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PC Control 808 Touch Control 809 Touch Control

Program version PC Control 1.0
Touch Control 5.808.0110 and 5.809.0110

Instructions for Use

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Although all the information given in these instructions has been checked with great care, errors cannot be entirely excluded. Should you notice any mistakes please inform the author at the address given above.

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1 Introduction

These instructions give you a comprehensive overview of the functions of the **Touch Control** software and the **PC Control** software for operating the **808 Titrand** and the **809 Titrand**. The **Touch Control** has a touch-sensitive screen and, together with a Titrand, forms a "stand alone" titrator. The Touch Control can also be used to control up to three Titrands. The **PC Control** software is installed on a computer to control up to three Titrands via a USB connection.

Figure 1 shows the versatility of the Titrand system. On the left is a Touch Control for operating an 808 Titrand and an 801 Magnetic Stirrer. To the right of it is a computer with the PC Control software which is being used to control an 809 Titrand and an 804 Titration Stand with an 802 Rod Stirrer.



Fig. 1: The Titrand system

The documentation for the 808/809 Titrando system consists of the following printed instructions:

- **Installation Instructions for the 808 Titrando and 809 Titrando**, which describes the installation of the titration system and gives the specifications of the Titrandos (8.808.1103).
- **Instructions for Use for the 808 and 809 Touch Control and for the PC Control software**, in which the operation of the titration system by using the Touch Control and PC Control software is described (8.808.1303).
- **Tutorial for the 808 and 809 Touch Control**, which provides a simple introduction to the operation of the Titrando system with the Touch Control (8.808.1403).
- **Tutorial for the PC Control software**, which provides a simple introduction to the operation of the Titrando system with the PC Control software (8.808.1503).

These documents as well as the following are available as PDF files. Please contact your Metrohm representative.

- Instructions for complying with FDA Guideline 21 CFR Part 11 (**Titrando Compliance Guide**), which provides a step-by-step description of the configuration of the Titrando system if work is to be carried out in accordance with the FDA Guideline 21 CFR Part 11 – *Electronic Records; Electronic Signatures* (8.808.8013).
- **System Assessment Report** based on electronic data and electronic signatures; Final Rule 21 CFR Part 11.
System: Titrando 808 or 809 with Touch Control (8.808.8023)
System: Titrando 808 or 809 with PC Control (8.808.8033)
- Description of the PC/LIMS report (**Titrando PC/LIMS Report Guide**), in which the contents of the PC/LIMS report as produced by the Titrando system are described in detail (8.808.1603).

Further up-to-date information about the Titrando system can be found on the Internet under www.titrando.com.

Information about special applications can be found in our "**Application Bulletins**" and "**Application Notes**"; these can be obtained free of charge from your local Metrohm agency or downloaded from the Internet under www.metrohm.com. Various **monographs** on the subjects of titration techniques and electrodes are also available.

1.1 Instrument description

There are two different ways of operating the Titrando system: with **Touch Control** the operation is via a touch-sensitive screen. A computer with installed **PC Control** software is a version with several additional features which directly utilize the communications and storage facilities of a PC. Both programs have a context-sensitive **online help** function.

The appearance and operation of the two versions are almost identical; this means that if you work with Touch Control then you can also use the PC Control software without any problems and vice-versa. Methods, determinations, sample data silos, result silos and backups are **100% compatible**.

These Instructions for Use describe the operation of the Titrando system with both Touch Control and the PC Control software. If the description applies to only one of these versions then this is indicated in the text.

The most important features of the PC Control which are not found in the Touch Control are these:

- Sample data silo table with all sample data in a separate window.
- Follow-me help (the help text for the current dialog is always shown in a separate window) .
- Manual operation is carried out in a separate window.
- Import of Titrino methods
- Audit trail (protocol of user actions)

1.2 Information about these Instructions for Use

**Attention!**

Please study these instructions carefully before you start to use the Titrando system. The instructions contain information and warnings that must be observed by the user in order to guarantee the safe use of the instrument. Please keep these instructions near the instrument so that they are always to hand when required.

1.2.1 Organization

These Instructions for Use for the 808 Touch Control, the 809 Touch Control and the PC Control software provide you with a comprehensive overview of the installation and operation of the programs. Measures to be taken to remedy problems and the technical data of the Touch Control are also provided.

The instructions are arranged as follows:

Introduction

Description of the instrument and general information about these Instructions for Use

Installation

Installation of the PC Control software and Touch Control setup, description of the Touch Control parts and controls

Operation

Operating principles of Touch Control and PC Control, description of all the functions of the Titrando system (system settings, creating, storing and loading methods, carrying out determinations, viewing and recalculating determination data, statistical calculations, report printouts, manual operation of the Titrando systems

Parameters

Detailed description of all method parameters

Troubleshooting

Description of possible faults and their remedies

Annex

Technical data, description of the Remote Box and USB-RS 232 Box, standard accessories, optional accessories, warranty and declaration of conformity





Index

In order to find the information you require about the Touch Control or PC Control you should either use the **Contents** or the **Index**.

Please also observe the information given in the separate **Installation Instructions** for the 808 Titrando and 809 Titrando (8.808.1103).

1.2.2 Notation and pictograms

The following notation and pictograms are used in these Instructions:

9	Numbers of the parts and controls see illustrations in <i>Section 2.1</i> .
	Instructions carry out the instructions step by step.
User	Parameters, input values Parameters and values for parameters, dialog title. Menu, menu item in the PC Control software.
[Next]	Button on the user interface. Fixed key on the Touch Control.
<Ctrl>	Key on the computer keyboard.
	Danger/Warning This symbol indicates a possible risk of injury to the user and possible damage to the instrument or its components.
	Attention This symbol indicates important information that you should read before continuing.
	Information This symbol indicates additional information and tips which may be of particular use to you.

2 Installation

This section describes how you can install the **PC Control** software on your computer and/or how to start up the **Touch Control**. The setup of the titration system with peripheral devices such as stirrers and dosing devices is given in the Installation Instructions for the 808 Titrand and 809 Titrand (8.808.1103).

2.1 Installation of the PC Control software

Connecting the computer to the Titrand is described in the Installation Instructions for the 808 Titrand and 809 Titrand.

2.1.1 System requirements

The PC Control software should be installed on a PC with the following minimum performance features:

- Processor: Pentium III
- Main memory: 128 MB RAM
- Free memory space: 50 MB for program files
- CD-ROM drive
- Connection: one free USB slot (type A)

Microsoft **Windows 2000** or **Windows XP** must be used as the operating system.



Attention!

*The **installation of PC Control** must be made by the "Administrator". When using the NTFS file system make sure that the intended users have full rights of access to the PC Control program folder and the subfolders it contains. Check this under Windows Explorer in the security settings which are defined in the properties of the PC Control folder. If you want to select other folders for Card 1 and Card 2, e.g. on a network drive (see Section 3.11) then the user must also have full rights of access to these folders.*

Windows XP: *The security settings described above are only accessible when the option "Use simple file sharing" has been switched off under Windows Explorer in the menu Tools/Folder options/View.*

2.1.2 Installing the program

- ☞ When the **installation CD** is inserted the program "Setup.exe" should start automatically. If not, start it manually.
- ☞ During the initial installation the license agreement appears. You should read through it and then confirm your agreement with a mouse-click on **[Yes]**.
- ☞ You must then define the folder to be used for the installation of the PC Control software on the hard disk. If necessary, you can use **[Browse...]** to select a different folder from that shown as default. Confirm the target folder with **[Next >]**.
- ☞ Now select the program folder in which the program symbol is to appear: **[Next >]**.
- ☞ Before the copying process starts you can check the shown settings and, if necessary, correct them using **[< Back]**.
- ☞ All program files are then copied and the successful conclusion of the installation is shown. Exit the installation program with **[Finish]**.

During the installation and subsequent operation the following subfolders will be created in the program folder:

backup	Internal backup system
bin	Program files
Card1, Card2	Standard folders for the memory cards Card 1 and Card 2 (see <i>Section 3.11</i>) In Card1 a folder Examples will be created with examples of methods and determinations (see <i>Section 3.11</i>).
data	Memory location for all current data and settings
Files	Folder for the memory location Internal Memory The files in the internal memory are protected in the file archive.metr. All other files in this folder are temporary and not visible in the PC Control file manager.
jre	Program files
lib	Program files
log	Folder for log files
MethodTemplates	Folder for method templates
res	Program files



Note!

*You should only manage the PC Control files with the **file manager of the PC Control software**. If you use Windows Explorer for this then there is the risk that you might no longer find the files in PC Control as the folder structure is not compatible.*

If you want to replace an existing PC Control software version by a new installation then, after the start of "Setup.exe", select the option "Repair or install over existing installation". In this way all the user data (system settings, user lists, titrants, sensors and other system-specific data, methods, results, determinations, sample data silos and result silos) are retained. This applies also for the internal memory containing methods (see also *Section 3.11*).

The menu "Modify, repair, or remove program" only appears if a version of the PC Control software is already installed on the PC.

A USB dongle ("authorization plug") is supplied with the full version of the PC Control software. Insert this in any USB slot (type A) on your computer or Titrandos.

2.1.3 Demo version

You can use all the functions of the PC Control software without the dongle for a period of **100 days** after the initial installation. When this period has expired it will no longer be possible to start any determinations. You can, however, still use such a PC Control installation to create and manage methods and to view and reprocess determinations.

2.1.4 Registration

After the installation please fill in the enclosed registration form and send it to Metrohm. In this way you will participate in our update service.

Absender _____ Name _____ Firma/Company _____ Abteilung/Department _____ Strasse/Address _____ Postleitzahl, Ort/Postal Code, City _____ Telefon/Phone _____ Fax _____ E-Mail _____	 Metrohm AG Oberdorfstrasse 68 CH-9101 Herisau Schweiz/Switzerland	Programmversion/Version of program _____ Kaufdatum/Purchase date _____ Windows Version <input type="checkbox"/> Windows 2000 <input type="checkbox"/> Windows XP Anzahl Titrandos/ <input type="checkbox"/> Waage <input type="checkbox"/> LIMS Number of Titrandos _____ Balance Wünsche/ Features you miss _____ <i>Die Metrohm-Software-Lizenzbedingungen nehme ich zur Kenntnis.</i> <i>I recognize the Metrohm software license conditions.</i> Unterschrift/Signature _____ <div style="text-align: right;">8.808.8007</div>
--	--	--

2.1.5 Deinstallation of the PC Control software

To deinstall the PC Control software start the program "Setup.exe" on the installation CD. Alternatively, you can start the Windows installation program to remove PC Control under Start/Settings/Control panel/Add or remove programs.

Select the option **[Remove]** and confirm the following safety query.

In this program-guided deinstallation of the PC Control software all the user data (system settings, user lists, titrants, sensors and other system-specific data, methods, results, determinations, sample data silos and results silos) are retained.

If you want to save the system settings and user data for a later PC Control installation in another place then you should use the backup function of the PC Control software (see *Section 3.11.6*).

A new installation of the PC Control software is the only way of making the system accessible again if it is impossible for a user to log in because, for example, even the Administrator has forgotten the password or no Administrator has been defined (see *Section 3.7.5*). In this case before the new installation you should delete the file archive.metr in the Data folder (see *Section 2.1.2*). After the new installation you should load the last backup (see *Section 3.11.6*).

**Note!**

*You should make a **backup** at **regular intervals** in order to avoid data loss. For the Touch Control we recommend – depending on how frequently you alter methods or system settings – making a backup every week to every month. For the PC Control software the period should be in accordance with that usually used for data security backups in your company.*

2.2 Setting up the Touch Control

2.2.1 Packaging

The Touch Control and its specially packed accessories are supplied in very protective special packaging. Please store this packaging in a safe place; it is the only way in which the safe transport of the instrument can be guaranteed.

2.2.2 Checks

Please check that the delivery is complete and undamaged immediately on receipt (compare with delivery note and list of accessories given in *Section 6.4*). If transport damage is evident please refer to the information given in *Section 6.8.1*.

2.2.3 Location

The Touch Control has been designed for internal laboratory use and should not be used in explosion-endangered locations.

Place the instrument on a suitable vibration-free laboratory bench, protected as much as possible from corrosive atmospheres and contact with chemicals.

Choose a location where the temperature is usually between +5 °C and +45 °C. The instrument should be protected against excessive variations in temperature and direct sunlight.

Connecting the Touch Control to the Titrando is described in the Installation Instructions for the 808 Titrando and 809 Titrando.

2.3 Touch Control parts and controls

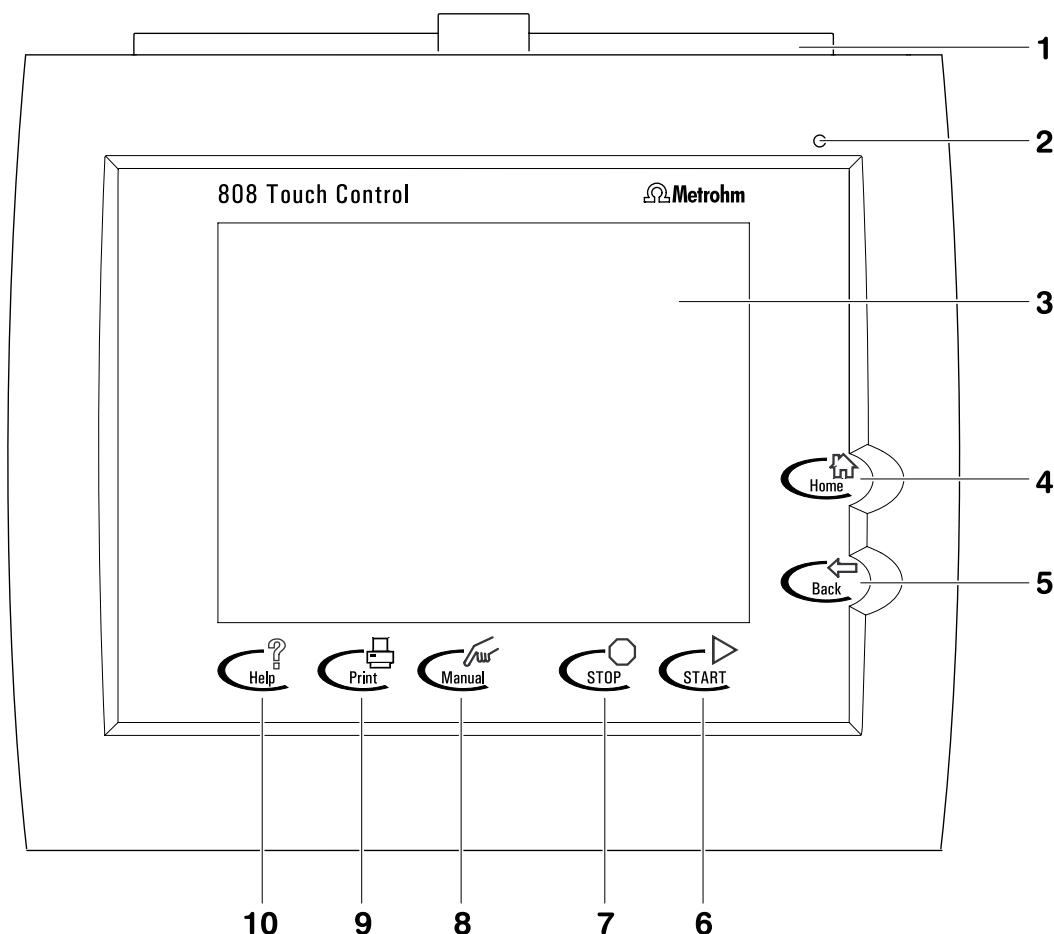


Fig. 2: Front view of the Touch Control

1 Protective cover for card slots

Accommodates two PCMCIA or CompactFlash memory cards.

2 “ON” LED

Lights up when instrument is switched on.

3 Touch Screen display

Shows the changing dialog.

4 Fixed key [Home]

Changes to main dialog.

5 Fixed key [Back]

Changes to previous dialog.

6 Fixed key [START]

Starts the current method.

7 Fixed key [STOP]

Stops the run.

8 Fixed key [Manual]

Opens the dialog for manual operation of the titration system.

9 Fixed key [Print]

Opens the print dialog for manual printout of a report.

10 Fixed key [Help]

Opens the context-sensitive help.

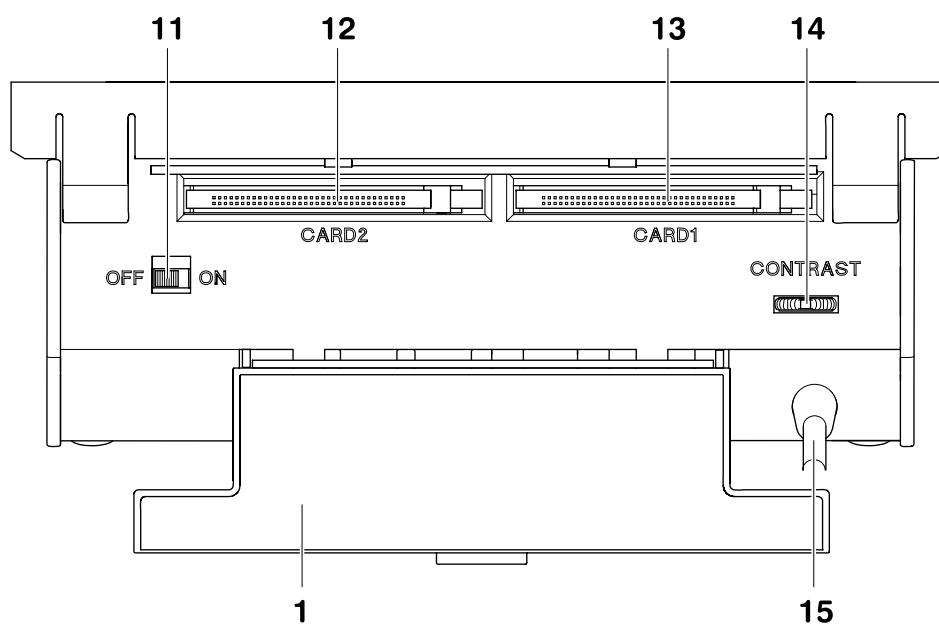


Fig. 3: Rear view of the Touch Control

1 Protective cover for card slots

Must be closed during operation to protect the electronics from splashes.

11 On/Off switch

Touch Control must be shut down properly by switching it off before the current supply is interrupted.

12 Card slot 2

Accommodates one PCMCIA or CompactFlash memory card.

13 Card slot 1

Accommodates one PCMCIA or CompactFlash memory card.

14 Contrast controller for display

15 Connection cable

for connecting the Touch Control to the Titrando ("Controller" connection).

3 Operation

The most important points concerning the operation of the Touch Control and PC Control are described in this section. As the appearance of the **operator interface** and the functions are almost identical, only the **PC Control** operator interface is shown. If individual functions are only available in **Touch Control** or in the PC Control software then this is indicated accordingly in the text.

The arrangement of the program and the **operating concept** are identical for Touch Control and the PC Control software. In **Touch Control** operation is carried out via a touch-sensitive screen (Touch Screen), in **PC Control** the software is operated by using a mouse and the PC keyboard. This results in several system-specific operating possibilities.

3.1 Operating principles: Touch Control

3.1.1 Switching Touch Control on and off

A Touch Control which is properly connected to a Titrando is switched on and off with ON/OFF switch **11** on the rear panel of the instrument.



Attention!

*The Touch Control must be **shut down properly** by **switching it off** with the ON/OFF switch on the rear panel of the instrument before the current supply is interrupted. Otherwise there is the risk that data may be lost. As power is provided to the Touch Control via the Titrando, the Titrando must never be separated from the mains supply (e.g. by switching it off via a multiple outlet strip) before the Touch Control has been switched off. When the Touch Control is **switched on** all the other peripheral devices (e.g. printer) must already be switched on.*

We recommend the following procedure:

- ☞ Connect all the instruments (Titrando and peripheral devices) to the mains supply via a **multiple outlet strip with mains switch**.
- ☞ When **switching on** first switch on the multiple outlet strip with the Touch Control switched off. Then switch on the Touch Control.
- ☞ When **switching off** proceed in the reverse order. First switch off the Touch Control. Then switch off all the peripheral devices via the multiple outlet strip switch.

3.1.2 Setting the display contrast of the Touch Control

Knob **14** for setting the contrast of the Touch screen is located on the rear panel of the instrument. Move it in one direction and hold it tight when it reaches the stop in order to increase or reduce the contrast.

- ☞ Use the fixed key **[Help]** in the main dialog to open the online help. Set the contrast so that the scroll bar surface is light gray and the margins to the left and below are dark gray (see Section 3.3.2).

3.1.3 Operating the Touch Screen

The whole screen surface is touch-sensitive. Just touch some of the buttons on the screen to see how to operate the Touch screen. You can always return to the main dialog by touching **[Home]**.

In order to **activate** an element on the Touch Control user interface just touch the screen with your fingertip, finger nail, the eraser of a pencil or a stylus (special tool for operating Touch screens); see below:

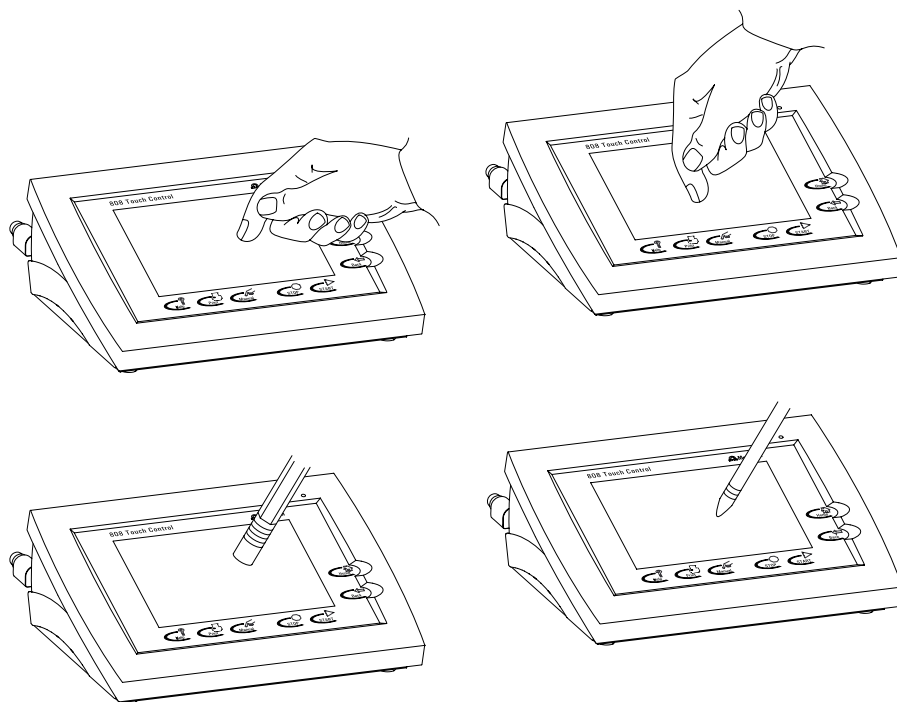


Fig. 4: Different ways of navigation on the Touch Screen



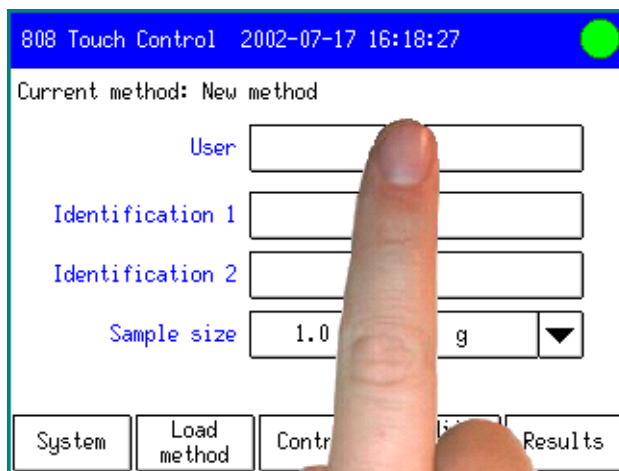
Attention!

Never touch the Touch screen with a pointed or sharp object such as a ballpoint pen.

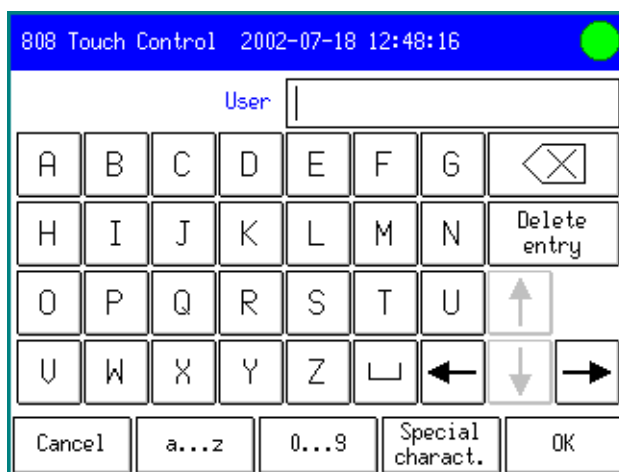
If you use the standard settings then touching an active operating element creates a sound.

3.1.4 Entering text and numbers using Touch Control

☞ Just touch an input field, e.g. **User** in the main dialog, to open the **Text editor**.



In the text editor the name of the parameter is shown in front of the input field.

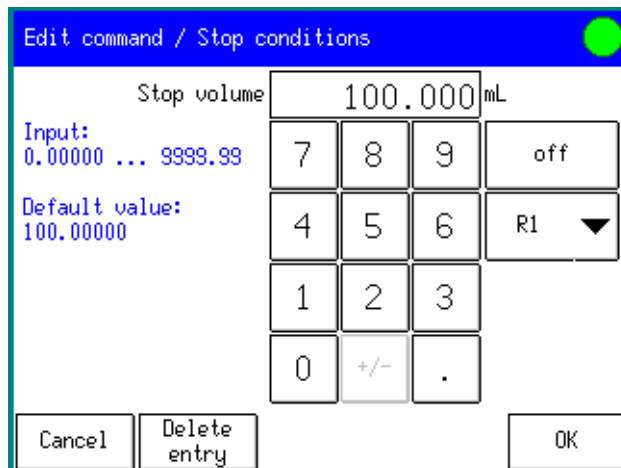


☞ Touch the required character. Apart from the capital letters which first appear, there are also sets of characters with lower case letters, numbers and mathematical signs as well as three blocks of special characters. You can switch to the required set of characters with the **[a...z]**, **[0...9]** and **[Special characters]** buttons and between the blocks of special characters with **[More]**. The backspace button **[X]** deletes the character in front of the cursor. **[Delete entry]** deletes the whole text. With the arrow buttons the cursor can be positioned in the text.

☞ Accept your entry with **[OK]** or **[Back]**, or reject it with **[Cancel]**.

In input fields for numerical values the **number editor** will open on the Touch Screen. The required value is entered directly via the indicated keys. A stop is automatically used as the decimal separator.

- ☞ For example, in the main dialog touch the input field for the **Stop volume** in a titration command (see *Section 3.16*).



To the left of the block of numbers you can see the **input range** that applies for the parameter together with its **default value**. If not only numbers but also **special values** (e.g. **off**) can be entered for a parameter then the corresponding buttons will be shown to the right of the block of numbers. For many method parameters it is also possible to enter a result which has previously been defined in the method sequence as a value. The result variable can be selected under **[R1]** (see *Section 4.4.6*).

- ☞ Touch the required number or special value. The whole entry can be deleted with **[Delete entry]**.
- ☞ Accept your entry with **[OK]** or **[Back]**, or reject it with **[Cancel]**.

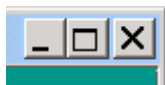
To make the entry of texts and numbers easier you can also connect an external PC keyboard with a USB connection to a Titrando system with Touch Control (see *Section 3.10.9*).

3.2 Operating principles: PC Control

3.2.1 Starting and stopping the PC Control software



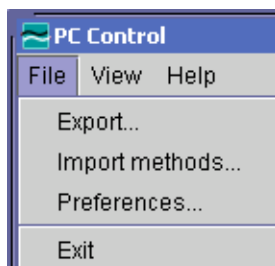
A double-click on the **PC Control icon**, which is automatically copied onto the Windows desktop during installation, starts the program. Alternatively you can start the program in the menu Start/Program Files/Metrohm/PC Control or execute the file PcControl.exe under C:\Program Files\Metrohm\PC Control\bin (installation with the default path) with a double-click. After the program start the main dialog window opens (see Section 3.3).



The program can be closed by either clicking on **[x]** (close) in the top right-hand corner of the program window or by clicking on the menu item **Exit** in the **File** menu. When the PC Control software is started the program window cannot be closed.

3.2.2 Operating the PC Control software

The **PC Control** program is operated within the main dialog window in exactly the same way as Touch Control. All the elements of this program window as well as the fixed keys can be activated or selected with a mouse-click.



PC Control also has a **menu bar** via which the specific PC Control functions can be selected.

In addition, the controls of the main dialog display can be accessed and operated via the **PC keyboard**. A cursor is provided; this can be moved from one item to the next by using the tab key. An item selected in this way is activated by the space bar. Input fields can be edited directly.

3.3 User interface and controls

3.3.1 User interface of the Touch Control and PC Control

In both cases the user interface consists of the **dialog window** itself and the **fixed keys**.

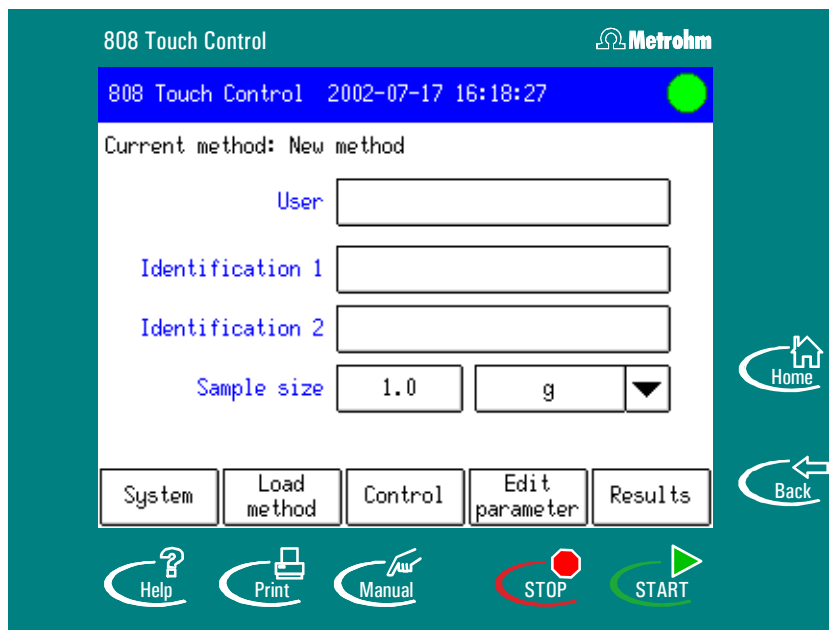


Fig. 5: Touch Control user interface

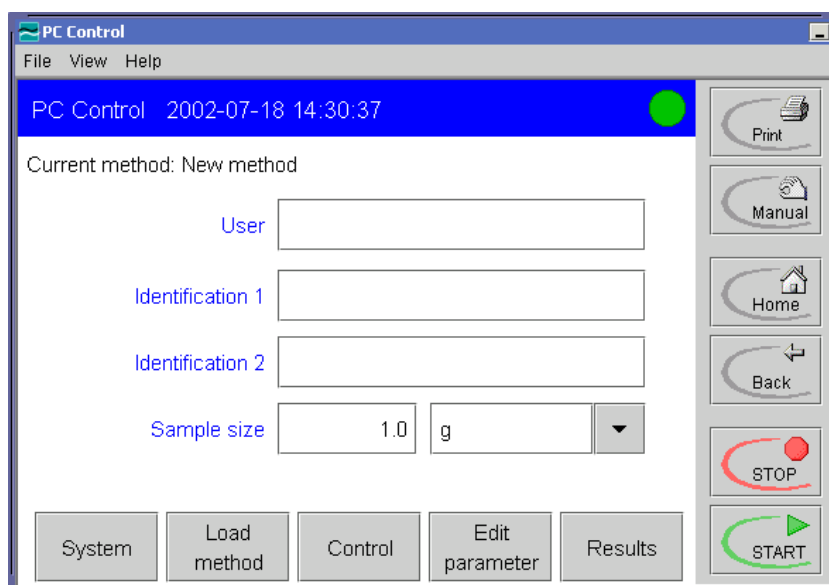

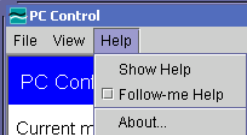














Fig. 6: PC Control user interface

The PC Control program has an additional **menu bar**.

3.3.2 Controls of the Touch Control and PC Control

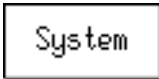
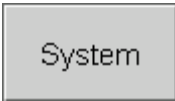
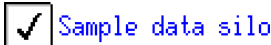



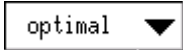
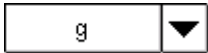


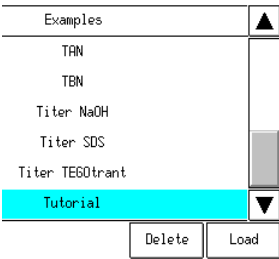
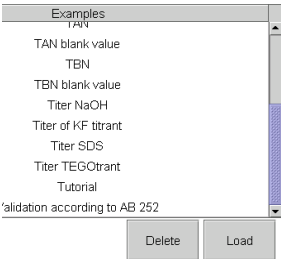
Both the Touch Control and the PC Control software systems have changing controls within the dialog window and fixed keys outside the dialog window which are accessible at all times. The following table lists the functions of all the controls:

<i>Fixed keys</i>		
<i>Touch Control</i>	<i>PC Control</i>	<i>Fixed key function</i>
		Opens the context-sensitive online help function (see Section 3.3.3).
		Opens the print dialog for the manual printout of the reports (see Section 3.23).
		Opens the dialog for the manual operation of the titration system (see Section 3.24). With the PC Control a separate dialog window is opened.
		Stops the determination sequence. The command which is currently being processed will be stopped immediately and the results page will be shown (see Section 3.20.3). The following commands (e.g. calculations, REPORT commands) will not be carried out.
		Starts the current method; this will then be processed (see Section 3.20).
		Switches to main dialog.
		Switches to previous dialog.



Note!

The settings made in a dialog window with **PC Control** will only be stored when the dialog is exited with **[Back]** or **[Home]**.

Dialog elements		
Touch Control	PC Control	Fixed key function
		Active buttons are indicated by a frame. Inactive buttons are shown in gray.
		Tip or click on a checkbox to activate it.
		Use the scroll bar in order to navigate quickly through lists or longer text displays. To move up and down in the list push the scroll bar up and down with your finger or with the left-hand mouse key pressed down.
 	 	<p>The combo box can be recognized by the arrow to the right of the text. In an open combo box the element currently selected is shown with a background bar. Select the required element in the list with the finger or mouse. This entry will then be transferred directly to the input field.</p> <p>If the input field and arrow are separated by a line then this means that you can also make your own entries. In the Touch Control you can open the text editor by touching the input field. In PC Control you can click directly on the input field and enter text. The selection list is opened with the arrow.</p>
		In the selection list the selected line is indicated by a light blue bar. You should first mark the line to be selected and then activate the button for the function you want to apply to the selected element.

3.3.3 Online help

These instructions are chiefly intended to describe the procedure for configuring the system, carrying out a determination and evaluating and storing the data. For further details about the individual parameters, e.g. input ranges, you should use the context-sensitive **online help**, which will rapidly provide you with the information you require at any point.

In **Touch Control** you can open the online help with the **[Help]** fixed key. In the **PC Control** software the online help is opened with the <F1> key on the computer keyboard or started by clicking on the menu item **Show help** in the **Help** menu. If you also activate the item **Follow-me help** in this menu then the help window will be updated each time that the dialog is changed.

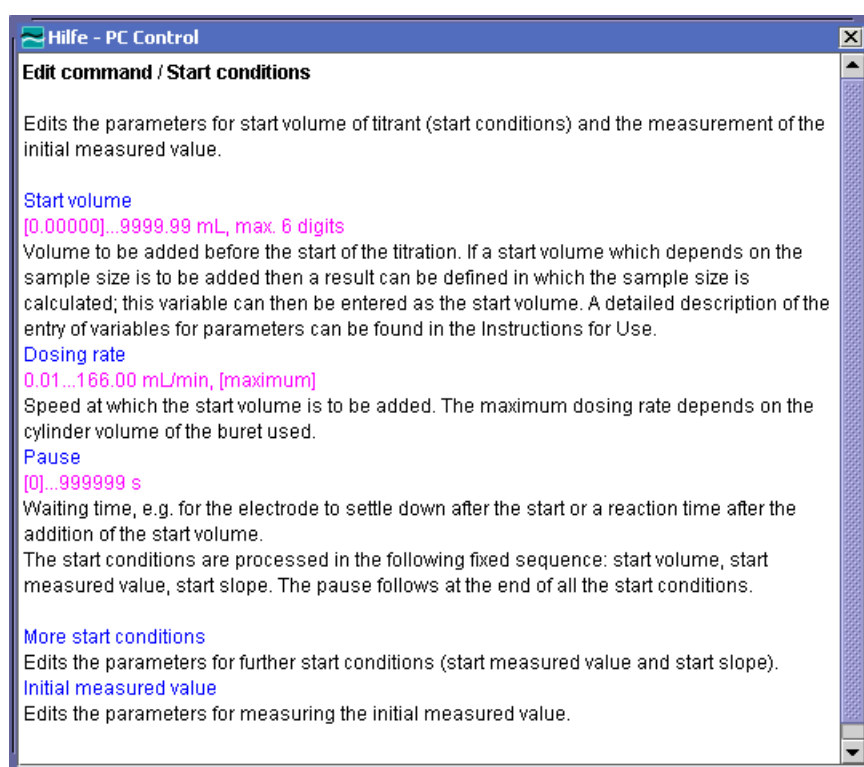
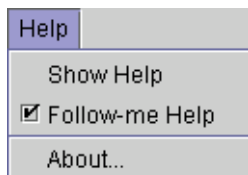


Fig. 7: Online help, PC Control

The following markings apply to the online help for Touch Control and PC Control:

Blue text	Parameters and buttons which are explained.
Violet text	Input values for the parameters.
[Value]	Default value for a parameter.

3.4 Program structure

The program structure is arranged so that the most important functions can be accessed with only a few clicks or touches on the buttons. Functions which are not often used in routine operation, such as changing the system settings or editing individual parameters in a method, can be found in lower dialog levels. In order to provide an overview of the structure of the program we have summarized the most important functions in the following diagram:

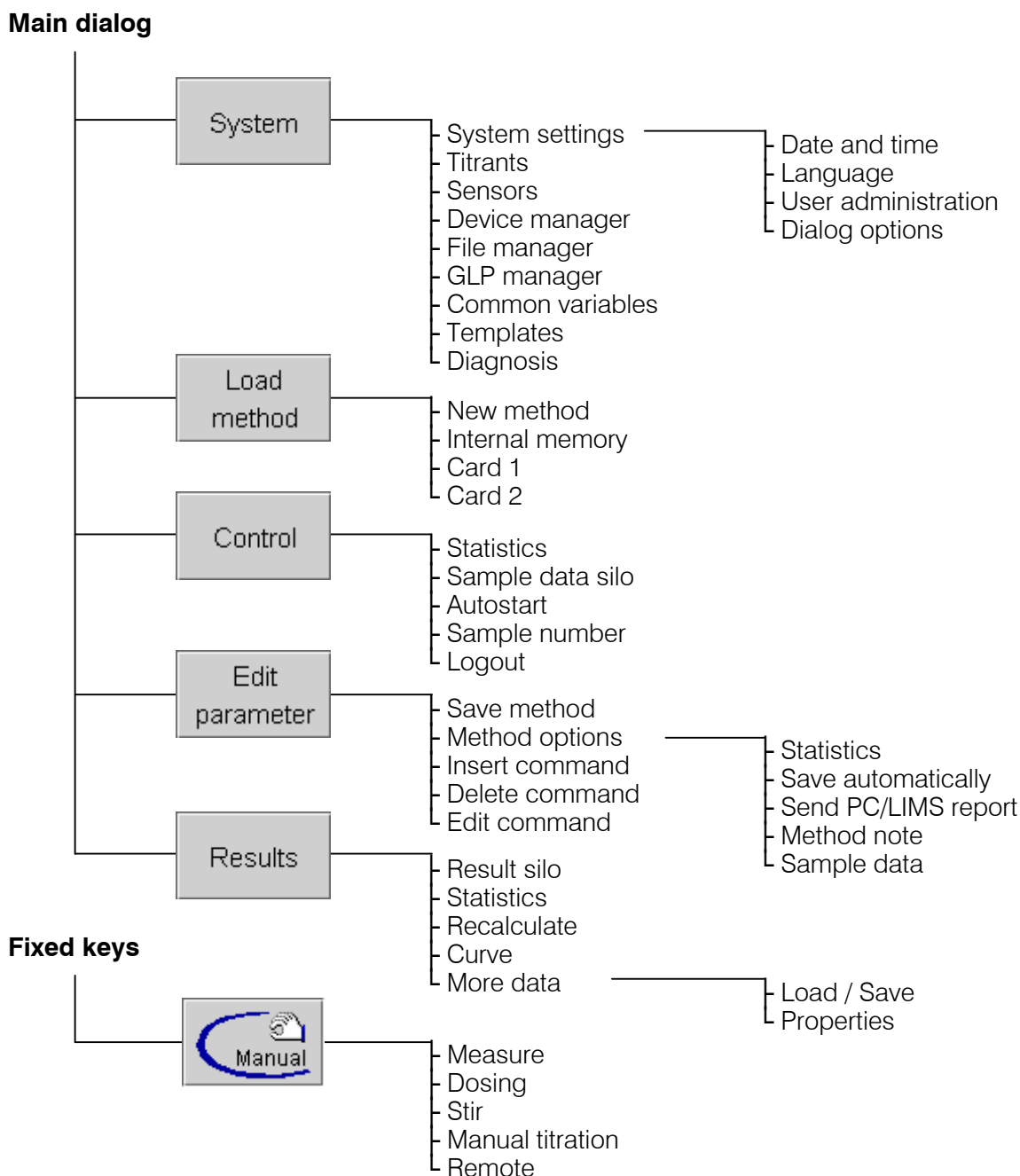
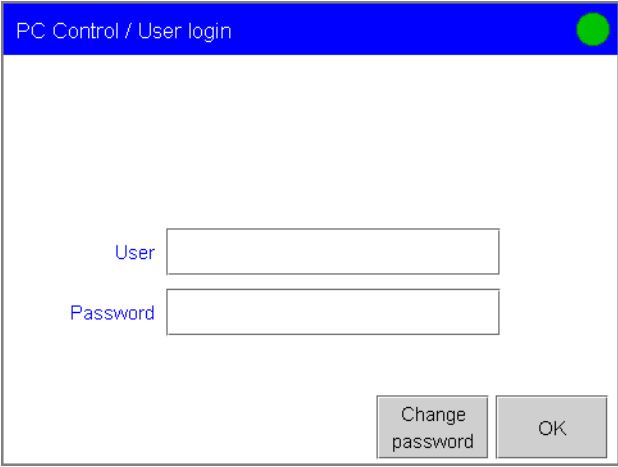


Fig. 8: Program structure

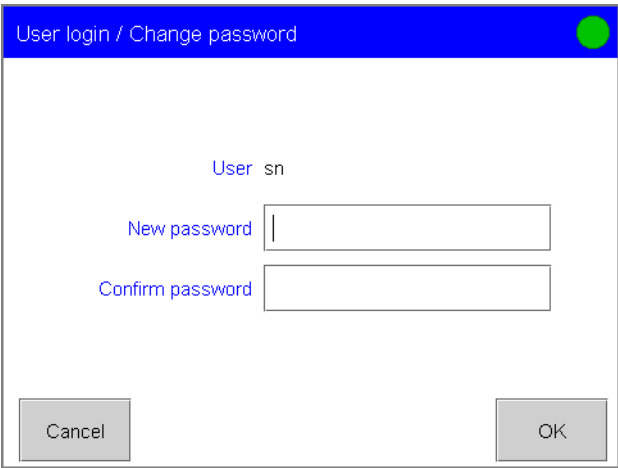
3.5 Login

Depending on how your Titrando system is configured, you may have to use the **User login** function before you can work with the system. User administration is carried out by a user with administrator rights (see *Section 3.7.5* to *Section 3.7.7*). There are two different ways of identifying the user: by the **entry of the user name** or by using an **identification card**, on which the user name and the routine dialog settings are stored. If a **password** is required for identification then this will be requested on login in both cases.

