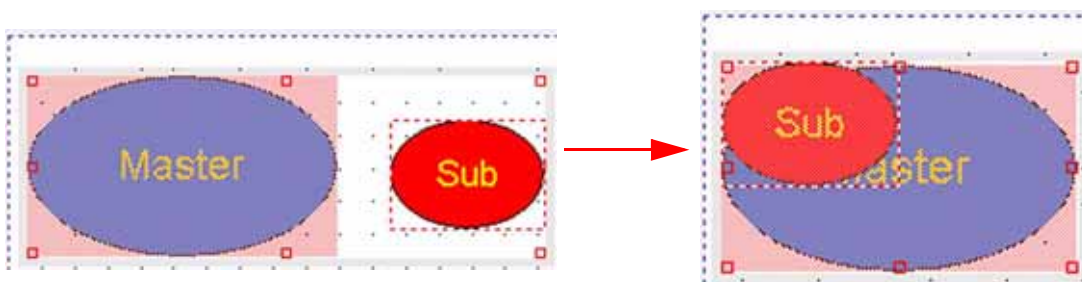
- Define a “Master” object and a “Sub” object.
- Select the “Master”. Thereby, the “Master” will be enclosed by its box.
- Keep the **<Ctrl>** key pressed and click on the “Sub”. Both objects will be enclosed by one common box. This indicates, that they now belong together. The “Sub” can now be adjusted relative to the “Master” in different ways as follows.



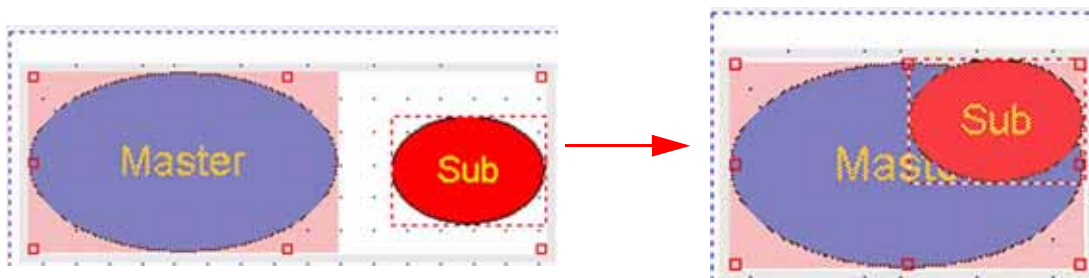
- Use the **Adjust down** button  to arrange the “Sub” at the bottom of the common box.



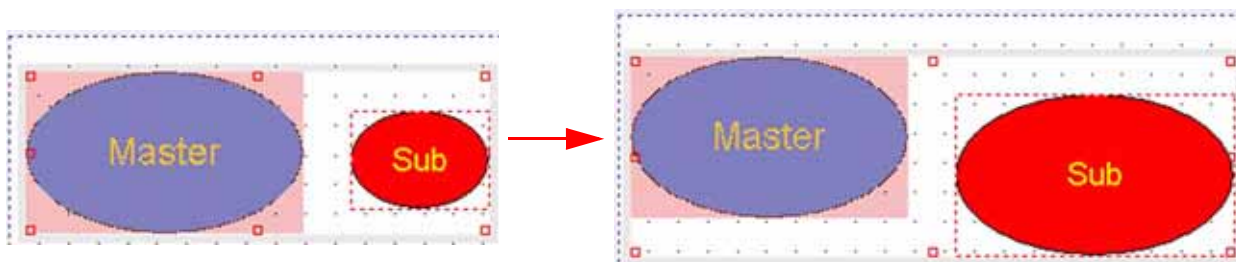
- Use the **Adjust up** button  to arrange the “Sub” on top of the common box.




- Use the **Adjust left** button  to arrange the “Sub” at the left edge of the common box.

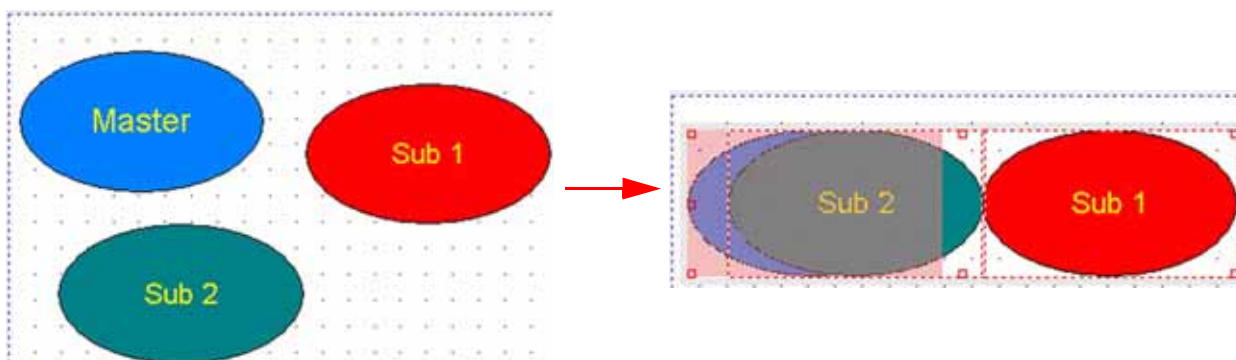


- Use the **Adjust right** button  to arrange the “Sub” at the right edge of the common box.



- Use the **Adjust size** button  to conform the size of the “Sub” to that predefined by the “Master”.

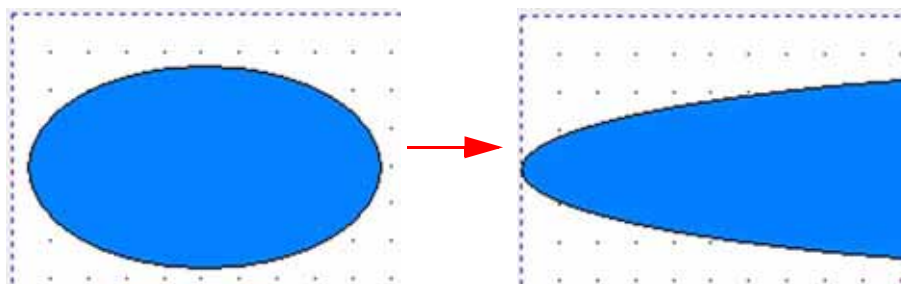
Furthermore, it is possible to adjust more than one “Sub” to a “Master”.