In the following example the user must identify himself/herself by entering a name and password.

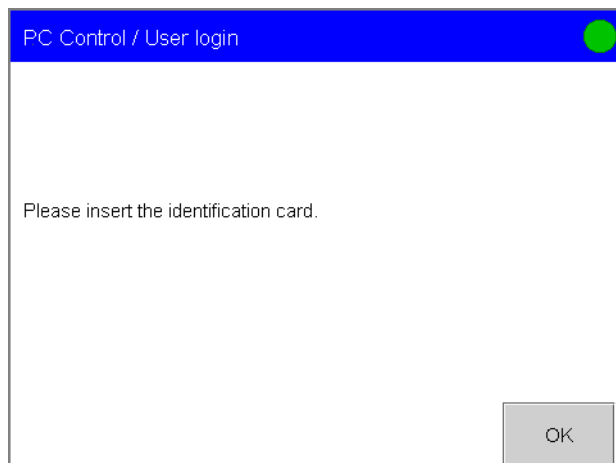


The first time that you log in you must first define your password with **[Change password]**:



- ☞ First enter the password under **New password** and enter it again under **Confirm password** for confirmation. Please note that this password can not be used multiple times.
- ☞ Enter your **password** in the login dialog. If the user is defined in the list of users and if the correct password has been entered then the main dialog will open.

If you have to identify yourself with an identification card then you will be requested to insert it.








In **Touch Control** you must always insert your identification card in Card slot 1. In **PC Control** ask your system administrator to tell you the drive to be used. If a password additionally has to be entered then the corresponding dialog will be opened automatically; otherwise the main dialog will open directly.

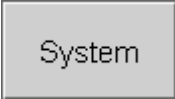
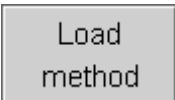

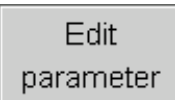
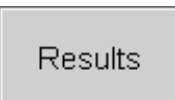
3.6 Main dialog and structure of the dialog windows

This section provides an overview of the structure of the dialog windows and the various dialog elements. The user interface without the fixed keys **[Help]**, **[Print]**, **[Manual]**, **[STOP]**, **[START]**, **[Home]** and **[Back]** is known as the **dialog window** (or just dialog):

- In the **status line** (blue bar) the titles of the previous dialog and current dialog are normally shown. Only in the main dialog the type of instrument and the actual date and time are shown in this status line. In the live display (see *Section 3.20.4*) the name of the current method is shown.
- In the right top corner the current **status** of the system is shown:

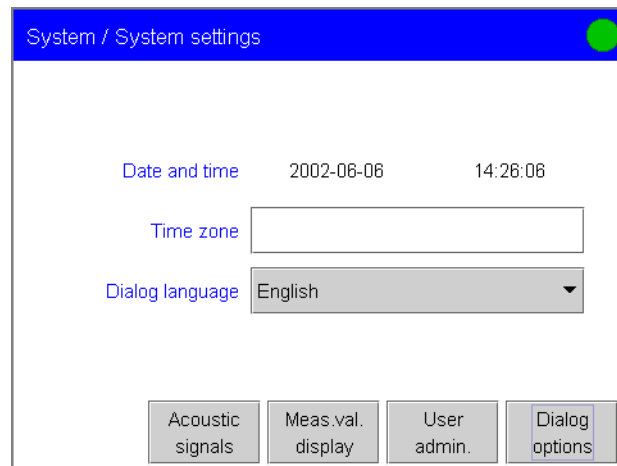
	Instrument in normal working condition (ready), i.e. a determination can be started.
	A determination sequence has been started. [START] and [Print] are not active now.
	The determination sequence has been interrupted manually with [Hold] or automatically. It can be restarted with [Continue] .
	A run has been started in the "Manual operation" dialog window.
	A fault has occurred during the manual operation of the System.

- In the **main dialog** you can enter or select the **user** if you are not working with login (see *Section 3.7.5* and *Section 3.5*). You can also edit the **sample data** (see *Section 3.19.1*).
- The buttons at the lower margin of the dialog change their function according to the dialog shown. They are usually used to open a new dialog. You can open the following dialogs from the **main dialog**:

	Instrument-specific system settings, titrant and sensor management, management and configuration of peripheral devices, file management, GLP functions, edits system-specific variables, creates various templates, diagnostic functions and software updates.
	Loads a method from the method memory and creates a new method.
	Switches statistics on/off, switches sample data silo on/off, deletes sample data silo (Touch Control only), autostart, sample number, system logout and deletes statistics.
	Edits method command list and the parameters of the current method.
	Shows the results of the current determination, recalculation and re-evaluation of the current determination, views, saves and loads determination data, views statistics results and results silo.

3.7 System settings

A range of system-specific settings and configurations is described in this section. You should first select the dialog language and set the date and time. You can also configure the dialog for routine use and create a list of users. You can make various settings concerning the measured value display and output of acoustic signals.



3.7.1 Selecting the dialog language

- ☞ Open the dialog **System/System settings**.
- ☞ Open the combo box **Dialog language** with the arrow and select the language.
- ☞ Exit the dialog with **[Home]** so that the setting applies to all dialogs. (From this particular dialog you can also return to the main dialog with **[Back]**.)

With **PC Control** you should end the program and then restart it after the dialog language has been changed.

3.7.2 Setting the date, time and time zone

PC Control and **Touch Control** show date and time according to ISO standard 8601.

- ☞ Open the dialog **System/System settings**.

With **PC Control** the date and time will be taken directly from the operating system of your computer. The change from Summer to Winter time and vice versa is made automatically.



Note!

In order for the **Summer /Winter time** to be taken into account in the **Windows** time display you must activate the checkbox **Automatically adjust clock for daylight saving changes** under System settings in the menu Date/Time Properties under Time zone.

With **Touch Control** you should set the date and time as follows:

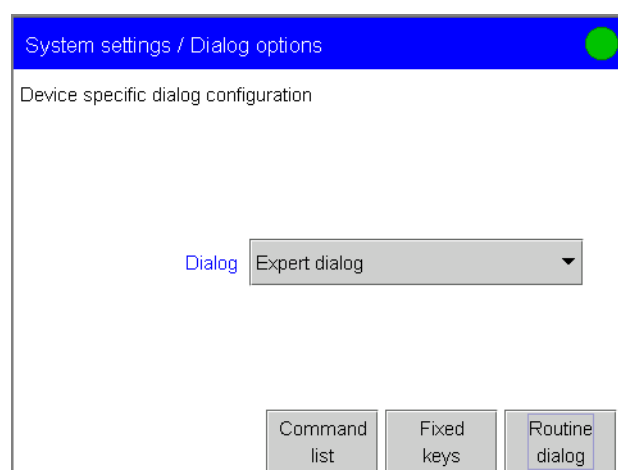
- ☞ Open the date editor by touching the input field for the **date**.
- ☞ Enter the actual date in the format year (4-place)-month-day. The hyphens are already present. Confirm the entry with **[OK]**.
- ☞ Open the editor for the **time** by touching the input field for the time.
- ☞ Enter the actual time in the format hours:minutes:seconds. The entry should be made in the 24-hour format. The colons already exist. Confirm the entry with **[OK]**.

By entering a **time zone** the time information becomes unambiguous. You can enter the time zone for both PC Control and Touch Control. It is printed out in the report header together with the date and time.

- ☞ In the **time zone** input field you should enter the time zone based on UTC (Universal Time) or an unambiguous city name (e.g. -05:00 or New York).

3.7.3 System-specific dialog options

The functions which a user can access can be configured specifically for the system. You can define which method commands and fixed keys can be used, and whether the system is to be operated in expert dialog (all functions accessible) or in routine dialog (individual functions disabled). The buttons to be disabled in routine dialog can also be system-specifically defined. If an identification card is to be provided for each user (see *Section 3.7.6*) then the routine dialog settings can also be stored user-specifically on the card.



If you are not working with login then you can system-specifically choose whether the system is to be operated in **expert dialog** or **routine dialog**. In expert dialog all functions are accessible. In routine dialog you can disable individual functions under **Dialog options /Routine dialog**.

- ☞ Select either **Routine dialog** or **Expert dialog** under **Dialog** in **System settings/Dialog options**.
- ☞ Exit the dialog with **[Home]** so that the setting applies to all dialogs.



Note!

If you have selected **routine dialog** and the dialog **System settings/Dialog options** is disabled for routine dialog then you can change back to expert dialog by entering **Metrohm** as the user in the main dialog. If you are using login then a user who works with expert dialog must log in.

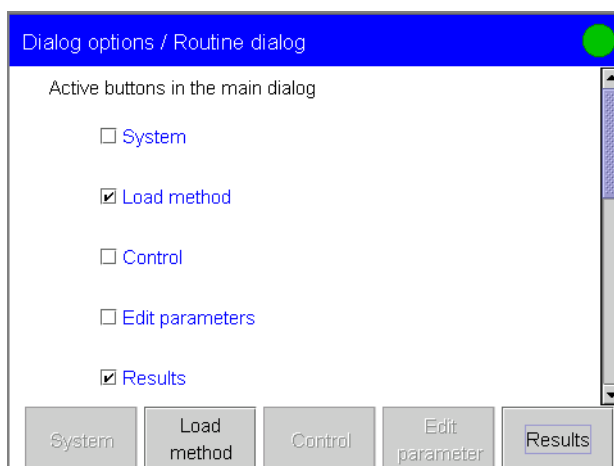
The selection of **method commands** (list of commands) and the **fixed keys** ([Print] and [Manual] only) which can be used can only be opened when the system is being operated in expert dialog.

- ☞ Open the **Dialog options/Command list** dialog.
- ☞ Disable the checkboxes for the command groups which are not to be used. These will then be shown in gray in the method editor for the selection of the commands. These settings apply to both expert dialog and routine dialog.
- ☞ Open the **Dialog options/Fixed keys** dialog. Only the [Print] and [Manual] (manual operating of the titration system) fixed keys can be disabled.
- ☞ Disable the checkboxes for the fixed keys which are not to be used. These settings apply to both expert dialog and routine dialog.

3.7.4 Routine dialog: disabling functions

A standard configuration which is suitable for routine dialog is stored: methods can be loaded but not altered or newly created. Determination data (results) can be viewed and saved, but not modified. You can adapt this standard configuration as follows:

- ☞ Open **Dialog options/Routine dialog** in order to deactivate those buttons which are to be disabled in the main dialog and live display. With PC Control you can also disable individual menus. This dialog can only be opened when the system is being used in expert dialog.



- ☞ Deactivate the checkboxes for the functions which are to be disabled in routine dialog.

You can disable individual functions in the corresponding dialogs with the buttons at the lower margin of the dialog window (**[System]**, **[Load method]**, **[Control]**, **[Edit parameter]** and **[Results]**). In order for the button to be active the corresponding checkbox must be activated above.

- ☞ Open the dialog in which you wish to **disable buttons** and deactivate the checkboxes for the buttons that are to be disabled for routine dialog.

You can also disable buttons in several subdialogs. These are indented so that you can see which buttons belong to which dialog.

3.7.5 User administration

You can draw up a system-specific **list of users** who can operate the titration system. You can use this list in two different ways: if you work with **login**, i.e. if each user must log into the system before starting work, then only those users entered in the list can log in. The user who is currently logged in is shown in the main dialog and cannot be edited. If you work without login then in the main dialog you can select the user from those entered in the list and document the user of the titration system in this way. The user name is printed out in all reports containing determination data and stored in the determination file. Each file always contains the name of the user who created it and the name of the last user to edit it.

The name of the user, the dialog that the user can use to operate the system and the status of the user are shown in the **user list**. If you work with login then this dialog is only accessible to users with administrator rights.

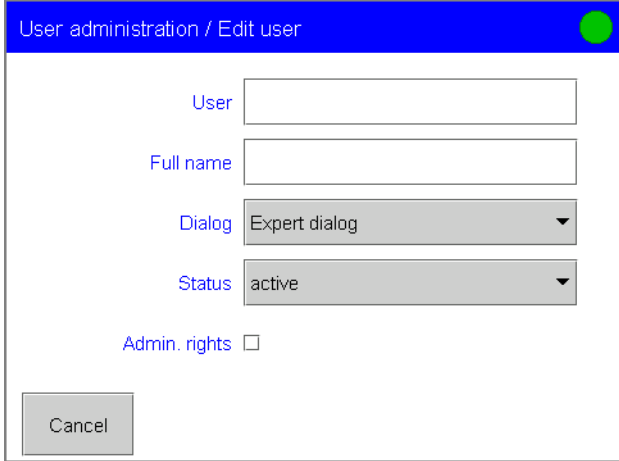
- ☞ Open the dialog **System settings/User administration**.

System settings / User administration		
User	Dialog	Status
Administrator	Expert dialog	active
em	Expert dialog	active
km	Routine dialog	active
ps	Routine dialog	active
sn	Expert dialog	active
wz	Routine dialog	active
<div> <div>Login options</div> <div>Create ID card</div> <div>New</div> <div>Delete</div> <div>Edit</div> </div>		

The user list is initially empty.

- ☞ Use **[New]** to define all the users who are allowed to operate the system.

The dialog in which the **user data** can be entered is opened automatically with **[New]**. For an existing user this dialog can be opened with **[Edit]**. Existing users can be removed from the list with **[Delete]**. If you work with login and password protection then it is no longer possible to delete users. The list of users can only be printed out in a context-sensitive situation from the dialog **System settings/User administration** and its subdialogs by using the **[Print]** fixed key. This means that only users with administrator rights can print out this list.



- ☞ Enter an unambiguous identification under **User**, for example the in-house abbreviated form of the name or the personnel number. Each user name can only appear once in the list of users.
- ☞ Under **Full name** enter the proper name of the user, i.e. given name and family name.
- ☞ Select the **Dialog** in which the user is to operate the system.

This setting is only effective when login is used. In **Expert dialog** all functions are accessible. For **Routine dialog** the system-specific routine dialog configuration is normally used (see *Section 3.7.3*). If each user is to have separately defined routine dialog settings then you can produce an identification card for each user on which these settings are stored (see *Section 3.7.6*). During login the dialog settings stored on the card will be loaded automatically.

The **user status** normally remains **active**. It is a good idea to deactivate a user when, for example, he or she is absent for a long time or is no longer authorized to use the system. This user can then no longer log into the system until the **active** status is reactivated.

- ☞ You should activate the **Administrator rights** checkbox for each user who is to have access to the user administration.

**Attention!**

If you work with **Login** then **User administration** is only accessible to users with administrator rights. This means that you must ensure that at least two users have administrator rights so that one of them is almost always available. Keep the rights of access for a user with administrator rights in a safe place so that it is accessible in an emergency. The last user to have administrator rights cannot be deleted.

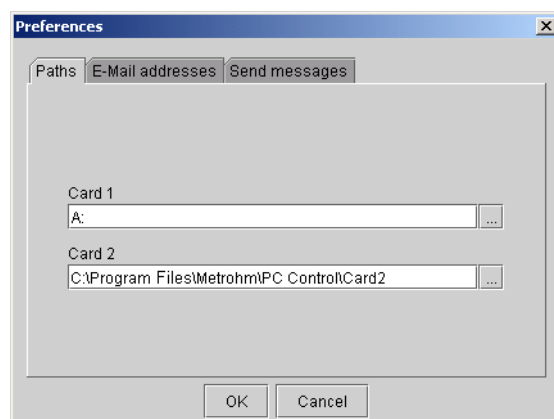
3.7.6 Producing an identification card

If you have selected the version **Login via identification card** under **User administration/Login options** (see Section 3.7.7) then you must provide each user with an identification card. The identification card has the **User name** and the current **routine dialog settings** stored on it (see Section 3.7.4).

During login with an identification card a check is made that the user is present in the list of users and whether expert dialog or routine dialog is to be used. After a successful login the routine dialog settings stored on the card are loaded into the system. These define the buttons and functions that are accessible to the user if routine dialog is used.

If you wish to provide separate routine dialog settings for each user then, before you produce the identification card for the particular user, you must always adapt the routine dialog settings for the user under Dialog options/Routine dialog (see Section 3.7.4). These **user-specific routine dialog settings** are stored on the identification card with the name of the user.

With **Touch Control** the identification card is always produced in **Card slot 1**. Insert the data card into Card slot 1 (13, see Fig. 3: Rear view of the Touch Control). With **PC Control** you must define the drive in which the identification card is to be used under **Paths** for **Card 1** in the menu **File/Preferences** (see Section 3.11).



Select the diskette drive if you want to use diskettes as identification cards. You can also use a card drive with PCMCIA FlashCards or CompactFlash cards, or USB FlashCards. With external drives you must always check how to recognize when a storage process has been com-

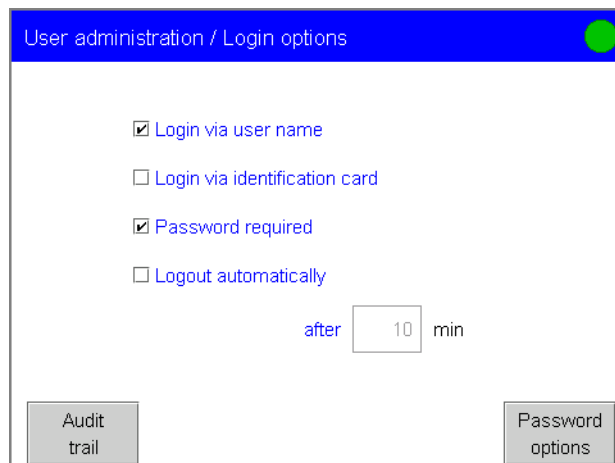
pleted in the instruction manual for the drive. This is usually indicated by an LED. If you use the PCMCIA card drive of a laptop computer then you should always trigger "Remove hardware" in the operating system before removing a card from the drive. This is the only way that you can be sure that the data has been stored when you remove the card.

- ✎ Insert a card in the drive and produce an **identification card** for each user by selecting the user from the list of users and start the transfer of data to the card with **[Create ID card]**.

3.7.7 Editing login options

There are various ways of logging in to the system: either the user name is requested or identification is carried out by using an identification card (see Section 3.7.6). It is also possible to combine both versions.

- ✎ Open the dialog **User administration/Login options**.



- ✎ Activate the checkbox(es) for the **login option(s)** that you wish to use.



Attention!

*If you select **Login via identification card** then you must produce an identification card for each user (see Section 3.7.6).*

Once you have selected a login option you can then make further settings for logging in:

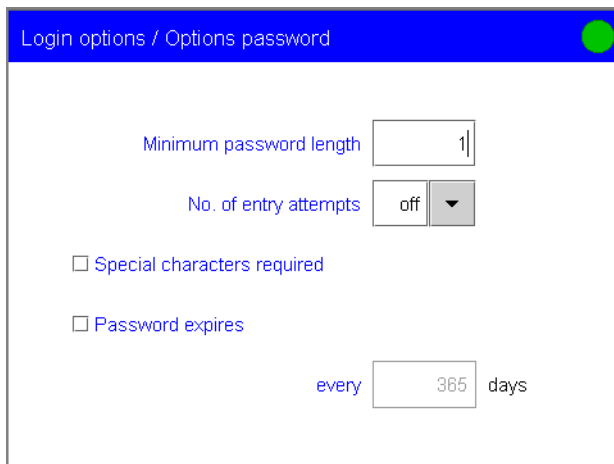
- ✎ If a password is to be requested as well as the user name then you must activate the **Password required** checkbox. If this function is switched on then it is no longer possible to delete users from the list of users; they can only be deactivated. This is a requirement for complying with **FDA Guideline 21 CFR Part 11**. The various settings for entering a password are carried out under **Password options** (see p. 34).
- ✎ Activate the **Logout automatically** checkbox if the user is to be logged out of the system automatically after a certain time has

elapsed. Enter the interval after which the logout is to take place automatically.



Note!

When you exit this dialog (**User administration/Login options**) with **[Back]** or **[Home]** after you have activated one of the login options **Login via user name** or **Login via identification card** then you will automatically find yourself in the login dialog and will have to log into the system. This means that you must make sure that you have first defined all the users and produced the identification cards before you activate login.

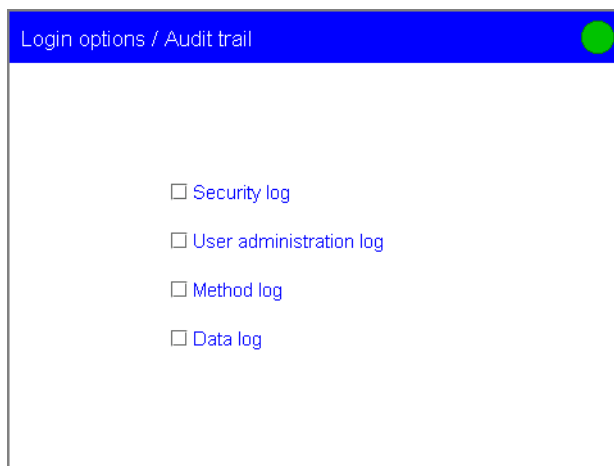


☞ You should now edit the password options. You can define a **minimum length** for the passwords to be used. This will be checked when a user enters a new password. After the maximum **Number of entry attempts** during login the user will be automatically deactivated and can only be reactivated by a user with administrator rights. The use of certain **Special characters** in the password can be demanded (see **online help**). You can also define a time limit after which the password must be altered. Changing a password, it is not possible to choose one which was already used before.

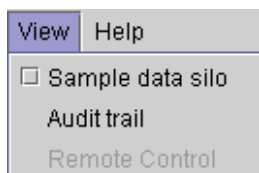
In the **Titrand Compliance Guide** there is a step by step description of the necessary procedure for complying with **FDA Guideline 21 CFR Part 11**.

3.7.8 Audit trail (PC Control only)

In the **Audit trail** all user actions are recorded together with the user name, date and time. Recording an audit trail is important for using PC programs to meet the requirements of **FDA Guideline 21 CFR Part 11**.



☞ Under **System/System settings/User administration** in the dialog **Login options/Audit trail** activate the checkboxes for the data to be protocolled in the audit trail. The actions which should be protocolled can be found in the **online help**. In order to meet the requirements of **FDA Guideline 21 CFR Part 11** for an audit trail you must activate all the options.



You can also use the audit trail function specifically to record the data which interest you.

To view the recorded data you should open the menu item **Audit trail** in the **View** menu.
















































Audit trail						
File Filter						
No		Date	User	Category	Action	Details
1		2002-07-12 16:44:30	sn	Admin	Change audit t. opt.	Security log off --> on
2		2002-07-12 16:44:30	sn	Admin	Change audit t. opt.	User administration log off --> on
3		2002-07-12 16:44:30	sn	Admin	Change audit t. opt.	Method log off --> on
4		2002-07-12 16:44:30	sn	Admin	Change audit t. opt.	Data log off --> on
5		2002-07-12 16:44:45	sn	Admin	Change login options	Login via user name off --> on
6		2002-07-12 16:44:45	sn	Security	Logout	
7		2002-07-12 16:44:47	sn	Security	Login	
8		2002-07-12 16:45:09	sn	Admin	New user	ps Peter Schneider Expert dialog Status active Admin. rights on
9		2002-07-12 16:45:26	sn	Security	Logout	
10		2002-07-12 16:45:27	sn	Security	Login	
11		2002-07-12 16:45:48	sn	Data	Edit titrant	NaOH Titer 1.015 --> 1.001
12		2002-07-12 16:46:50	sn	Data	Edit sensor	Unitrode with Pt1000 Slope 100.0 --> 99.6
13		2002-07-12 16:47:32	sn	Method	Delete	Messen Konzentration.mmth Card 1
14		2002-07-12 16:48:11	sn	Data	Edit common variable	CV01: Density --> 2.785
15		2002-07-12 16:49:15	sn	Method	New	Dynamic Titration pH V2
16		2002-07-12 16:49:44	sn	Method	Edit	New method V0 03 REPORT Raw data off
17		2002-07-12 16:49:54	sn	Method	Edit	New method V0 03 REPORT Line between sections on
18		2002-07-12 16:51:19	sn	Method	Edit	New method V0 04 REPORT Mode 2
19		2002-07-12 16:51:19	sn	Method	Insert command	New method V0 01 REQUEST
20		2002-07-12 16:51:49	sn	Method	Edit	New method V0 04 REPORT Determination properties on
21		2002-07-12 16:52:51	sn	Method	Save	Determination of NaOH V1 Internal memory
22		2002-07-12 16:52:55	sn	Security	Logout	
23		2002-07-12 16:53:00	ps	Security	Login	
24		2002-07-12 16:53:15	ps	Method	New	Empty method
25		2002-07-12 16:53:24	ps	Method	Insert command	New method V0 01 WAIT
26		2002-07-12 16:53:36	ps	Method	Start	New method V0
27		2002-07-12 16:54:08	ps	Method	Stop	New method V0
28		2002-07-12 16:54:26	ps	Method	Start	New method V0
29		2002-07-12 16:54:40	ps	Method	Skip command	New method V0 WAIT
30		2002-07-12 16:54:40	ps	Method	Stop	New method V0
31		2002-07-12 16:54:42	ps	Method	Start	New method V0
32		2002-07-12 16:54:52	ps	Method	Manual stop	New method V0
33		2002-07-12 16:55:15	ps	Method	Delete command	New method V0 01 WAIT
34		2002-07-12 16:55:18	ps	Method	Insert command	New method V0 01 CALC
35		2002-07-12 16:55:41	ps	Method	Edit	New method V0 01 CALC Calc. formula C00
36		2002-07-12 16:55:41	ps	Method	Edit	New method V0 01 CALC Result name R1
37		2002-07-12 16:55:59	ps	Data	Edit sample data	Sample size 1.0 --> 1.2
38		2002-07-12 16:56:22	ps	Method	Edit	New method V0 01 CALC Result unit g
39		2002-07-12 16:56:22	ps	Method	Edit	New method V0 01 CALC Result name Probeneinmass
40		2002-07-12 16:56:24	ps	Method	Start	New method V0
41		2002-07-12 16:56:26	ps	Method	Stop	New method V0
42		2002-07-12 16:56:48	ps	Data	Edit sample data	Sample size 1.2 --> 1.15
43		2002-07-12 16:56:49	ps	Data	Recalculate	Probeneinmass 1.2 g --> Probeneinmass 1.15 g




Fig. 9: Audit Trail

The first column shows the **number of the entry**. The second column shows a **symbol** which classifies the entry:  for information about actions which are neither security-relevant nor alter the determination data;  for actions such as logging in and out of the system, changes to the login options and alterations to the determination data such as recalculations;  for errors which may occur such as entering an incorrect password during login. The third column shows the **date**; the fourth column gives the **user** who carried out the action. The fifth column shows the **category** to which the entry belongs. The categories for which actions should be entered in the audit trail can be defined under **Login options/Audit trail** (see p. 35). The sixth and seventh columns show the **action** and **details** of the action. For alterations to a method the method name and version (e.g. V1) are always shown un-

der details. V0 is shown for new methods which have not yet been saved. Behind this the number and name of the command are shown. The old value and new value, separated by an arrow, are always shown for alterations to variables or parameters.

Only users with administrator rights can export the audit trail as a text file. This means that the audit trail can be archived and made available for inspection whenever necessary. This is done by opening the menu item **Export** in the **File** menu and entering the path and file name with the extension **.txt**. When the audit trail is exported its contents will be deleted. The audit trail window is closed with **Close**.

To **print** the audit trail click on the symbol  in the symbol bar.

Quick filters can be used on the audit trail entries. Click on a cell in the table which meets the filter criterion. In the **Filter** menu click on **Quick filter** or on  in the symbol bar. You can use the quick filter in succession for various entries. To show all the entries again click on **Show all** in the **Filter** menu or on  in the symbol bar. You can update the list with  so that new entries are also shown. The audit trail window is not automatically updated "live". When the audit trail window is opened the table is updated automatically.

In the **Titrand Compliance Guide** there is a step by step description of the necessary procedure for complying with **FDA Guideline 21 CFR Part 11**.

3.7.9 Measured value display

This setting refers only to the display of the measured values in the determination sequence (live display) and in manual operation (Manual Control). The values are always stored with their full resolution.

- ☞ Open the dialog **System settings/Measured value display**.
- ☞ Select **Number of decimal places** with which pH values and potentials are to be shown in the measured value display.

3.7.10 Acoustic signals

- ☞ Open the dialog **System settings/Acoustic signals**.
 - **Show a message**: each time that a message appears on the screen a short beep will be heard. This informs the user that the message must be confirmed. This function is switched off by deactivating the checkbox.
 - **Button contact** (Touch Control only): each time that a button is touched on the Touch Screen this will be confirmed by a beep. If you touch an inactive area of the Touch Screen then no beep will be heard.
- ☞ Exit the dialog with **[Home]** in order to accept the settings.

If you touch or click on a fixed key which should not be used at the moment (e.g. **[START]** when a determination is running) a beep will be heard to indicate an error.

3.8 Titrants

This section describes how you can draw up a list of titrants used in the system. These titrants can be used in intelligent type dosing units or intelligent type exchange units or in so-called non-intelligent exchange and dosing units. **Intelligent exchange and dosing units** have a built-in datachip on which **data about the reagent and the unit** can be stored. When the exchange or dosing unit is attached to the Titrand, this data is read off automatically by the Titrand and entered in the **list of titrants**. You can also store the titrant data for reagents which are used in non-intelligent exchange or dosing units in the list of titrants.

The following **reagent data** is stored in the list of titrants:

- Titrant name
- Concentration with unit
- Comment
- Titer with unit
- Statistical information about last titer determination
- Period of validity for titer (with date for next titer determination)
- History of the last 10 titers
- Working life (with preparation date and expiry date)

The following **exchange or dosing unit data** is also stored:

- Designation (name)
- Ordering number (read in automatically for intelligent exchange or dosing units)
- Serial number (read in automatically for intelligent exchange or dosing units)
- Cylinder volume (read in automatically for intelligent exchange or dosing units)
- Serial number of the cylinder (read in automatically for intelligent exchange or dosing units; however, must be re-entered if the cylinder is changed)
- Length and diameter of the tubing and port occupancy of the dosing unit
- Parameters for preparing the exchange or dosing unit
- Time interval for carrying out a GLP test at regular intervals

Each titrant is identified in the system by an unambiguous titrant name.

☞ Open the dialog **System/Titrants**.

System / Titrants			
Titrant	Cyl.	Type	Dos.device
AgNO3	5 mL	EU	
EDTA	10 mL	DU	
HCl	20 mL	IEU	D1
NaOH	10 mL	IDU	
<div> <div>New</div> <div>Delete</div> <div>Edit</div> </div>			

In the **list of titrants** the **name**, **cylinder volume** and **type**, i.e. exchange unit (**EU**) or dosing unit (**DU**) are given for every configured titrant. Intelligent exchange or dosing units are indicated by **IEU** and **IDU** and the data is shown in green (magenta if the line has been selected). With intelligent exchange or dosing units the **dosing device connection** is shown (together with the name of the Titrandos if several Titrandos are connected) when the unit is attached.

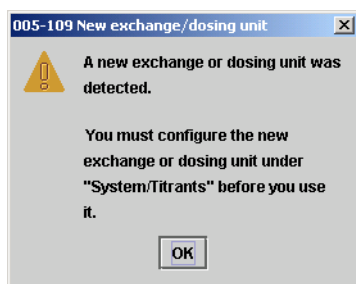
If data is read off from the datachip of an intelligent exchange or dosing unit then a check is made whether the titrant list already contains a titrant in the same type of exchange or dosing unit with the same serial number. If this is the case then the older data record will always be overwritten by the new data record, no matter whether the data record in the titrant list of the system or on the datachip is the most recent one.

You can configure a new titrant with **[New]** (see *Section 3.8.1* and *Section 3.8.2*). With **[Delete]** titrants can be removed from the list. You can also delete titrant data for intelligent exchange or dosing units (even when these have just been attached). These will be entered in the list again the next time that the corresponding unit is attached and the data read in. **[Edit]** opens the dialog for entering titrant data.

3.8.1 Configuring a titrant in a new intelligent exchange or dosing unit

- ☞ Attach the **new exchange unit** to the Titrando or Dosimat or attach the **new dosing unit** to the Dosino (see Installation Instructions for 808 Titrando and 809 Titrando and Instructions for Use for the Dosino).

When the exchange or dosing unit has been recognized the following message will appear:



If you are working with the default settings for the dosing connections (see Section 3.8.6) then you will also be requested to carry out the "Prep" function in order to rinse all the tubing (see Section 3.24.2).

- ☞ Open the dialog **System/Titrants**.
- ☞ Open the **dosing device selection list**, in which new exchange or dosing units are recognized, with **[New]**. Only one dosing device will normally be shown, unless you have attached several new exchange or dosing units.
- ☞ Confirm the selection with **[Select]**.

The dialog in which you can enter the **titrant data** opens automatically.

- ☞ Enter the titrant data as described in Section 3.8.3.

3.8.2 Configuring a titrant in a new non-intelligent exchange or dosing unit

A non-intelligent exchange or dosing unit does not need to be attached for the titrant data to be entered.

- ☞ Open the dialog **System/Titrants**.
- ☞ Use **[New]** to open the **dosing device type selection**. Select the exchange unit (for Titrando or Dosimat) or dosing unit (for Dosino).

The dialog in which you can enter the **titrant data** opens automatically.

- ☞ Enter the titrant data as described in Section 3.8.3.

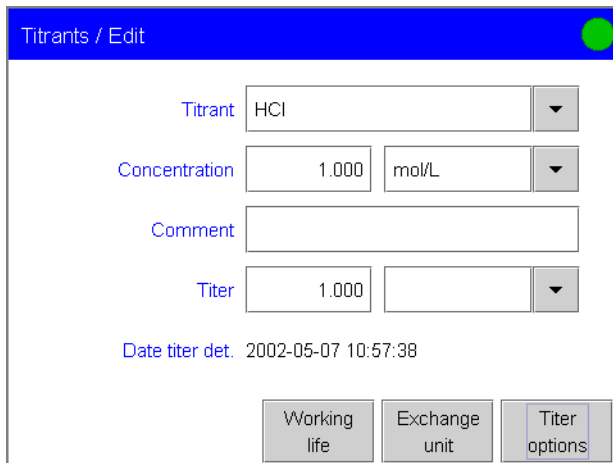
3.8.3 Editing titrant data

- ☞ Open the dialog **Titrants/Edit** by either configuring a new titrant (see Section 3.8.1 and Section 3.8.2) or selecting an existing titrant from the list and modifying it with **[Edit]**.



Note!

*If you are using an intelligent exchange or dosing unit and have selected a titrant for a titration or dosing command in the method, then at the **START** of the determination sequence a check will be made whether you are using the **correct titrant**.*



- ☞ Enter an unambiguous titrant name under **Titrant** or select a name from the selection list.
- ☞ Enter the **Concentration** of the titrant and its units.

The titrant concentration can be calculated as the variable **CONC** in the result calculations (see Section 4.4.3). This is done by selecting a titrant in the titration command for the method (see Section 4.1). In a following calculation command you can calculate the concentration of this titrant.

- ☞ You can add a **Comment** to each titrant.

Normally the **Titer** is automatically determined and assigned. To do this you must draw up a method for the titer determination (see Section 3.15.2 and Section 3.16) and select a titrant in the titration command (see Section 4.1). In a following calculation command you can assign the variable **TITER** to this titrant (see Section 4.4.1). Alternatively you can enter the value for the titer manually. If you alter the titer or the concentration of a titrant in a loaded determination at a later date and would then like to recalculate the determination with the corrected value then you must alter the value in the determination data under **View data/Titrant data** (see Section 3.18.1).

- ☞ You can also enter a **unit** for the titer. This unit is not taken into account in the calculations.

The **date** and time of the **titer determination** are entered automatically on assignment or entry of the titer. If a new titrant is entered then the entry date will be given as the date of the titer determination.

3.8.4 Titer determination options and data

Detailed information about the titer determination is shown under **Titrants/Edit/Titer options**. Under **Titer method** the method with which the titer was determined is shown. If the titer has been entered manually then **manual** will be shown. The user who was logged in when the titer was assigned or entered manually is shown under **User**.

For automatically assigned titers the number of titer determinations is shown together with the absolute and relative standard deviation if the mean value of the determinations has been saved as the titer (see Section 4.4.1).

Edit titrant / Titer options

Titrant: HCl

Titer method Titer HCl

User sn

Statistics titer determination

n (titer det.) 5

s +/- 0.00080

s rel 0.08 %

Validity History

You can monitor the **time interval** after which the titrants titer must be redetermined.

☞ Open the dialog **Titer options/Validity** and activate the checkbox for **Monitoring**.

Titer options / Validity

Titrant: HCl

Date titer determ. 2002-05-16

☒ Monitoring

Validity of titer 999 days

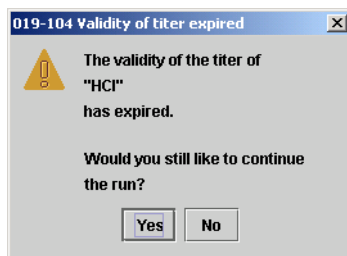
Next titer determ. 2005-02-08

Action Display message ▼

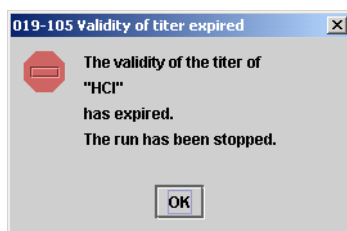
- ☞ Enter either the **time interval for the validity of the titer** or the **date for the next titer determination**. When either the time interval or the date is edited the other value will be updated automatically.
- ☞ Select an **Action** to be carried out when the time interval has expired. If the titrant is used in the current method then the time interval will be checked at each START of a determination.

When the monitoring interval has expired one of the following **actions** can be selected and carried out:

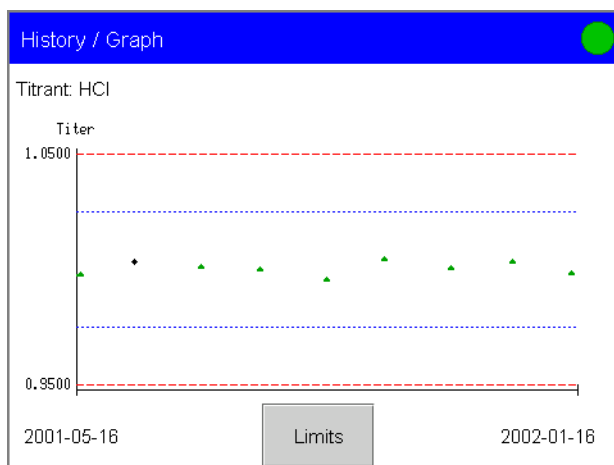
- **Display message:** a message is shown. You can choose whether you want to continue with the determination or cancel the run. If you carry out the run then the fact that the monitoring interval had expired when the determination was carried out will be documented in the determination data. The message can be viewed under **Results/More determination data/Messages** (see Section 3.18.2).



- **Document message:** the fact that the monitoring interval had expired when the determination was carried out will be documented in the determination data. The message can be viewed under **Results/More determination data/Messages** (see Section 3.18.2).
- **Cancel determination:** the determination sequence will stopped and the following message shown:



Under **Titer options/History** the date, time and values of the last ten titer determinations are shown in a table. Titrants which have been determined automatically are shown in green, manually entered titer values are shown in black and marked with **(m)**. With **[Graph]** you can open a graph in which the titer values are plotted against the date of the titer determination. With **[Delete history]** you can delete the complete history if, for example, the reagent is changed or a new bottle is opened. If multiple determinations (Statistics) have been carried out in order to calculate the titer then only one entry will be made in the history.



This graph corresponds to a control chart on which both **warning limits** and **intervention limits** are shown for the titer determinations. The values for these warning limits and intervention limits can be entered under **Graph/Limits**. No automatic action is taken when these limits are infringed.

3.8.5 Exchange unit and dosing unit

Under **Edit titrant/Exchange unit** and **Edit titrant/Dosing unit** you can enter data concerning the unit used with the reagent.

Edit titrant / Exchange unit

Titrant: HCl

Name

Order number 8.3026.220

Serial number 11180070

Cylinder volume 20 mL

Serial no. cyl. 277

GLP test

PREP param.

Tubing param.

The data which can be entered here varies according to whether or not an intelligent exchange or dosing unit is used.

- ☞ You can enter a **Name** for the buret.
- ☞ With intelligent exchange or dosing units the **Order number** and **Serial number** are read in automatically. The data can be entered manually for non-intelligent units.
- ☞ With intelligent exchange or dosing units the **Cylinder volume** is read in automatically. The data can be selected for non-intelligent units. If you have selected a titrant for a titration or dosing command in the method then the **cylinder volume** will be checked during the run. This also checks whether the correct buret is being used.

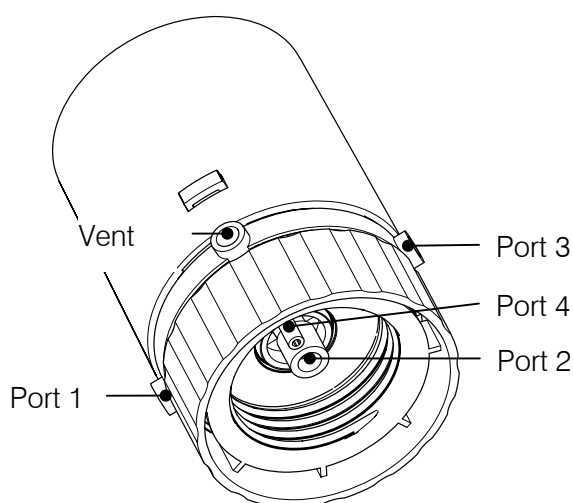
**Note!**

If you are using an intelligent exchange or dosing unit and have selected a titrant for a titration or dosing command in the method then during the run a check will be made that you are using the **correct titrant**.

☞ With intelligent exchange or dosing units the **serial number of the cylinder** is read in automatically. It can also be entered manually, e.g. after the cylinder has been exchanged. The serial number can be entered manually for non-intelligent units. With new cylinders it is printed on the cylinder.

3.8.6 Tubing parameters and parameters for the preparation procedure

Under **Exchange unit/Tubing parameters** or **Dosing unit/Tubing parameters** you can enter the lengths and diameters of the connected tubing. With the dosing unit you can also alter the port occupancy. These parameters are important for correctly carrying out the **preparation** (PREP command) and **emptying** (EMPTY command) functions for the dosing unit, as the volumes of the tubing connections must be taken into consideration (see Section 3.24.2).



Dosing unit / Tubing parameters			
Titrant: NaOH			
	Port	Length in cm	Diameter in mm
Dosing port 1	Port 1	40.0	2.0
Dosing port 2	Port 3	0.0	2.0
Filling port	Port 2	25.0	2.0
Special port	Port 4	0.0	2.0

Fig. 10: Dosing unit port occupancy and tubing connections

The default values for the **tubing parameters** of the exchange unit and dosing unit have already been entered; these represent the dimensions of the standard tubing supplied. If you do not make any changes to the tubing then you do not need to alter the tubing parameters.

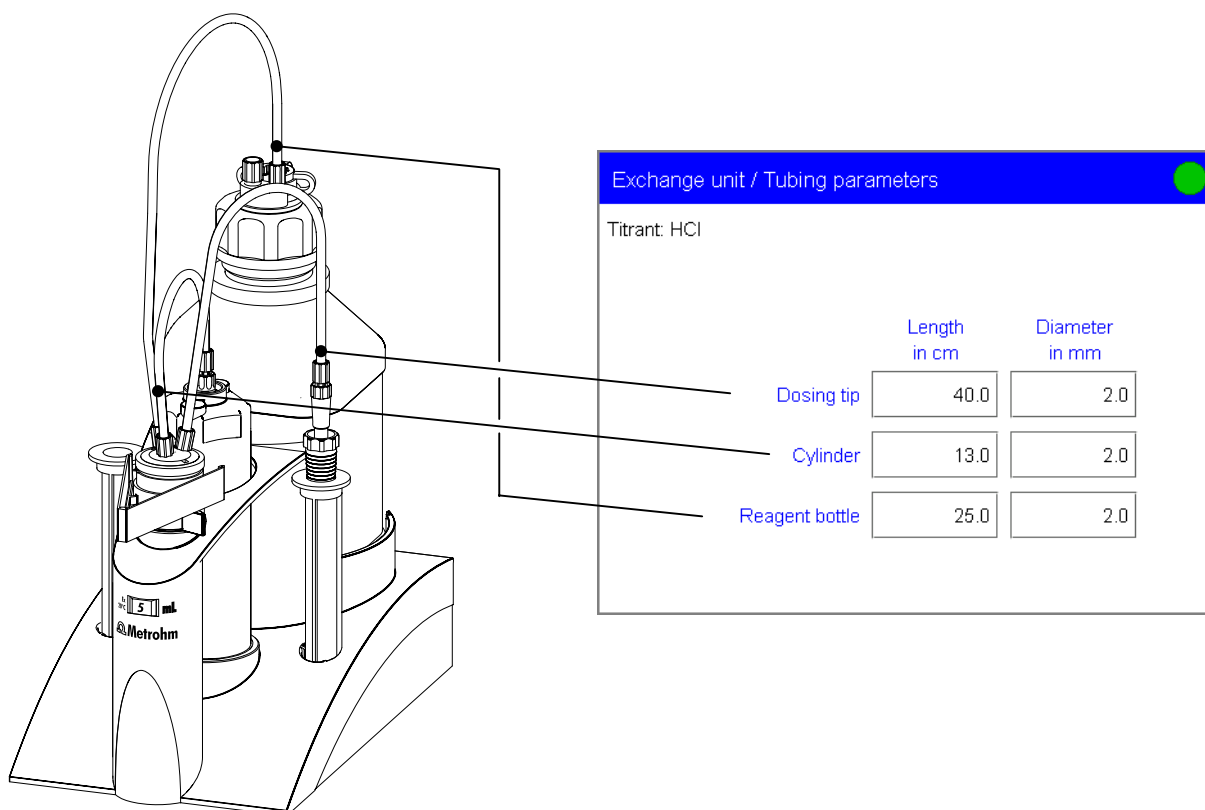


Fig. 11: Exchange unit tubing connections

Under **Exchange unit/PREP parameters** and **Dosing unit/PREP parameters** you can enter the parameters for carrying out the **preparation** (PREP command) and **emptying** (EMPTY command) functions. The preparation function is used to rinse the burets if they have not been used for a long time. When this function has been carried out all the tubing and the cylinder will be filled with reagent. These parameters are different for exchange units and dosing units.

You should carry out the **preparation** function (PREP command) before you start up the exchange unit for the first time as well as when the unit has not been used for a long time. The PREP function can be found under **manual operation**; this can be started with the **[Manual]** fixed key (see Section 3.24.2). For each dosing device (MSB) you can define when a message is to be shown to remind you that the PREP function must be carried out for the particular dosing device under **Device manager** (see Section 3.10.4).

Exchange unit / PREP parameters
●

Titrant: HCl

Volume

cyl.v.
▼

mL

Cycles

2
▼

Dosing rate

maximum
▼

mL/min

Filling rate

maximum
▼

mL/min

- ☞ Enter the **Volume** of reagent which is to be dosed in during a rinsing cycle. The default value is the **cylinder volume**, i.e. the contents of one cylinder is dosed in during a rinsing cycle. You can also enter a different volume.
- ☞ Select the number of **Cycles** to be carried out during the preparation function. At least two rinsing cycles should be carried out in order to remove all the air bubbles.
- ☞ Enter the **Dosing rate** and the **Filling rate** to be used during the PREP function for drawing in and ejecting the reagent. Lower dosing rates should be entered for substances with higher viscosities.

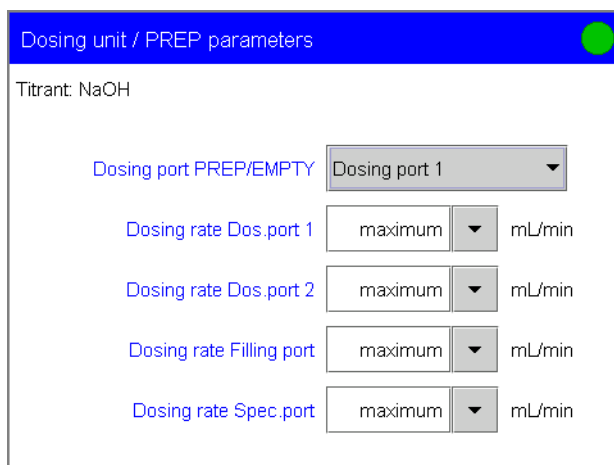
The **maximum dosing rate** and **maximum filling rate** for the exchange unit depend on the cylinder volume:

<i>Cylinder volume</i>	<i>Max. rate</i>
1 mL	3.00 mL/min
5 mL	15.00 mL/min
10 mL	30.00 mL/min
20 mL	60.00 mL/min
50 mL	150.00 mL/min

You can always enter a value between 0.01 and 166.00 mL/min independent of the cylinder volume. When the function is carried out the rate will be reduced automatically to the highest possible value.

For the **dosing unit** you should carry out the **preparation** function (PREP command) before each series of samples or approx. once per day. The parameters apply to the **preparation** (PREP command) and **emptying** (EMPTY command) functions. The preparation and emptying functions can be found under **manual operation** which can be started with the **[Manual]** fixed key (see Section 3.24.2). For each dosing device (MSB) you can define when a message is to be shown to remind

you that the PREP function must be carried out for the particular dosing device under **Device manager** (see Section 3.10.4).



- ☞ Select the **Dosing port** via which the first cylinder contents are to be ejected during preparation and emptying.
- ☞ Enter the **Dosing rates** for all the ports to be used during the preparation and emptying functions for drawing in and ejecting the reagent. Lower dosing rates should be entered for substances with higher viscosities.

The **maximum dosing rate** and **maximum filling rate** for the dosing unit depend on the cylinder volume:

<i>Cylinder volume</i>	<i>Max. rate</i>
2 mL	6.64 mL/min
5 mL	16.60 mL/min
10 mL	33.20 mL/min
20 mL	66.40 mL/min
50 mL	166.00 mL/min

You can always enter a value between 0.01 and 166.00 mL/min independent of the cylinder volume. When the function is carried out the rate will be reduced automatically to the highest possible value.

3.8.7 Monitoring the GLP test

You can monitor the **time interval** after which a **GLP test** must be carried out again for the buret. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.)

- ☞ Open the dialog **Exchange unit/GLP test** or **Dosing unit/GLP test**. Enter the date of the last GLP test to have been carried out and activate the **Monitoring** checkbox.
- ☞ Enter either the **GLP test interval** or the **date of the next GLP test**. If the time interval or date is altered then the other parameter will be updated automatically.
- ☞ Select an **Action** to be taken when the time interval has expired (see *Section 3.8.4*).

3.8.8 Monitoring the working life

You can monitor the **time interval** after which the **reagent** must be replaced. This is a very good idea when your reagent has a limited working life. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.) For documentation purposes you can enter the preparation date without monitoring the time interval.

- ☞ Open the dialog **Edit titrant/Working life**. Enter **Preparation date** for the reagent or the date on which the bottle was opened and activate the **Monitoring** checkbox.
- ☞ Enter either the **Working life** or **Expiry date** of the reagent. If the time interval or date is altered then the other parameter will be updated automatically.
- ☞ Select an **Action** to be taken when the working life has expired (see *Section 3.8.4*).

3.9 Sensors

This section describes how you can draw up a list of the sensors used in the system.

The following **sensor data** is stored in the list of sensors:

- Sensor name
- Sensor type
- Comment
- Measuring input to which the sensor is connected.
- Calibration data (for pH and ISE sensors only – ISE=Ion-Selective Electrode)
- Calibration interval (for pH and ISE sensors only)
- Limit values for the calibration data (for pH and ISE sensors only)
- Working life (with starting date and expiry date)

Each sensor in the system is identified by an unambiguous sensor name.

☞ Open the dialog **System/Sensors**.

System / Sensors	
Sensor	Sensor type
pH electrode	pH electrode
Unitrode with Pt1000	pH electrode
Ag-Titrode	Metal electrode
Metal electrode	Metal electrode
Fluoride electrode	ISE electrode
NTC sensor	Temp. sensor
Temperature sensor	Temp. sensor
<div> <div>New</div> <div>Delete</div> <div>Edit</div> </div>	

The **name** and **type** of each configured sensor are shown in the **list of sensors**. Four standard sensors are already defined in the list and cannot be deleted: **pH electrode**, **Metal electrode**, **Fluoride electrode** and **Temperature sensor**.

You can configure new sensors with **[New]** (see Section 3.9.1). Sensors can be removed from the list with **[Delete]**. **[Edit]** opens the dialog for entering sensor data.

3.9.1 Configuring a new sensor

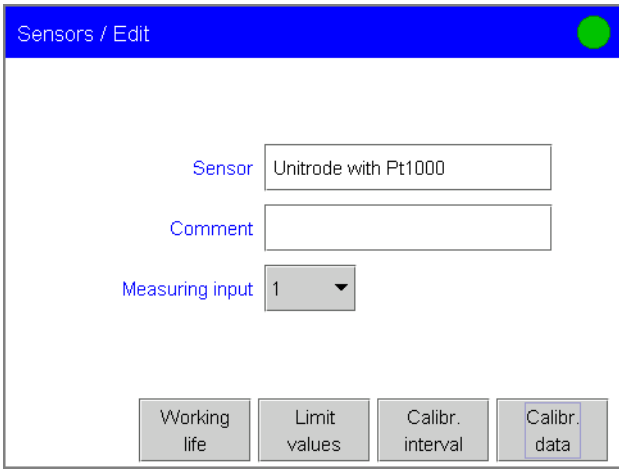
- ☞ Open the dialog **System/Sensors**.
- ☞ Use **[New]** to open the **selection of the sensor type**. Select the sensor type (**pH electrode**, **Metal electrode**, **ISE electrode**, **Other sensor** or **Temperature sensor**).
- ☞ If you select **ISE electrode** then the ion for which the electrode is selective will be requested automatically. Select the **Ion**. You can also select **Custom** as the ion and then enter a name and select the charge for your "own" ion.

The dialog in which you can enter the **sensor data** opens automatically. The sensor data vary according to the sensor type. Calibration data, calibration interval and calibration data limits are only stored for pH electrodes and ISE electrodes.

- ☞ Enter the sensor data as described in *Section 3.9.2*.

3.9.2 Editing sensor data

- ☞ Open the dialog **Sensors/Edit** by either configuring a new sensor (see *Section 3.9.1*) or selecting an existing sensor from the list and modifying it with **[Edit]**.



- ☞ Enter an unambiguous name for the sensor under **Sensor**. For ISE electrodes the ion whose concentration can be determined with the sensor is also shown.
- ☞ You can enter a **Comment** for each sensor.
- ☞ Select the **Measuring input** to which the sensor is or will be connected. If your Titrand only has a single measuring interface (Input 1) then you should select Measuring input 1. Whether a sensor is actually attached to a particular measuring input is not checked automatically.

3.9.3 Calibration data (for pH and ISE electrodes only)

Detailed information about calibrations is given under **Edit sensor/Calibration data**. For pH electrodes the **Slope** is given in % and the electrode zero point **pH (0)** is shown. For ISE electrodes the **Slope** is given in mV; the electrode zero point **E (0)** and the blank concentration **c (blank)** are also shown. The calibration date is entered automatically after a calibration has been carried out (see *Section 4.6*).

Under **Calibration temperature** the temperature at which the calibration was carried out is shown. If the temperature was measured and entered manually during the calibration then this is indicated by **manual**. If the temperature was measured with a connected temperature sensor then the type of sensor (**Pt1000** or **NTC**) will be shown. The **Calibration date** is entered automatically together with the time. When a sensor is entered into the list for the first time the date of entry will be given as the calibration date.

Under **Calibration method** the method used to calibrate the sensor is shown. If the calibration data has been entered manually then **manual** will be shown here. The user who carried out the calibration or entered the calibration data manually is shown under **User**.

Edit sensor / Calibration data

Sensor: Unitrode with Pt1000

Slope 100.1 %

pH (0) 6.997

Calibration temp 25.0 °C (manual)

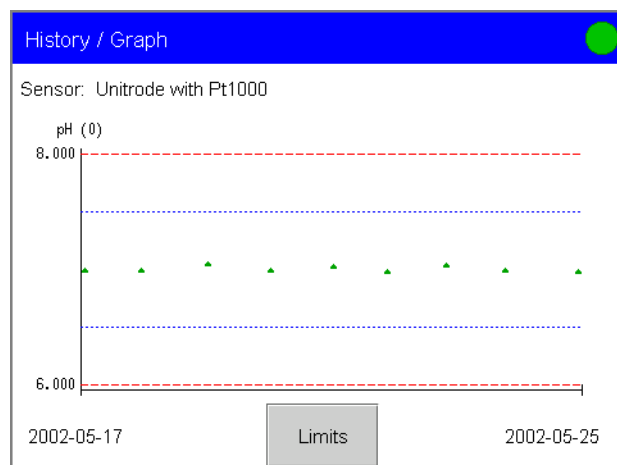
Calibration date 2002-05-17 15:23:38

Cal. method pH calibration

User sn

History

Under **Calibration data/History** the calibration data, dates and times of the last ten calibrations are shown in the form of a table. Calibration data which have been determined automatically is shown in green, manually entered calibration data is shown in black and marked with **(m)**. With **[Graph slope]** and **[Graph pH (0)]**, or **[Graph E (0)]** you can open a graph in which the slope or pH (0) for pH electrodes or E (0) for ISE electrodes is plotted against the calibration date. If a sensor has to be replaced then you can delete the complete history with **[Delete history]**.



This graph corresponds to a control chart on which both **warning limits** and **intervention limits** are shown for the calibration data. The values for these warning limits and intervention limits can be entered under **Graph/Limits**. No automatic action is taken when these limits are infringed.

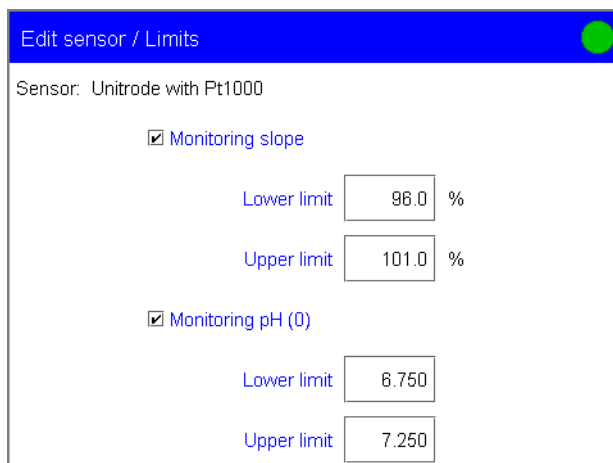
3.9.4 Monitoring the calibration interval (for pH and ISE electrodes only)

You can monitor the **time interval** after which the **sensor** must be **re-calibrated**. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.) For documentation purposes you can enter the starting date without monitoring the time interval.

- ☞ Open the dialog **Edit sensor/Calibration interval** and activate the **Monitoring** checkbox.
- ☞ Enter either the **Calibration interval** or **Next calibration** date. If the time interval or date is altered then the other parameter will be updated automatically.
- ☞ Select an **Action** to be taken when the time interval has expired (see *Section 3.8.4*).

3.9.5 Calibration data limits (for pH and ISE electrodes only)

You can define **Limits** for the calibration data; these will then be monitored when a calibration is carried out (see *Section 4.6*). During the calibration run you can decide whether to accept the calibration data even though the limits have been infringed.



☞ Activate the checkboxes for the calibration data you wish to monitor (slope, pH (0) or E (0)).

☞ Enter the **Lower limit** and **Upper limit** for the calibration data.

3.9.6 Monitoring the working life

You can monitor the **time interval** after which the **sensor** must be replaced. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.) For documentation purposes you can enter the starting date without monitoring the time interval.

☞ Open the dialog **Edit sensor/Working life**. Enter the date that the sensor was used **for the first time** and activate the **Monitoring** checkbox.

☞ Enter either the **Working life** or **Expiry date**. If the time interval or date is altered then the other parameter will be updated automatically.

☞ Select an **Action** to be taken when the working life has expired (see *Section 3.8.4*).

3.10 Device manager

This section describes the configuration of the Touch Control, Titrando and the connected **peripheral devices**. The installation of the hardware is described in the Installation Instructions for the 808 Titrando and 809 Titrando. You should first connect all the peripheral devices and then configure them in the device manager.

☞ Open the dialog **System/Device manager**.

System / Device manager	
Device name	Device type
PC Control	PC Control
Titrando 1	808 Titrando
Balance Laboratory 1	Balance
PC Laboratory 1	PC/LIMS
Barcode reader	Barcode reader
<div> <div>New</div> <div>Delete</div> <div>Edit</div> </div>	

The device list gives the name and type of every configured instrument. **PC Control** or **Touch Control** and the connected **Titrandos** with the dosing devices, stirrers and remote boxes connected to the MSB are entered automatically in the list. If you are using a Touch Control then the printer, PC keyboard, barcode reader and the USB-RS 232 box will also be automatically recognized and entered in the list with their default settings. No parameters can be edited for the USB-RS 232 box. The devices used for carrying out a determination are stored together with the determination data (see Section 3.18.4).

You can configure new devices with **[New]** (see Section 3.10.1). **[Delete]** removes devices from the list. Devices which are recognized automatically cannot be deleted from the list while they are still connected. **[Edit]** opens the dialog for entering the device data.



Note!

After you have configured peripheral devices in the device manager you should shut down the system and then restart it.

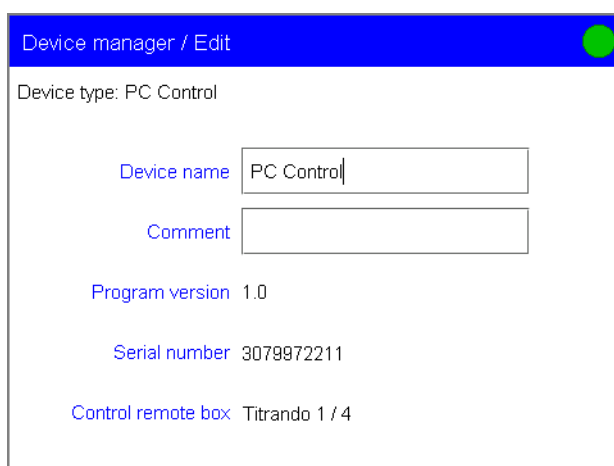
3.10.1 Configuring a new device

- ☞ Open the dialog **System/Device manager**.
- ☞ Use **[New]** to open the **device selection** window. Select the device type (**Printer** (Touch Control only), **Balance**, **PC/LIMS**, **PC keyboard** (Touch Control only), **Barcode reader** or **Titrandos**). With the exception of the Titrandos you can only log in one device of the same type. A maximum of three Titrandos can be logged in even if they are not connected. In this way it is possible to write methods for various Titrandos even when the hardware is currently not available. The new device is entered in the list.
- ☞ Enter the device data as described in *Section 3.10.2*.

3.10.2 Editing device data

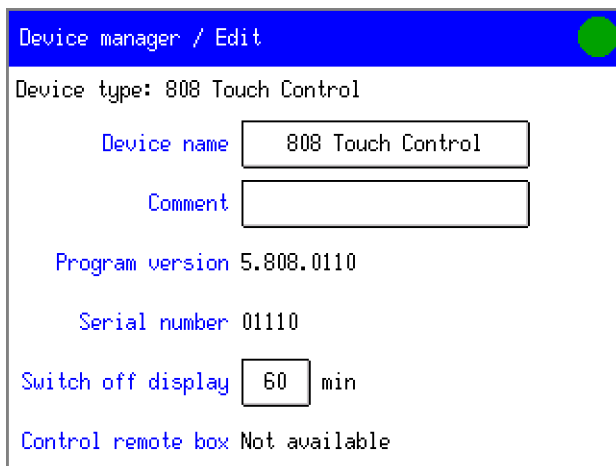
The data stored for a device depends on the type of device.

- ☞ Open the dialog **Device manager/Edit** by selecting the device to be configured from the list and activating **[Edit]**.
- ☞ You can enter a **Device name** for each device.
- ☞ You can enter a **Comment** for each device.



3.10.3 PC Control and Touch Control

With the **PC Control** software the **Program version**, **Serial number** of the USB dongle ("authorization plug") or demo version, if no dongle is connected, and the **Control remote box** are shown. The Control remote box is the interface at which, for example, lines for controlling a sample changer during the determination sequence can be set and scanned automatically (see *Section 6.2*). The first remote box to be recognized after system start-up will always be used as the control remote box. Titrandos 1/4 means that the remote box is connected to MSB connection 4 on Titrandos 1 (name of the Titrandos).



Device manager / Edit

Device type: 808 Touch Control

Device name: 808 Touch Control

Comment:

Program version: 5.808.0110

Serial number: 01110

Switch off display: 60 min

Control remote box: Not available

With **Touch Control** the **Program version** and **Serial number** of the Touch Control are shown.

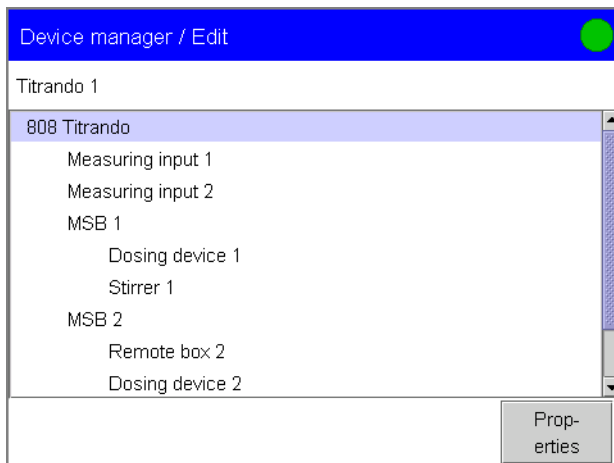
☞ Under **Switch off display** enter the time after which the display illumination is to be switched off automatically when the system has not been used.

As with the PC Control, the **Control remote box** connection is shown (see p. 57).

The **Device name** of the PC Control or Touch Control is printed out in the standard report header.

3.10.4 Titrandos

The measuring inputs and the devices connected to the MSB connection are automatically shown in a table for the **Titrandos** which are connected (**plug and play**). In the following example the Titrandos has two measuring interfaces. A dosing device and a stirrer are connected to MSB 1. As this is an 808 Titrandos, dosing device 1 is the internal dosing device (see Installation Instructions for the 808 Titrandos and 809 Titrandos). A dosing device and a remote box are connected to MSB 2. With Titrandos that are not connected (see Section 3.10.1) only the **Device name** and **Comment** can be edited.



Device manager / Edit

Titrandos 1

808 Titrandos
Measuring input 1
Measuring input 2
MSB 1
Dosing device 1
Stirrer 1
MSB 2
Remote box 2
Dosing device 2

Properties

☞ Select the connection or device to be configured and open the corresponding dialog with **[Properties]**.

For connected **Titrandos** the **Program version** and **Serial number** are shown.

For the **Measuring inputs** the **ADC type** (Analog-Digital Converter) and **Serial number** of the measuring interface are shown.

☞ You should select the **Sensor type** for the temperature sensor to be connected to this measuring input. If you use an NTC sensor then you must set two further parameters that can be obtained from the technical specifications of the sensor: the nominal resistance at 25 °C (**R (25 °C)**) and the **B value** referring to measurements of the resistance at 25 °C and 50°C. The default values apply to Metrohm sensors with an NTC sensor. If no B-value is given for your sensor then you can retain the default value. B-values of other NTC sensors are frequently based on different reference temperatures (usually 25 °C / 50 °C – 100 °C). When entering the B-value the influence of the second reference temperature is negligible in comparison with the measuring accuracy of an NTC sensor.

For the **MSB connections** you can define when the request to carry out a **preparation** function (PREP command) for connected dosing devices is to be displayed. The preparation of the burets is described in *Section 3.24.2*. For a description of the parameters please consult the **online help**.

For connected **dosing devices** the **Dosing device type** and, for type 8xx dosing devices, the **Serial number** are shown.

For connected **stirrers** the **Stirrer type** and **Serial number** are shown.

No properties can be shown or edited for the connected **remote boxes**.

3.10.5 Printer (Touch Control only)

A **printer** can only be configured for the **Touch Control**. When a printer is connected it is automatically entered in the device list with default parameters. Printer models which can be currently connected can be found on the Internet under www.titrando.com.

☞ Select the **printer type**. If you are using a printer with a resolution of 360 dpi (e.g. Epson) then the text will be printed out somewhat smaller than with printers with a resolution of 300 dpi (e.g. Canon or HP).

☞ Select the **paper format** (DIN format **A4** or US format **Letter**).

☞ Deactivate the **Color** checkbox if your printout is to be black/white (not for HP LaserJet).

The **PC Control** software automatically uses the **Windows standard printer**. If you want to use a different printer then you must define it as the standard printer in the operating system under Settings/Printer.

3.10.6 Balance

Connecting a **balance** to the Titrando or PC is described in the Installation Instructions for the 808 Titrando and 809 Titrando. In the device manager you must configure the serial interface used to connect the balance.

☞ Select the **Balance type**.

The following table shows the balance type to be selected for various **balance models**:

<i>Balance</i>	<i>Balance type</i>
AND balance with RS 232 interface (OP-03)	AND
Mettler AB, AG (LC-RS25), AM, PM Mettler interface 011, 012 or 016	Mettler
Mettler AT	Mettler AT
Mettler AX, MX, UMX, PG, AB-S	Mettler AX
Ohaus Voyager, Explorer, Analytical Plus	Ohaus
Precisa balance with RS 232C interface	Precisa
Sartorius balance with RS 232C interface	Sartorius
Shimadzu BX, BW	Shimadzu

☞ Select the **RS 232 interface** that the balance is connected to. If you are operating the Titrando with the **PC Control** software then select the serial interface (COM) of the PC to which the balance is connected. All the COM interfaces of the PC will be shown. If you are operating the Titrando with the **Touch Control** then select the RS 232 interface at the **USB-RS 232 box** which is used to connect the balance.

☞ Edit the parameters for the interface on the PC or at the USB-RS 232 box to which the balance is connected under **Edit device/Port parameters**. The settings on the balance must agree with these settings. For a description of the parameters please con-

sult the **online help**. A detailed description of the handshake is given in *Section 6.3*.

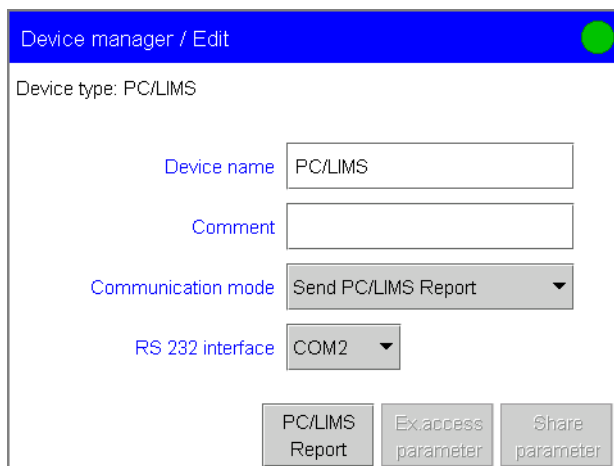
The sample size is transferred as a number with up to ten places, sign and decimal point. Units transmitted by the balance will also be transferred. Control characters will not be transferred. With some balances it is also possible to transmit the sample identification and method from the balance as well as the sample size. When editing the sample data in the sample data silo all the data can be transmitted from the balance (see *Section 3.19.3*). In some cases a special input unit may be necessary; this can be supplied by the balance manufacturer.

In order to do this the following addresses for the identifications and methods must first be selected:

<i>Balance</i>	<i>Method</i>	<i>Identification 1</i>	<i>Identification 2</i>
Sartorius (input unit)	METH or 27	ID.1 or 26	ID.2 or 24
Mettler AT (input unit)	D (Mthd)	C (ID#1)	B (ID#2)
Mettler AX	Label for ID which con- tains the method name: METHOD	Label for ID which con- tains Identifi- cation 1: ID1	Label for ID which con- tains Identifi- cation 2: ID2

3.10.7 PC/LIMS

You can connect and configure a computer (**PC/LIMS**) to which a report in ASCII format containing all the data of a determination (PC/LIMS report) can be transmitted. You can also select **Share system** in one system in order to make the data accessible to a second system. Connecting a computer to a system with Touch Control is described in the Installation Instructions for the 808 Titrando and 809 Titrando.



In order to **transmit a PC/LIMS report via a serial interface** you must configure the system in the following way:

- ☞ Select **Communication mode "Send PC/LIMS Report"**.
- ☞ Select the **RS 232 interface** via which the report is to be transmitted. If the Titrando is being controlled with the **PC Control** software then select the serial interface (COM) of the PC via which the report is to be transmitted. All the COM interfaces of the PC will be shown. If the Titrando is operated by the **Touch Control** you should select the RS 232 interface at the **USB-RS 232 box**, to which the computer which the report is to be transmitted to, is connected.
- ☞ Open the dialog **Edit device/PC/LIMS Report** and deactivate the **File** checkbox.
- ☞ Under **Edit device/Port parameter** you should edit the parameters for the interface at the PC or USB-RS 232 box, to which the computer which the report is to be transmitted to, is connected. The settings for the interface to which the report is to be transmitted must be identical with these settings. A description of the parameters can be found in the online help. A detailed description of the handshake is given in *Section 6.3*.
- ☞ End the PC Control program or switch off the Touch Control and then restart the system.

A detailed description of the contents of the PC/LIMS report is given in the Titrando **PC/LIMS Report Guide**.

In order to **save a PC/LIMS report as a text file** you must configure the system as follows:

- ☞ Open the dialog **Edit device/PC/LIMS report** and activate the **File** checkbox (corresponds to default setting).

When you save the PC/LIMS report as a file then it does not matter which communication mode is selected. The **File** checkbox is automatically active when the **Communication mode** is not "**Send PC/LIMS-Report**" as in this case the RS 232 interface is already occupied with a different function.

- ☞ Select the **memory** in which the files are to be stored and the **group** (see *Section 3.11.4*).

The file is either saved automatically at the end of a determination (see *Section 3.16.9*) or manually with the **[Print]** fixed key (see *Section 3.23.1*). A detailed description of the contents of the PC/LIMS report is given in the Titrando **PC/LIMS Report Guide**.

If you want to select **Share system** in one system in order to make the data accessible to a second system then the systems must be configured as follows:

System in which a memory is to be shared (System 1):

- ☞ Select "**Share system**" under **Communication mode**.

- ☞ Select the interface to be used for transmitting data under **RS 232 interface**.
- ☞ Open the dialog **Edit device/Share parameters** and select the **memory** which is to be shared.

System which is to be able to access the shared system (System 2):

- ☞ Select the **Communication mode "External system access"**.
- ☞ Select the **RS 232 interface** via which the data is to be transferred.

No further parameters need to be entered. The communication parameters are fixed and cannot be altered by the user. Data exchange can take place between a computer with PC Control and a Touch Control (in both directions) or between two computers with PC Control.

- ☞ Switch off both systems and restart System 1 first, then System 2.

When saving and loading files you can now use the file manager in System 2 to select the memory which is to be shared in System 1 as **Shared memory**.

3.10.8 Transmitting messages as E-Mails

If you are using **Touch Control** to operate your titration system to which a computer with Internet access and PC Control software is connected, messages (all warnings with the symbol **!** and error messages with the symbol **X**) can be sent as E-Mails. Connecting a computer to a system with Touch Control is described in the Installation Instructions for the 808 Titrando and 809 Titrando. If you are operating the titration system with the **PC Control** software you can send the messages directly from the computer if it has an Internet connection.

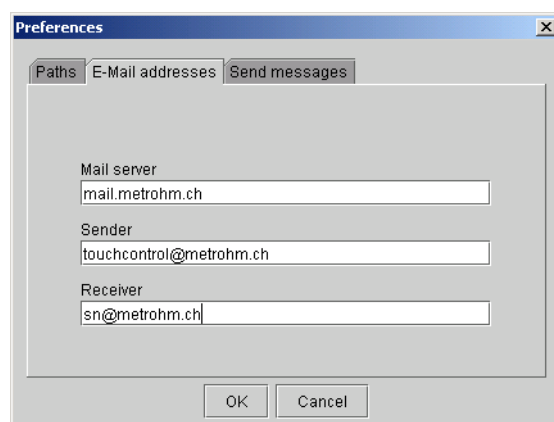
Configuration of Touch Control and PC Control if the titration system is to be operated with **Touch Control**:

Touch Control:

- ☞ Under **Device manager/Edit** select **Communication mode "External system access"** for the PC/LIMS.
- ☞ Select the **RS 232 interface** to be used for data transfer.
- ☞ Open the dialog **Edit device/Access parameters** and activate the **E-Mail** checkbox.
- ☞ If the default settings are retained then **messages will only be sent when the system is running** (BUSY), i.e. when a determination or sample series has been started. If you also want to send messages in the normal working condition (READY) then this checkbox must be deactivated.

PC Control on a connected computer:

- ☞ Under **Device manager/Edit** select the **Communication mode "Share system"** for the PC/LIMS. No share parameters need to be set.
- ☞ Select the **RS 232 interface** via which data transfer is to take place.
- ☞ In the menu **File/Preferences** enter the **Mail server** under **E-Mail addresses** and the following E-Mail addresses: E-Mail address to be given as the **Sender** in the E-Mail (this address must have the format of an E-Mail address, but does not need to be identical to an existing E-Mail account); E-Mail address of the **Receiver** who is to receive the messages. The **Mail server** can be found in the settings of your E-Mail program.



No further parameters need to be entered. The communication parameters are fixed and cannot be altered by the user.

- ☞ Switch off both systems and restart them again.

Configuration of **PC Control** if the system is being operated by the PC Control software:

- ☞ Under **File/Preferences** enter the addresses in **E-Mail addresses** as described above.
- ☞ In the menu **File/Preferences** activate the **E-Mail** checkbox under **Send messages**.
- ☞ If the default settings are retained then **messages will only be sent when the system is running** (BUSY), i.e. when a determination or sample series has been started. If you also want to send messages when no analysis is running (READY) then this checkbox must be deactivated.

3.10.9 PC keyboard (Touch Control only)

An external **PC keyboard** can be connected to a Titrando system with Touch Control to make the input of texts easier.

☞ Select the country-specific key occupancy under **Keyboard layout**.

When the PC keyboard is selected the unambiguous identification of the manufacturer (**Vendor ID**) and the **USB address** will be shown automatically.

For entering texts and numbers with the PC keyboard the appropriate text and number input dialog must be opened on the Touch Control. Only the following keys on the PC keyboard have a function :

<i>PC keyboard key</i>	<i>Function in text or numerical input dialog of the Touch Control</i>
Escape	Cancel
Numbers, letters and special characters	Enters the corresponding character
Numbers, letters and special characters + Shift	Enters the corresponding character
Tab (⇧)	Confirms the input and closes the text or numerical input dialog
Backspace, ⌫	Deletes the character in front of the cursor
Delete	Deletes the input
Return (↵)	Starts a new line in multi-line text input
Arrow keys (← →)	Moves the cursor to the left or right by one character
Arrow keys (↑↓)	Moves the cursor up or down by one line in multi-line text input
Numbers and characters on the number block	Enters the corresponding character
Enter on the number block	Confirms the input and closes the text or numerical input dialog

3.10.10 Barcode reader

A **barcode reader** can be connected to the Titrando system to read in sample data or other texts. When a barcode reader is connected to a Titrando system with Touch Control then it is automatically entered into the device list with default parameters. Barcode reader models which can currently be connected can be found on the Internet under www.titrando.com.

- ☞ Select the **Barcode input target** for the barcode character string. For PC Control **Active input field** means that the contents of the barcode will be written into the input field in which the cursor is currently located. With Touch Control **Active input field** means that the barcode string will be written into the **Input field** of an opened text or numerical input dialog. For the input targets **Method**, **Identification 1**, **Identification 2** and **Sample size** (value only) the location can be anywhere in the dialog, the read-in string will be written automatically into the selected input field. Only numerical entries will be accepted for the sample size. Strings which contain characters other than numbers and decimal separators will be ignored.
- ☞ With Touch Control you can also select the country-specific key occupancy for the emulation of the PC keyboard under **Keyboard layout**. This setting must be identical to that on the barcode reader (see barcode reader documentation).