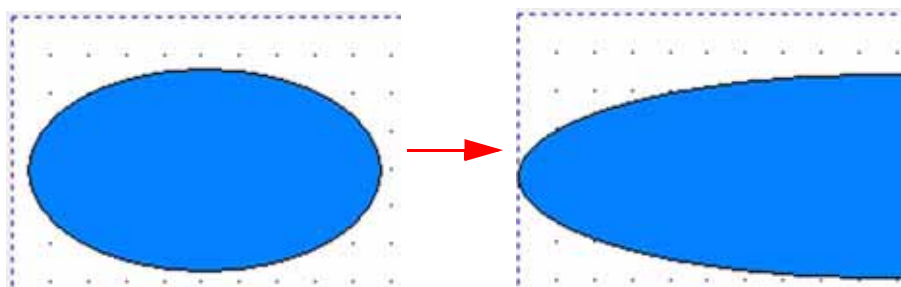
1. Select the “Master”.
2. Keep the **<Ctrl>** key pressed while selecting the “Subs”.
3. Click the **Align** command of interest.


Adjust objects relative to the page margins

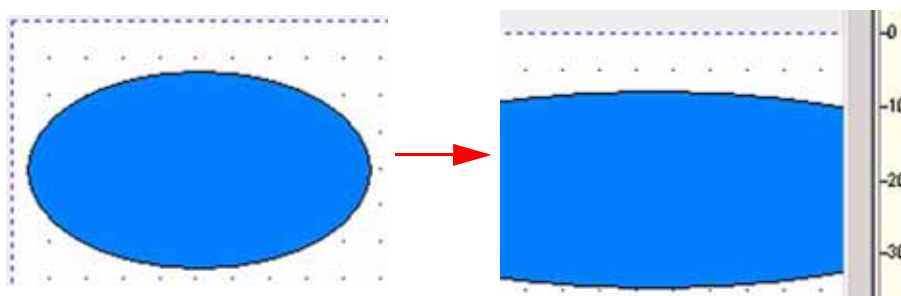
The following three commands serve to adjust objects relative to the page margins.




1. Select the object(s) to be adjusted.
2. Press the  button. The selected object will be stretched and spans the entire page width.



1. Select the object(s) to be adjusted.
2. Press the  button. The selected object will be stretched and spans the left half of the page. The right half of the page remains untouched, e.g. stays empty.

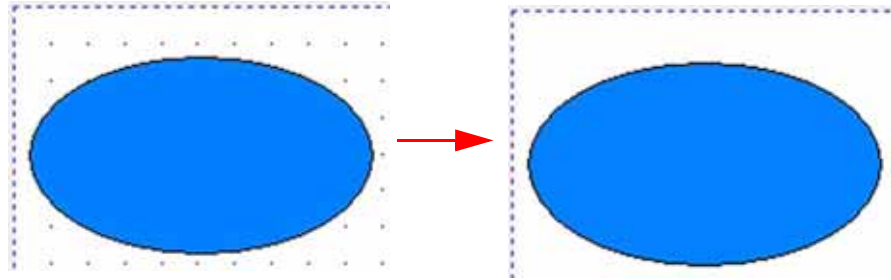



1. Select the object(s) to be adjusted.
2. Press the  button. The selected object will be stretched and spans the right half of the page. The left half of the page remains untouched, e.g. stays empty.

If objects are locked, they can not be adjusted, see topic **Context Menu** on page 4-47. You can adjust an (unlocked) object while another locked object is placed within the stretching area. It will be stretched in the background, whereas the locked object remains untouched in the foreground.


After selecting an object, you can switch between the three different stretching modes, e.g. first stretch an object to the left half of the page. Then simply click the respective button to stretch it to the right half of the page.

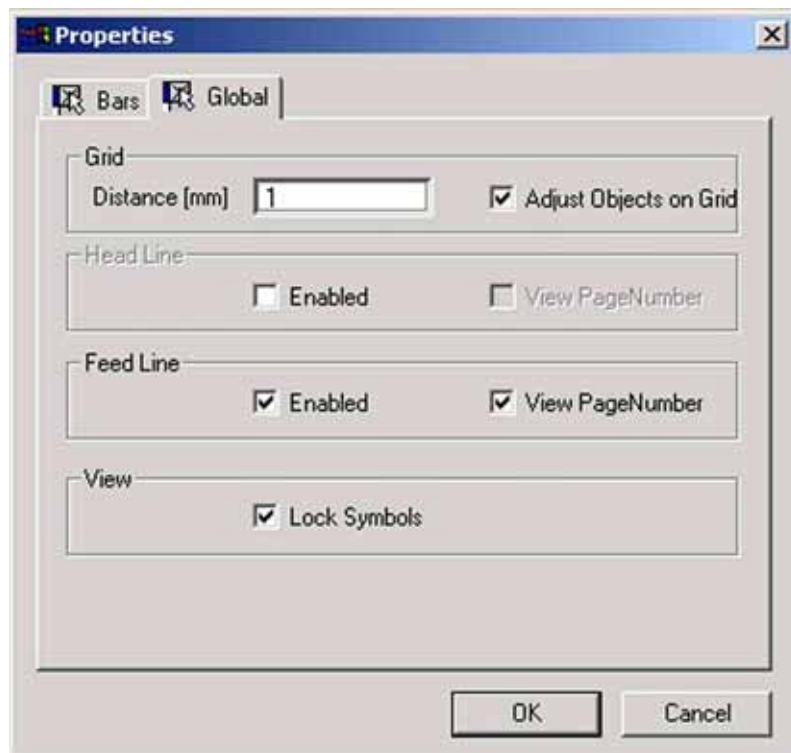
Switch on/off the guiding lines





- Press the  button to let the guiding lines of the working grid appear or disappear (toggle command).

Changing the appearance of the guiding lines

1. On the Basic toolbar, press the **Options** button  (see topic **Basic Toolbar** on page 4-20).
2. Select the **Global** tab.




3. At **Distance** regulate the distance between two guiding lines (in mm):
either type in an integer value between 1 and 10 or use .
4. If you mark the **Adjust objects on grid** checkbox, the guidelines can be
shown and hidden via the toggle command . If the checkbox is unmarked, the toggle command is inactive and the guidelines are not visible.
5. At **Head Line** and **Feed Line**, mark the **Enable** checkbox to insert a header/footer into the working grid. If the checkbox is unmarked, no header/footer will be inserted.
6. At **Head Line** and **Feed Line**, mark the **View Page Number** checkbox to insert a page number into the header/footer. If it is unmarked, no page number will be inserted. The **Enable** and **View Page Number** checkboxes can be used independently: a page number can be displayed without a header or footer. A header or footer can be displayed showing no content.