When the barcode reader is connected to a Titrando system with Touch Control then the unambiguous identification of the manufacturer (**Vendor ID**) and the **USB address** will be shown automatically.

When a string has been transmitted by the barcode reader and accepted then this will be confirmed by an acoustic signal. If a Touch Control is used for operating the Titrando system then data should only be read in when the system is in the normal operating status (Ready), i.e. when no determination is running.

3.11 File manager

The **File memory** of the Touch Control and PC Control has the following arrangement:

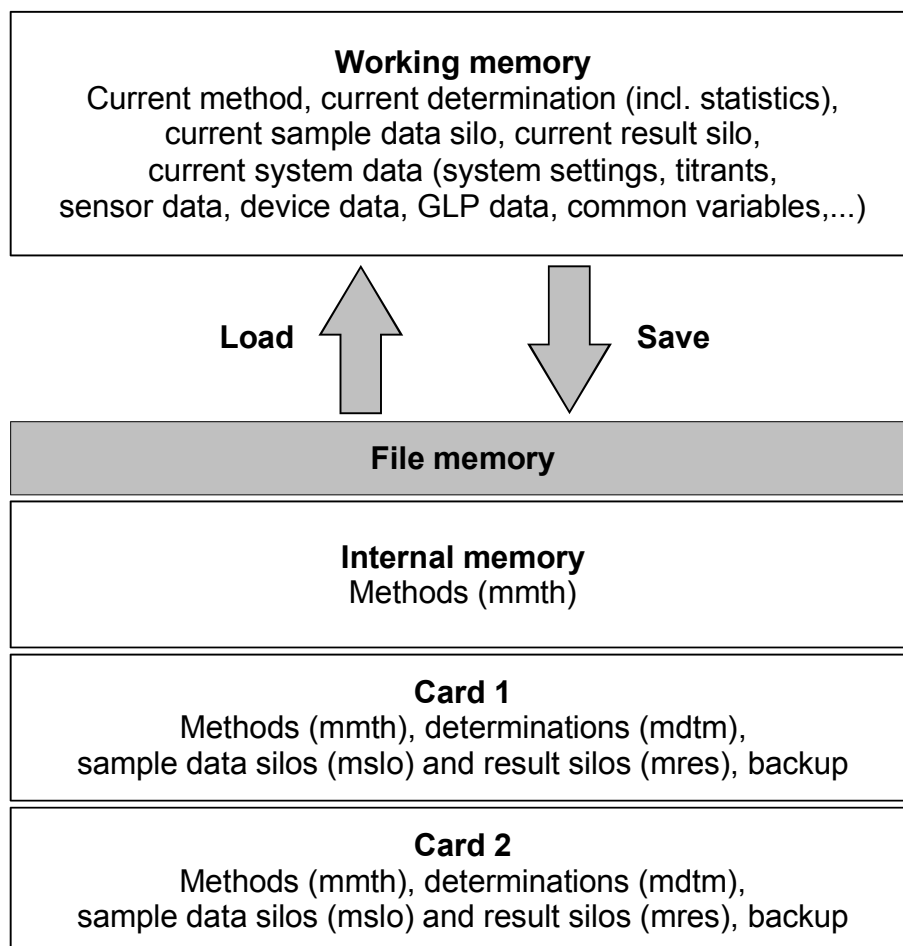
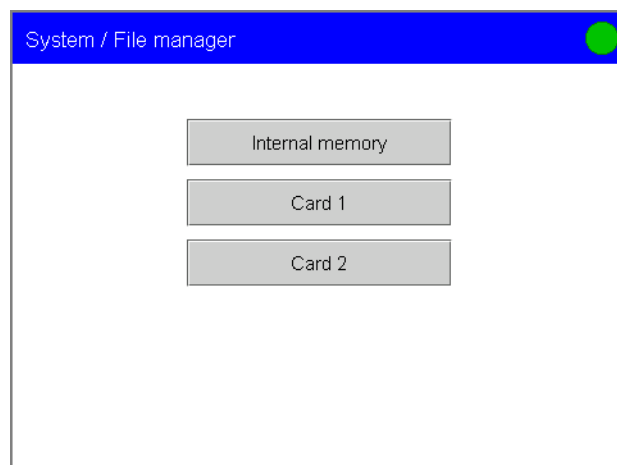


Fig. 12: Data memory arrangement

In the **File manager** you can **load, delete, copy, rename and write-protect** methods, determinations, sample data silo files and results silo files as well as edit the **File properties** of each file. You can also produce a **backup** (safety copy) containing all stored data and settings on a card and reload them.

 Open the dialog **System/File manager**.



You can select the memory to be used for the files. **[Card 1]** and **[Card 2]** are inactive when the memory cannot be accessed. With **Touch Control** the cards must be inserted before you open the file manager. If neither card can be accessed then the dialog **System/File manager** will be skipped.

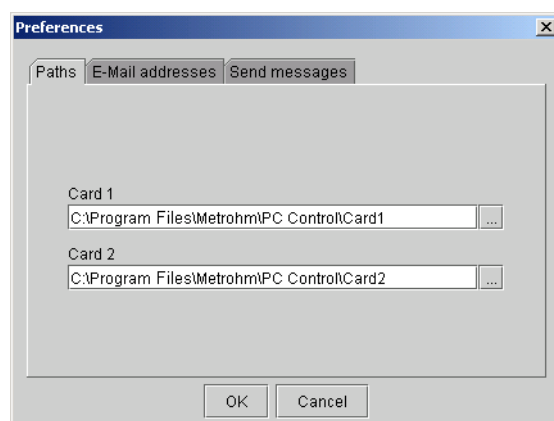
With the **Touch Control** the card slots for the PCMCIA cards are located on the rear of the instrument (see Fig. 3: Rear view of the Touch Control).



Note!

With **Touch Control** it is possible to access only one card drive at a time and not both simultaneously. For example, if an identification card (see Section 3.7.6) is inserted in Card slot 1 then Card slot 2 cannot be used. You should first remove the card from the one slot before inserting another card into the other slot.

With **PC Control** you can define folders in **File/Preferences** under **Paths** for **Card 1** and **Card 2**. These can be folders on a hard disk, a network drive or any removable data carrier. It must be possible to access the drive when the path is being defined.



If you retain the default settings then folders in the PC Control installation folder are selected for **Card 1** and **Card 2**. The example files (**Examples**) are stored in the folder for **Card 1**.

**Note!**

In **PC Control** the **file groups** correspond to folders. **Card 1** and **Card 2** each have only one level for groups and folders. The file names must be unambiguous for all groups (folders) in a memory location. You should only manage the PC Control files with the file manager of the PC Control software. If you use Windows Explorer for this then there is the risk that you might no longer find the files in PC Control as the folder structure is not compatible.

With **PC Control** if you store files or a backup in the folders selected for Card 1 or Card 2 then the following **Folder structure** will be created automatically:

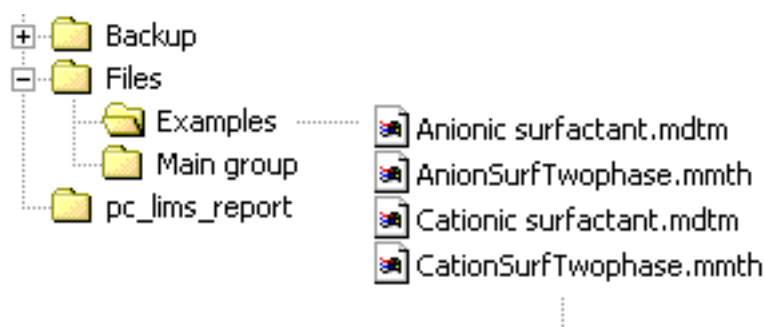
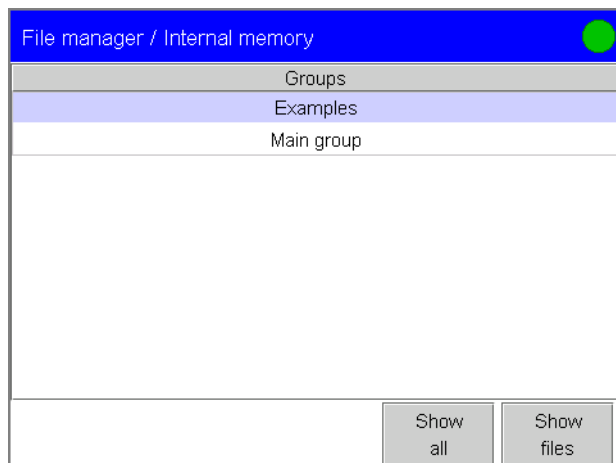


Fig. 13: PC Control: Folder structure for Card 1 and Card 2

All the files which belong to a backup are stored in the **Backup** folder. All the files which can be seen in the file manager of the PC Control under **Card 1** and **Card 2** are stored in groups (subfolders) in the **Files** folder. The subfolder (group) **Examples** is present in the standard folder for Card 1 (see above). The example files are stored in this folder. The **Main Group** folder is created as soon as a file is stored without entering a new group. The **pc_lims_report** folder is created when you store a PC/LIMS report as a file without entering a new group.

The files in the internal memory are protected and cannot be accessed via the Windows Explorer. All methods which are stored in the internal memory can only be exchanged by using the file manager of the PC Control software. File transfers in the file manager are documented in the audit trail (see Section 3.7.8).

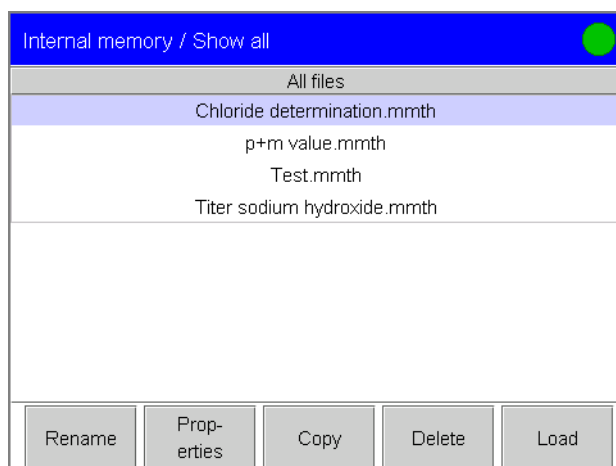
☞ Open the **Internal memory**. The file groups in the internal memory are shown.



You can arrange your files in the **file groups**. All the **files names** in each file memory must be **unambiguous**, i.e. you cannot save a file in different groups with the same file name.

From the list of files you can print out a **list with all the files** in these groups with the **[Print]** fixed key.

☞ Open the list of files containing all the files with **[Show all]** or the list of files for the selected group with **[Show files]**. Only methods can be stored in the internal memory. Methods have the file extension .mmth.



You can load the selected file into the working memory with **[Load]**. The list of files remains open. You can remove the selected file from the list with **[Delete]**. From the list of files you can use the **[Print]** fixed key to print out a **list with all the shown files**.

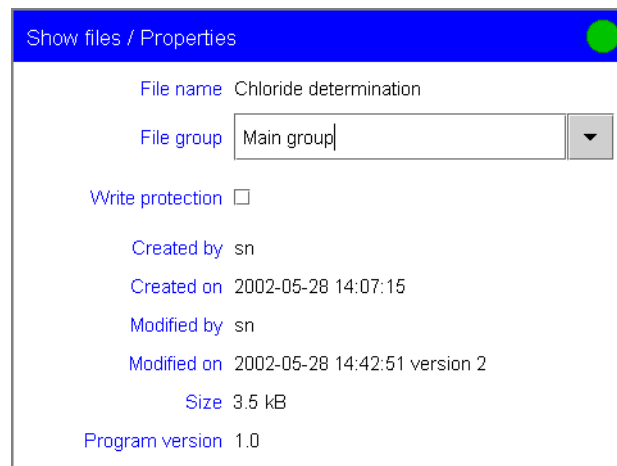
3.11.1 Copying files

- ☞ Select the file to be **copied** in the list of files and open the selection of the file memory with **[Copy]**.
- ☞ Select the **file memory** into which the file is to be copied. You can only select a file memory which can currently be accessed. If the required memory cannot be accessed (**Card 1** or **Card 2**) then you should exit the file manager and define the path for the card (for **PC Control** – see p. 68) or insert a card into the required card slot (for **Touch Control**) and then copy the file.

The **file group** is retained, i.e. the group will be newly created in the file memory into which the file is copied if it does not already exist there.

3.11.2 File properties

- ☞ Select the file in the list of files whose **Properties** you wish to edit and open the dialog **Show files/Properties**.



Various file properties are shown in this dialog.

- ☞ You can select a different **File group** or enter a new file group in which the file is to be stored. In this way the file can be "regrouped" in the same memory.
- ☞ You can activate **Write protection** for the file. As long as write protection is switched on the file cannot be saved under the same name, deleted, regrouped or renamed. The write protection in PC Control is independent of the write protection in Windows Explorer under Properties.

The following data is also shown:

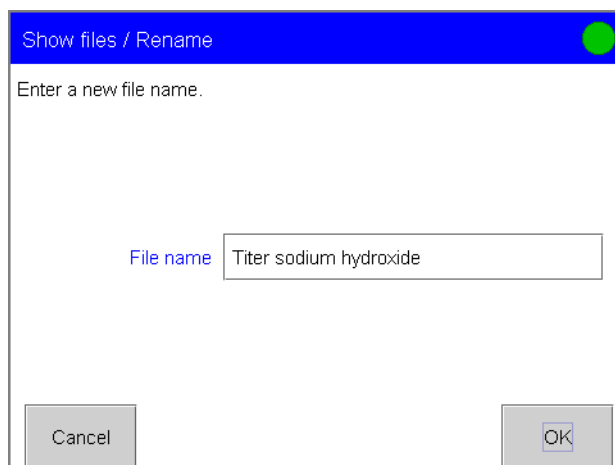
- **User** who **saved the file for the first time**.
- **Date** and time at which **the file was saved for the first time**.
- **User** who was the **last to save the file**.
- **Date** and time at which **the file was saved for the last time**.
- **Version** of the file. The version is increased by one each time that the file is saved under the same file name. The version is retained when the file is copied and loaded in a different system.
- The approximate **Size** of the file in kB.
- **Program version** with which the file was saved for the last time.

File properties can only be printed out in a context-sensitive situation from the dialog **Show files/Properties** with the **[Print]** fixed key.

3.11.3 Renaming a file

☞ Select the file to be **renamed** in the list of files and open the dialog for entering the new file name with **[Rename]**.

☞ Enter the new **File name**.

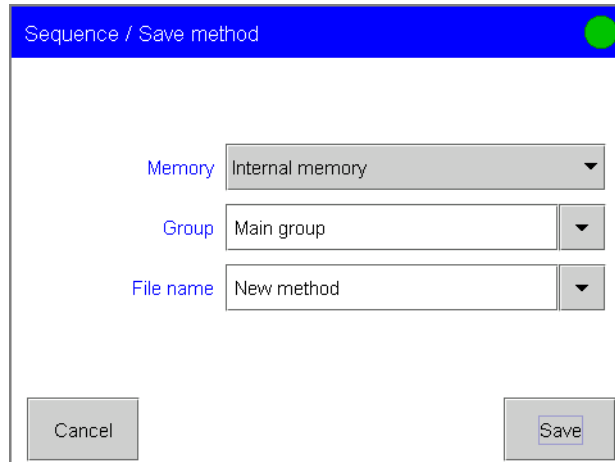


Apart from the alteration of the file name the file properties are not affected by the renaming.

3.11.4 Saving a file

Files are not saved from the file memory but via the dialogs in which the files can be edited. Saving a file using a method as an example is described below.

☞ Open the dialog for saving the file from the main dialog with **[Edit parameters]** and **[Save method]**.



- ☞ Select the memory in which the file is to be stored under **Memory**. Methods can be saved in the **Internal memory**, on **Card 1** or **Card 2** or on a different external memory (PC Control). All other files can only be stored on **Card 1** or **Card 2**.
- ☞ You can arrange your files by storing them in different groups. Enter the **Group** in which the file is to be saved. You can also select the group from the list of existing file groups. If the file has already been saved then the group in which it has been stored will be proposed. All the **files names** in each memory must be **unambiguous**, i.e. you cannot save a file in different groups with the same file name.
- ☞ Enter a **File name**. If the file has already been saved then the name under which it has been stored will be proposed. The file is saved with **[Save]**. The file will not be saved with **[Cancel]** and **[Back]**.

3.11.5 Card 1 and Card 2

No only methods but also determinations, sample data silo files and results silo files can be stored on **Card 1** and **Card 2**. Safety copies (backups) can also be stored on the cards (see *Section 3.11.6*). The **type of file** can be recognized by the file extension: mmth for methods, mdtm for determinations, mslo for sample data silos and mres for results silos.

- ☞ If you are operating the Titrando system with **Touch Control** then insert the **CompactFlash card with the methods** (6.6048.000 or 6.6049.000 with its adapter) into Card slot 1.
- ☞ Open the **Card 1** memory. The file groups on Card 1 are shown.

On the cards you can also open lists of files with **[Show all]** or **[Show files]** in exactly the same way as for the internal memory (see *p. 70*).

- ☞ Open the dialog **Card 1/Card info**. Various information about the card is shown in this dialog. Please note that with **PC Control** this information refers to the drive defined under **File/Preferences/Paths**, for example your computer hard disk.
- ☞ You can switch on **Write protection** for the card by deactivating the **Card shared** checkbox. If 'enable' is deactivated it is no longer

possible to save, delete and rename files on the card. With **PC Control** the write protection applies to the folder defined for the card under **File/Preferences/Paths**.

The following information about the card is shown:

- The **Label** of the card or data carrier which was entered when the data carrier was formatted or entered later under Properties in Windows Explorer.
- **Storage capacity** (total space), **Used memory** and **Free memory** for the card, or for the whole data carrier under PC Control.

3.11.6 Backup and recovery

You can use the **Backup** function to easily create a safety copy containing all the data and settings of your system.



Note!

Make a **Backup** at **regular** intervals in order to avoid data loss, e.g. caused by voltage variations. For Touch Control we recommend an interval of between one week and one month, depending on how frequently you alter your methods or system settings. For the PC Control software the interval should correspond to the normal data security practice in your company.

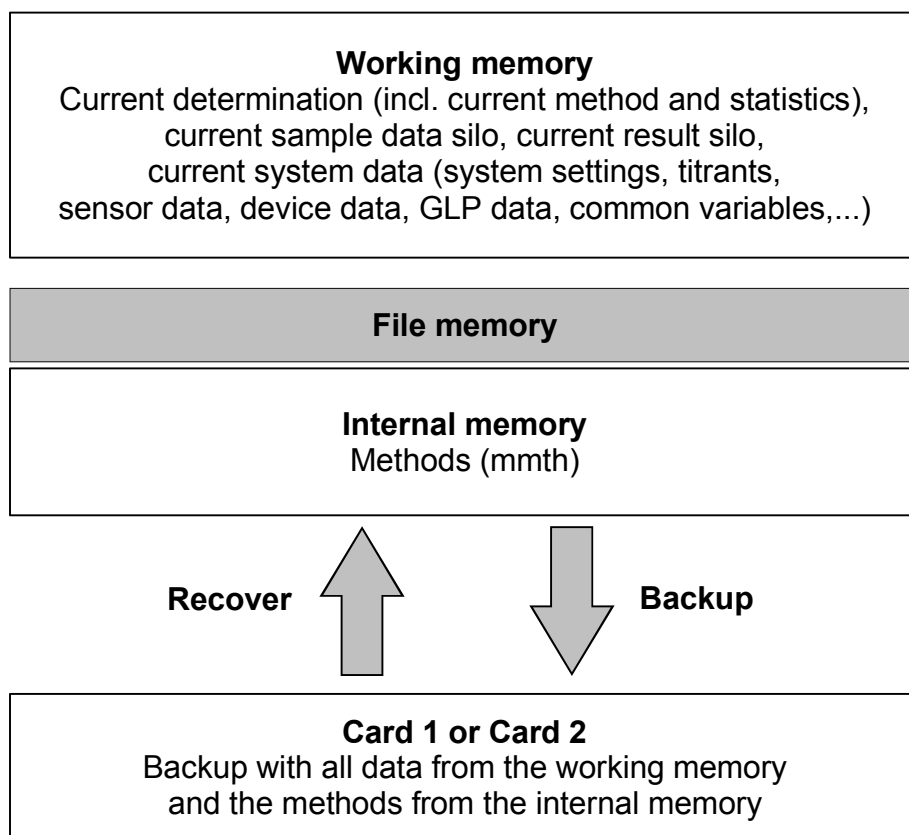


Fig. 14: Data transfer Backup/Recovery

Touch Control:

- ☞ Insert the card on which you want to make your safety copy in **Card slot 1 or 2** of the Touch Control.

PC Control:

- ☞ Select the **Folder** or drive on which you want to make your safety copy under **File/Preferences/Paths**.

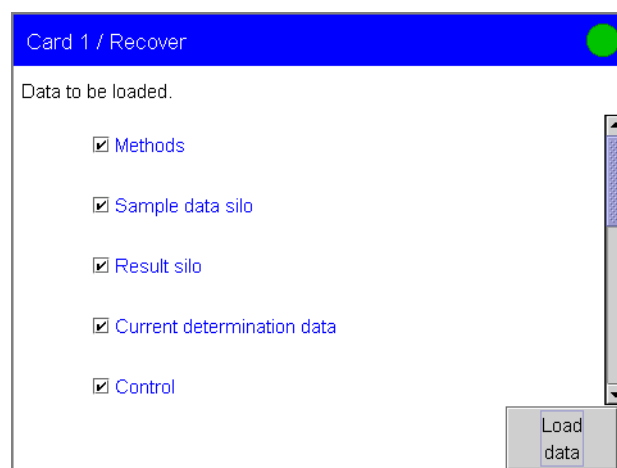
You can now open the file manager and start the backup.

- ☞ Open the **Card 1** or **Card 2** memory in the file manager
- ☞ Start data storage with **[Backup]** and answer the query "Do you want to start the backup?" with **[Yes]**.

Only one backup can be stored on each card. If you try to create a new backup on a card which already contains an older backup then this first backup will be overwritten.

You can load the backup data into your system with the **Recover** function. During the backup all your data is saved and, in the recover function, you can select individual data blocks to be loaded from the safety copy.

- ☞ Open the **Card 1** or **Card 2** memory in the file manager
- ☞ With **[Recover]** you can open the dialog for selecting the individual data blocks.



The following data blocks can be loaded individually:

- **Methods** (from the internal memory): all method stored in the internal memory as a file.
- **Sample data silo**: current sample data silo from the working memory.
- **Result silo**: result silo from the working memory.

- **Current determination data:** all the data for the current determination and the current method with which the determination was carried out.
 - **Control:** settings under control.
 - **User list** under System settings/User administration and settings for each user.
 - **System settings/User administration:** all system settings including device-specific dialog configuration and dialog options for the list of commands and fixed keys, device-specific settings for the user administration (login options, password options and audit trail).
 - **Titriments:** all titrant data.
 - **Sensors:** all sensor data.
 - **Device data** (Touch Control only): all data from the device manager.
 - **GLP data:** all data from the GLP manager. Please note that the GLP data cannot be loaded if you load the safety copy on a different system.
 - **Common variables:** all common variables.
 - **Templates:** all templates for sample data, result templates, remote lines, custom calibration buffers and report header.
 - **Routine dialog settings:** current routine dialog settings under Dialog options/Routine dialog.
- ☞ Deactivate the checkboxes for the data blocks which you do not wish to recover and load the activated data blocks with **[Load data]**.

You can also load a backup from Touch Control in PC Control and vice versa. When a Touch Control backup is loaded in PC Control then the device data is ignored.

- ☞ After the recovery you must shut down the **PC Control software** and then **restart** it, or switch **Touch Control off and then on again**.

3.12 GLP manager

In the **GLP manager** you can document data for various GLP tests. The results of the automatic system tests carried out after START are also documented. You can also draw up a list containing the test tools which you use and enter a service interval for having routine maintenance carried out by a Metrohm service technician.

Further information about quality management and validation is also given in the documentation series **Quality Management with Metrohm** and **Application Bulletin AB 252** (Validation of Metrohm titrators (potentiometric) according to GLP/ISO 9001). An example of a method for carrying out a validation according to AB 252 (**Validation according to AB 252**) is stored under Examples (see *Section 3.15.1*).

☞ Open the dialog **System/GLP manager**.

System / GLP manager		
Test	Last test	Next test
Automat. system test	2002-05-29	Power on
GLP test measurement	2002-04-30	2002-10-31
GLP test titration	2002-04-30	2002-10-31
System validation	2002-04-30	2002-10-31
<div> <div>Test tools</div> <div>GLP tests HW/SW</div> <div>System validat.</div> <div>Service interval</div> <div>View test data</div> </div>		

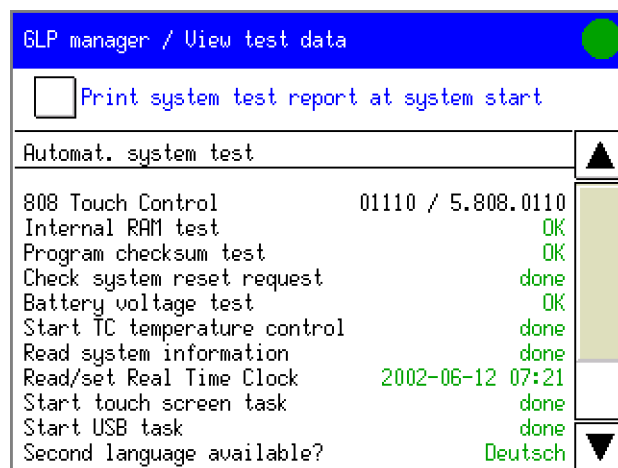
The table shows the last time that each test was carried out and when the next test is to be carried out. A test is entered in the list the first time that it is documented. The following tests can be documented: a **GLP test for measurement**, a **GLP test for titration** and the **system validation**.

You can view the results of the selected test with **[View test data]**.

3.12.1 Automatic system test

The system test is carried out automatically each time that the Touch Control is switched on or each time that the PC Control software is started.

- ☞ Select the line **Automatic system test** in the table and open the results page for the test with **[View test data]**.
- ☞ You can automatically print out the results of the automatic system test each time that the system starts up by activating the **Print system test report at system start** checkbox.



With Touch Control (see example) the test is very comprehensive. The result of each test is shown in **green** if no error has occurred. If a result is shown in **red** then an error occurred when the corresponding test was carried out. Switch the system off and then on again. If the error still occurs please consult Metrohm Service.

3.12.2 Service interval

You can monitor the **time interval** after which the Titrando system must be serviced again.

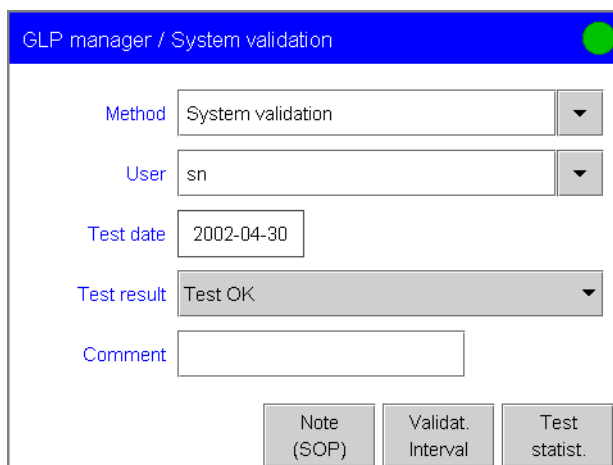
- ☞ Open the dialog **GLP manager/Service interval**. Enter the date upon which the last service was carried out and activate the **Monitoring** checkbox.
- ☞ Enter either the **Service interval** or date for **Next service**. If the time interval or date is edited then the other parameter will be updated automatically.

When the service interval has expired then the corresponding message will appear at the START of a determination; this will also be documented in the determination data (see Section 3.18.2).

3.12.3 System validation

You can document the **System validation** results here and also define the time interval after which validation must be carried out again.

- ☞ To document the results of a system validation open the dialog **GLP manager/System validation**.



- ☞ You can select or enter the **Method** used for the system validation. Only methods in the internal memory will be shown in the selection list. You can also enter or select the **User** who carried out the validation from the selection list (see *Section 3.7.5*).
- ☞ Enter the **Test date** for the last validation and select the **Test result**.
- ☞ You can enter a **Comment** for each test.
- ☞ Open the dialog **System validation/Test statistics**. You can document the **statistical data** for the last system validation here. Please consult the **online help** for a description of the individual parameters.

You can monitor the **time interval** after which a **system validation** must be carried out again. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.)

- ☞ Open the dialog **System validation/Validation interval**. Enter the date on which the last system validation was carried out and activate the **Monitoring** checkbox.
- ☞ Enter either the **Validation interval** or the date for the **Next validation**. If the time interval or date is edited then the other parameter will be updated automatically.
- ☞ Select an **Action** to be carried out when the time interval has expired (see *Section 3.8.4*).

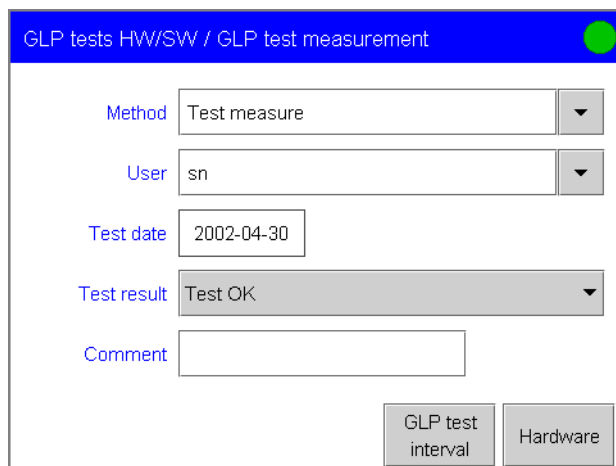
The validation interval will always be monitored at the START of a determination.

If you want you can enter a short note under **System validation/Note (SOP)**, e.g. a summary of the SOP (standard operating procedure) according to which the system validation was carried out.

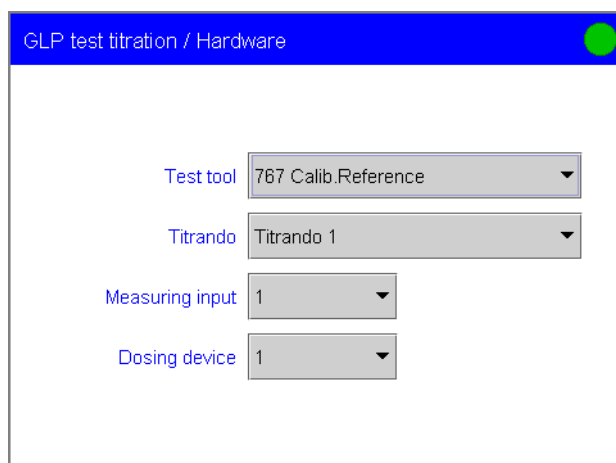
3.12.4 GLP tests for measurement and titration

You can document the **GLP tests for measurement and titration** here.

- ☞ Open the dialog **GLP manager/GLP tests HW/SW** (HW = hardware, SW = software).
- ☞ Select **[GLP test measurement]** or **[GLP test titration]** according to which GLP test you wish to document.



- ☞ For both tests you can select or enter the **Method** with which the test is to be carried out. Only methods in the internal memory will be shown in the selection list. You can also enter or select the **User** who carried out the test from the selection list (see Section 3.7.5).
- ☞ Enter the **Test date** for the last test and select the **Test result**.
- ☞ You can enter a **Comment** for each test.
- ☞ Open the dialog **GLP test measurement/Hardware** or **GLP test titration/Hardware**.



- ☞ Select the **Test tool** (list under **GLP manager/Test tools**), **Titrando** (configured in Device manager), **Measuring input** and **Dosing device** (GLP test titration only) used for the test.

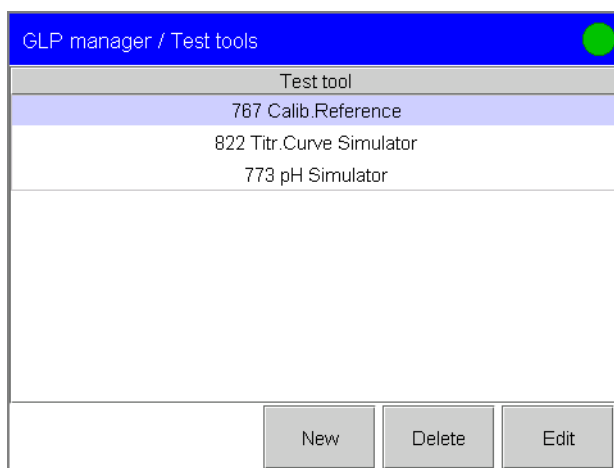
You can monitor the **time interval** after which a **GLP test** must be carried out again. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.)

- ☞ Open the dialog **GLP test measurement/Test interval** or **GLP test titration/Test interval**. Enter the date on which the last GLP test was carried out and activate the **Monitoring** checkbox.
- ☞ Enter either the **GLP test interval** or the date for the **Next GLP test**. If the time interval or date is edited then the other parameter will be updated automatically.
- ☞ Select an **Action** to be carried out when the time interval has expired (see *Section 3.8.4*).

The GLP test interval will always be monitored at the START of a determination.

3.12.5 Test tools

You can create a **list of test tools** to be used in the tests in the GLP manager.



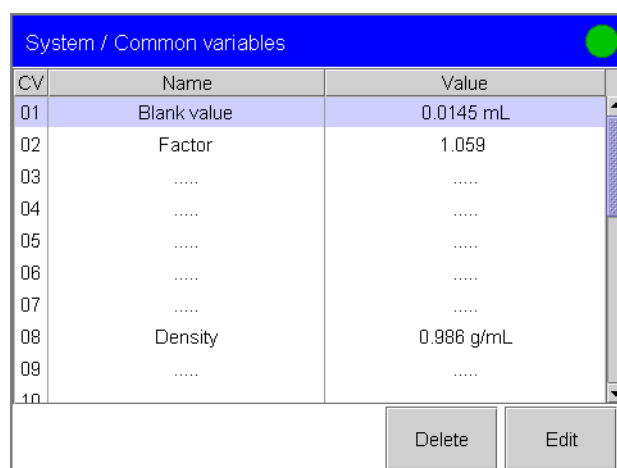
The list already contains definitions of some test tools.

You can add and edit new test tools with **[New]**. Test tools can be removed from the list with **[Delete]**. The dialog for entering the data for the new tool is opened with **[Edit]**. You can enter a name and comment for each test tool.

3.13 Common variables

Up to 25 **device-specific, method-independent variables** can be stored in the system. These variables can be calculated as **CV01** to **CV25**. Common variables are always used when a result from one determination carried out with Method A is to be used in a determination carried out with Method B. Typical uses are in the determination of a **Blank value** or the content of a standard solution to be taken into consideration when calculating the content in a sample. Common variables can also be automatically requested during the course of a determination (see *Section 4.9.3*). This allows the entry of additional data for the sample which can be used in calculations, e.g. the density, etc.

☞ Open the dialog **System/Common variables**.



CV	Name	Value
01	Blank value	0.0145 mL
02	Factor	1.059
03
04
05
06
07
08	Density	0.986 g/mL
09
10

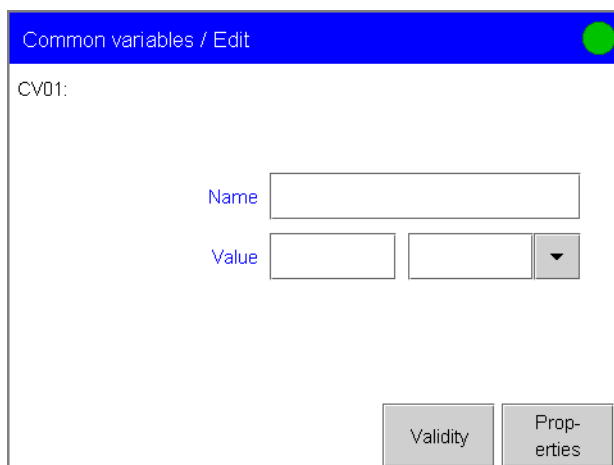
The list of common variables contains the name and values for all 25 common variables. Variables to which no value has yet been assigned are indicated by ".....". The selected common variable is deleted with **[Delete]**. **[Edit]** opens the dialog for entering the common variable and monitoring its validity.

3.13.1 Editing common variables

There are three basic ways of editing a common variable: the common variable is edited either under **Common variables/Edit** or entered manually in a **request** in the determination sequence or the variable is automatically assigned to a result in the determination sequence in a **result calculation**.

Editing common variables manually:

☞ Select the common variable to be defined or edited from the list and open the dialog **Common variables/Edit**.



☞ Enter a name for the common variable under **Name**.

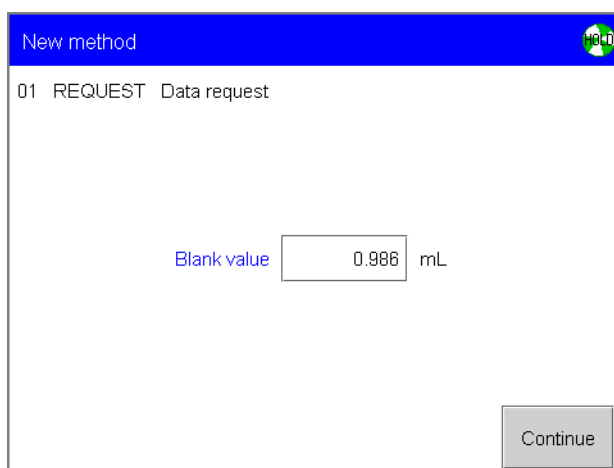
☞ Enter the **Value** and the unit of the common variable.

The name and unit will be shown automatically when the value of the common variable is asked for with a REQUEST command (see below).

Requesting a common variable during a determination sequence:

☞ Define a **REQUEST command** in the method as described in Section 4.9.3.

☞ Define the variable that you want to request (**CV01** to **CV25**) under **Common variable** in the parameter dialog for the REQUEST command. During the determination sequence you can then enter the value of the common variable. The name and unit will be shown in the request. They can be altered under **System/Common variables** (see above).



If you wish to output the common variable as a result then you must define a CALC (calculation) command in the method and calculate a result $RX = CVXX$ (see Section 4.4.1).

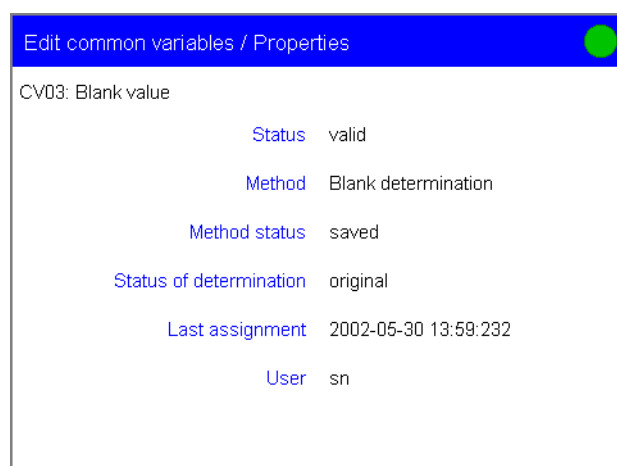
Automatic assignment of a result to a common variable, e.g. for a blank value determination :

- ☞ Define a **CALC (calculation) command** in the method in which the result (e.g. the blank value) to be assigned to the common variable is calculated. This can also be the mean value of a multiple determination (see *Section 3.21* and *4.4.1*).
- ☞ In the parameter dialog activate the **Save result as common variable** checkbox in the CALC command under **Edit result/Result options** and select the **Variable (CV01 to CV25)** to which the result is to be assigned. The name and unit of the value will also be assigned to the common variable as well as the value.

In further determinations you can use this result (e.g. the blank value) as a common variable (CV01 to CV25, selected as above) in calculations.

3.13.2 Properties of common variables

Under **Edit common variables/Properties** detailed information about the common variables is shown. The **Status** of the common variable can either be valid or invalid. The value is invalid when no value has been entered or when the time interval for the validity has expired (see *Section 3.13.3*). The method with which the result has been assigned to the common variable is shown under **Method**. If the common variable has been edited manually then **manual** will be shown. **Method status** and **Determination status** are only shown when the common variable is to be assigned automatically in the determination sequence with a CALC command. The date and time of the last alteration of the value of the common variable are shown under **Last assignment**. The user who was logged in when the common variable was assigned or manually edited is shown under **User**.



3.13.3 Monitoring the validity

You can monitor the **time interval** after which the common variable must be assigned a new value. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.)

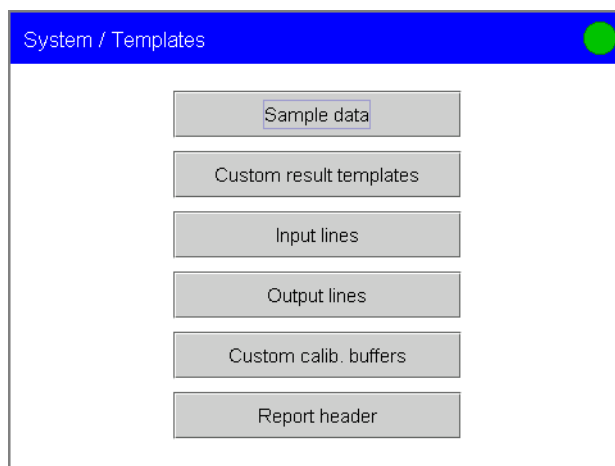
- ☞ Open the dialog **Edit common variables/Validity** and activate the **Monitoring** checkbox.
- ☞ Enter either the time interval for the **Validity** of the common variable or the date for the **Next assignment**. If the time interval or date is edited then the other parameter will be updated automatically.
- ☞ Select an **Action** to be carried out when the time interval has expired (see *Section 3.8.4*). The validity of the common variable will be checked on each START of a determination if the particular common variable is to be used in the method.

When the validity of the common variables is being monitored then the date for the **Next assignment** will be shown under **Common variables/Edit**.

3.14 Templates

You can define **system-specific templates** for sample data, result calculations, remote lines, calibration buffers and the report header. You can use these templates when editing the corresponding data.

☞ Open the dialog **System/Templates**.

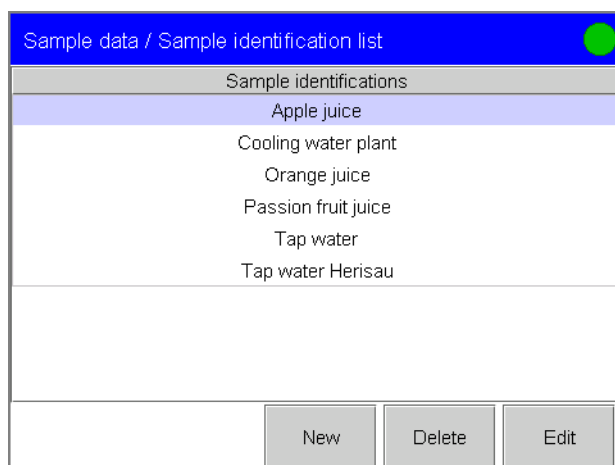


3.14.1 Sample identification list

You can create a system-specific list with templates for sample identifications. You can select from this list when entering the sample data **Identification 1** and **Identification 2** in the main dialog, during a sample data request (REQUEST command) or in the sample data silo (see Section 3.19). The **sample identification list** makes it easier for you to enter frequently used sample identifications. It may be a good idea to define the unchanging part of the identification as a template and to add the variable part during sample data input.

☞ Open the dialog **Templates/Sample data**.

☞ Open the list of templates for the sample identifications with [**Sample identification list**].



- ☞ Use **[New]** to define all sample identifications which are to be available for selection one after the other.

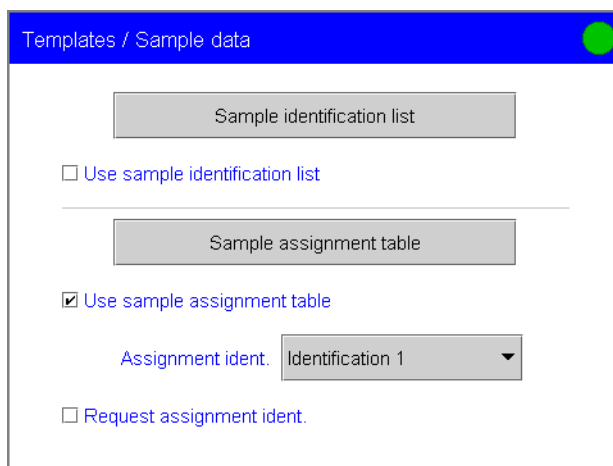
The dialog in which you can enter the templates for **sample identifications** is opened automatically with **[New]**. For an existing template this dialog can be opened with **[Edit]**. Existing sample identifications can be removed from the list with **[Delete]**.

- ☞ Exit the dialog with **[Back]** and activate the **Use sample identification list** checkbox so that you can select from the templates when entering the sample data.

3.14.2 Sample assignment table

If you use the **sample assignment table** then you can be sure that the samples will be processed with the **correct method**. In the sample assignment table a sample identification is assigned to a particular method. Samples with an identification which appears in this table can only be processed by the assigned method. This means that no mistakes can occur. The user enters the sample identification and at the START of the determination the correct method is loaded automatically.

- ☞ Open the dialog **Templates/Sample data**.



- ☞ Use **[Sample assignment table]** to open the list of sample identifications with their assigned methods.

Sample data / Sample assignment table	
Sample ident.	Method
Apple juice	Formol number
Cooling water plant *	p+m value
Mineral water	Chloride determination
Orange juice	Formol number
Passion fruit juice	Formol number
Tap water	Water hardness
<div> <div>New</div> <div>Delete</div> <div>Edit</div> </div>	

☞ You can define new sample assignments with **[New]**.

The dialog in which you can enter the templates for **sample identifications** is opened automatically with **[New]**. This dialog can be opened with **[Edit]** for an existing template. Existing sample identifications can be removed from the list with **[Delete]**.

Sample assignment table / Edit	
Identification	<input type="text"/> ▼
Memory	Internal memory ▼
Method	<input type="text"/> ▼
<div>Cancel</div>	

- ☞ Enter the **Identification** for the sample assignment. You can also select an identification from the sample identification list (see Section 3.14.1). You can enter an * as a wildcard at the beginning or end of the character string. In this way, for example, you can append a running number which will be ignored during the method assignment (see example **Cooling water plant ***). Upper and lower case letters will be differentiated in the comparison.
- ☞ Enter the **Memory** from which the method is to be loaded. Data memories which cannot be currently accessed can also be entered.
- ☞ Enter the name of the **Method** with which the sample is to be processed. If the method is already stored in the memory selected above then it can also be selected.
- ☞ Exit the input dialog and activate the **Use sample assignment table** checkbox under **Templates/Sample data**. Determinations can now only be carried out when the assignment identification has been entered and is present in the sample assignment table.

- ☞ Choose whether **Identification 1** or **Identification 2** is to be used for the **Assignment identification** in order to load the correct method.
- ☞ You can also request the assignment identification automatically after the START. If the **Request assignment identification** checkbox is activated then the method with which the sample is to be processed will only be loaded when the assignment identification is entered and confirmed with **[Continue]**.

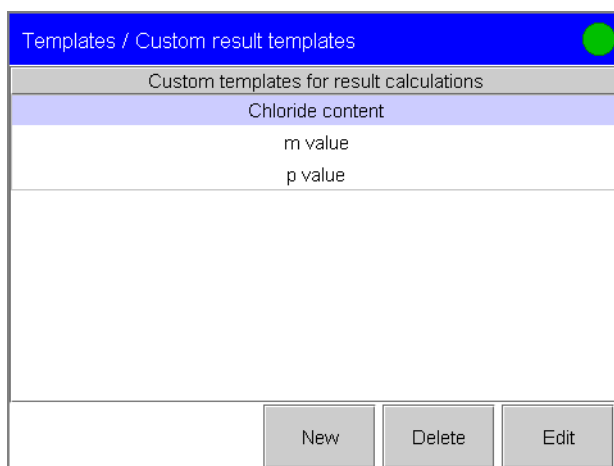

Note!

*If you have activated **Use sample assignment table** then you can no longer define the method to be used for processing the sample in the **sample data silo**. If methods have already been defined then they will be ignored.*

3.14.3 Custom results templates

Templates can be created for editing result calculations in the methods; these can be loaded when editing CALC commands.

- ☞ Open the dialog **Templates/Custom result templates**.



With **[New]** you can define new templates. Existing templates can be removed from the list with **[Delete]** or altered with **[Edit]**.

- ☞ Use **[New]** to open the edit dialog for a new result template.

Custom result templates / Edit

Result name

R

Calc. formula R

Decimal places

2

Result unit

%

Note

Note for wizard

Result options

Creating result templates is carried out in the same way as editing the result calculations in the CALC command (see *Section 4.4.1*). A **Note for wizard** can also be entered. This note will be shown when the template is loaded during the creation of a new result in the CALC command.

Further special features when creating result templates are described in *Section 4.4.3*.

3.14.4 Input lines

Binary patterns can be defined for **scanning remote lines** with the **SCAN command** (see *Section 4.8.1*) during the determination sequence; these can then be selected when editing the parameters.

 Open the dialog **Templates/Input lines**.

Templates / Input lines

Signal name	Input signal
Sample ready	***1****

New

Delete

Edit

You can define new templates with **[New]**. Existing templates can be removed from the list with **[Delete]** or edited with **[Edit]**.

One template is already defined: **Sample ready**: *****1****** waits for the corresponding signal from a connected sample changer to indicate that this is ready.

☞ Use **[Edit]** to open the edit dialog for the template **Sample ready**.

To input the binary pattern please consult the **online help**.

3.14.5 Output lines

Binary patterns can be defined for **setting remote lines** with the **CTRL command** (see *Section 4.8.2*) during the determination sequence or manually under manual operation (see *Section 3.24.5*); these can then be selected when editing the parameters.

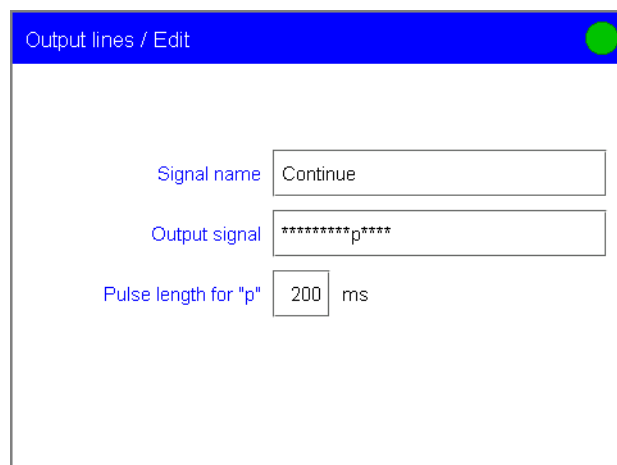
☞ Open the dialog **Templates/Output lines**.

Signal name	Output signal
Continue	*****p****
Init	0000000000000000
Start Dosimat	*****p*****

You can define new templates with **[New]**. Existing templates can be removed from the list with **[Delete]** or edited with **[Edit]**.

Three templates are already defined: **Continue: *****p****** sends a continuation pulse to a connected sample changer, **Init: 0000000000000000** initializes the remote interface, **Start Dosimat: *****p******* starts a connected 665, 725, 765 or 776 Dosimat with an activation pulse (6.2139.000 Cable).

☞ Use **[Edit]** to open the edit dialog for the template **Continue**.



Output lines / Edit

Signal name: Continue

Output signal: *****p****

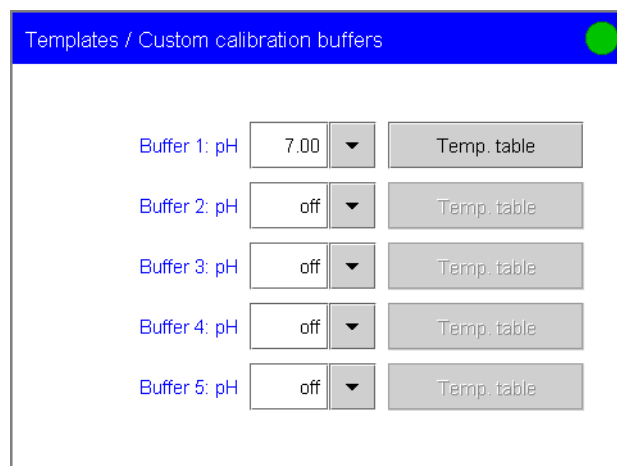
Pulse length for "p": 200 ms

You can also set pulses for the lines by entering a **p** in the binary pattern. The pulse length is defined under **Pulse length for "p"**. The pulse length can only be entered for signals which are defined as templates. If you define a signal directly in the CTRL command (see *Section 4.8.2*) or in manual operation (see *Section 3.24.5*) then a fixed pulse length of 200 ms will be used. To input the binary pattern please consult the **online help**.

3.14.6 Custom calibration buffers

You can define five of your own calibration buffers which can then be used for **calibration with automatic buffer recognition**. The buffer series can be selected in the **CAL** (calibration) command as the **Custom** buffer series (see *Section 4.6*).

☞ Open the dialog **Templates/Custom calibration buffers**.

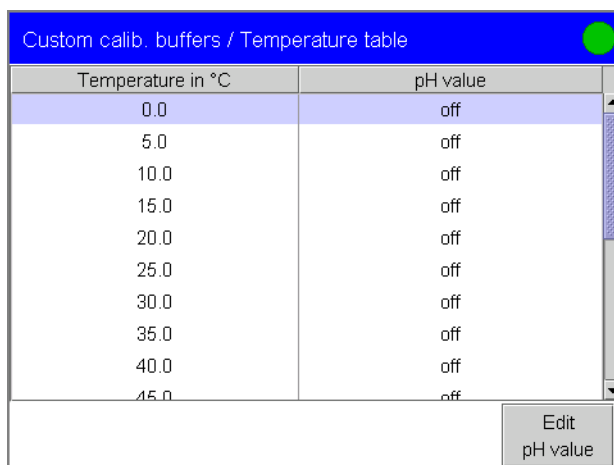


Templates / Custom calibration buffers

Buffer 1: pH	7.00	▼	Temp. table
Buffer 2: pH	off	▼	Temp. table
Buffer 3: pH	off	▼	Temp. table
Buffer 4: pH	off	▼	Temp. table
Buffer 5: pH	off	▼	Temp. table

☞ Enter the pH of the first buffer under **Buffer 1**.

☞ Use **Temp. table** to open the temperature table for this buffer. The temperature table shows the pH values for the buffer at temperatures from 0 to 95 °C.



Temperature in °C	pH value
0.0	off
5.0	off
10.0	off
15.0	off
20.0	off
25.0	off
30.0	off
35.0	off
40.0	off
45.0	off

Use **[Edit pH value]** to enter the pH value for the temperature range in which your pH measurements will later be carried out. In the dialog **[Temperature table/Edit pH value]** you can change directly to the next temperature. If you do not know the pH values for individual temperatures then these will be automatically calculated by linear interpolation.

You can select your own buffer calibration series in the **CAL command** (calibration) as **Buffer type: Custom**.


3.14.7 Report header

You can enter a text here (max. four lines each with 46 characters) which will always be printed out in front of the standard report header (see Section 3.23).



Enter the text for your **Report header**. If you want to print out the Metrohm logo to the right of the text then activate the **Print logo** checkbox.

The settings shown above will produce a report header which looks like this:

Metrohm AG 9100 Herisau Switzerland		 Metrohm
PC Control PC Control Laboratory 1	Serial number 3079972211 Printed	Program version 1.0 2002-06-03 11:00:27

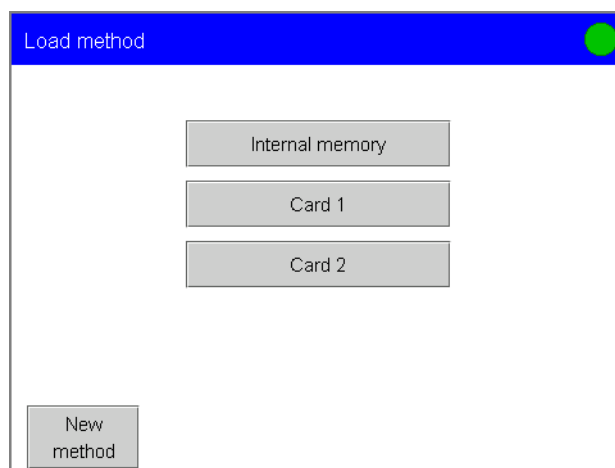
3.15 Loading methods

The sequence of a **determination** is defined in the **method**. In the **Load method** dialog you can load methods from a file memory or **method templates** for creating new methods.

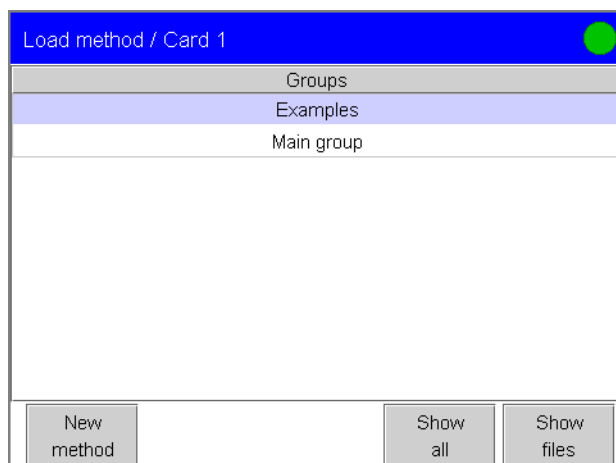
3.15.1 Loading a method

With Touch Control and PC Control the methods can be stored in the internal memory, on Card 1 and on Card 2 (see also *Section 3.11*). In a new system no methods are stored in the internal memory which is why the following example describes **loading a method from Card 1**, on which the methods provided as examples are stored.

- ☞ With **Touch Control** insert the supplied data card containing the examples of methods (6.6048.000) in Card slot 1.
- ☞ From the main dialog open the dialog **Load method** and select **[Card 1]** as the file memory.

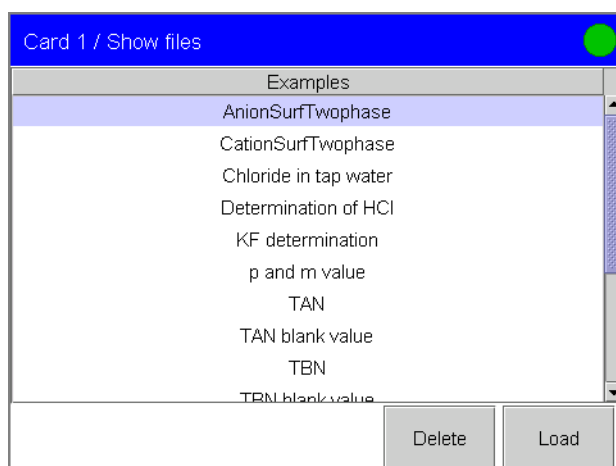


The selection of the file memory will be skipped if neither of the cards can be accessed and only the internal method memory is accessible. If several **file groups** exist on the card then a list showing the existing **groups** will be displayed:



The selection of the group will be skipped if only one group is present in the selected memory.

- ☞ Select the group **Examples** and open the file list for this group with **[Show files]**. With **[Show all]** you can open the list of files containing all the methods in the selected memory.



- ☞ Select a method from the list, e.g. **Determination of HCl** and load it into the working memory with **[Load]**. When the file has been loaded the program will jump automatically to the main dialog. If the method contains a **Note** which is displayed when the method is loaded then this can be closed with **[Continue]**. You can edit the method with **[Edit parameters]** (see Section 3.16).



Note!

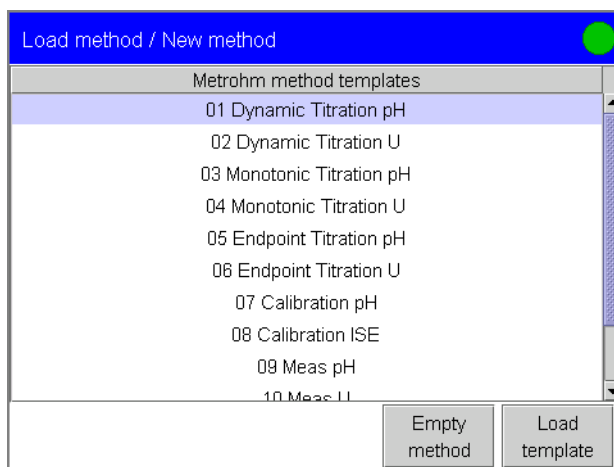
*The data of the current **determination** will be **deleted** if a new method is loaded.*

You can use the procedure described above to load methods from all available file memories. The selected file can be removed from the list of files with **[Delete]**. If you have activated **Write protection** for the method in the **File manager** under **Show files/Properties** then it cannot be deleted.

3.15.2 Creating a new method

If you wish to create a new method then you can either load a **method template** from the selection list and adapt it to meet your requirements or load an **"empty" method** in which no sequence of commands has yet been defined.

☞ From the main dialog open the dialog **Load method** and then open the list of method templates with **[New method]**.



The individual templates are described on the following pages. The commands in the method templates have standard parameters. These standard parameters are suitable for most titrations.



Note!

*If you would like to test a **new titration method** then select the **Dynamic titration pH or U** template. Dynamic titration is suitable for practically all standard applications and you only have to adapt individual parameters in special cases.*

No results have been defined yet in the calculations (see Section 4.4.1).

☞ Select a method template from the list and load it with **[Load template]** or load a method template in which no sequence of commands has yet been defined with **[Empty method]**. When the file has been loaded the program will jump automatically to the main dialog. You can edit the method with **[Edit parameters]** (see Section 3.16). This method has the name **New method**. You can change this name when you save the method (see Section 3.16.10).

The following **method templates** can be selected:

<i>Method template</i>	<i>Command sequence</i>	<i>Application</i>
01 Dynamic titration pH	DET pH (dynamic titration) CALC REPORT (result report and titration curve)	Dynamic reagent addition , for rapid equivalence point titrations, large volume increments in the flat part of the curve; small increments near the EP, many measuring points near the EP. For all standard titrations (acid/base titrations, precipitation titrations, redox titrations).
02 Dynamic titration U	DET U (dynamic titration) CALC REPORT (result report and titration curve)	
03 Monotonic titration pH	MET pH (monotonic titration) CALC REPORT (result report and titration curve)	Reagent addition with constant volume increments , relatively few measuring points near the EP. For titrations with relatively high signal variations or a suddenly occurring potential jump, very flat potential jumps, slow titrations (non-aqueous titrations, certain redox titrations, surfactant determinations).
04 Monotonic titration U	MET U (monotonic titration) CALC REPORT (result report and titration curve)	
05 Endpoint titration pH	SET pH (endpoint titration) CALC REPORT (result report and titration curve)	Titration to a predefined endpoint . For rapid routine determinations , titration to particular standards and titrations in which an excess of titrant must be avoided (p+m values, pH adjustment).
06 Endpoint titration U	SET U (endpoint titration) CALC REPORT (result report and titration curve)	
07 Calibration pH electrode	CAL pH (calibration of a pH electrode) REPORT (result report with calibration data and titration curve)	Calibration of pH electrodes.
08 Calibration ISE electrode	CAL Conc (calibration of an ISE sensor) REPORT (result report with calibration data and titration curve)	Calibration of ion-selective electrodes.
09 Measure pH	MEAS pH (pH measurement) CALC REPORT (result report and measurement curve)	pH measurement.

<i>Method template</i>	<i>Command sequence</i>	<i>Application</i>
10 Measure U	MEAS U (potential measurement) CALC REPORT (result report and measurement curve)	Potential measurement.
11 Measure temperature	MEAS T (Temperature measurement) CALC REPORT (result report and measurement curve)	Temperature measurement with a temperature sensor (Pt1000 or NTC).
12 Measure concentration	MEAS Conc (concentration measurement) CALC REPORT (result report and measurement curve)	Ion concentration measurement with an ion-selective electrode.

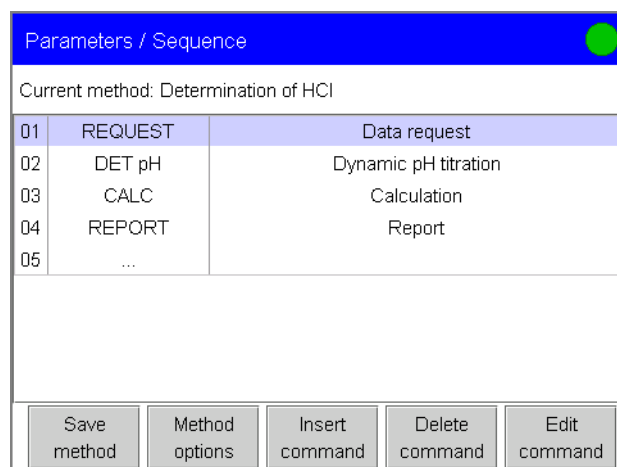

Note!

If you have no **printer** connected to your system then you should delete all **REPORT commands** from the list of commands.

3.16 Editing parameters

Here you can define and edit the **method commands** which are processed successively during a **determination**. The **current method** loaded in the working memory will always be edited.

☞ From the main dialog use **[Edit parameters]** to open the **list of commands** for the current method. If you have loaded a method (see *Section 3.15.1*) then the list of commands will already contain a sequence of method commands. If you have used **[Empty method]** to create a new method (see *Section 3.15.2*) then the list of commands will still be empty.



Parameters / Sequence		
Current method: Determination of HCl		
01	REQUEST	Data request
02	DET pH	Dynamic pH titration
03	CALC	Calculation
04	REPORT	Report
05	...	
<div> <div>Save method</div> <div>Method options</div> <div>Insert command</div> <div>Delete command</div> <div>Edit command</div> </div>		

In the **list of commands** the **command number**, **command name** and the **command comment**, which you can edit yourself, are shown for each command. The last command line is always empty. It can neither be deleted nor edited.

With **[Insert command]** you can insert a new method command in the list in front of the selected command (see *Section 3.16.2*). With **[Delete command]** the selected command is removed from the list. You can edit the parameters for the selected command with **[Edit command]** (see *Section 3.16.1*).

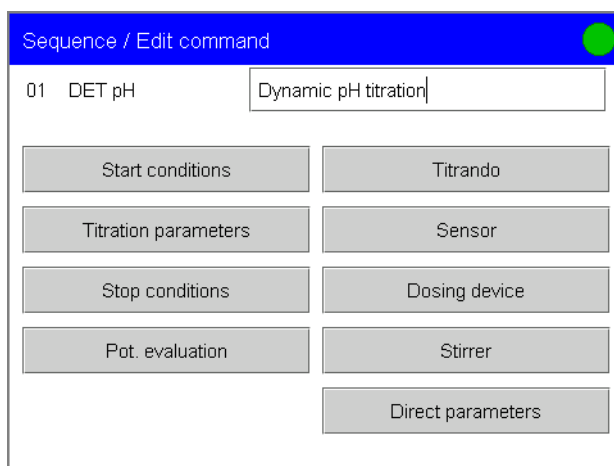
In the dialog **Sequence/Method options** you can make settings which apply to the whole method and not just to individual commands. With **[Save method]** you can store the method in one of the memories (internal memory, Card 1, Card 2) (see also *Section 3.11* and *Section 3.16.10*).

3.16.1 Editing commands

The edit dialog differs greatly according to the number of **parameters** which can be edited in a method command. For example, the REQUEST command requires only a single dialog level for parameter input. Editing a titration (e.g. DET pH) is considerably more complex, although standard titrations can be carried out with the standard para-

meters and parameters only need to be altered for special applications or instrument configurations. In a CALC command up to nine results can be defined; a calculation formula is entered for each result and various options are defined (see *Section 4.4.1*). An **overview of all commands and parameters** can be found in *Section 4*. The **input range** for all parameters can be found in the **online help**.

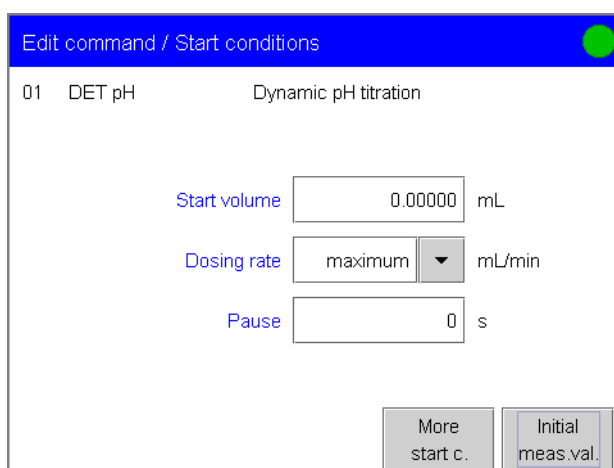
☞ Select the command in the list for which you want to edit the parameters and open the edit dialog with **[Edit command]**. In the example shown the command **DET pH** has been selected.




Note!

The **Titrande** button will only be shown when several Titrands have been logged in to the device manager.

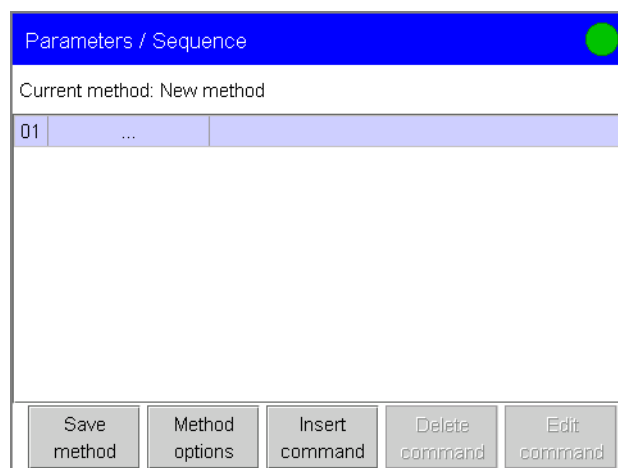
☞ Open the edit dialog for the start conditions with **[Start conditions]**.



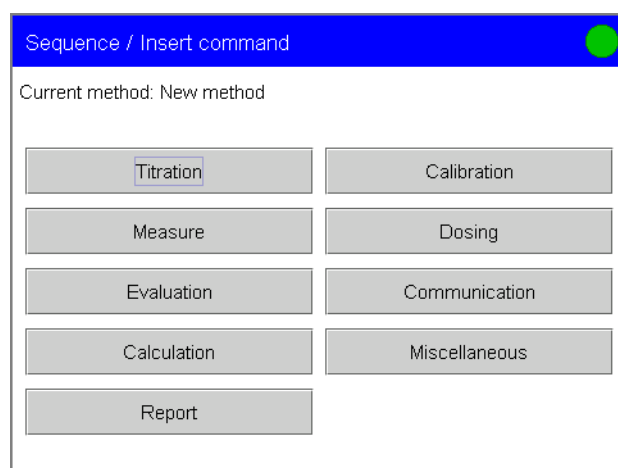
For many parameters (e.g. **Start volume** and **Pause**) you can enter a numerical value directly, with other parameters (e.g. **Dosing rate**) you can use the arrow to the right of the input field to alternatively select a "special value" from the combo box. It is often only possible to choose between various settings in a combo box (e.g. **Measuring input** under **Edit command/Sensor**).

3.16.2 Insert command

A method may contain a sequence of max. 99 commands. You can use **[Insert command]** to insert a new method command in front of the selected line. In the example shown a new "empty" method is being edited.



☞ Use **[Insert command]** to open the dialog **Sequence/Insert command**.



The method commands are arranged in different groups. An **overview of all commands and parameters** can be found in *Section 4*. The individual commands are also described in the **online help**.

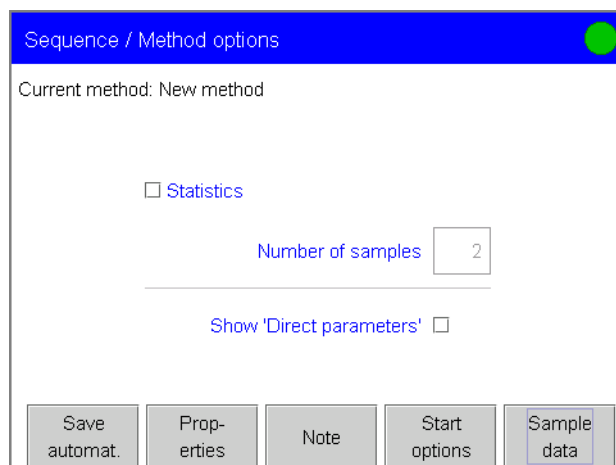
☞ Select the group from which you wish to insert a command. For **Calculation** and **Report** the command is inserted directly. For all other groups the command selection list is opened for you to select a command.

After a command has been inserted the list of commands is automatically shown again. The inserted command is shown as selected so that you can use **[Edit command]** directly to edit the parameters of the newly inserted command (see *Section 3.16.1*). You can insert a maximum of nine titrations or measurements and nine calculations. There is no limit to the number of other commands (up to 99 in one method).

3.16.3 Method options

Method options are settings which apply to the method as a whole and not to an individual command. For example, you can switch **Statistics** on and off, **Show direct parameters** on and off, **automatically save the determination at the end of the run**, enter a **Note** and make the **settings for sample data input**.

☞ Open the dialog **Sequence/Method options**.



3.16.4 Statistics

If you want to statistically evaluate certain **results** which have been calculated during the determination sequence by using a **CALC** command then you must make the following settings:

- ☞ Activate the **Statistics** checkbox if statistical calculations are to be carried out.
- ☞ Enter the **Number of samples** on which the statistics are to be based. For example, if you carry out a three-fold determination then you should enter **3**.

The results to be calculated in a determination on which statistical calculations are to be carried out are defined in the corresponding **CALC command** (see *Section 4.4.1*).

3.16.5 Direct parameters

Direct parameters can be defined for many method commands; they are then shown in a table when the parameter dialog is opened and can be edited directly. The direct access ("**Quick Access**") to the edit dialog for selected method parameters simplifies the editing of parameters which need to be changed frequently.

- ☞ Activate the **Show direct parameters** checkbox and use **[Home]** to return to the main dialog. Now open the **Direct parameter list** with **[Edit parameter]**.

Parameters			
Current method: New method			
01	DET pH	Titration rate	optimal
01	DET pH	Stop volume	100.000 mL
01	DET pH	Stirring rate	8
Save method		Sequence	Edit parameter

The above example shows the direct parameters for a DET pH titration with standard settings. The parameters that are to be shown in the direct parameter list can be selected for each command in which direct parameters are available (see *Section 4*) under **Edit command/Direct parameters**.

You can open the edit dialog for the selected command with **[Edit parameter]** and then edit the parameter. The **command list** is opened with **[Sequence]**. **[Save method]** is used to store the method in one of the file memories (internal memory, Card 1, Card 2) (see also *Section 3.11* and *Section 3.16.10*).

3.16.6 Sample data

In the method you can adapt the **Title of the sample identifications 1** and **2** which are shown in the main dialog. You can also define the **Sample size unit** or a **Fixed sample size**. The sample size can then no longer be edited in the main dialog. If you define **Sample size limits** then these will be monitored during the determination after START and at the end of the determination.

Method options / Sample data	
Title	
<input checked="" type="checkbox"/> Identification 1	Identification 1
<input checked="" type="checkbox"/> Identification 2	Identification 2
<hr/>	
<input type="checkbox"/> Fix sample size	
Sample size	1.0 g
Limits smpl size	

If you do **not want to show an identification** in the main dialog you can deactivate the checkbox for the corresponding identification. If you

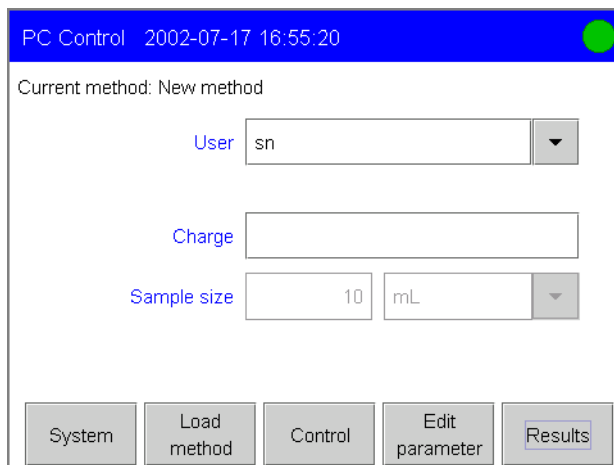
want to enter different method-independent titles for the identifications, e.g. batch number, density, etc. then you can enter your own titles under **Title**. These titles will be updated in the main dialog and when the sample data is requested with a REQUEST command (see *Section 4.9.3*).

For the **Sample size** you can either enter a **unit** or select one; this will be shown in the main dialog but can still be altered later. The unit will be updated each time that the method is loaded in the main dialog.

If you always use the same amount of sample for your determinations then you can define a **Fixed sample size** in the method. The sample size is shown in the main dialog and can no longer be edited.

☞ Enter, for example, "Charge" as the **Title** for **Identification 1** and deactivate the checkbox for showing **Identification 2**. Activate the **Fixed sample size** checkbox and enter "10 mL" as the **Sample size**. Use **[Home]** to return to the main dialog.

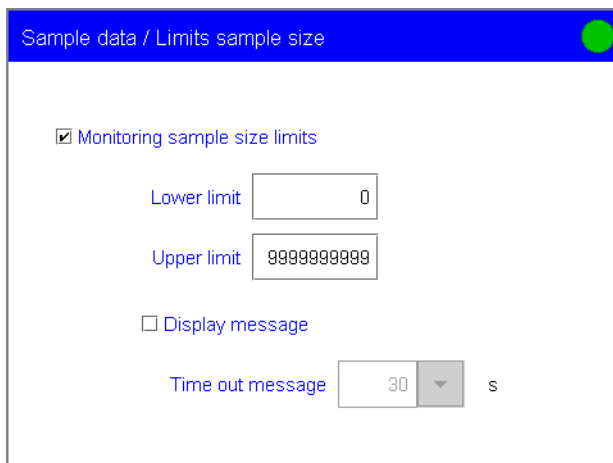
The main dialog will now appear as shown below:



Only Identification 1 is shown with the title "Charge". The fixed sample size "10 mL" is shown and cannot be edited.

You can also define the **limits for the sample size** which will then be monitored in the determination sequence.

☞ Open the dialog **Sample data/Sample size limits** and activate the **Monitoring sample size limits** checkbox.



☞ Enter a **Lower limit** and an **Upper limit** for the sample size.

The limits will not be monitored when the sample size is entered in the main dialog, but at the START of the determination and at its end, when an automatic sample data request is made with a REQUEST command (see Section 4.9.3), and on recalculating a determination (see Section 3.18.8). It does not matter whether the sample size has been entered in the main dialog "by hand", transmitted by a balance or barcode reader or entered in the sample data silo. When monitoring is switched on and the limits for the sample size are infringed then an **entry in the message list** for the determination will be made automatically (see Section 3.18.2).

Activate the **Display message** checkbox if a message is to be shown during a determination sequence to indicate that the sample size limits have been infringed. You then have the choice of continuing the run or of canceling it. This **Message** can be provided with a **Time out**, i.e. it will vanish automatically when the given time has elapsed and the run will be continued automatically.

3.16.7 Start options and note

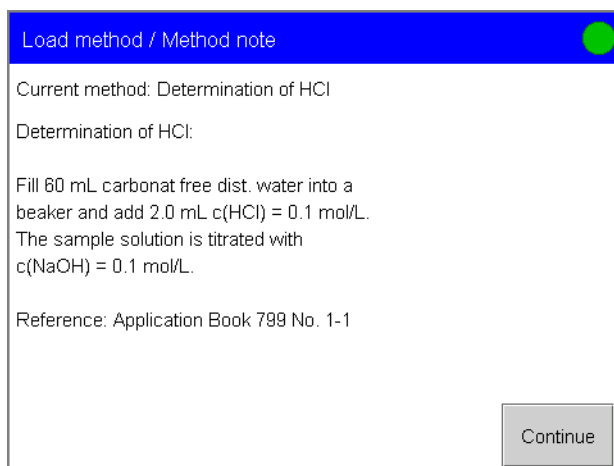
Under **Method options/Start options** you can switch off the **Start check**, which is carried out automatically after the START of a determination. This avoids delays after the START. The Start check verifies whether all devices, titrants and sensors which are necessary for the run are present and whether monitoring intervals for the titrants and sensors used have expired.



Note!

*We recommend that you only switch **Start check** off when the titration must be started directly after the START of the determination. For example, this is the case with **very rapid reactions** such as enzyme-catalyzed reactions. Otherwise the determination sequence could be interrupted because e.g. devices, titrants or sensors are not present and available for the determination. If the Start check is switched off then the monitoring intervals for titrants and sensors will be checked during the run.*

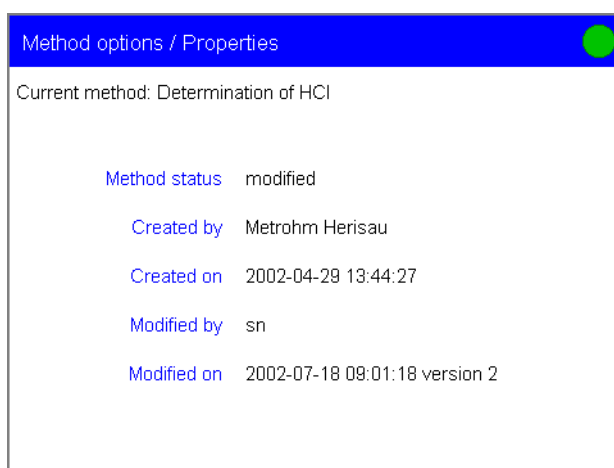
Under **Method options/Note** you can enter a short description of the method. If you activate the **Automatically after loading the method** checkbox under **Note/Display options** then the note will be shown after the method has been loaded. The note is concluded with **[Continue]**. You can use this function to provide the user with further important information about carrying out the determination. For example, after loading the method example **Determination of HCl** the following note will be displayed:



This function should not be used when the method is loaded automatically when processing a sample data silo (see *Section 3.19.3*).

3.16.8 Properties

The properties of the current method are shown under **Method options/Properties**.



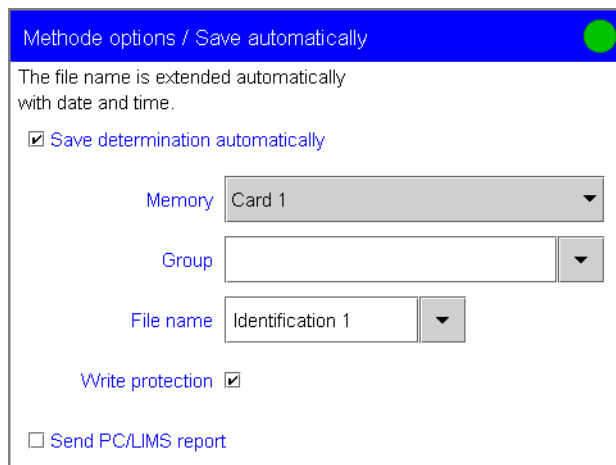
An explanation for the individual entries can be found in the **online help** (see also *Section 3.11.2*). The method shown as the example has already been saved twice (**version 2**). In comparison to the stored version 2 further parameters have been edited, so that the **Method status** is not **saved** but **modified**.