Object Toolbar

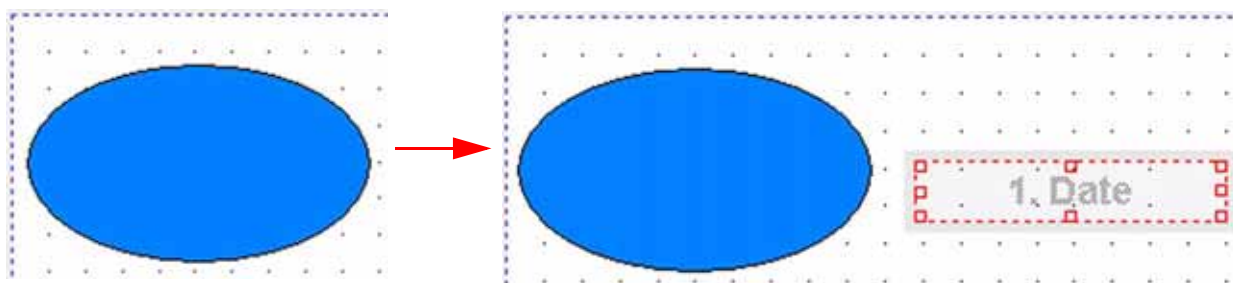



Arrow icon

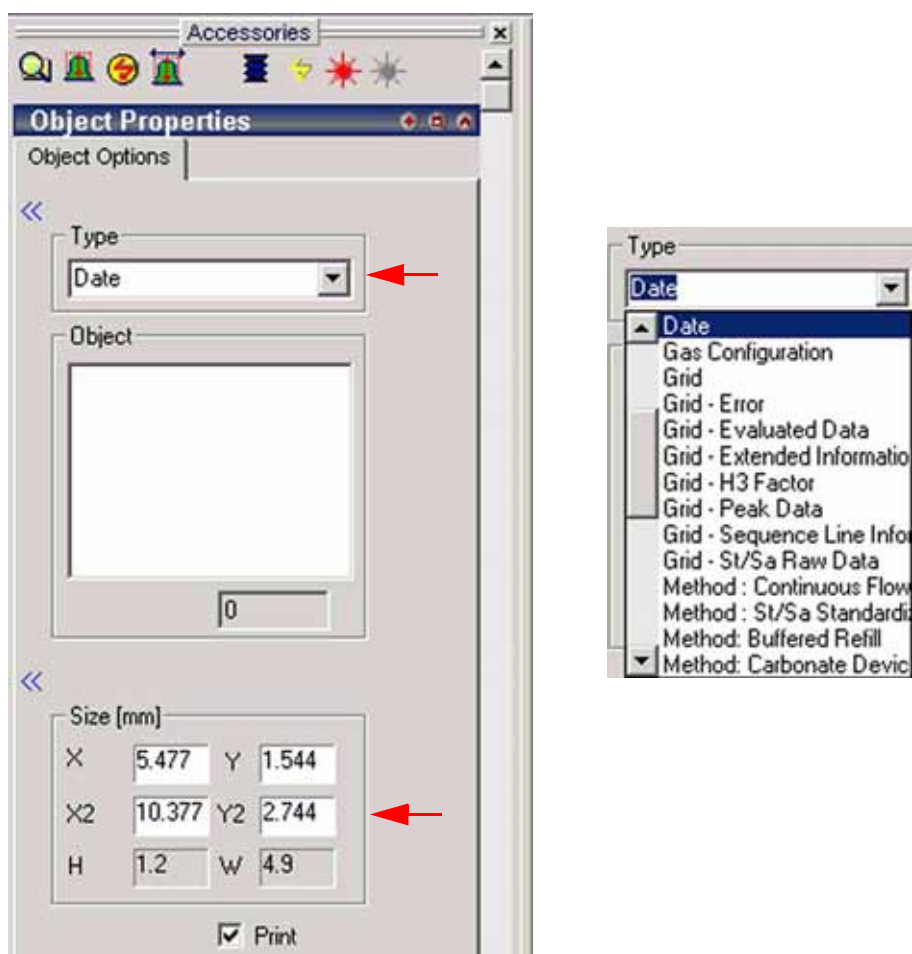
- Press the **Arrow** icon  to perform a lot of actions on the working grid.

Insert Acquisition Time

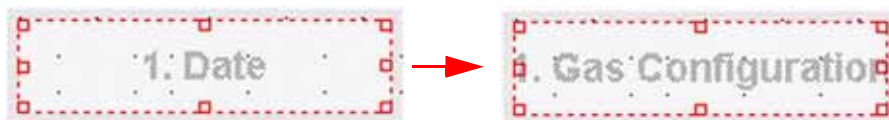
It is possible to insert the time of data acquisition into the working grid.



- Press the **Acquisition Time** icon . The mouse pointer turns into a crosshair cursor.
- Click on the position within the working grid, where you want the new box to appear.
- Drag the crosshair cursor until the final size of the box is reached.
- The box may contain different texts (e.g. "1. Date").



5. From the **Type** pull-down menu, choose between various entries (default: Date, which leads to the text “1. Date” within the box).



E.g. Choosing Gas Configuration leads to the text “1. Gas Configuration” within the box, etc.

6. The actual size of the box is displayed below (in mm). When the size is changed via the sizing handles at its edge, these modifications will also be displayed.

Insert Isodat Object

- To insert various Isodat objects into the working grid, press the **ISO** icon



Insert Result File Name


- To insert the name of a Result File into the working grid, press the

Result File Name icon .



Insert Text File

- To insert an *entire text file* into the working grid, press the **Text File** icon




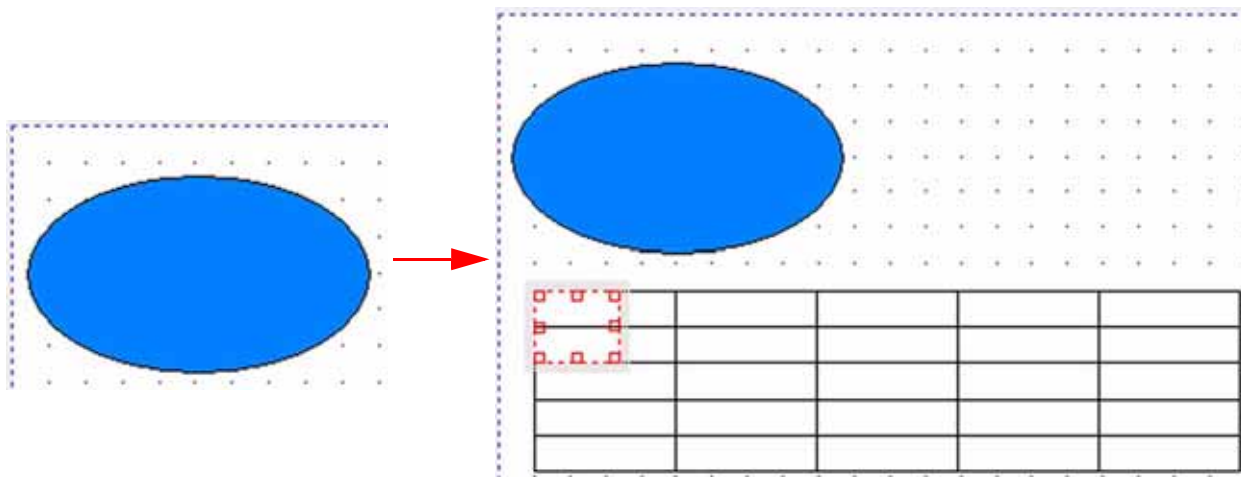
. However, to insert *text*, use the **Text** icon .

Insert Text

- To insert text into the working grid, press the Text icon  (see **Inserting a Text Object** on page 4-42). However, to insert an entire text file, use the Insert Text File icon  described above.

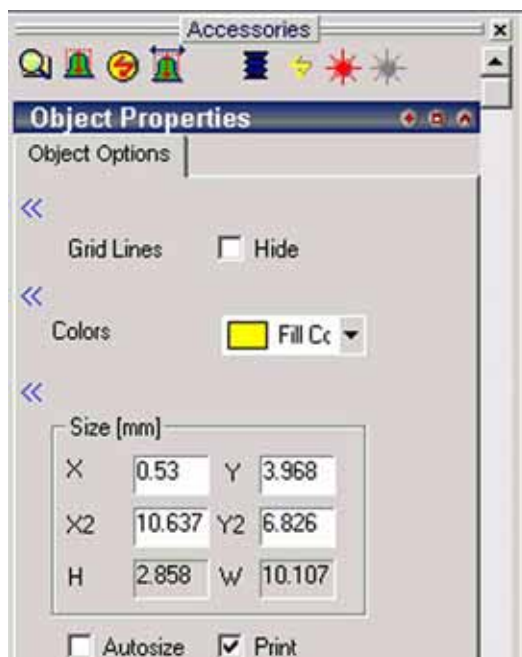
Insert Grid

- To insert a *grid* into the actual working grid, press the Grid icon . The mouse pointer turns into a crosshair cursor.

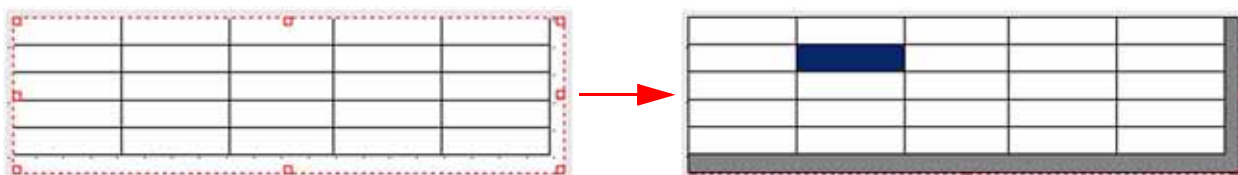


- Click on the position within the working grid, where you want the new grid to appear.
- Drag the crosshair cursor to generate the grid, i.e. a table (default: 5 rows and 5 columns).
- To increase the size of the box that contains the grid drag its sizing handles. The box should enclose the grid.

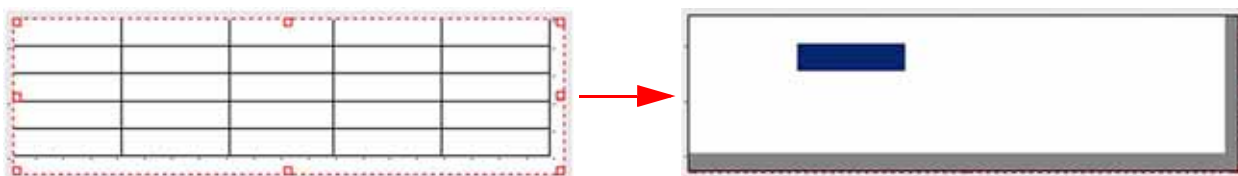
Alternative: Mark the **Autosize** checkbox. The box will automatically enclose the grid. It is impossible then to modify the box dimensions by dragging the sizing handles.



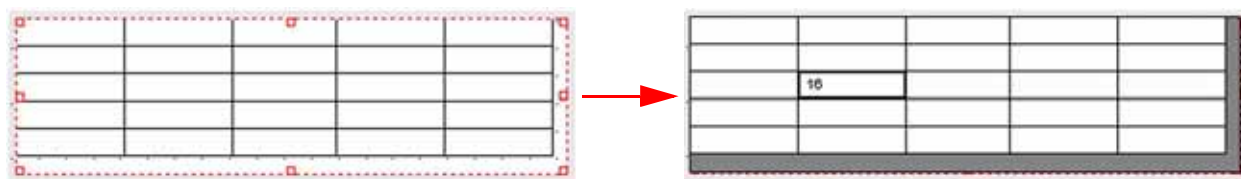
5. Mark the **Hide** checkbox to hide the lines within the new grid (i.e. table).
6. At **Colors**, select a fill color for the new grid.
7. At **Size**, the dimensions of the box enclosing the grid is displayed.
8. Mark the **Autosize** checkbox to let the grid be enclosed by the box.