Information about the first person to save the method and when it was first saved (**Created by** and **Created on**) is given together with the last person to save the method and when it was last saved (**Modified by** and **Modified on**). Each time that the method is saved under the same name the version number is increased by one, even when the method is saved in a different memory.

3.16.9 Saving the determination automatically and sending a PC/LIMS report

In the method you can define that the **determination data** is to be saved automatically at the end of the determination sequence and/or saved or transmitted as a **PC/LIMS report**.

- ☞ Open the dialog **Method options/Save automatically** and activate the **Save determination automatically** checkbox.



Methode options / Save automatically

The file name is extended automatically with date and time.

☒ Save determination automatically

Memory Card 1

Group

File name Identification 1

Write protection ☒

☐ Send PC/LIMS report

- ☞ Under **Memory** select the memory in which the determinations are to be stored. Determinations can only be stored on **Card 1** or **Card 2** and not in the internal memory (see *Section 3.11*). Enter the **Group** in which the determinations are to be stored.

If you have retained the standard settings for the **File name** then it will be made up of the first 16 characters which you have entered for **Identification 1** and the **determination time** (date and time): Identification 1-YYYYMMDD-hhmmss. For the first 16 characters of the file name you can also select **Identification 2** or enter a different text. The date and time will be appended so that the file name is always unambiguous.

If the **Write protection** checkbox is activated then the saved determination files will be automatically write-protected and therefore protected against accidental alterations or alterations by unauthorized persons. This function is switched on by default so that the **original data** is also retained.

If the **Send PC/LIMS report** checkbox is activated then an ASCII report containing all the important data of the determination will be transmitted automatically at the end of the determination. The settings for transmit-

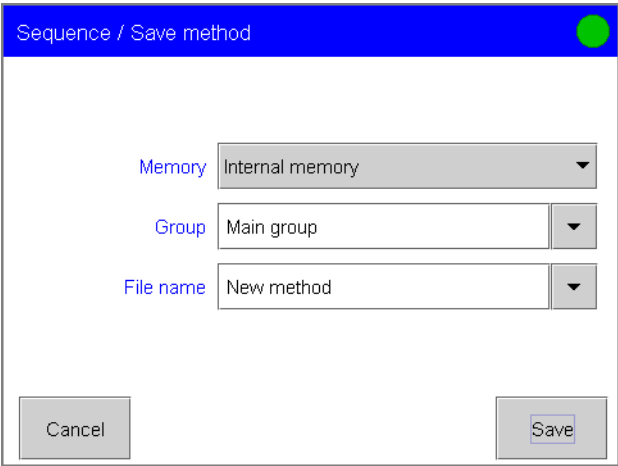
ting and saving the PC/LIMS report are made in the device manager under **Edit device/PC/LIMS report** (see *Section 3.10.7*). The file name corresponds to the name of the determination preceded with PC_LIMS_Report-. I.e. the format is PC_LIMS_Report-Identification 1-YYYYMMDD-hhmmss.txt if you keep the default settings for the **File name** under **Save determination automatically**. The date and time correspond to the determination time. A detailed description of the contents of the PC/LIMS report can be found in the Titrando **PC/LIMS Report Guide**.

3.16.10 Save method

You can save the current method in one of three memories (see *Section 3.11*).

- ☞ From the main dialog use **[Edit parameter]** to open the **command list** for the current method. If the use of direct parameters has been switched on (see *Section 3.16.5*) then the **direct parameter list** will be opened; the method can also be saved from here.
- ☞ Use **[Save method]** to open the dialog for selecting the memory, file group and file name.

If you have created a new method (see *Section 3.15.2*) and this has still not been saved then the dialog **Sequence/Save method** will look like this:



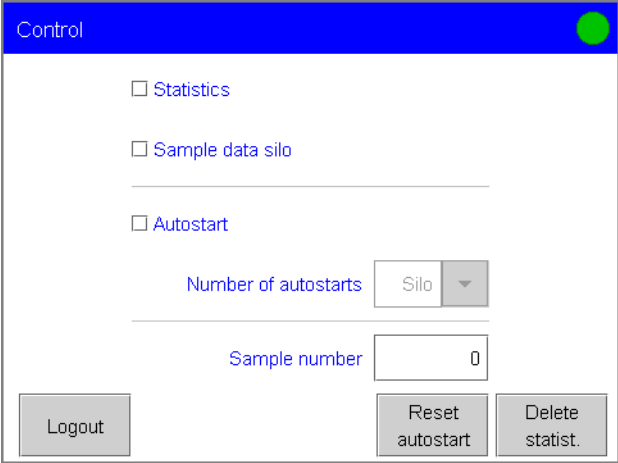
- ☞ Under **Memory** select the memory in which the method is to be saved. Methods can be saved in the **Internal memory**, on **Card 1** or **Card 2** or in a different external memory (see *Section 3.11*). Even if the method has been loaded from a card the default setting remains **Internal memory**.
- ☞ In order to arrange your methods they can be stored in different groups. Enter the **Group** in which the method is to be saved. You can also select the group from the list of existing file groups. If the method has already been stored then the group in which the method has already been stored will be proposed. In each memory all the **file names** must be **unambiguous**, i.e. you cannot save a file in different groups with the same name.

- ✎ Enter a **File name** for the method. If the method has already been stored then the name under which the method has already been saved will be proposed. The method is saved with **[Save]**. With **[Cancel]** and **[Back]** the method is not saved.

3.17 Control

This is where various **settings** for a determination run or for processing a series of samples are made. If you are working with login (see Section 3.7.7), then you can use **[Logout]** in this dialog to log out of the system. The login dialog will then be shown.

☞ From the main dialog open the **Control** dialog.



The **Sample number** is primarily used for documentation. Each time that a determination is started with START it is increased by one. Each time that the system is started (by starting the PC Control software or switching on Touch Control) it is reset to zero. You can also enter a sample number yourself.

3.17.1 Statistics

In the **Control** dialog you can switch **Statistics** on and off for individual determinations. Whether this checkbox is activated when the dialog is opened depends on whether statistics has been activated in the method under **Method options** (see Section 3.16.4). When a method is loaded the setting under Control is updated automatically.



Note!

*If you activate **Statistics** in the method under **Method options** then **Statistics** under **Control** will be activated automatically.*

This button is chiefly required to enable an "**urgent sample**" to be inserted while a series of samples is being processed without it being included in the statistics calculations. If you process the "urgent sample" with the same method as the sample series then you only have to switch the statistics button off while the urgent sample is being processed and then on again after it has been processed. If the "urgent sample" has to be processed with a different method then proceed as follows:

- ☞ Save the current sample series determination on a card (see *Section 3.18.5*) and load the method for the "urgent sample" (see *Section 3.15.1*).
- ☞ Carry out the determination for the "urgent sample" (see *Section 3.20.1*).
- ☞ Load the last determination in the sample series that you have previously saved (see *Section 3.18.6*). The method used and the statistics table will also be loaded together with the determination. The statistics button under **Control** and the statistics counter will have the same status as they had before the interruption to the sample series.
- ☞ Continue with the processing of the sample series.

You can view the statistics table under **Results/Statistics** (see *Section 3.21*). With **[Delete statistics]** you can delete the statistics table under **Control**. When the number set in the statistics counter (number of samples to be used to calculate the statistics) in the method under **Sequence/Method options** is the same as the actual number shown in the current statistics counter (number of processed samples) then the next time that the method is started the statistics table will be **automatically deleted**.

The statistics table will be **automatically deleted** when you use **[Load method]** from the main dialog to load a method into the working memory (see *Section 3.15.1*). It does not matter whether this is the same method that was previously loaded. If you use either the **sample data silo** (see *Section 3.19.3*) or the **sample assignment table** (see *Section 3.14.2*) then a check will be made whether the method is the same (file name is the same) as that which is already loaded in the working memory. Only when this is a different method will the new method be loaded and the statistics deleted.

When a determination is loaded the method with which the statistics are to be calculated is also loaded (see *Section 3.18.6*); this means that the current statistics are deleted when a determination is loaded.

3.17.2 Sample data silo

Under **Control** you can switch on the use of the sample data silo. The **sample data silo** is a table in which the sample data for a sample series can be entered and stored. If you have activated the **Sample data silo** checkbox then at each START of a determination the sample data will be taken from the silo memory. You can then open the sample data table in the main dialog with **[Sample data silo]**. The input of the sample data is described in *Section 3.19.3*.

With **Delete silo** (**Touch Control** only) you can delete all the lines in the current silo. The settings made under **Sample data silo/Properties** are retained.

3.17.3 Autostart

The autostart function is used for processing a sample series. If the **Autostart** checkbox is activated then a new determination will be started automatically when a determination has ended until the set **Number of autostarts** has been reached. The number of autostarts can also correspond to the number of samples defined in the sample data silo (see Section 3.19.2).

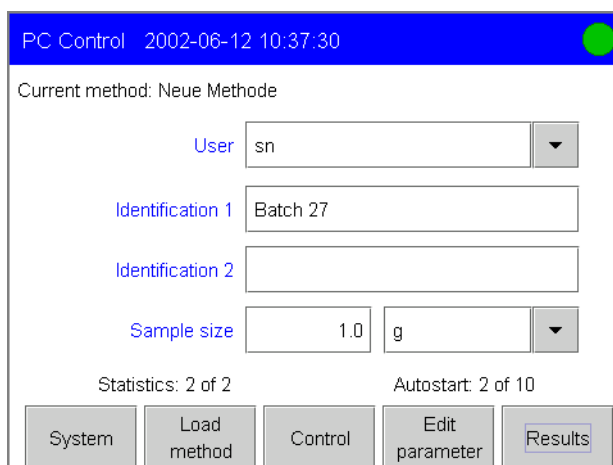


Note!

The **autostart function** is only suitable for **special applications**, e.g. multiple determinations in the same titration beaker where the determinations are carried out in succession without the user having to take any actions. If you are using a **sample changer** from which the Titrando is automatically started then the number of samples is defined in the sample changer. The autostart function of the Touch Control or PC Control is not used for such applications.

If you deactivate the **Autostart** checkbox while a determination is running then the current determination will be concluded but no new START will take place. With **[Reset Autostart]** you can reset the autostart counter, i.e. the number of autostarts which have already been carried out in a series, to zero.

The current **statistics status** and the current **autostart status** will be shown in the main dialog when these functions have been switched on.



PC Control 2002-06-12 10:37:30

Current method: Neue Methode

User: sn

Identification 1: Batch 27

Identification 2:

Sample size: 1.0 g

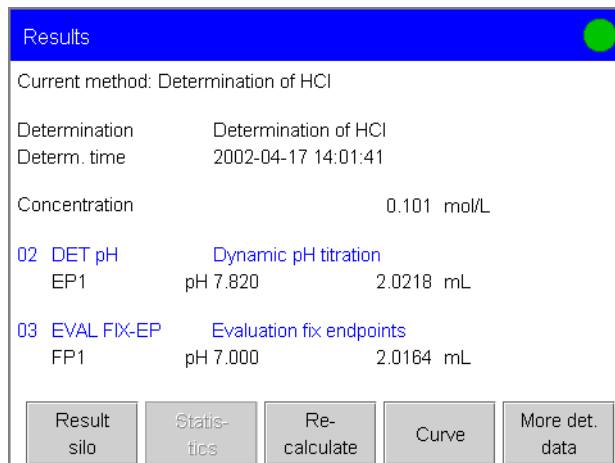
Statistics: 2 of 2 Autostart: 2 of 10

System Load method Control Edit parameter Results

3.18 Results and more determination data

The most important **details of the current determination** (method used to carry out the determination, name of the determination, determination time), the **calculated results** (result name and result with unit) and the **raw data** (e.g. endpoints or final measured values) are shown under **Results**.

☞ From the main dialog open the **Results** dialog.



From this dialog you can use **[More determination data]** to view **further data about the current determination** (measuring point lists, details of the endpoints, messages produced during the determination, properties of the determination, devices used, etc.). Under **Results/More determination data** you can **load and save determinations**. For the current determination you can use **[Curve]** to view the titration or measurement curves and **[Recalculate]** to recalculate and re-evaluate the determination.

From the results dialog you can also open the **Result silo**, a table with results which have been stored (see Section 3.22), and the **Statistics table** (see Section 3.21).



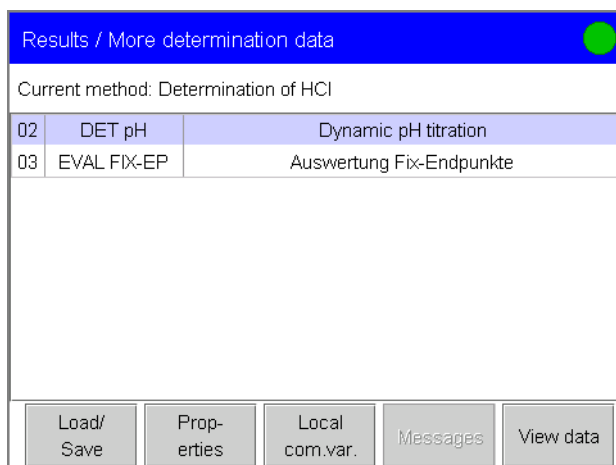
Note!

*The data of the current **determination** will be **deleted** if a new method is loaded.*

3.18.1 More determination data

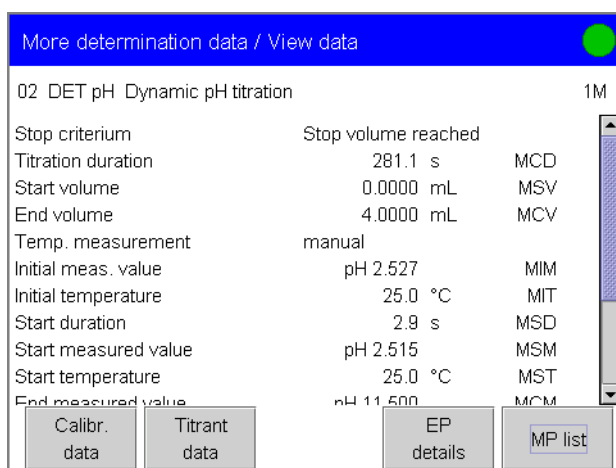
Under **Results/More determination data** a list containing all the method commands which produce raw data (DET, MET and SET titrations, MEAS measurements and CAL calibrations) and evaluations (EVAL commands) is shown.

☞ Open this list with **[More determination data]**.



Under **View data** the **raw data** and **variables** for titrations and measurements are shown. Details of evaluations are shown.

☞ Select a titration, measurement or evaluation and open the dialog **More determination data/View data**.



The **[Calibration data]** and **[Titrant data]** buttons are only shown for loaded determinations. With **[EP details]** you can view details of the endpoints and open the **measuring points list** with **[MP list]**.

In the first line the command and the command identification are shown (in the above example **1M**, i.e. the first titration/measurement command). The command identification is used for the unambiguous assignment of the variables to a mode. If only one titration or measurement is carried out in a determination then the command identification does not need to be given.

Below this is a list of raw data and variables. The abbreviation of the variable is shown for variables which can be used in calculations. The individual variables are described in *Section 4.4.3*. In addition to the variables, the **Stop criterion** used to stop the titration or measurement (manual stop, stop volume reached, error, etc.) and the type of **temperature measurement** (Pt1000, NTC or manual) are shown.

- ☞ With **[MP list]** you can view the **measuring point list** for a titration or measurement.

View data / MP list		
02 DET pH Dynamic pH titration		1M
Volume [mL]	Meas.value [pH]	ERC
0.00000	2.515	0.0
0.01000	2.513	6.3
0.02000	2.513	6.7
0.03000	2.515	7.4
0.45200	2.618	9.2
0.94800	2.783	12.8
1.31600	2.972	18.2
1.53400	3.140	24.9
		<input type="button" value="View"/>

With the **[Print]** fixed key you can print out the complete **measuring point list with all its columns**.

- ☞ With **[View]** you can choose which quantities are to be shown in the three columns. The quantities which can be selected depend on the titration or measuring mode. The settings are stored separately and system-specifically for each mode (DET, MET, SET, MEAS).
- ☞ From the dialog **More determination data/View data** you can use **[EP details]** to view more data about the equivalence points or endpoints. This button is only available for the titration modes (DET, MET, SET).

View data / EP details		
02 DET pH Dynamic pH titration		1M
Endpoint 1		
Volume	2.0218 mL	EP1
Measured value	pH 7.820	EM1
ERC	85.0	EF1
Time	162.4 s	ED1
Temperature	25.0 °C	ET1

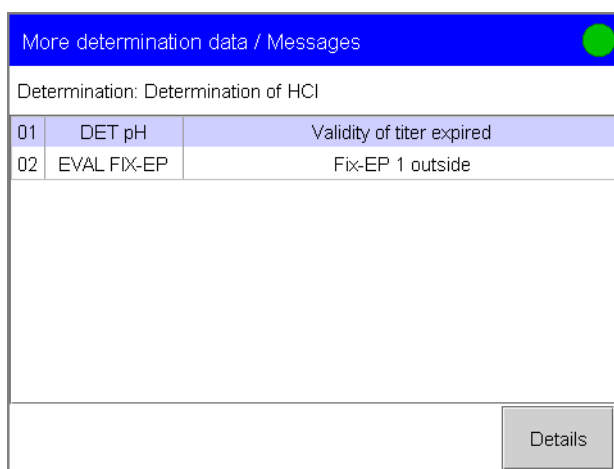
The individual variables are described in *Section 4.4.3*. The **ERC** (**E**quivalence point **R**ecognition **C**riterion) is a measure of the size of the jump in the titration curve. The ERC found is compared with EP criterion defined in the method for the **evaluation of the titration curve** (see *Section 4.1.1*). The ERC is therefore an important quantity if you have to adapt the parameters for the evaluation of the equivalence points.

The **[Calibration data]** and **[Titrant data]** buttons in the dialog **More determination data/View data** are only present when the de-

termination has been loaded. In these dialogs the sensor data and titrant data which were used at the time when the determination was carried out are shown. The **concentration** and **titer** of the titrant can be subsequently altered here. When a loaded determination is recalculated (see *Section 3.18.8*) the values used for the variables TITER and CONC (concentration) are not the values entered under **System/Titrants** but the values shown here under **View data/Titrant data**. The **Calibration data** cannot be altered at a later date.

3.18.2 Messages

If **Messages** are produced during a determination sequence then these will be shown under **More determination data/Messages**. The **[Messages]** button in the dialog **Results/ More determination data** is only active when messages have been entered during the run.



With **[Details]** you can show the unambiguous identification number of the message, the time when the message was produced during the run and the message text for the selected message.

3.18.3 Local common variables

The **[Local common variables]** button in the dialog **Results/More determination data** is only present when the determination has been loaded. In this dialog the list of common variables as they were at the time when the determination was carried out is shown. The common variables can be edited. When a loaded determination is recalculated (see *Section 3.18.8*) the values used for the common variables CV01 to CV25 will not be those stored under **System/Common variables**, but the values shown here under **More determination data/Local common variables**. This does not result in an alteration of the list of common variables stored under **System/Common variables**.

3.18.4 Determination properties

- ☞ Use **[Properties]** to open the dialog **More determination data/Properties** in the dialog **Results/More determination data**. Various details of the current determination are shown here. The abbreviation of the variable is shown for variables which can be used in calculations. The individual variables are described in *Section 4.4.3*.

More determination data / Properties		
User	Metrohm Herisau	
Sample number	18	%RN
Start counter	21	%SC
Determ. duration	347 s	DD
Method status	saved	
Determination	Determination of HCl	
Determination end	Regular without errors	
Status of deter.	recalculated loaded	
	version 1	
Recalculated by	sn	
Recalculated on	2002-06-12 11:17:33	
Used devices		
PC Control	P 1.0	S 30799722
809 Titrand	P 58090010	S 2196

The following data is shown for each determination:

- The user who was logged in when the determination was carried out is shown under **User**. If you are working with login and password protection (see *Section 3.7.7*) you can be certain that **only authorized users** can carry out determinations.
- Under **Sample number** the sample number entered at the end of the determination under **Control** is shown.
- The **Start counter** is, like the sample number, increased by one at each START of a determination. However, the start counter cannot be reset by the user. This therefore permits a check of the **uninterrupted documentation of all determinations**. You can see how often the Titrand system has been started from the start counter.
- The **Determination duration** is the time between the START of the determination and the proper end of the sequence or manual termination with **[STOP]**.
- Under **Method status** the status of the method which was used to carry out the determination is shown (see **online help**). The **Method name** is shown under **Results**.
- Under **Determination** the name of the determination will be shown if it has been saved.
- Under **Determination end** the way in which the determination was ended is shown (see **online help**).
- The **Determination status** shows the current status of the determination (see **online help**).

The following information will only be shown if the determination has been recalculated:

- **Recalculated by** shows the user who was logged in when the determination was recalculated for the last time.
- **Recalculated on** shows the date and time when the determination was recalculated for the last time.

The **devices** used for the determination sequence are shown for each determination. This means that you can document the devices used to carry out each determination.

- **Touch Control** with program version (P) and serial number (S) or **PC Control** with program version (P) and serial number (S) of the dongle (authorization plug). If no dongle is connected then Demo version will be shown.
- **Titrandos** or Titrandos with program number (P) and serial number (S).
- **Measuring input** (1 to 2) with ADC type and serial number.
- The connected devices (dosing device with exchange or dosing unit, stirrer, remote box) with serial numbers are shown for each **MSB** connection (1 to 4).

3.18.5 Save determination

You can **save** the **current determination** in one of the Card 1 or Card 2 memories. In this way you can store all the data for a determination. If you wish to save every determination then you can use the function **Save automatically** (see Section 3.16.9). Under **Sequence/Method options** you can define that all the determination data is to be saved at the end of each determination. If the data is saved automatically with the standard settings then each determination will be automatically **write-protected**. In this way your **original data** is **protected** and can neither be edited nor deleted.

☞ In the dialog **Results/More determination data** open the selection **Load/Save**.

☞ Open the dialog **Save**. The procedure for saving a file is described in Section 3.11.4. The file name **Identification 1-YYYYMMDD-hhmmss** is proposed as default. This means that the file name consists of the text entered as Identification 1 and the determination time. You can also enter any other file name you choose. The extension of the file name with the determination time has the advantage that the file names of all determinations are unambiguous.



Note!

*If **no determination data** is present because a new method has been loaded then the "empty" determination cannot be saved.*

The following data is stored for each determination:

- Calculated results.
- All raw data (measuring point lists, endpoints...) and variables produced during the determination.
- Determination properties.
- Statistics, if statistical calculations have been carried out.
- Method with which the determination was carried out.
- Common variables (values and properties of all common variables at the time of the determination).
- Most important titrant data for the titrants used.
- Most important calibration data for the sensors used.

**Note!**

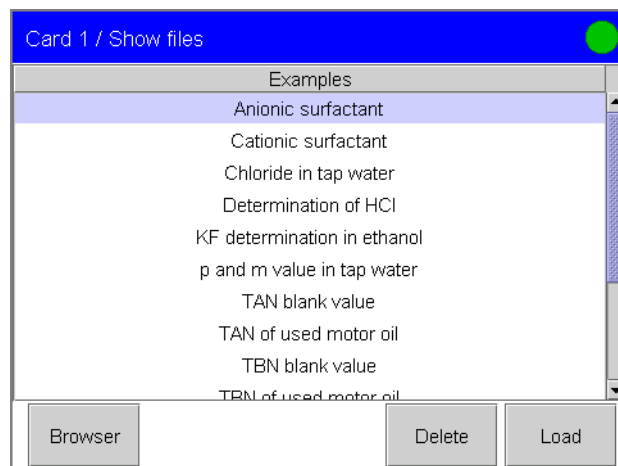
The data saved with each determination ensures that the data is traceable and that the documentation is GLP-conform.

3.18.6 Load determination data

You can load determination files into the working memory from Card 1 or Card 2.

- ☞ In the dialog **Results/More determination data** open the selection **Load/Save**. If no card is inserted then the **[Load]** button is inactive.
- ☞ Open the dialog **Load** and select **[Card 1]** or **[Card 2]**. **Touch Control**: the list of groups for this card is shown automatically (see Section 3.11).
- ☞ Use **[Show all]** to open the list of files containing all the files or **[Show files]** to open the list of files for the selected group (see Section 3.11). Only determination files will be shown.

In the following example the list of files for the determinations stored under **Examples** is shown. With **PC Control** these determinations are stored on Card 1 (see p. 68). For **Touch Control** they are stored on the supplied data card with the examples of methods (6.6048.000).



With **[Load]** you can load the selected file into the working memory. The program then changes automatically to the main dialog. With **[Delete]** you can remove the selected file from the list of files. If the determination has been automatically saved with write protection, or if **Write protection** has been activated for the determination in the **File manager** under **Show files/Properties** then it can no longer be deleted.


Note!

When you **load a determination** then the method with which the determination was carried out will be loaded automatically into the working memory. If you have made **alterations** to the **current method** which you would like to save then you should save the current method before loading the determination.

For loaded determinations the status **loaded** will be shown under **More determination data/Properties**.

The **determination browser** allows you to present the determination data in a clearer way. Not only the determination name is shown in the list but, for example, one of the sample identifications or the method used to carry out the determination and a result. You can also sort the determinations according to various criteria or use a filter. This makes it easier to find the required determination.

☞ Use **[Browser]** to open the browser for the determination files.


Note!

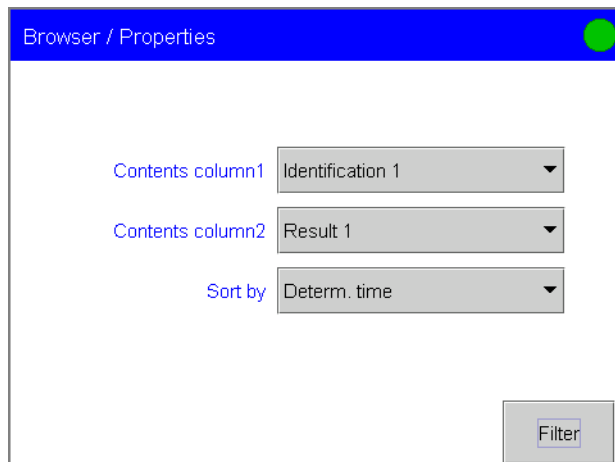
The determination browser always shows only the first **100 files** in the file list. This means that you should take care that not more than 100 files are contained in a single group when arranging the determinations.

Show files / Browser file list		
Sorted by Determ. time		15
No.	Identification 1	Result 1
1	Chloride in tap water	8.43 ppm
2	TBN blank value	0.0000 mL
3	TBN of used motor oil	10.090 mg/g
4	Titer of NaOH	0.9981
5	Determination of HCl	0.101 mol/L
6	p and m value	0.00 mmol/L
7	TAN blank value	0.0000 mL
8	TAN of used motor oil	3.097 mg/g
<div> <div>Prop- erties</div> <div>Delete</div> <div>Load</div> </div>		

In this list each line also corresponds to a determination. The first line shows the sorting criterion together with the total number of determinations. You can load the selected file into the working memory with **[Load]**. The program then changes automatically to the main dialog. You can remove the selected file from the list of files with **[Delete]**. In

the browser you can select the criteria according to which the list is to be sorted as well as the data to be shown in the list under **Browser/Properties**. You can also use filters on the list.

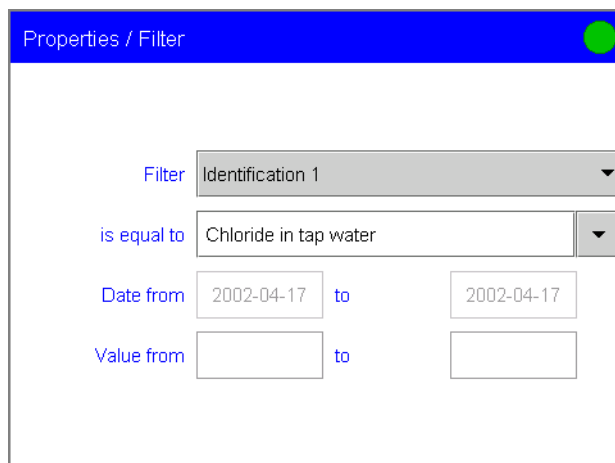
☞ Open the dialog with **[Properties]**.



☞ Select the **Contents** for **Column 1** and **Column 2**. In **Column 1** you can enter the sample data (Identification 1 or 2 or the sample size), determination time, method or the result name. In **Column 2** you can choose which result is to be shown. In this case the numbering of the results corresponds to the sequence in which the results are calculated in the determination sequence and not that of the result variables. Use **Sort by** to select the criterion according to which you want to sort the contents of the list.

You can set a **Filter** to show the determinations in the browser.

☞ Open the dialog **Properties/Filter**.

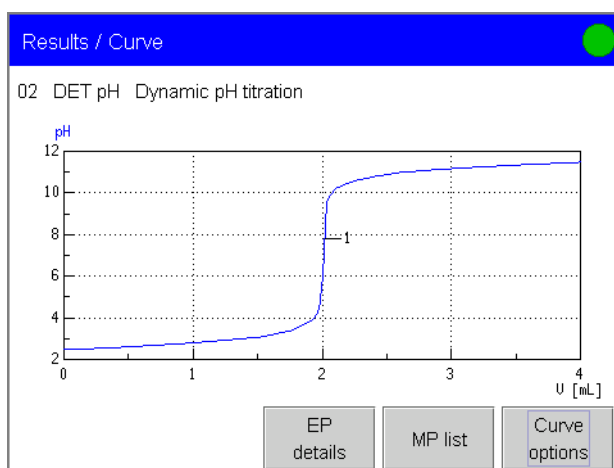


If you have selected a filter criterion under **Filter** then in the lines below you can enter the corresponding text or the time range or the range of values. Only one filter criterion can be active at a time. Only those determinations which meet the filter criterion will be shown in the **Browser file list**.

3.18.7 Curves

You can open all the curves of the current determination from the **Results** dialog.

- ☞ Use **[Curve]** under **Results** to open the curve view. If the determination contains several titrations, measurements or calibrations, i.e. modes in which a curve is produced, then a list showing these modes will first be opened. In this case you can select the required curve with **[Show curve]**.



You can alter the presentation of the curve with **[Curve options]**. You can view the **measuring point list** for the curve with **[MP list]**. With **[EP details]** you can view more data for the displayed equivalence points or endpoints. These dialogs are described in *Section 3.18.1*.

- ☞ Open the dialog **Curve/Curve options**.

The settings for the curve view are saved separately and system-specifically for each mode (DET, MET, SET, MEAS). They apply to the **curve view** under **results** and the **live display** in the modes DET, MET, SET and MEAS (see *Section 3.20.4*).

3.18.8 Recalculation and re-evaluation

You can **recalculate** the **results** of a determination if you have altered the evaluation parameters in a way that changes the recognized end-points or equivalence points, if you have altered the calculation itself (CALC commands) or if variables (e.g. the sample size, titer or common variables) have been altered.

The following commands in the method can be altered subsequently with the **[Recalculate]** button in the **Results** dialog:

- For titrations in the DET and MET modes the potentiometric evaluation will be carried out again. Under **Edit command/Pot. evaluation** you can alter the parameters for the equivalence point recognition (see *Section 4.1.1*) and use **[Recalculate]** to trigger the search for the equivalence points (EP) again. The newly recognized EPs will be shown in the results dialog.
- All subsequent evaluations (**EVAL commands**) will be carried out. Under **Parameters/Sequence** (see *Section 3.16*) you can alter the parameters for the **evaluations** EVAL FIX-EP (evaluation of fixed endpoints), EVAL pK/HNP (evaluation pK/HNP), EVAL MIN/MAX (minimum/maximum evaluation) and EVAL BREAK (evaluation of point of inflection) (see *Section 4.3*) or subsequently insert new evaluations.
- All **calculations (CALC commands)** will be carried out. You can edit the calculations under **Parameters/Sequence** (see *Section 3.16*) (change formulas, alter result variables, edit result options, etc.; see *Section 4.4.1*) or insert new calculations. If you subsequently alter the titrant for a titration in a method then the variables **TITER** and **CONC** of the "new" titrant will be used in the calculations. If a result of the variable TITER is assigned in a calculation then the titer of the "new" titrant will also be overwritten.



Note!

*An alteration of the **calibration data** under System/Sensors (see *Section 3.9.3*) cannot be taken into account in a recalculation. A change of the sensor in a method for a titration or measurement also has no influence on the measured data.*

The fact that a determination has been recalculated is shown under **More determination data/Properties** (see *Section 3.18.4*). The user who was logged in when the recalculation was carried out will also be documented together with the time of the recalculation.



Note!

*A **recalculation cannot be undone**. However, you can save the original data by saving the determination before it is recalculated (see *Section 3.18.5*). The best way of doing this is to use the function **Save automatically** (see *Section 3.16.9*).*

A method may be altered so much, e.g. by the insertion of further titration commands, that it is no longer possible to recalculate the determination.

Recalculating loaded determinations (see Section 3.18.6):

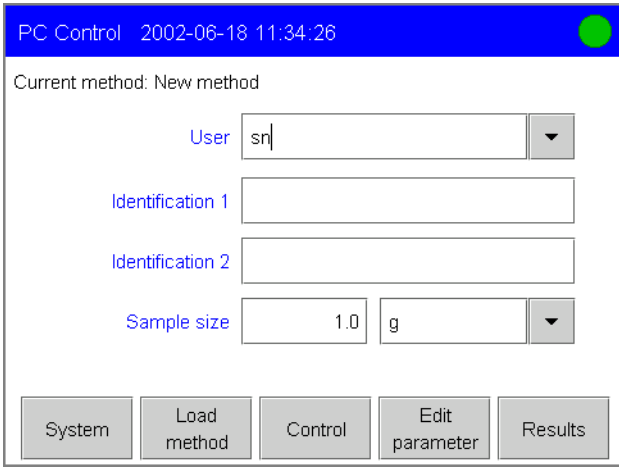
- With loaded determinations it is assumed that they have been carried out a long time ago and that the **titrant data** and **common variables** no longer coincide with those of the current system. This is the reason why the most important titrant data of the titrants used and the common variable list (local common variables) are stored together with each determination. When a loaded determination is recalculated this is the data which will be used and not that stored under **System/Titrants** or **System/Common variables**. If you want to recalculate the result of a loaded determination with a corrected common variable or a corrected titer then you must alter the corresponding values in the dialog **Results/More determination data** under **Local common variables** or **View data/Titrant data**. If you subsequently alter the titrant for a titration in a method then this alteration cannot be taken into account in the recalculation.
- If loaded determinations are to be recalculated and if a **titer** or a **common variable** is to be assigned in the recalculation then the variable **TITER** for the titrant configured under **System/Titrants** or the **common variable** configured under **System/Common variables** will only be overwritten after a query has been confirmed. If you subsequently alter the titrant for a titration in the method then this alteration cannot be taken into account in the recalculation.
- When loaded determinations are recalculated **no assignments in the result silo** are carried out.

3.19 Sample data

If you wish to process single samples then you can enter the identifications and sample sizes for the **current sample** directly in the **main dialog**. You can also program an **automatic sample data request** during the determination sequence with a REQUEST command. If you are processing **sample series** then it is a good idea to use the **sample data silo**. The sample data silo is a table in which you can store the identifications, sample size and method with which the sample is to be processed for up to 999 samples.

3.19.1 Sample data input in the main dialog

You can enter the **sample data** for the sample which is to be processed with the next START of a determination (current sample) in the main dialog. You can always access the main dialog with the **[Home]** fixed key. The sample data in the main dialog can also be entered "live", i.e. while a determination is running (see *Section 3.20.5*).



The screenshot shows a software window titled "PC Control 2002-06-18 11:34:26". Inside, it displays "Current method: New method". There are input fields for "User" (containing "sn"), "Identification 1", "Identification 2", and "Sample size" (containing "1.0" and a unit dropdown set to "g"). At the bottom, there are five buttons: "System", "Load method", "Control", "Edit parameter", and "Results".

☞ Under **Identification 1** and **Identification 2** you can enter sample-specific data.

The sample identifications can be calculated as the variables **CI1** and **CI2** (see *Section 4.4.3*). The titles of the sample identifications (**Title**) can be edited specifically for the method (see *Section 3.16.6*). Under **System/Templates/Sample data** you can create a **sample identification list**. You can then make a selection from this template when entering the identifications. This simplifies the input of frequently used texts for the identification. You can also enter the identifications with the aid of a barcode reader (see *Section 3.10.10*) or send them from a connected balance (see *Section 3.10.6*). With Touch Control we recommend the connection of a PC keyboard if long texts are to be entered as identifications (see *Section 3.10.9*).

☞ Enter the value and unit for the **sample size**.

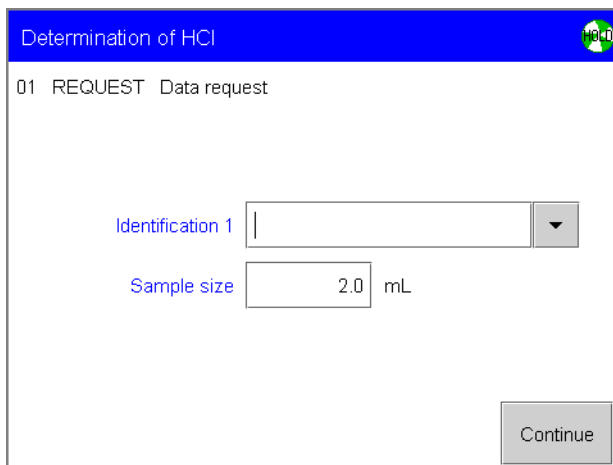
This value can be calculated as the variable **C00** (see *Section 4.4.3*). The sample size unit can either be selected from a list or entered directly. You can also send the sample size from a connected balance (see *Section 3.10.6*). You can define the **sample size unit** or a **fixed sample size** in the method (see *Section 3.16.6*). The sample size unit is shown in the main dialog, but can be edited. A fixed sample size cannot be entered in the main dialog. You can also define **sample size limits** in the method which will be monitored during the determination sequence (START of the determination and at the end of the determination) (see *Section 3.16.6*).


Note!

The **sample size limits** are not monitored during the input of the sample data in the main dialog.

3.19.2 Sample data request in the determination sequence

To make sure that the sample data input is not forgotten you can also request the sample data in the determination sequence with a REQUEST command. The automatic sample data request in the determination sequence is essential for back-weighing. In the method you can define which data (Identification 1 and/or 2, sample size) is to be requested (see *Section 4.9.3*).



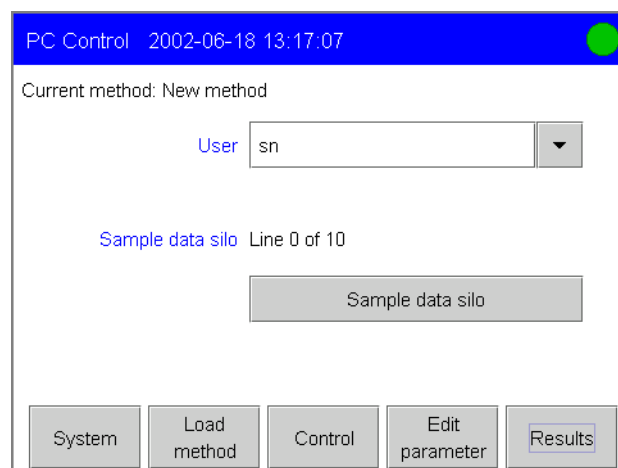
If the **Stop sequence** function is activated in a REQUEST command then the determination sequence will be stopped and must be continued when the sample data has been entered with **[Continue]**. If the stop sequence function is deactivated then the determination will continue in the background until the next titration, measurement or calibration command has been processed. The determination will then be stopped automatically and only continued when the sample data has been entered. In this way you can ensure that the sample data required for calculations which are to be carried out after the titration or measurement is actually available. In this case the sample data input is also confirmed with **[Continue]**.

If **sample size limits** have been defined in the method then these will be monitored when the entry has been confirmed with **[Continue]** (see *Section 3.16.6*). If a **fixed sample size** has been defined in the method then the sample size will be shown during the input of the sample data but cannot be edited (see *Section 3.16.6*).

3.19.3 Sample data silo

If you would like to use the sample data silo then you must activate the corresponding checkbox under **Control**. With **PC Control** you can also enter the sample data when the sample data silo has not been activated. You can open and close the table in the menu **View**. With **Touch Control** the sample data silo for the sample data input must be activated.

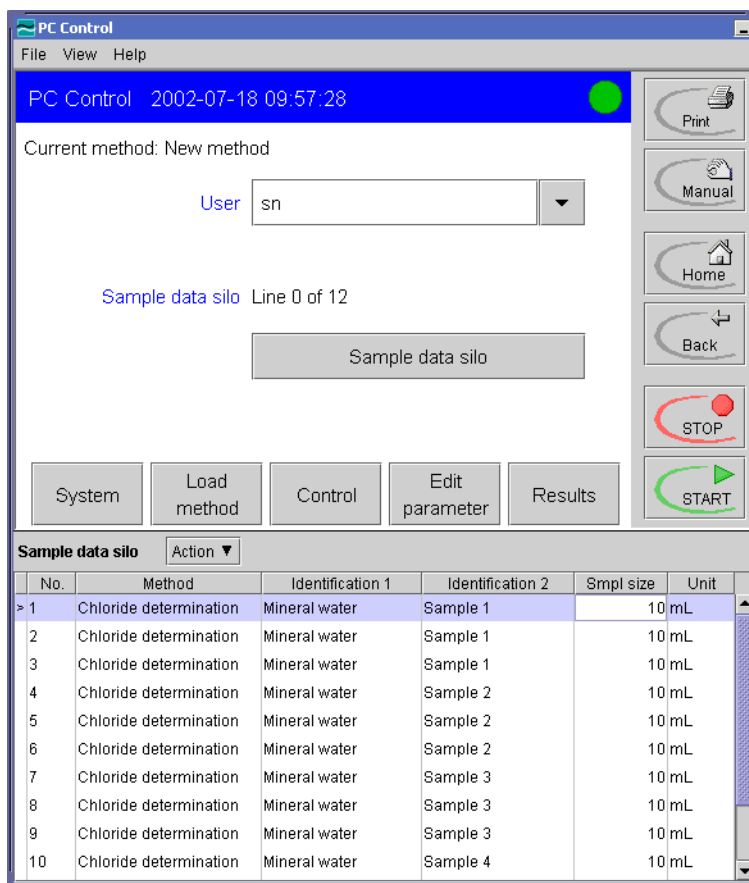
If the sample data silo is activated then in the main dialog the **[Sample data silo]** button will be seen instead of the input field for the sample data.



For the **sample data silo** the number of lines which have already been processed from the total number of lines in which sample data have been entered is shown in the main dialog.

☞ Open the sample data table with **[Sample data silo]**.

With **PC Control** the sample data table is shown beneath the open dialog window. The individual fields can be filled in directly. The silo line into which the weight is transmitted by a balance is indicated by the following character: **>**.



Click on **Action** in the title line of the sample data silo.

Insert line
Delete line
Delete all silo lines
Load sample data silo
Save sample data silo
Reset line number
Silo line for balance
Properties
Show Help
Close

You can use **Insert line** to insert a new silo line in front of the selected line, delete the selected line with **Delete line** and clear the whole of the current silo with **Delete all silo lines**. The settings under **Sample data silo/Properties** are retained.

You can use **Load sample data silo** to open the dialog for loading a sample data silo file from Card 1 or Card 2 (see p. 134) and **Save sample data silo** to open the dialog to save the current sample data silo on Card 1 or Card 2 (see Section 3.11.4).

When all the existing silo lines have been processed and you would like to refill the sample data silo then you can use **Reset line number** to set the first line back to No. 1. With **Silo line for balance** you can mark the selected silo line (>), into which the weight transmitted by a balance is to be entered. If the sample data input for the silo line is concluded automatically (see p. 132) then the marking will be automatically set in the next line.

With **Properties** you can open the dialog **Sample data silo/Properties** (see p. 132); **Show help** opens the online help for the sample data silo and **Close** is used to close the sample data table again.

With **Touch Control** a new dialog window is opened to show the sample data silo. Apart from the column with the line number, a maximum

of two further columns can be shown. The columns to be shown can be selected under **Sample data silo/Properties** (see p. 132).

Sample data silo			
No.	Identification 1	Sample size	
1	Mineral water	10 mL	
2	Mineral water	10 mL	
3	Mineral water	10 mL	
4	Mineral water	10 mL	
5	Mineral water	10 mL	
6	Mineral water	10 mL	
Load/Save		Prop-erties	Insert line
		Delete	Edit



Note!

Sample data silo files can be exchanged between **PC Control** and **Touch Control** as their contents are identical.

With **[Edit]** you can open the dialog in which the data for the selected line is to be entered. **[Delete]** is used to delete the selected silo line. With **[Insert line]** you can insert an empty silo line in front of the selected silo line.

The sample data is entered and processed line by line in ascending order. The **"active" line** which is currently being processed (current sample) has a yellow background with PC Control; with Touch Control it is indicated by the text being shown in green.

The input of the individual sample data (Identification 1, Identification 2, value and unit for the sample size) and the method is in principle the same for **PC Control** and **Touch Control**. In PC Control the data is entered directly into the table, in Touch Control a new dialog is opened for editing the silo line.

☞ With **Touch Control** open the edit dialog for the selected silo line with **[Edit]**. If you want to fill an empty sample data silo then this is the first empty silo line. In the first line you can see which line you are currently editing. The new line will only be saved when the entry is confirmed. As long as the line has not been saved **New sample** will be shown under the input field for the method name. In the edit dialog for the active line which is currently being processed **Current sample** will be shown in the same place. If several silo lines are already present you can use the **[+]** and **[-]** buttons to switch between the edit dialogs for the individual lines without having to return to the table.

You should now enter the sample data, irrespective of whether you are using **PC Control** or **Touch Control**.

- ☞ Under **Method** you can select the name of the method with which the sample is to be processed. You can use **Sample data silo/Properties** to define the **Method memory** (internal memory, Card 1, Card 2) from which the method is to be loaded. You can also enter the method name. If no method is entered then the current method in the working memory will be used. If you enter the same method in successive silo lines then the method will not be loaded separately for each determination.

If you have switched on the use of the **Sample assignment table** under **System/Templates/Sample data** then you cannot define a method in the sample data silo. If a method has already been entered before the sample assignment table is activated then this entry will be ignored.

- ☞ You can enter sample-specific data under **Identification 1** and **Identification 2**.

The sample identifications can be accounted as the variables **CI1** and **CI2** (see Section 4.4.3). The titles of the sample identifications (**Title**) can be edited specifically for the method (see Section 3.16.6). Under **System/Templates/Sample data** you can create a **sample identification list**. You can then make a selection from this template when entering the identifications. This simplifies the input of frequently used texts for the identifications. You can also enter the identifications with the aid of a barcode reader (see Section 3.10.10) or send them from a connected balance (see Section 3.10.6). With Touch Control we recommend the connection of a PC keyboard if long texts are to be entered as identifications (see Section 3.10.9).

- ☞ Enter the value and unit for the **sample size**. If you have retained the standard settings under **Sample data silo/Properties** then the silo line will be concluded with the sample size. With **PC Control** if you confirm the input of the value with **[Enter]** then a new silo line will be generated automatically. With **Touch Control** if you confirm the input of the value with **[OK]** then the program will automatically change to the edit dialog for the next silo line.

The value for the sample size can be calculated as the variable **C00** (see Section 4.4.3). The sample size unit can either be selected from a list or entered directly. You can also send the sample size from a connected balance (see Section 3.10.6). If you have defined a **sample size unit** (see Section 3.16.6) then this will be ignored in the sample data silo. The sample size unit entered in the sample data silo will always be used. If you have defined a **fixed sample size** (see Section 3.16.6) then this will be written into the corresponding silo line when the method is opened. The previously entered sample size (this is usually still the default value of 1.00 g) will be overwritten.

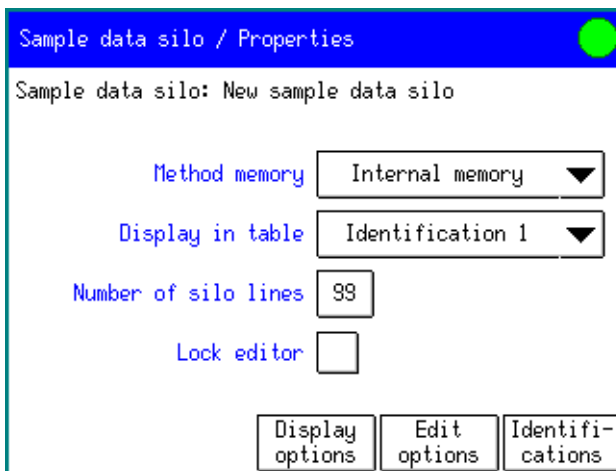
You can also define **sample size limits** in the method; these will be monitored in the determination sequence (see Section 3.16.6).

**Note!**

The **sample size limits** are not monitored during the input of the sample data in the sample data silo.

Properties of the sample data silo:

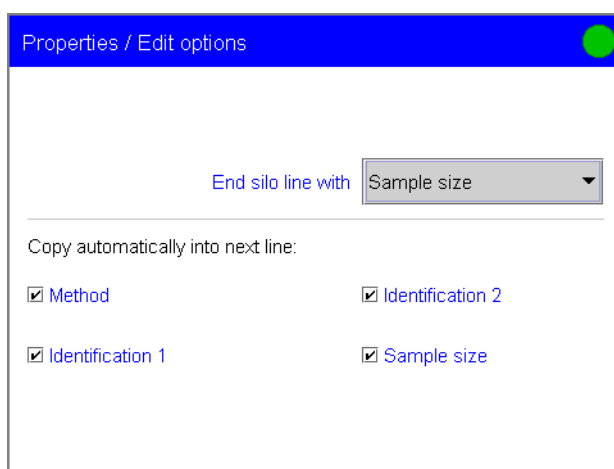
- ☞ Open the dialog **Sample data silo/Properties**. With **PC Control** this is done by selecting the menu item **Properties** under **Action** (see p 129). With **Touch Control** open the corresponding dialog from the sample data silo table with **[Properties]**.


**Attention!**

With **PC Control** the settings made under **Sample data silo/Properties** and its subdialogs will only become effective when the dialog is changed, e.g. with **[Back]**.

- ☞ Under **Method memory** select the memory from which the methods for carrying out the determinations are to be loaded if the sample data silo is being used.
- ☞ **Touch Control**: choose whether **Identification 1 or 2** and the **sample size** or only the **method** is to be shown in the silo table. With **PC Control** all the columns are always shown.

- ☞ You can enter the maximum **Number of silo lines** which are to be filled. When this number of lines has been entered the silo is full and no further lines can be added.
- ☞ You can **disable editing** the sample data in the sample data silo. This is a good idea when the sample data silo has been filled and you wish to prevent data from being altered while the silo is being processed.
- ☞ **Touch Control**: open the dialog **Properties/Show options** and deactivate the checkboxes for the sample data you do not want to use. These will then no longer be shown in the edit dialog for the individual samples.
- ☞ Open the dialog **Properties/Edit options**. In this dialog you can make the settings for editing the sample data table.



- ☞ Select whether the silo line is to be automatically concluded with **Sample size**, **Identification 1** or **Identification 2**. When the corresponding entry is confirmed with **[OK]** or **[Enter]** then the program switches automatically to editing the next line. You can also conclude the sample data input for a silo line **manually**. With **Touch Control** the **[New sample]** button will be shown in the edit dialog (**Sample data silo/Edit**). With **[New sample]** you can open the edit dialog for a new sample. With **PC Control** a new silo line will be generated when the sample size is confirmed with **[Enter]**.
- ☞ If you have to enter similar data for each sample then you can **automatically copy into the next line** the data which is identical for each sample. Deactivate the checkboxes for the data which is not to be copied into the next line.
- ☞ Under **Properties/Identifications** you can define the **Titles** of the Identification 1 and Identification 2 columns in the sample data table.

Save sample data silo:

Sample data silo files can only be saved on Card 1 or Card 2.

- ☞ Open the selection **Load/Save** in the dialog **Sample data silo**. If no card is present then the **[Save]** button is inactive.
- ☞ Open the dialog **Save**. The procedure for saving a file is described in *Section 3.11.4*

Load sample data silo:

Sample data silo files can only be loaded from Card 1 or Card 2.

- ☞ Open the selection **Load/Save** in the dialog **Sample data silo**. If no card is inserted then the **[Load]** button is inactive.
- ☞ Open the dialog **Load** and select **[Card 1]** or **[Card 2]**. **Touch Control:** the list of groups for this card will be shown automatically (see *Section 3.11*).
- ☞ Use **[Show all]** to open the list of files containing all the files or **[Show files]** open the list of files for the selected group (see *Section 3.11*). Only sample data silo files will be shown.

You can load the selected file into the working memory with **[Load]**. The program then switches automatically to the main dialog. You can remove the selected file from the list of files with **[Delete]**.

3.20 Determination sequence

This section provides a description of how to **carry out a determination**, i.e. how to process a **single sample** or a **sample series**. The determination sequence is defined in the method. When a determination is started the current method is processed line by line. The current sample data is used for calculations.

3.20.1 Carrying out a single determination

If you wish to process a single sample then proceed as follows:

- ☞ Load the **method** with which the sample is to be processed (see *Section 3.15.1*).
- ☞ Enter the **sample data** in the main dialog (see *Section 3.19.1*).
- ☞ Start the determination sequence with the **[START]** fixed key.



When a determination has been started a check is first made that all **devices** which are necessary are connected and ready for use and whether all the titrants are present. All the **monitoring intervals** for the titrants, sensors and common variables are also checked. Then all the **method commands** are processed in succession. The dialog changes automatically to the **live display** (see *Section 3.20.4*). While a determination is being carried out this is indicated by a **moving symbol** in the status line. When all the method commands have been processed the determination is concluded and the program switches automatically to the **Results** dialog (see *Section 3.18*). Only if you alter the live parameters, edit the sample data silo (Touch Control only) or if the manual control window is open (Touch Control only) will there be no automatic switch to the results display at the end of the determination. You can see when the determination is finished from the status display at the top right corner.

If you wish to save the results of the determination in the **result silo** then they will be copied into the result silo at the end of the determination (see *Section 3.22*).

If you have switched on the use of the **sample assignment table** (see *Section 3.14.2*) then a check will be made at START whether the identification which has been selected as the assignment identification is present in the sample assignment table. If this is so then the assigned method will be loaded automatically and the determination itself will be started. If the automatic request for the assignment identification is switched on this will be requested first.

3.20.2 Processing a sample series

You can use the following functions when processing sample series:

Statistics for multiple determinations:

- ☞ Activate the **Statistics** checkbox in the method under **Options/Method** and enter the **Number of samples** whose results are to be used for the statistical calculations. You can carry out the determinations individually (see Section 3.20.1) or use the sample data silo for entering the sample data (see below).



Note!

*Only results which have been produced with the same **method** can be used in the statistics. Please note the information given about deleting the statistics table in Section 3.21.2).*

Sample data silo: in the sample data silo you can enter the sample data for a whole sample series and process the series in succession.

- ☞ Activate the use of the **sample data silo** under **Control** (see Section 3.17.2).
- ☞ Enter the **sample data** in the sample data silo. You can also edit the sample data silo "live", i.e. while a determination is being carried out. You can define the **method** used to process each sample in the sample data silo. This is not necessary if all samples are to be processed by the same method. In this case the current method in the working memory will be used.



There are various ways of starting the determination of a sample series.

- You can start the sequence for each individual determination with the **[START]** fixed key.
- You can use the **autostart** function, which can be activated under **Control** (see Section 3.17.3). In this case the next determination will be started automatically after the end of the previous one.
- If a **sample changer** is connected (see Installation Instructions for 808 Titrand and 809 Titrand) then this can transmit a signal for starting the determination of each sample to the Titrand via a remote box (see Instructions for Use for the sample changer).

If a **method** is entered in the sample data silo then this method will first be loaded and then the determination sequence will be started.

When a determination has been started a check is first made that all **devices** which are necessary are connected and ready for use and whether all the titrants are present. All the **monitoring intervals** for the titrants, sensors and common variables are also checked. Then all the **method commands** are processed in succession. The dialog changes automatically to the **live display** (see Section 3.20.4). While a determination is being carried out this is indicated by a **moving symbol** in the

status line. When all the method commands have been processed the determination is concluded and the program switches automatically to the **Results** dialog (see *Section 3.18*). Only if you alter the live parameters, edit the sample data silo (Touch Control only) or if the manual control window is open (Touch Control only) will there be no automatic switch to the results display at the end of the determination. You can see when the determination is finished from the status display at the top right corner. The sample data from the processed sample data silo line is copied into the determination file and the line in the sample data silo is deleted.

If you wish to save the results of the determination in the **result silo** then they will be copied into the result silo at the end of the determination (see *Section 3.22*).

If you have switched on the use of the **sample assignment table** (see *Section 3.14.2*) then a check will be made at START whether the identification which has been selected as the assignment identification is present in the sample assignment table. If this is so then the assigned method will be loaded automatically and the determination itself will be started. If methods have been entered for the sample data in the sample data silo then these entries will be ignored.

3.20.3 Stopping determinations manually



A determination can be stopped at any time with the **[STOP]** fixed key. The command which is being processed will be stopped and no further commands will be carried out. The program will switch automatically to showing the **Results** (see *Section 3.18*).

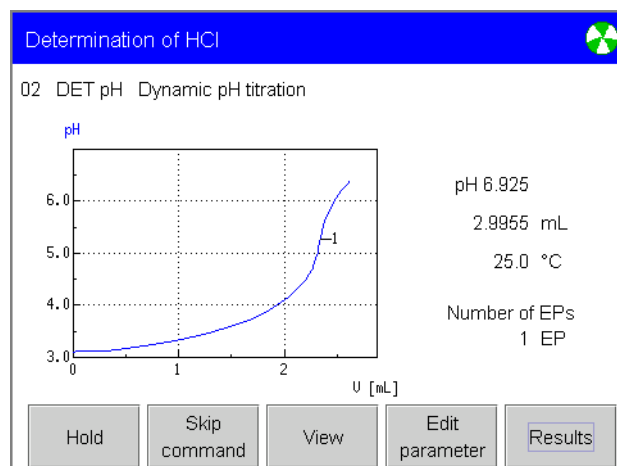
If the **autostart** function is switched on (see *Section 3.17.3*) then the processing of the whole series will be stopped and no further automatic START will be carried out.

If you do not want to stop the whole determination sequence but only want to stop a command then you should use the function **[Skip command]** in the live display (see *Section 3.20.4*). This is particularly useful when you want to stop a titration because the required equivalence point has already been found. All the following commands, e.g. calculations and report printouts, will still be carried out.

3.20.4 Live display

In each method command which is processed in the determination sequence and which lasts for a certain time the step which is currently being carried out is indicated. The name of the current **method** is shown in the **status line** (blue bar). In the first line the line number, **command name** and **command comment** are shown for the command which is currently being processed.

The **titration or measurement curve** is shown for titrations and measurements (DET, MET, SET, MEAS). If you have selected the presentation of **Curve & measured values** under **View** then to the right of the curve you will see the number of equivalence points or endpoints (EP) which have been recognized in addition to the measured values. The endpoints are marked on the curve.



With **[Results]** you can open the results display. The data for the method commands which have already been carried out will be shown. The **Results** dialog and its subdialogs will not be updated during the sequence as long as they are open. If you want to view the most recent results you must exit the dialog and then reopen it.

With **[Edit parameter]** you can edit the live parameters, i.e. the method parameters which can be altered while a sequence is being processed (see Section 3.20.6).

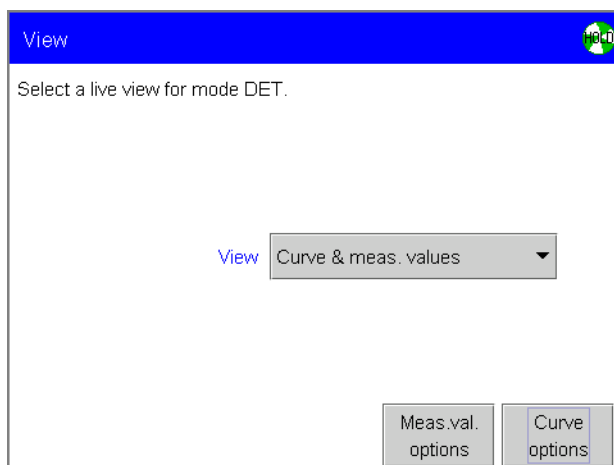
The button in the center has various functions. For titrations and measurements you can use **[View]** to make settings for displaying the curve and the measured values (see below). In the live display for all commands you can switch to the main dialog with **[Sample data]**.

With **[Skip command]** the method command which is currently being processed will be stopped. The sequence will be continued with the next command. If a titration or measurement (DET, SET, MET, MEAS) is stopped with **[Skip command]** then the determination data will show **Manual stop** as the stop criterion.



With **[Hold]** you can halt the determination at any time. The system is then in the HOLD status (status display in the top right corner). The button marking then changes to **[Continue]**. You can use **[Continue]** to continue the sequence.

☞ Use **[View]** to open the dialog for a titration or measurement in the live display in order to alter the settings for showing the curve and measured values.



You can choose whether you would like to display the curve with the measured values to the right of it (default setting), only the curve (larger, fills the whole display), only the measured values (large) or the curve with the sample data to the right of it.

You can alter the appearance of the curve with **[Curve options]** (see *Section 3.18.7*). The settings for the curve display are stored separately and system-specifically for each mode (DET, MET, SET, MEAS). They apply to the **curve display** under **results** and the **live display** for the DET, MET, SET and MEAS modes.

With **[Measured value options]** you can alter the display of the measured values. A maximum of three different values can be shown at the same time. The values which can be selected vary with the mode (DET, MET, SET, MEAS).

The CAL (**calibration**) command has a special sequence and is described in *Section 4.6*.

For the ADD (**dosing**) command the volume to be added (set volume) and the volume already added are shown. For the PREP (**preparation**) and EMPTY (Dosino only) commands the piston movements and the valve settings are shown.

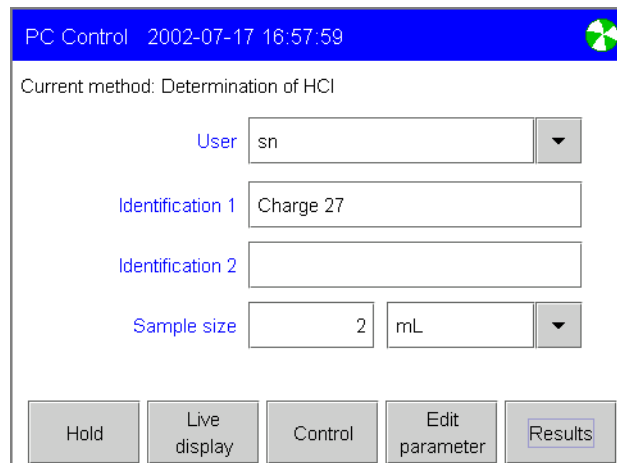
For the **SCAN** command the signal which is being waited for is shown.

For the WAIT (**waiting time**) command the remaining waiting time is shown, possibly together with a message which can be defined in the method.

For all other command a text is either shown or they are carried out so quickly that no special live display is available (e.g. evaluations, calculations, etc.).

3.20.5 Main dialog "live"

The appearance of the main dialog changes slightly when a determination has been started.



The **sample data** can also be entered "live", i.e. while a determination is being carried out (see *Section 3.19.1*). In calculations the sample data which has been entered in the main dialog at the time when the calculation is carried out (CALC command) is always used.

No device-specific settings can be carried out "live"; this is why the **[System]** button is not available. It is also not possible to load or create methods. The **[Load method]** button is also not available.



With **[Hold]** you can halt the determination at any time. The system is then in the HOLD status (status display in the top right corner). The button marking then changes to **[Continue]**. You can then use **[Continue]** to continue the sequence.

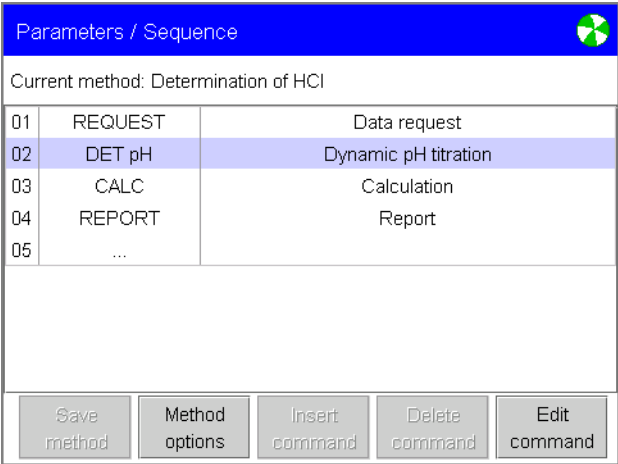
You can switch to the live display with **[Live display]**, i.e. to showing the method command which is currently being processed (see *Section 3.20.4*).


With **[Control]** you can alter the settings for the determination sequence (see *Section 3.17*). Several functions are not accessible "live". The settings for **Statistics** and **Sample data silo** cannot be altered. If you deactivate the **Autostart** checkbox while a determination is being carried out then the current determination will be concluded but no new START will be carried out. The sample number cannot be edited. If you are working with login (see *Section 3.7.7*) then you can log out of the system with **[Logout]** even when a determination is being carried out. The logout dialog will then be shown immediately. The determination continues to run in the background. It can be stopped with the **[STOP]** fixed key. All other functions are only accessible again after a new user has logged in.

3.20.6 Live parameters

Certain method parameters can be edited while a determination is being carried out. Whether a parameter can be edited "live" is given in *Section 4* for each parameter.

☞ Open the **Edit parameter** dialog while a determination is currently being carried out.



Parameters / Sequence 

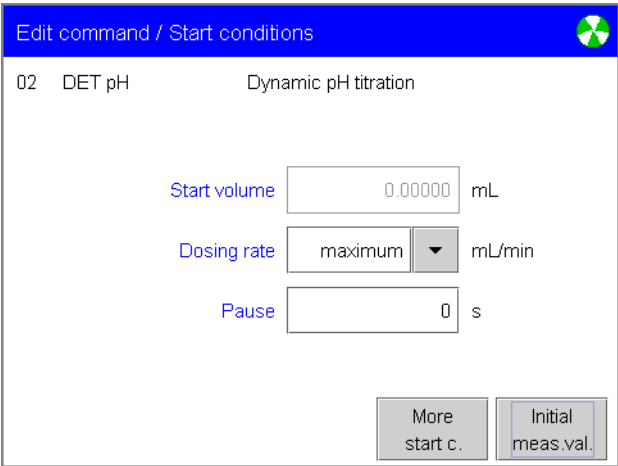
Current method: Determination of HCl


01	REQUEST	Data request
02	DET pH	Dynamic pH titration
03	CALC	Calculation
04	REPORT	Report
05	...	

Save method Method options Insert command Delete command Edit command

The **[Edit command]** button is active for a command in which live parameters can be edited. The sequence, i.e. the sequence of commands, cannot be altered. This is why the **[Delete command]** and **[Insert command]** buttons are inactive. Under **Method options** only the **Save automatically** function is accessible (see *Section 3.16.9*). The method cannot be saved while a determination is being carried out.

☞ As an example, open the dialog for editing the **Start conditions** for a titration in the DET mode (see *Section 3.16.1*).



Edit command / Start conditions 

02 DET pH Dynamic pH titration

Start volume mL

Dosing rate mL/min

Pause s

More start c. Initial meas.val.

Only parameters which it is possible to edit while a determination is being carried out can be edited.

The edited parameters are immediately taken into account in the determination sequence. However, for example, if you alter the start conditions after the start volume has already been added then these alterations will only be taken into account the next time that the method is started.

**Note!**

*If the **sample data silo** is used and a different method is loaded for the next sample then the live alterations will be lost.*

3.21 Statistics

If you have carried out statistical calculations in your determinations then you can open the statistics table in the **Results** dialog with **[Statistics]**. This table contains the statistical results for a multiple determination. A maximum of nine results calculated in a single determination can be statistically evaluated. A statistics series can contain a maximum of 20 determinations, i.e. samples.

If you wish to have statistical calculations carried out on the results then you must activate the **Statistics** checkbox in the method under **Sequence/Method options** and enter the **Number of samples** (see Section 3.16.4).

The results in a determination for which statistical calculations are to be carried out must be defined in the corresponding **CALC command** (calculation) (see Section 4.4.1).

If you have not yet carried out a determination with statistical calculations you will find a short description in the **Tutorial** for Touch Control and PC Control.

Results / Statistics	
Current method: New method	
Determinations 3 of 3	
Result name	Mean
Content (mmol/L)	99.80 mmol/L
Voume HCl	5.1 mL
<div> <div>Add determ.</div> <div>Details</div> </div>	

The number of determinations which have already been carried out is shown above the table (actual statistics counter) together with the total number of determinations to be carried out (set statistics counter). The name of the result and the mean value are shown in the table for each result for which statistical calculations are to be carried out.

With **[Details]** you can display the statistics results for the selected result and the table with the individual results of all the determinations. With **[Add determination]** you can also add a sample to the series later. This is a good idea if one determination in the series was so incorrect that it cannot be accepted.



Note!

*If you **recalculate** a **determination** then the statistics calculations for the determination will also be recalculated.*

3.21.1 Statistical information about the result

☞ Select a result in the statistics table and open the dialog **Statistics/Details**.

Statistics / Details		
Result name: Content (mmol/L)		SMN1
Mean	99.80 mmol/L	n=03
s +/-	0.112 mmol/L	
s rel	0.11 %	
No.	Sample size	Result
1	5.1 mL	99.93 mmol/L
2	5.5 mL	99.72 mmol/L
3	4.8 mL	99.78 mmol/L
<div> <div>Sample data</div> <div>Determ. on/off</div> <div>Result on/off</div> </div>		

The name of the result and the variable for the mean value (in this example SMN1) are shown under **Details** for each result for which statistical calculations have been carried out (see *Section 4.4.1*). The **Mean** value and the absolute (**s +/-**) and relative (**s rel**) standard deviations are also shown above the table. The number of individual results used for the calculation of the mean value is shown to the right of the mean value. The number of the determination, the sample size saved with the determination data and the value for the unit are shown in the table for each result.

If results cannot be calculated for a determination then **Invalid** will be shown in the table for these results, which will be ignored in the statistical calculations. **n** (number of results used for calculating the statistics) will therefore be reduced by the corresponding number of results.

You can use [**Result on/off**] to remove individual results from the statistical calculations. The value for this result will then be indicated by an *. With [**Determination on/off**] you can remove all the results of a determination from the statistical calculations. In this case all the entries in the corresponding line will be indicated by an *. The statistical results will be recalculated immediately. If you wish to assign a mean value to a **common variable** or to the variable **TITER** (see *Section 4.4.1*) then you must recalculate the determination (see *Section 3.18.8*). You can use the same buttons to deactivate these actions again.

Identification 1, **Identification 2** and the **Sample size** of the determination selected in the table are shown under **Details/Sample data**.

3.21.2 Delete statistics table

You can delete the whole statistics table under **Control** with **[Delete statistics]**. When the number in the set statistics counter (number of sample to be used to calculate the statistics) in the method under **Sequence/Method options** is the same as the number shown in the actual statistics counter (number of processed samples) then the next time that the method is started the statistics table will be **automatically deleted**.

The statistics table will be **automatically deleted** when you use **[Load method]** from the main dialog to load a method into the working memory (see *Section 3.15.1*). It does not matter whether this is the same method that was previously loaded. If you use either the **sample data silo** (see *Section 3.19.3*) or the **sample assignment table** (see *Section 3.14.2*) then a check will be made whether the method is the same (file name is the same) as that which is already loaded in the working memory. Only when this is a different method will the new method be loaded and the statistics deleted.

3.21.3 Adding a determination to a statistics series

If you wish to add a further sample to a statistics series because, for example, a different sample has to be removed from the statistics, you can increase the set statistics counter under **Results/Statistics** with **[Add determination]**. This does alter the **Number of samples** defined in the method under **Sequence/Method options**. When the required number of determinations has been carried out the set statistics counter defined in the method will again apply to the next statistics series.

The number of determinations by which the set statistics counter has been increased is shown above the table in brackets. This information is also shown in the main dialog and in the statistics report.

Results / Statistics	
Current method: New method	
Determinations 5 of 3 (+2)	
Result name	Mean
Content (mmol/L)	99.80 mmol/L
Voume HCl	5.0 mL
<div> <div>Add determ.</div> <div>Details</div> </div>	

3.22 Result silo

The result silo is a **table** in which you can store the **results of up to 99 determinations**. A maximum of nine results from a single determination can be stored in the result silo. This table is used to provide a clear overview of, for example, the results of all determinations carried out on a particular day. As the display is not large enough to show all the data at the same time, it is better to print out the result silo (see *Section 3.23*). If you have stored results in the result silo when carrying out determinations (see *Section 4.4.1*) then the result table can be opened in the **Results** dialog with **[Result silo]**.

The results which are to be calculated in a determination and stored in the result silo are defined in the corresponding **CALC command** (calculation) (see *Section 4.4.1*).

Results / Result silo		
Sorted by Determ. time		9 of 99
No.	Identification 1	Result 1
1	HCl Sample 1	99.93 mmol/L
2	HCl Sample 2	99.72 mmol/L
3	HCl Sample 3	99.76 mmol/L
4	Charge 27	3.15 mmol/L
5	Charge 27	2.99 mmol/L
6	Charge 27	2.87 %
7	Charge 28	4.32 %
8	Charge 28	4.19 %
<div> <div>Load/Save</div> <div>Properties</div> <div>Delete all</div> <div>Delete</div> <div>Details</div> </div>		

The criterion according to which the results in the table have been sorted is shown above the table together with the number of determinations (of max. 99) from which results have been stored in the result silo. If a filter has been used then this number will normally be higher than the number of lines in the table. One line always corresponds to one determination in the table.

The following details of the determination can be viewed with **[Details]**:

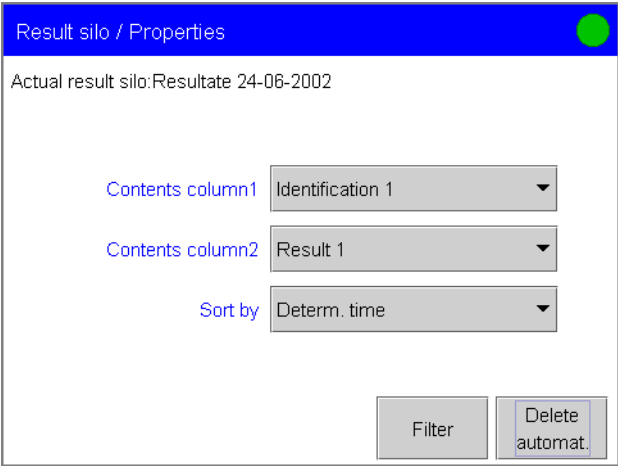
- User who carried out the determination.
- Method with which the determinations was carried out.
- Determination time (date and time).
- Sample data (Identification 1 and 2, sample size).
- Results which have been calculated in the determination sequence and stored in the result silo.

The selected determination line can be deleted from the result silo with **[Delete]**. **[Delete all]** deletes all the lines.

3.22.1 Result silo properties

Under **Result silo/Properties** you can choose the criteria according to which the list is to be sorted and which data is to be shown for each determination. The line number is always shown.

☞ Open the dialog with **[Properties]**.



☞ Select the **Contents** of **Column 1** and **Column 2**. In **Column 1** you can display the sample data (Identification 1 or 2, or sample size), determination time, method or the name of the result. In **Column 2** you can select the result to be shown. The numbering of the results corresponds to the order in which the results were calculated in the determination sequence and stored in the result silo and not that of the result variables. Use **Sort by** to select the criterion according to which the contents of the list are to be sorted. If the field for the sorting criterion remains "empty" then the entry will be shown at the end of the table.

With **[Delete automatically]**, you can define when the contents of the result silo is to be deleted automatically. You can set it so that the first (oldest) silo line will be deleted when the result silo is full and a new determination is to be entered. All lines can be deleted automatically when the titration system is switched on, when a new sample series is started with the autostart function switched on (see *Section 3.17.3*) or when the result silo is saved (see *Section 3.22.2*).

You can use **filters** for the display of the result silo table.

☞ Open the dialog for selecting the filter criteria under **Result silo/Properties** with **[Filter]**.

Properties / Filter

Filter

Identification 1

is equal to

Charge 27

Date from


to

Value from

to

If you have selected a filter criterion under **Filter** then in the lines below you can enter the corresponding text or the time range or the range of values. Only one filter criterion can be active at a time. Only those determinations which meet the filter criterion will be shown in the **result silo table**:

Results / Result silo

Sorted by Determ. time9 of 99

No.	Identification 1	Result 1
1	Charge 27	3.15 mmol/L
2	Charge 27	2.99 mmol/L
3	Charge 27	2.87 %

Load/Save

Properties

Delete all

Delete

Details

The fact that a filter is active is indicated by the filter symbol in the top right-hand corner.

3.22.2 Saving and loading the result silo

Save result silo:

Result silo files can only be saved on Card 1 or Card 2.

- ☞ Open **[Load/Save]** in the dialog **Results/Result silo**. If no card is present then the **[Save]** button will be inactive.
- ☞ Open the **Save** dialog. The procedure for saving a file is described in Section 3.11.4.



Note!

*Not all determination data are saved with a result silo. If you want to save determination data of all determinations, use the option **Save determination automatically** (see Section 3.16.9).*

Load result silo:

Result silo files can only be loaded from Card 1 or Card 2.

- ☞ Open **[Load/Save]** in **Results/Result silo**. If no card is present then the **[Load]** button will be inactive.
- ☞ Open the **Load** dialog and select **[Card 1]** or **[Card 2]**. **Touch Control**: the list of groups for the card will be shown automatically (see Section 3.11).
- ☞ Use **[Show all]** to open the list of all the files or **[Show files]** to open the list of files for the selected group (see Section 3.11). Only result silo files will be shown.

You can use **[Load]** to load the selected file into the working memory. The program will switch automatically to the main dialog. You can remove the selected file from the list of files with **[Delete]**.

3.23 Print

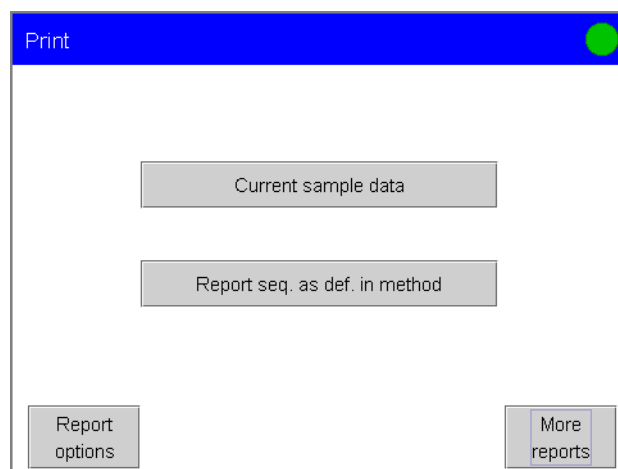
In principle there are two ways of printing a report in Touch Control and PC Control:

- Manual printout with the **[Print]** fixed key (see below).
- Printout during the determination sequence with a **REPORT command** (see *Section 4.5*).

How to connect a printer to a Titrando system with **Touch Control** is described in the Installation Instructions for the 808 Titrando and 809 Titrando. The configuration of the printer is described in *Section 3.10.5*. The **PC Control** software automatically uses the **Windows standard printer**. If you want to use a different printer then you must define it as the standard printer in the operating system under System control/Printer.

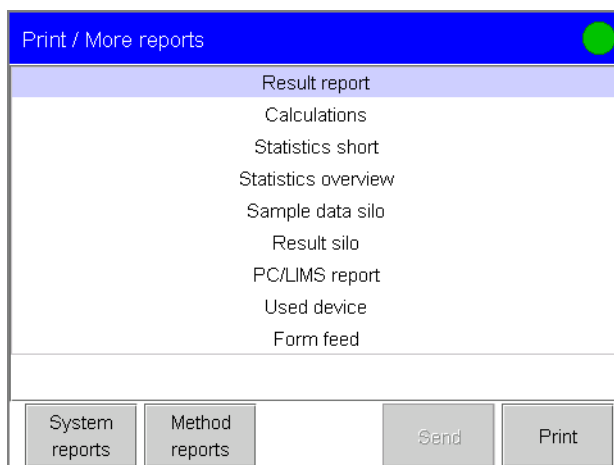
You can use the **[Print]** fixed key to rapidly print out **context-sensitive** reports for the dialog which is currently open. You can also print out all other reports which are available. The **[Print]** fixed key is inactive while a determination is being carried out (BUSY).

☞ Open the **Print** dialog from the main dialog with the **[Print]** fixed key.



The sample data is entered in the main dialog, which is why you can print out the sample data from the main dialog in a context-sensitive situation with **[Current sample data]**. All REPORT commands in the current method can be executed with **[Report seq. as def. in method]**. With **[More reports]** you can open a list containing all the available reports. You can make general settings for printing out the reports with **[Report options]**.

☞ Open the dialog **Print/More reports**. The first list shows the reports for the current determination.

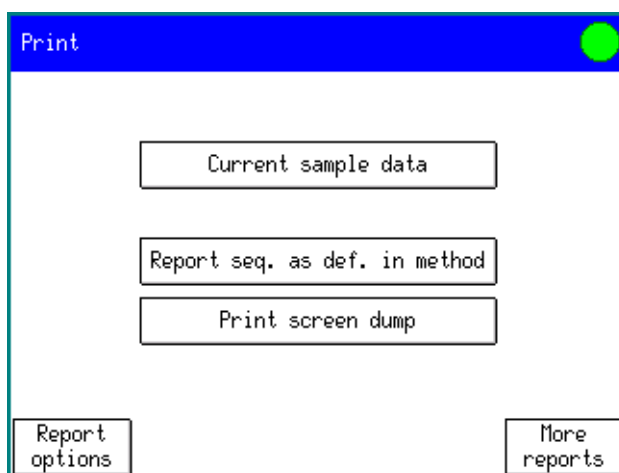


The selected report can be printed out with **[Print]**. The **[Send]** button is only active when **PC/LIMS report** has been selected. **[Method reports]** opens the list of reports for the current method. The list containing all the reports about the system-specific data is opened with **[System reports]**.

If the **[Print]** fixed key is used then the reports will always be printed out with the **default settings**. If you wish to print out a report with different settings then you should define a REPORT command in the method and adapt the parameters for the report (see *Section 4.5*). The report defined in the method is printed out with **[Print] [Report sequence as defined in method]**.