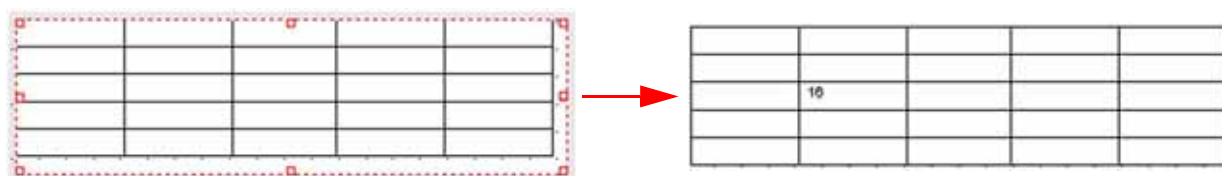
9. A double-click on the new grid leads to the design shown right.



10. If you marked the **Hide** checkbox before, the double-click leads to the design shown right, i.e. the lines are hidden.




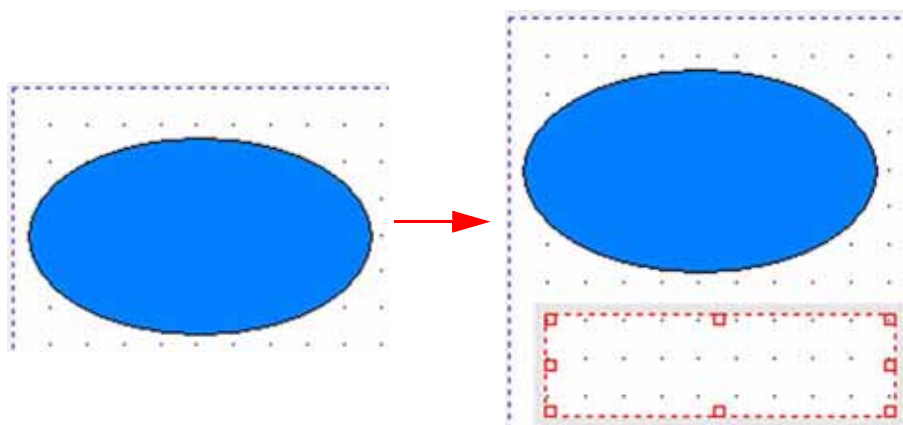
11. A further click on the grid allows values to be typed into its cells.



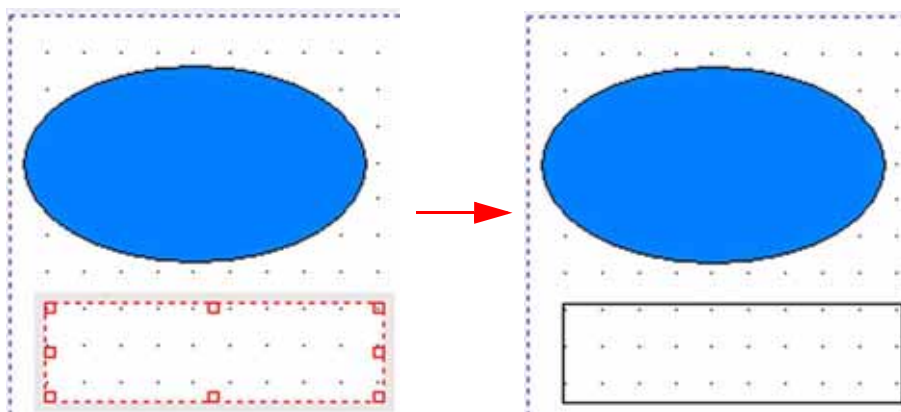
12. Finally, click on the surrounding working grid.

Insert a simple object

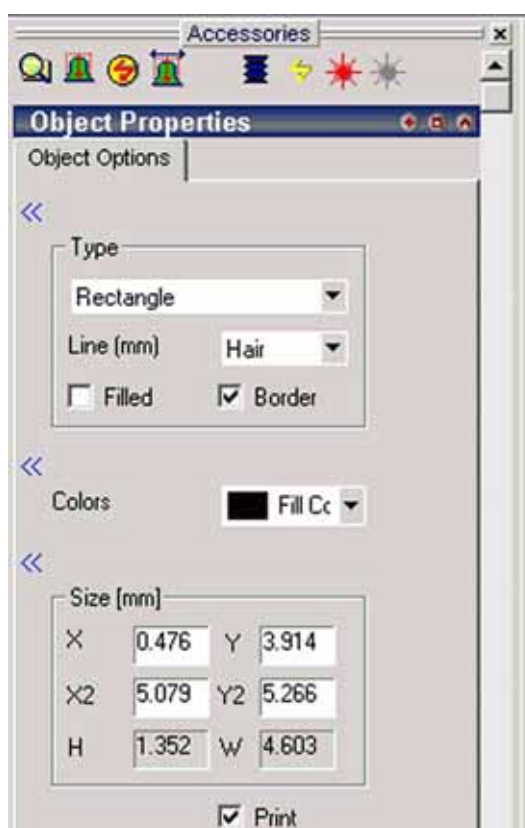
1. To insert a simple object, i.e. without text, into the actual working grid, press the **Simple** icon . The mouse pointer turns into a crosshair cursor.



2. Click on the position within the working grid, where you want the simple object to appear.
3. Drag the crosshair cursor to generate the simple object.




4. **Click** on the working grid to see the simple object just inserted.

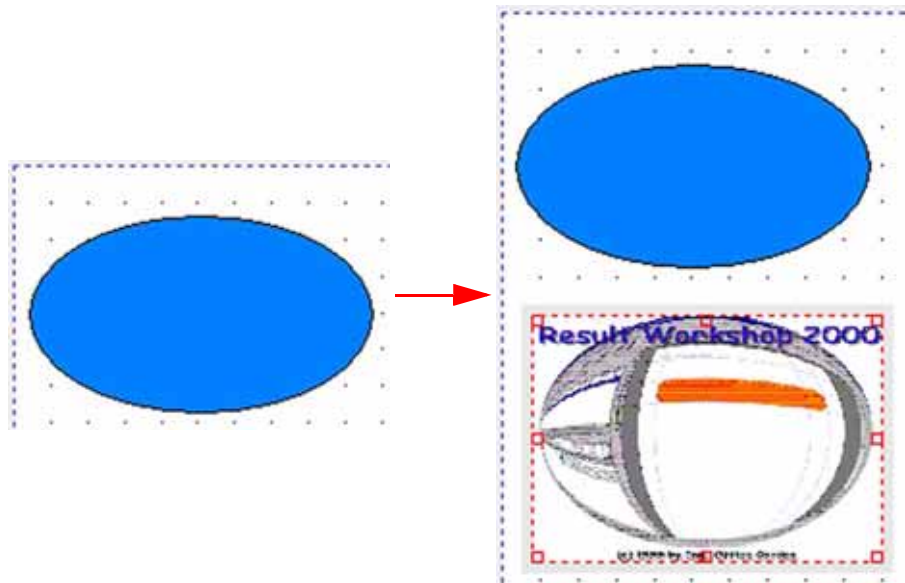


5. At **Type**, choose between a variety of geometric shapes to be displayed (default: rectangle).
6. At **Line**, define the thickness of the surrounding line between 0.1 mm and 10 mm. “Hair” is even thinner than 0.1 mm.
7. Mark the **Filled** checkbox to fill the geometric shape with a fill color defined below. If it is unmarked, the shape will not be filled at all.

8. Select a **Fill Color** to fill the geometric shape with. Additionally, select a Line Color for the line limiting the shape outwards.
9. At **Size**, define the dimensions of the geometric shape. If you modify its dimensions by dragging the sizing handles, these changes will be displayed there.


Insert a Graphic

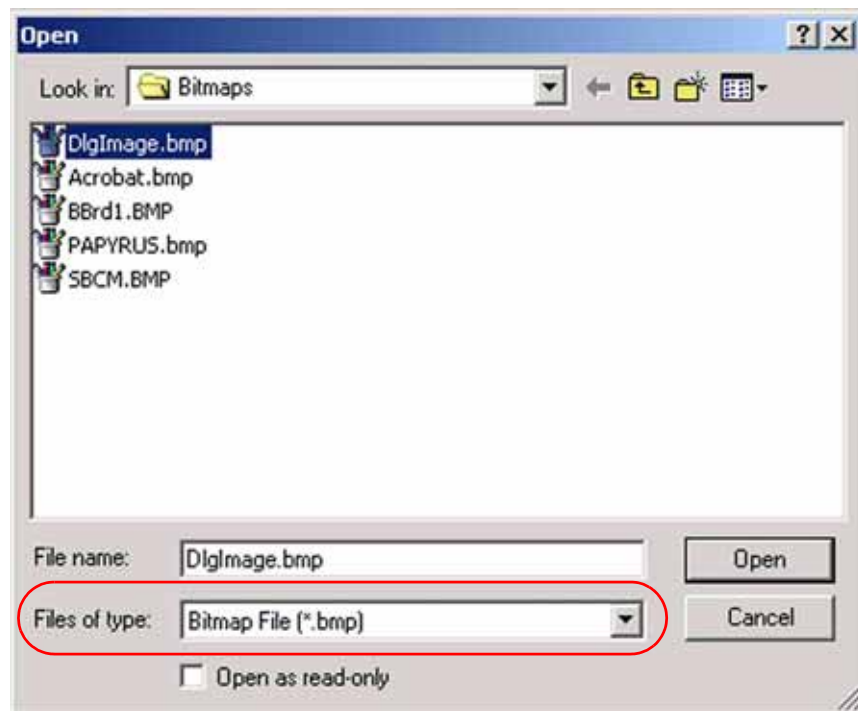
1. To insert a graphic into the working grid, press the **Bitmap** icon . The mouse pointer turns into a crosshair cursor.



2. Click on the working grid, where you want the graphic to appear.
3. Drag the crosshair cursor to generate the box that encloses the graphic. The default graphic shown above appears.



4. Press the  symbol to search another graphic to be displayed instead.



Usually, bitmaps related to Isodat 2.0 are stored in a folder of their own, e.g. Finnigan\ISODAT NT\Global\Databases\Bitmaps.

5. Select the bitmap (*.bmp) to be displayed instead of the default graphic.

Note. Only bitmap files (*.bmp) are supported.

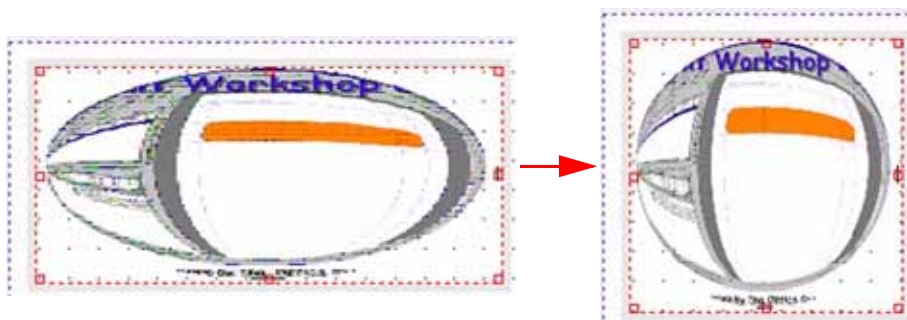
6. Confirm by **Open**.


The bitmap appears on the working grid and its name is displayed in the



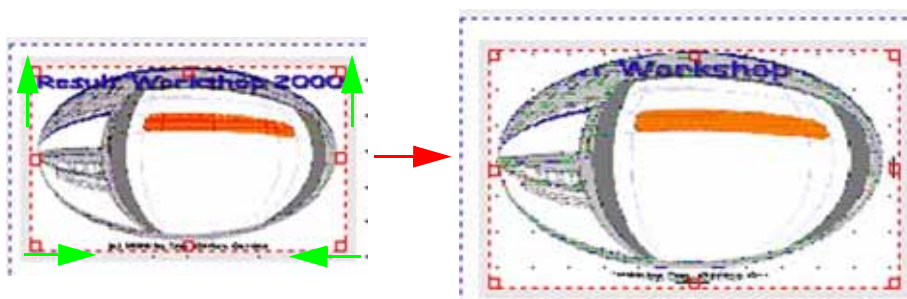
entry field:

7. The graphic is shown above the **Shade** checkbox.
8. Mark the **Shade** checkbox to assign a shade color to the graphic. The shade color will be defined below.



9. Press the  button to turn a highly asymmetric graphic into a regular one.

Note. At *Size*, the dimensions will change to $X2 = Y2$.



10. Mark the **Round** checkbox to erase graphic text that is located outside the contours of the graphic. Some rectangular graphics will be displayed with oblate rounded edges.



11. At **Colors**, select a shade color.

Note. The **Shade** checkbox must be marked for the shade color to take effect.

12. At **Size**, define the dimensions of the graphic. If you modify its dimensions by dragging the sizing handles, these changes will be displayed there.

Inserting Objects into the Working Grid

Via simple drag&drop, various types of objects can be placed onto the working grid, e.g. text objects, graphical objects.

Inserting a Text Object

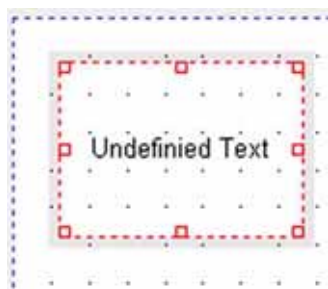
1. To place a text object (i.e. a text box) onto the working grid, press the

Text Object icon  on the *Object* toolbar.

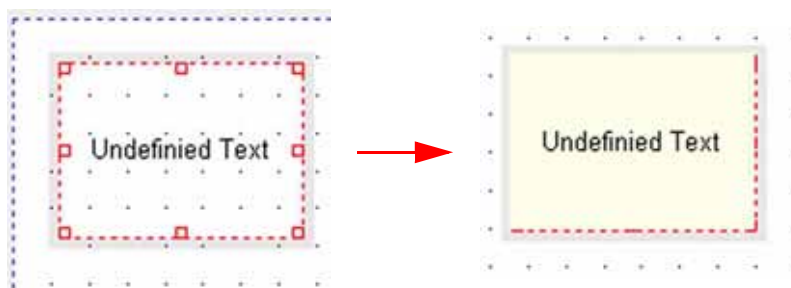
2. When you move your mouse pointer towards the working grid, it turns to a cross-hair cursor.
3. Keep the left mouse button pressed and drag the cross-hair cursor.
4. Release the left mouse button. A text object appears on the working grid.

Current Page : 1 Page Format : 190X271mm Objects : 1  Zoom : 1.000

Note that on the Status bar, the number of objects in the working grid has increased from 0 to 1.



5. Adjust the dimensions of the text object by dragging its sizing handles.
6. To adjust its position left-click into the box and keep the left mouse button pressed. Move the text object to its intended position. Finally, release the left mouse button.

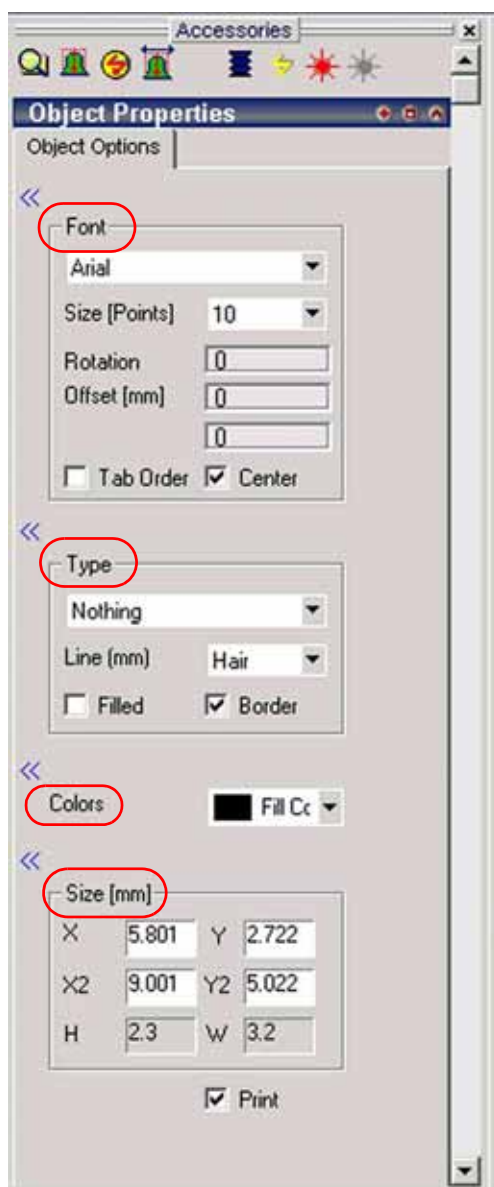


7. To assign a significant text to the text object double-click into it. The text object turns into yellow and the text becomes editable.
8. Type a significant text and click somewhere outside the box.

Changing the Properties of Objects

After *inserting* an object onto the working grid (e.g. a text object, see topic **Inserting Objects into the Working Grid** on page 4-42), you can change its properties using the *Object Properties* box at the “Accessories” toolbar.

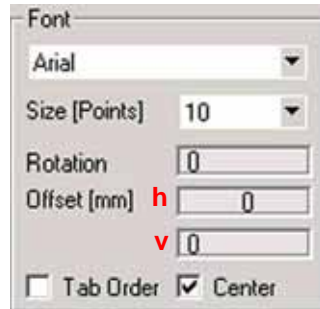
As long as an object is selected (e.g. a text object), *Object Properties* shows its actual properties:



The properties are arranged in groups: *font*-, *type*-, *colors*- and *size*-related ones.

- Use the << buttons to selectively mask particular groups of information.

Changing Font Properties



1. Choose a **font** from the list above (default: Arial).
2. Choose a font **size** between 0 points and 127 points from the list below (default: 10 points).
3. Choose a value in ° between 0 and 360 to **rotate** the text within the object (default: 0°, i.e. no rotation).
4. To choose a **horizontal offset** (h) in mm between 0 and 1000, double-click into the upper entry field and type a value. Alternatively, use



to increase or decrease the value. Using



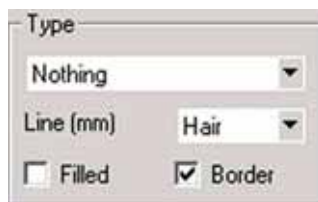
in the right corner of the entry field will **only increase** the value, while in the left corner of the entry field will **only decrease** it.

The text will be moved horizontally within the object. The default is 0, i.e. the text appears at the **left** edge of the object. When the offset exceeds the object dimensions, the text is moved outside the object and can not be seen.

5. To choose a **vertical offset** (v) in mm between 0 and 1000, analogously use the lower entry field.
6. The text will be moved vertically within the object. The default is 0, i.e. the text appears at the upper edge of the object. When the offset exceeds the object dimensions, the text is moved outside the object and can not be seen.

Note. When the Center checkbox is marked, rotation and offset changes will not take effect. Instead, the text will always stay centered. You must unmark this checkbox for the rotation and offset values to take effect.

Changing Type Properties

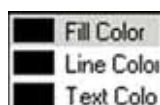


1. From the pull-down menu, select a **geometric structure** to be placed into the object (e.g. a circle). As default, “Nothing” is proposed, i.e. the object is displayed without a geometric structure incorporated.
2. From the **Line** pull-down menu, select a value between 0.1 mm and 10 mm for the thickness of the geometric structure's lines. The default value “Hair” is even thinner than 0.1 mm.
3. Mark the **Filled** checkbox to fill an enclosed geometric structure with a fill color. Black is proposed as default fill color. Geometric structures without enclosure, e.g. lines, can not be filled.

Changing Color Properties

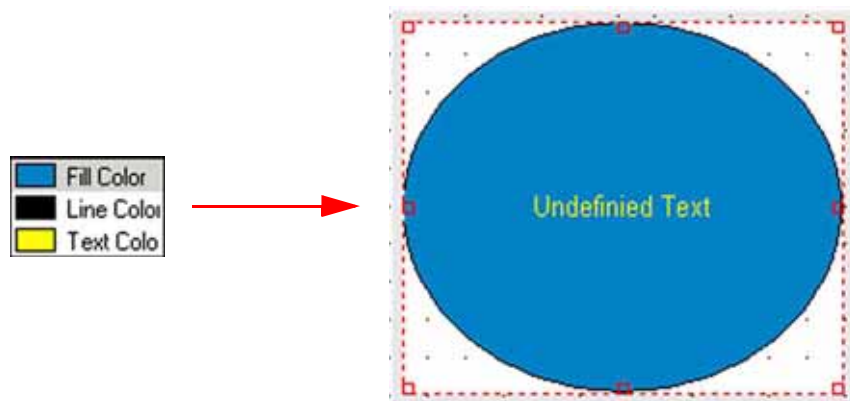


1. Press the  arrow.



2. Choose between fill color, line color and text color. Black is the default color for any of the three types.
3. **Clicking** on each line opens a collection of basic and custom colors. Make your choice and confirm by **OK**.
 - A **fill color** can be used in case of **enclosed** geometric structures (e.g. a circle). Geometric structures without enclosure, e.g. lines, cannot be filled, i.e. any fill color will have no effect.
 - A **line color** can be used for any geometric structure.
 - A **text color** can be used for any text.

Example for fill, line and text colors



Changing Size Properties

Size [mm]			
X	4.18	Y	4.604
X2	9.974	Y2	9.499
H	4.895	W	5.794

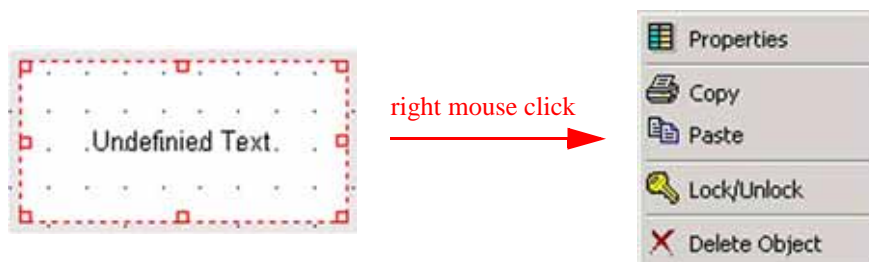
☒ Print

It is possible to change the dimensions of the chosen object by typing the intended values in the entry fields.

If you, on the contrary, drag an object's size handles, the values in the entry fields will be modified.

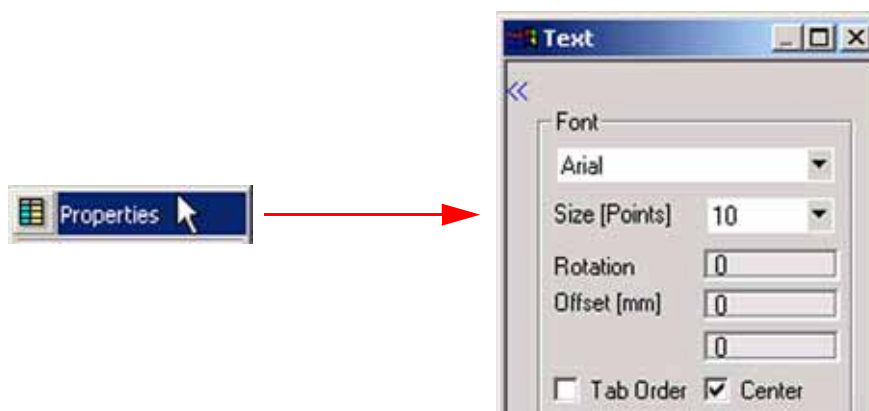
Context Menu

The properties of inserted objects can alternatively be changed as follows:



1. Select an object.
2. Press the right mouse button. The context menu appears.

Properties Command



- Select **Properties**. The Accessories toolbar appears. Usually this toolbar is displayed left to the working grid and shown or hidden via **Option > Accessories** (see topic **Accessories Toolbar** on page 4-4).

Copy and Paste Commands

Use these commands to duplicate objects, especially complex ones.

1. Select **Copy**  .
2. Anywhere select **Paste**  .



3. The object is duplicated even though only two-fold text can be seen.
4. Keep the left mouse button pressed and drag the new object to its intended place.

Lock/Unlock Command

Use this command to fix or unfix the position of objects. This immobilization may be especially helpful in case of an entire group of objects in order to preserve their positions relative to each other.

To select several objects together one after another keep the <Ctrl> key pressed. Afterwards it is sufficient to click Lock/Unlock once to lock/unlock all objects selected. A locked object can not be deleted.

1. Select **Lock/Unlock** .



2. The position of the selected object is fixed (see the key symbol).
3. Clicking **Lock/Unlock** again will unfix its position (the key symbol disappears).

Delete Object Command

1. Press **Delete Object** .
2. The selected object will be deleted unless it is locked.

Alternative: Use the **Delete** button on the Page toolbar (see topic **Page Toolbar** on page 4-22).

Chapter 5

Miscellaneous Features

This chapter contains the following topics:

- Acquisition Mode and Workspace Mode

5.1 Acquisition Mode and Workspace Mode

Principle: The well-known dialectic discrimination between “Dual Inlet” Mode and “Continuous Flow Mode” as applications has been abandoned. Instead, only one Acquisition Mode exists encompassing both of them.

In addition to Acquisition Mode, a nearly identical Workspace Mode is available. Workspace Mode allows creation of new elements (i.e. Isodat methods, GC methods, AS methods, sequences, Excel templates) and even evaluation during data acquisition. Any tools and files known from Acquisition Mode are available in Workspace Mode as well. However, only data acquisition is impossible in the latter.



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