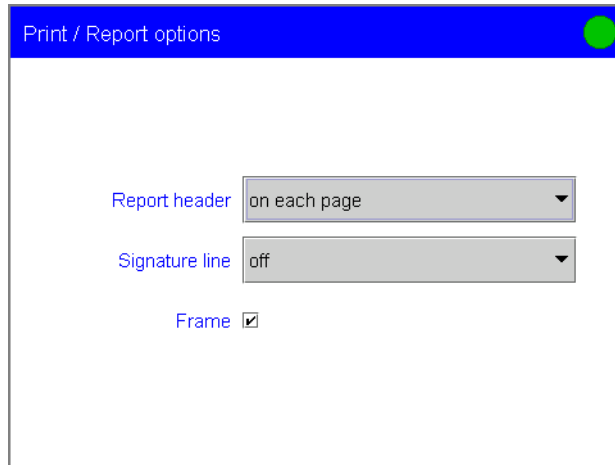
With **Touch Control** you can also print out a **screen dump** of the current dialog.

☞ Touch the **[Print]** fixed key.



☞ With **[Print screen dump]** you can activate the "print screen" function. The next time that you touch the **[Print]** fixed key the current screen contents will be printed out.

☞ Open the dialog for the report configuration with **[Report options]** in the **Print** dialog.



Print / Report options

Report header on each page ▼

Signature line off ▼

Frame ☒


In the **Report header** the type, serial number and program version of the software (Touch Control or PC Control), the device name which you can enter in the device manager for Touch Control or PC Control, and the printout date with time zone are printed out. You can also define your own report header under **System/Templates/Report header**; this will be printed out in front of the standard report header (see *Section 3.14.7*). Under **Report header** you can choose whether the report header is to be printed out on every page, on the first page of the report only or not at all. The **Signature line** gives you the possibility of signing the report together with the date. You can choose whether the **Signature line** is to be printed out on every page, on the first page of the report only or not at all. If the **Frame** checkbox is activated then a frame will be printed round each report page.

The following **reports** can be printed out with the **[Print]** fixed key:

	<i>Report</i>	<i>Contents</i>
<i>Print / More reports</i>		
Results (current determination)	Result report	Determination properties, sample data, raw data, i.e. endpoints, final measured values, results of evaluations (EVAL), calculated results, short statistics, messages produced during the determination.
	Curve	Context-sensitive only ; from the curve display (settings for the curve printed are adopted from the display).
	Measuring point list	Context-sensitive only ; from the measuring point list display.
	Calculations	Details of the calculations carried out during the determination sequence (details of every result from the CALC commands, calculated variables and calculated results with the shown accuracy).
	Used devices	All the devices used in the determination sequence as defined under More determination data/Properties .
Statistics	Statistics short	Summary of the statistics calculations. The number of results, the mean value, absolute and relative standard deviation are printed out for each result.
	Statistics overview	Detailed statistics table, landscape format. The sample data and all individual results are printed out for each determination. The number of results n, the mean value, absolute and relative standard deviation are printed out for each result.
Sample data	Current sample data	Context-sensitive only ; from the main dialog. The sample data is also printed out in the result report.
	Sample data silo	Sample data silo properties, landscape format, table with all sample data entered in the sample data silo.

	<i>Report</i>	<i>Contents</i>
Result table	Result silo	Result silo properties, landscape format, table with all results stored in the result silo.
<i>Print / More reports / Method reports</i>		
Current method	Method sequence	Method properties, list with all method commands.
	Parameters full	Method properties, method options, all method commands with all their parameters. All parameters which no longer have their default settings will be printed out bold . All parameters which have been modified in comparison to the stored version of the method are indicated by an * .
	Titration and measuring parameters	Method properties, all titration and measurement commands (DET, MET, SET, MEAS) with all parameters. All parameters which no longer have their default settings will be printed out bold . All parameters which have been modified in comparison to the stored version of the method are indicated by an * .
	Modified parameters	Method properties, all method commands with parameters which have been modified in comparison to the stored version of the method.
	Non default parameters	Method properties, all method commands with parameters which no longer have the default settings.
<i>Print / More reports / System reports</i>		
System settings	System settings	System settings, settings for acoustic signals and measured value display.
	Dialog options	Dialog options, settings for list of commands and fixed keys, routine dialog settings
	User list	Context-sensitive only ; list of all the users defined in the system under user administration.

	<i>Report</i>	<i>Contents</i>
Titrants	Titrant list	List of all the titrants configured in the system.
	All titrant data short	The most important titrant data for all configured titrants.
	All titrant data full	All titrant data for all configured titrants.
	Titrant data short	Context-sensitive only ; from edit dialog for the titrant. The most important titrant data for the titrant which is currently being edited.
	Titrant data full	Context-sensitive only ; from edit dialog for the titrant. All titrant data for the titrant which is currently being edited.
Sensors	Sensor list	List of all the sensors configured in the system.
	All sensor data short	The most important sensor data for all configured sensors.
	All sensor data full	All sensor data for all configured sensors.
	Sensor data short	Context-sensitive only ; from edit dialog for the sensor. The most important sensor data for the sensor which is currently being edited.
	Sensor data full	Context-sensitive only ; from edit dialog for the sensor. All sensor data for the sensor which is currently being edited.
Device manager	Device list	List of all devices configured in the system.
	All device properties	Properties of all the devices configured in the system.
	Device properties	Context-sensitive only ; from edit dialog for the device. Properties of the device which is currently being edited.
GLP manager	GLP data	All data stored in the GLP manager.
Common variables	Common variable list	List of all the common variables defined in the system.

	<i>Report</i>	<i>Contents</i>
	All common variable properties	Properties of all the common variables defined in the system.
	Common variable properties	Context-sensitive only ; from edit dialog for the common variable. Properties of the common variable which is currently being edited.
Templates	Templates sample data	Sample identification list, sample assignment table.
	Result template list	List of all results templates.
	All results templates details	Details of all results templates.
	Result template details	Context-sensitive only ; from edit dialog for the result template. Details of the result template which is currently being edited.
	Input/Output lines	List of all defined templates for input lines and output lines.
	Custom calibration buffers	Temperature tables for all defined custom calibration buffers.
Audit trail	Audit trail	Audit trail table (PC Control only). Can also be printed out from the audit trail window with  .

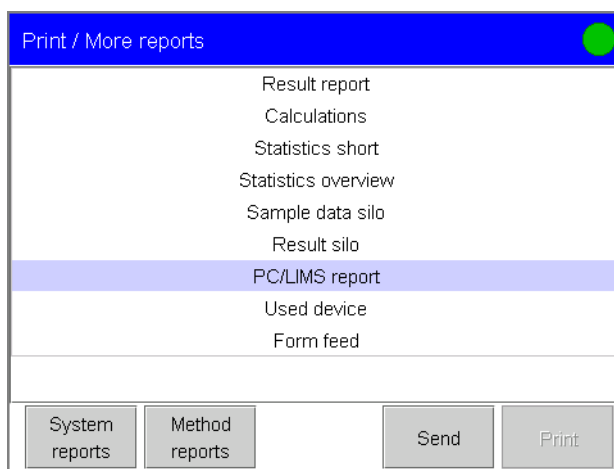
**Note!**

Some tables (statistics overview and sample data silo) are always printed out in **landscape format**, as otherwise the data could not be printed out on a single page. For PC Control you must select the Windows-specific **Printer setting: portrait**, as printout in landscape format is automatic.

3.23.1 Sending or saving a PC/LIMS report

You cannot only automatically send or save a **PC/LIMS report** (ASCII report containing all the most important data of a determination) at the end of a determination (see *Section 3.16.9*), you can also do this manually with the **[Print]** fixed key. The settings for sending and saving the PC/LIMS report are made in the device manager under **Edit device/PC/LIMS report** (see *Section 3.10.7*). A detailed description of the contents of a PC/LIMS report can be found in a separate document, the **Titrande PC/LIMS Report Guide**.

☞ Use the **[Print]** fixed key to open the **Print** dialog and then **[More reports]** to open the list of reports for the current determination.



☞ Select the **PC/LIMS report** in the selection list and send it to the connected PC or save it as a text file with **[Send]**.

3.24 Manual control

The **sensors**, **dosing devices**, **stirrers** and **remote boxes** connected to the Titrando can also be **controlled manually**. The manual control of devices which are not being used in the run is also possible during a determination sequence (BUSY). The dialog for manual control of the titration system is opened with the **[Manual1]** fixed key. With PC Control a new dialog window is opened so that the PC Control dialog window and the Manual control dialog window are open side by side.

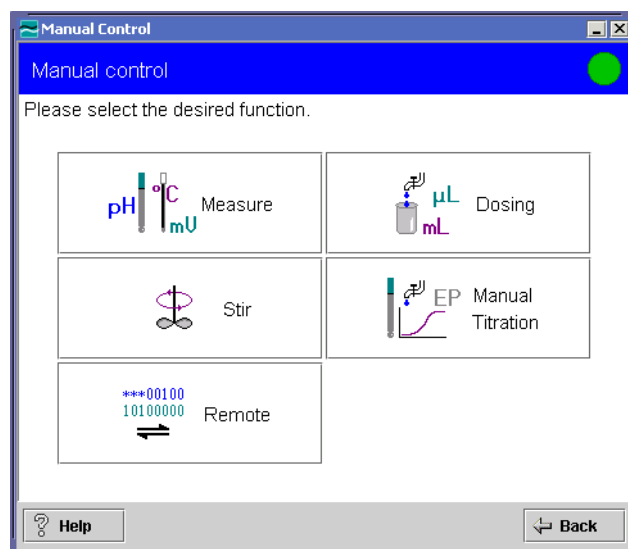


Note!

*The following manual runs can normally be aborted by touching the red button **[Stop]** given in the dialog. For that purpose you should stay in the respective dialog until the manual run is finished.*

PC Control:

☞ Click on **[Manual1]**.

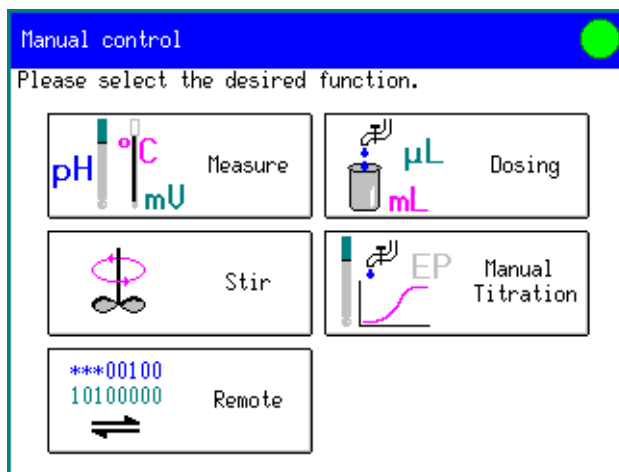


You can open the **online help** for manual control with **[Help]**. In manual control **[Back]** switches to the previous dialog. The Manual control dialog window is closed with **[x]** (close). You can also close the window when a manual run has been started and is not yet finished. In manual control you can recognize when a run has been started by the corresponding symbol in the status line (see Section 3.6).

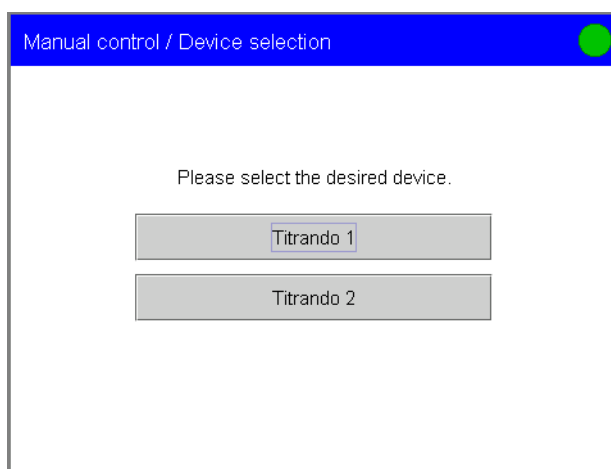
Touch Control:

With Touch Control the manual control dialog covers the last dialog to have been opened. You can switch back to this dialog with the **[Back]** fixed key.

☞ Touch the **[Manual1]** fixed key.



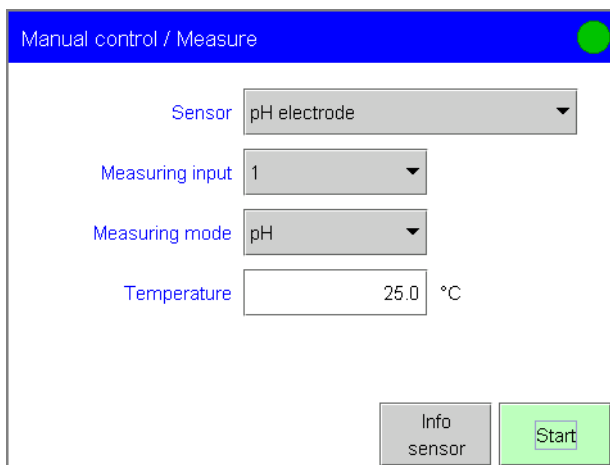
If several Titrando's are connected then, after selecting the function (**[Measure]**, **[Dosing]**, **[Stir]**, **[Manual titration]** or **[Remote]**), you must select the **Titrando** to be used.



The device name is shown on the button. The connected Titrando's are configured under **System/Device manager** (see *Section 3.10.4*).

3.24.1 Measure

☞ Select the **[Measure]** function in the **Manual control** dialog.



☞ First select the **sensor** to be used for the measurement. All the sensors defined under **System/Sensors** will be shown.

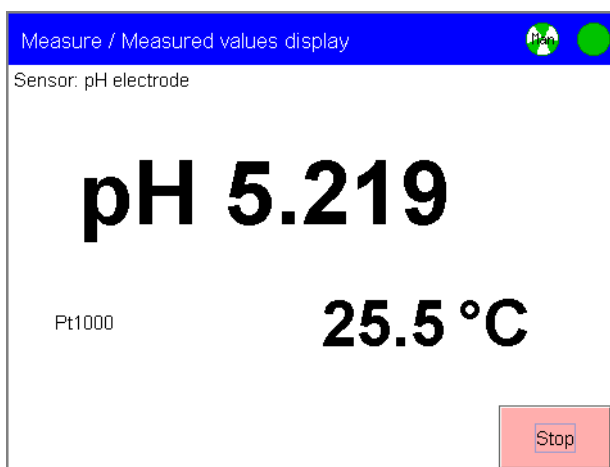
☞ Select the **Measuring input** to which the sensor is connected.

☞ Select the **Measuring mode**. The measuring modes which are suitable for the connected sensor will be shown.

☞ If a temperature sensor is connected then the **temperature** will be measured automatically. You can also enter the temperature manually here. This temperature is used for automatic temperature compensation for pH measurements if no temperature sensor is connected. This parameter is not available for the measuring mode **T** (temperature).

The most important sensor data (**sensor name**, **comment**, **sensor type** and, for pH and ISE electrodes, the **calibration data**) are shown under **Measure/Info sensor**.

☞ In the **Measure** dialog the **[Start]** button is used to start the measurement and to switch to the **Measured values display**.

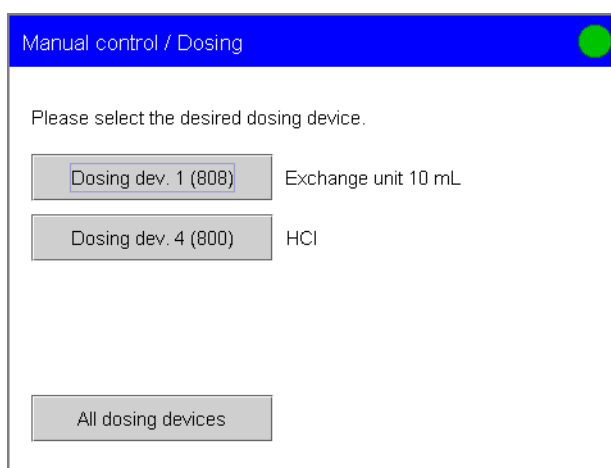


The measured values display shows the **current measured value** (updated every 500 ms), the type of temperature measurement (**Pt1000**, **NTC** or **manual**) and the **measurement temperature**. The measurement is terminated with **[Stop]**.

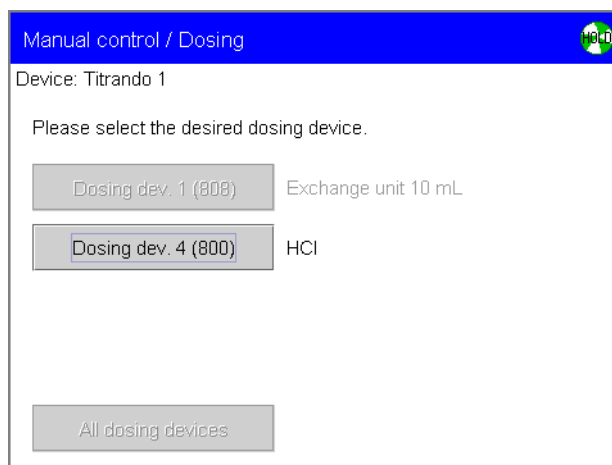
3.24.2 Dosing

The functions under **Manual control/Dosing** are chiefly important when you want to carry out **manual dosing** or when you want to **prepare** or **empty** dosing devices. You can also check which dosing devices are connected and which exchange or dosing units are attached.

- ☞ Select the **[Dosing]** function in the **Manual control** dialog. If several dosing devices are connected then the dialog for selecting a dosing device will be opened. If only one dosing device is connected then the properties of this dosing device will be shown directly (see below).



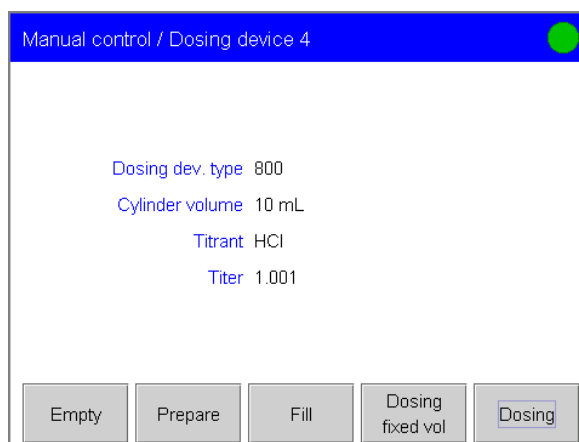
For every **dosing device** the **connection** (1 to 4) and the **type** are shown on the button. With type 8XX dosing devices with an intelligent exchange unit (IEU) or dosing unit (IDU) the **titrant** will be shown to the right. With type 6XX or 7XX dosing devices the cylinder volume of the EU or DU will be shown. If the EU or DU is not (correctly) attached to a connected dosing device then **---** will be shown. If a dosing device is busy with the determination sequence then it will be shown as inactive (gray).



With **[All dosing devices]** you can carry out the commands **Fill**, **Prepare** and **Empty** for several dosing devices at the same time.

☞ Select the **dosing device** to be controlled manually.

For type 8XX dosing devices with an intelligent exchange unit (IEU) or dosing unit (IDU) the data stored on the datachip of the IEU or IDU will be displayed.



For type 6xx or 7xx dosing devices you can select a titrant from the titrants configured under **System/Titrants**. Only those titrants which are suitable for use with the corresponding type of dosing device will be shown in the selection list, i.e. dosing units for Dosinos and exchange units for Dosimats. The cylinder volume is checked when dosing is carried out.

Manual control / Dosing device 1

Dosing dev. type 808

Cylinder volume 10 mL

Titrant NaOH

Titer 1.015

Prepare Fill Dosing fixed vol Dosing

Dosing:

Under manual control dosing will be carried out for as long as the **[Dose]** button is touched or clicked on.

☞ Use **[Dosing]** to open the dialog for manual dosing under **Manual control/Dosing device**.

Dosing device 1 / Dosing

Titrant: NaOH

Dosing rate dynamic mL/min

Filling rate maximum mL/min

1.4450 mL

Fill Dose

☞ Enter the **Dosing rate**. The maximum dosing rate depends on the cylinder volume of the buret used (see *Section 3.8.6*). **Dynamic** means that dosing will be carried out quicker and quicker until the maximum dosing rate has been reached (starting with 1 mL/min and then doubling the dosing rate every 1.5 s). **Dynamic** can only be selected when the buret is full, i.e. when either 0.0000 mL or a whole cylinder volume is displayed. If dynamic dosing is selected then the dosing rate cannot be altered while dosing is taking place.

☞ Enter the rate at which the buret is to be filled. The maximum **Filling rate** depends on the cylinder volume of the buret used (see *Section 3.8.6*).

☞ You can carry out manual dosing with **[Dose]**. The added volume is shown in the volume display. When a cylinder volume has been added the buret will be refilled automatically.

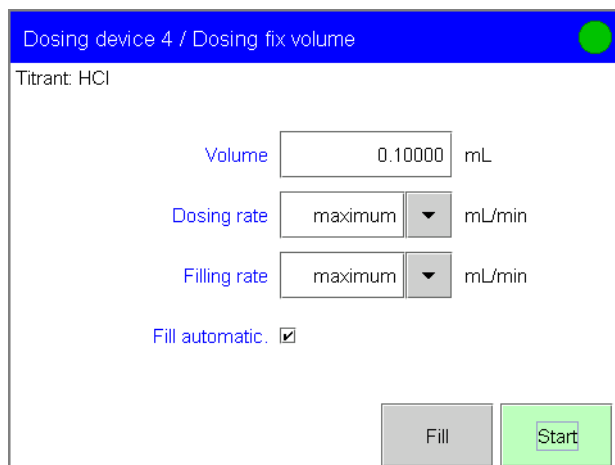
☞ You can refill the buret with **[Fill]**. The shown volume will be reset to 0.0000 mL.

If you exit the dialog with **[Back]** then the buret will be refilled and the valve switched to the change position.

Dosing fixed volume:

Under **Dosing device/Dosing fixed volume** you can add a specified volume.

☞ Open the dialog for dosing a specified volume under **Manual control/Dosing** with **[Dosing fixed volume]**.




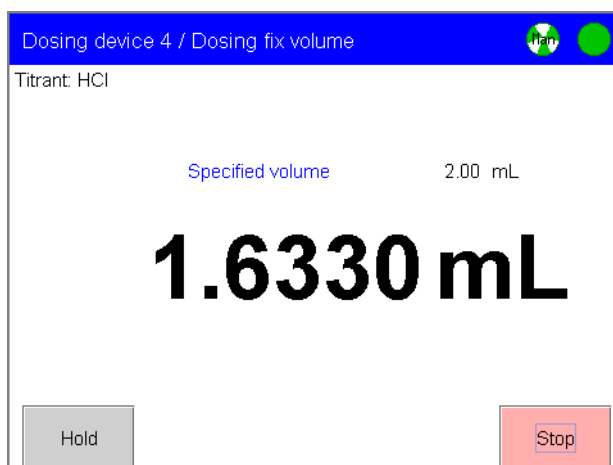
☞ Enter the volume to be added.

☞ Enter the **Dosing rate**. The maximum dosing rate depends on the cylinder volume of the buret used (see *Section 3.8.6*).

☞ Enter the rate at which the buret is to be filled. The maximum **Fill-ing rate** depends on the cylinder volume of the buret used (see *Section 3.8.6*).

If the **Fill automatically** checkbox is activated then the buret will be refilled automatically after dosing has been carried out and the added volume will be reset to 0.0000 mL in the volume display (see below). If the **Fill automatically** checkbox is deactivated then at each start the dosed-in fixed volumes will be added together. In the volume display (see below) there will be an additional **[Fill]** button. The added volume will only be reset to 0.0000 mL when the buret is refilled with **[Fill]** or the volume display is exited.

 **[Start]** is used to start the addition of the specified volume.



The volume to be added (specified volume) is shown above the **volume display**. The volume display shows the volume which has been added since the start of dosing.

[Stop] is used to stop the addition. You can use **[Hold]** to interrupt the addition and continue it with **[Continue]**.

Fill:

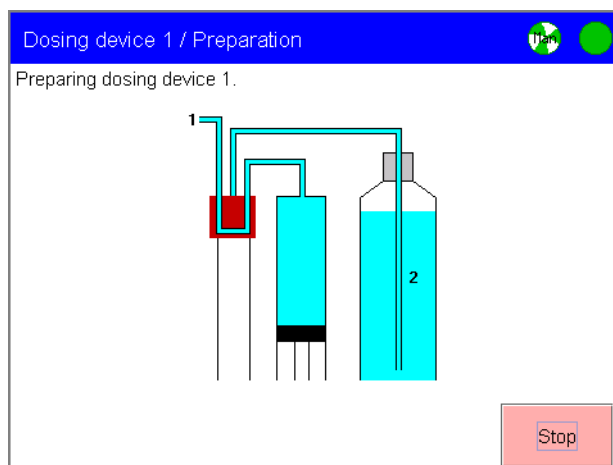
You can fill the buret manually with the **[Fill]** function. The piston and valve positions are shown during the filling process. Filling is carried out at the maximum filling rate.

Prepare:

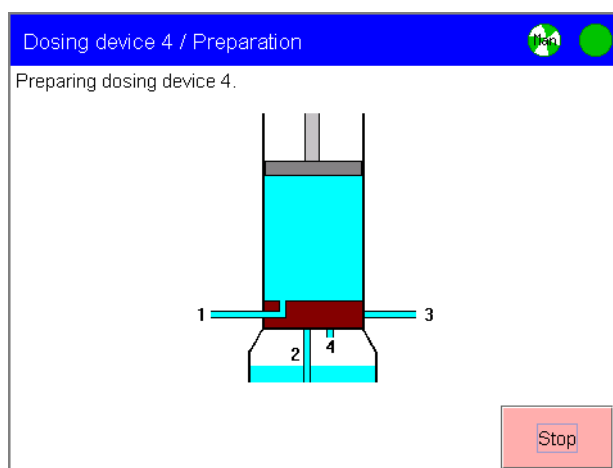
The **[Prepare]** function is used to rinse the cylinder and tubing of the exchange unit or dosing unit and refill them. The parameters defined for the titrant under **System/Titrants** and the tubing parameters will be used for rinsing (see *Section 3.8.6*). For every dosing device (MSB) you can use the **Device manager** to define when a message is to be shown to remind you that the dosing device has to be prepared (see *Section 3.10.4*).

 Start the preparation process with **[Prepare]**.

With an **exchange unit** you should carry out the prepare function before it is used for the first time and whenever the exchange unit has not been used for a long time.



With a **dosing unit** you should carry out the **Prepare** function (PREP command) before each sample series or about once every day.



Empty:

The **[Empty]** function can only be carried out with Dosino-type dosing devices. The Empty function empties the cylinder and all the tubing of the dosing unit. The parameters defined under **System/Titrants** for preparing the buret and the tubing parameters are used for emptying (see Section 3.8.6).

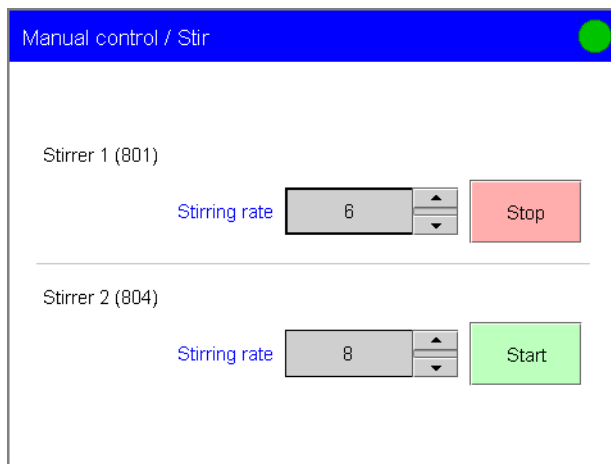
You can use the empty and prepare functions with a Dosino to change the reagent in a simple way without coming into contact with chemicals. Proceed as follows:

- ☞ Empty the dosing unit with **[Empty]**.
- ☞ Carry out the **[Prepare]** function using a suitable solvent to rinse the dosing unit.
- ☞ Empty the dosing unit with **[Empty]**.
- ☞ Carry out the **[Prepare]** function using the new reagent.

3.24.3 Stir

All the connected stirrers can be controlled manually.

☞ Select the **[Stir]** function in the **Manual operation** dialog.



The **connection** (1...4) and (in brackets) the **stirrer type** are shown for each **Stirrer**.

☞ You can increase the stirring rate with **[+]** or **[arrow up]** and decrease it with **[-]** or **[arrow down]**. The stirring direction changes as the sign changes. The stirring rate can also be altered while the stirrer is running. The default setting **8** corresponds to 1000 rpm (see Section 4.1.3, Fig. 21).

☞ **[Start]** starts stirring and **[Stop]** stops it.

If you have connected more than two stirrers then you can open the dialog for Stirrer 3 (and 4) with **[More stirrers]**.

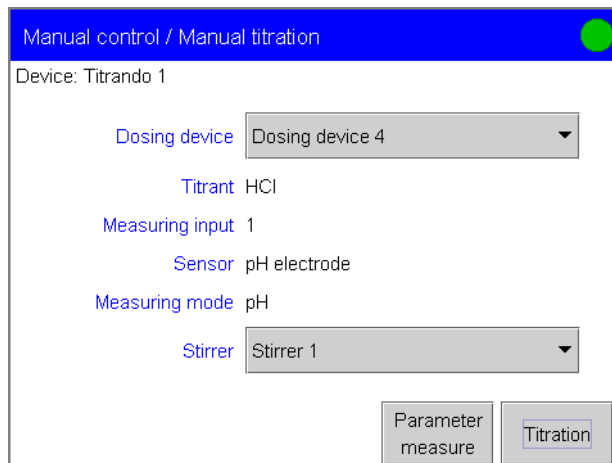
If you have started a stirrer manually then it will not be switched off automatically at the start of a determination. This means, for example, that you can switch on the stirrer before the start of a determination in order to dissolve the sample. The stirrer will continue to run during the determination until it is switched off in the determination sequence.

If a stirrer is used in the determination sequence it can nevertheless be controlled manually at the same time. You can, for example, use the manual control to reduce the stirring rate of a stirrer which has been started in the determination sequence.

3.24.4 Manual titration

Manual titrations can be carried out in the pH, U (mV), I_{pol} (mV), U_{pol} (μA), concentration and T (°C) modes.

- ☞ Select the **[Manual titration]** function in the **Manual control** dialog.

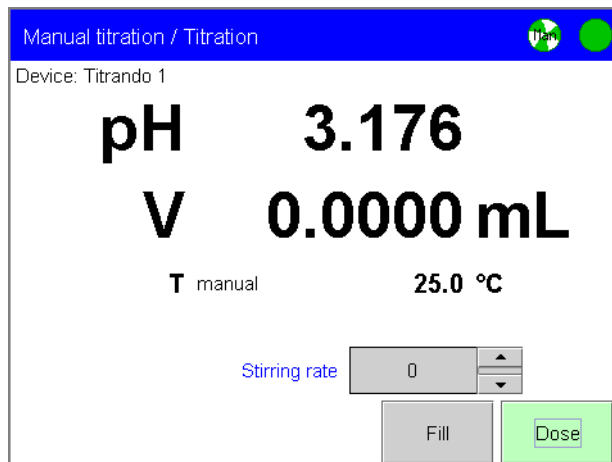


- ☞ Select the **Dosing device** to be used for the titration. With intelligent exchange or dosing units the **Titrant** contained in the buret will be displayed. With "non-intelligent" units the cylinder volume will be shown.

- ☞ Select the **Stirrer** to be used.

You can enter the **Measuring input**, **Sensor** and **Measuring mode** under **Manual titration/Parameter measure**.

- ☞ Use **[Parameter measure]** to open the edit dialog for the measurement parameters and enter these. The **measuring parameters** are described in *Section 3.24.1*.
- ☞ Use **[Titration]** to open the live display for the manual titration.



The live display shows the **current measured value** (updated every 500 ms), the added **volume**, the type of temperature measurement (**Pt1000**, **NTC** or **manual**) and the **measured temperature**.

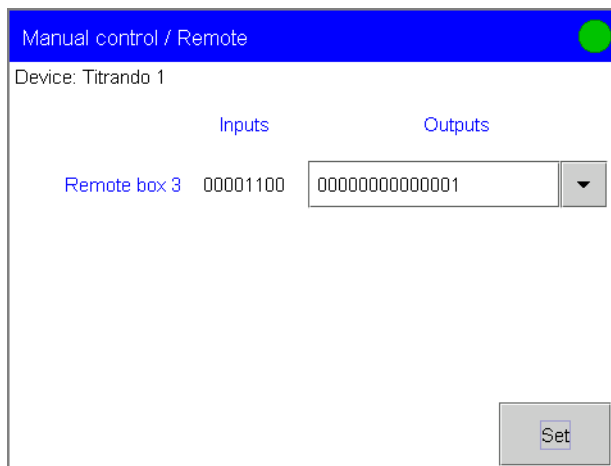
- ☞ You can increase the stirring rate with **[+]** or **[arrow up]** and decrease it with **[-]** or **[arrow down]**. The stirring direction changes as the sign changes (+ means counterclockwise and – means clockwise).
- ☞ You can carry out manual dosing with **[Dose]**. The buret will be refilled automatically when a cylinder volume has been added. Dosing will be carried out for as long as the **[Dose]** button is touched or clicked on. The addition is always **dynamic**, i.e. dosing will be carried out quicker and quicker until the maximum dosing rate has been reached (starting with 1 mL/min and then doubling the dosing rate every 1.5 s) .
- ☞ You can refill the buret with **[Fill]**. The shown volume will be reset to 0.0000 mL.

If you exit the dialog with **[Back]** then the buret will be refilled and the valve switched to the change position.

3.24.5 Remote

You can **set output lines** manually. The status of the **input lines** is scanned automatically.

- ☞ Select the **[Remote]** function in the **Manual control** dialog.



The current status of the input lines will be shown for each connected remote box. The output lines can be set. The input and output lines are always numbered from right to left starting with 0. Please consult the **online help** for entering the binary pattern. You can select binary patterns defined in the selection list under **System/Templates**.

- ☞ The binary patterns defined under Outputs are set with **[Set]**.

4 Parameters

All the **parameters for the method commands**, from which a list of commands can be constructed, are explained in this section. How you can insert an individual command in the list of commands is described in Section 3.16.2. The way of selecting a command from the list and editing it is described in Section 3.16.1.

With many numerical inputs you can also enter a **special value** (e.g. **off**) or a **result** that has previously been calculated (e.g. **R1**) instead of a number (see Section 4.4.5). With PC Control you can enter the special value with the arrow to the right of the input field (combobox). The result variables are entered directly via the PC keyboard. Numerical input for Touch Control is described in Section 3.1.4.

Parameters which are available as direct parameters (see Section 3.16.5) are marked with (d). For further **details about individual parameters**, e.g. the **input range** and **default values**, please use the context-sensitive **online help** (see Section 3.3.3).

4.1 Titrations

The following titration modes are available:

- **Dynamic equivalence point titrations (DET)** with dynamic incremental reagent addition for all standard titrations. The volume increments vary as a function of the slope of the curve. An attempt is made to achieve constant measured value alterations with each reagent addition. The optimal volume for dosing is determined from the measured value alterations of the previous reagent additions. Measured value acceptance is drift-controlled (equilibrium titration) or after a waiting period. Equivalence points are evaluated automatically (see Section 4.1.1).

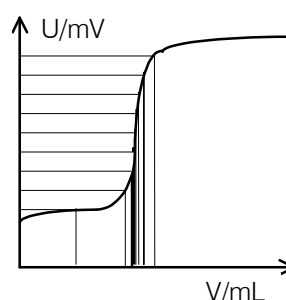


Fig. 15: Reagent addition for DET



Note!

As the reagent addition in DET depends on the measuring data, the titration curve should not vary too much from an **S-shaped curve**.

- **Monotonic equivalence point titrations (MET)** with reagent addition at constant volume increments for titrations with relatively high signal variations or suddenly occurring potential jump and for slow titrations or slowly responding electrodes. Measured value acceptance is drift-controlled (equilibrium titration) or after a waiting period. Equivalence points are evaluated automatically (see Section 4.1.1).

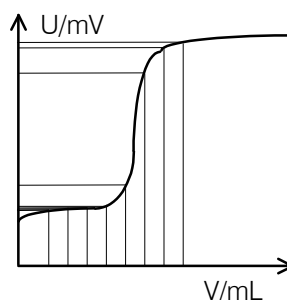


Fig. 16: Reagent addition for MET

- **Endpoint titrations (SET)** for rapid routine determinations by titration to a preset endpoint (e.g. titrations according to special standards) and titrations in which an excess of reagent must be avoided. The termination of the titration at the endpoint is either drift-controlled or after a waiting period. The volume that has been added when the endpoint is reached gives the calculable reagent consumption.

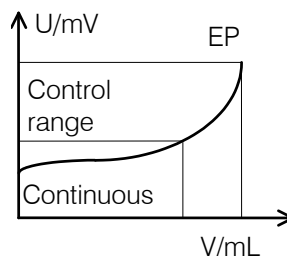


Fig. 17: Reagent addition for SET

The **measured quantities or modes** pH (potentiometric pH measurement), U (potentiometric voltage measurement), I_{pol} (voltammetric measurement with selectable polarization current) and U_{pol} (amperometric measurement with selectable polarization voltage) can be selected for all titrations.

4.1.1 Dynamic equivalence point titrations (DET) and monotonic equivalence point titrations (MET)

For equivalence point titrations in the DET and MET modes the parameters are identical except for a few exceptions. Both modes are described together here.

Start conditions

Under **Start conditions** the parameters for the initial addition of titrant and for the initial measured value (measured value before start conditions are processed) can be edited:

- **Start volume** (d): Volume that is added before the start of the titration. Under **Dosing rate** (d) you can enter the speed with which the start volume is to be added.
- **Pause** (d): Waiting period which is to elapse before the start of the titration after the start conditions have been fulfilled.
- **Start measured value** (d): Measured value at which the start volume addition is to be stopped. Under **Dosing rate** (d) you can enter the speed to be used until the start measured value or the start slope have been reached.
- **Start slope** (d): Slope (measured value per unit volume) at which the start volume addition is to be stopped. Under **Dosing rate** (d) you can enter the speed to be used until the start measured value or the start slope has been reached.

The start conditions are processed in succession: 1. Start volume, 2. Start measured value, 3. Start slope, 4. Pause.

Parameters for the **Initial measured value**:

- **Signal drift** (d): Drift, i.e. the alteration in the measured value per minute that has to be undercut for measured value acceptance.
- **Waiting time min.** (d): The minimum waiting period is only important for drift-controlled measurements. Measured value acceptance only takes place when the minimum waiting time has elapsed, even when the measured value drift has already been achieved. The drift continues to be checked while the waiting time is elapsing.
- **Waiting time max.** (d): If measured value drift is switched off or has not yet been achieved then the measured value will be accepted after the maximum waiting time has elapsed.

Titration parameters

Under **Titration parameters** you can edit the parameters for the titration procedure:

- **Titration rate** (d): Three predefined sets of parameters can be selected for the titration rate (see Table on p. 176). If individual titration parameters need to be adapted you should select the **user** setting and edit the individual titration parameters under **User defined Parameters**.

- **Temperature** (d): Manually entered titration temperature. If a temperature sensor is connected and the temperature measurement under **Sensor** is set to **automatic** or **continuous** (see Section 4.1.3) then the temperature will be measured continuously. The value is used for temperature compensation in pH measurements.

User defined Parameters

The **User defined Parameters** differ for dynamic equivalence point titrations (DET) and monotonic equivalence point titrations (MET).

User defined titration parameters for DET and MET

- **DET: Measuring point density** (d): A small value means small volume increments, i.e. a high measuring point density. The curve then shows all the finest details which also include noise; this could cause unwanted equivalence points to be found. A larger value, i.e. a smaller measuring point density, permits quicker titrations. If you are using a dosing device with a small cylinder volume then a smaller measuring point density value may be beneficial. However, you should also set a smaller measured value drift and a higher EP criterion at the same time.
- **DET: Minimum (volume) increment** (d): This smallest permitted volume increment is added at the start of the titration and with steep curves in the equivalence point region. Very small values should only be used if a low titrant consumption is expected, as unwanted equivalence points could be evaluated.



Note!

It is not advisable to select similar volumes for the minimum and maximum increments. For these applications monotonic equivalence point titration (MET) is more suitable.

- **DET: Maximum (volume) increment** (d): A maximum volume increment should be selected when the titrant consumption up to the equivalence point is expected to be very small, a start volume is to be added until just before the equivalence point is reached or if the change of direction in the potential jump region is very abrupt, as otherwise it is easy to add too large a volume in the equivalence point region. The value should not be less than 1/100 cylinder volume.
- **MET: Volume increment** (d): Volume to be added at each dosing step. The choice of the correct volume increment is a basic requirement for achieving high accuracy. A good guideline is 1/20 of the expected EP volume. For steep jumps the volume increment should tend toward 1/100 and for flat jumps toward 1/10 of the EP volume. Small volume increments are used for determining blank values or with very asymmetrical curves. The accuracy of the evaluation cannot be increased by using smaller increments as the measured value alterations between two measuring points are then of the same order of magnitude as the noise.
- **Dosing rate** (d): Rate at which the volume increment is added. The maximum dosing rate depends on the cylinder volume of the buret used (see Section 3.8.6).

- **Signal drift (d):** Drift, i.e. the alteration in the measured value per minute that has to be undercut for measured value acceptance. This type of titration is often known as an equilibrium titration. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the titration reaction occurs slowly or if the electrode has a slow response.


Note!

A **constant measured value** is often only achieved after a certain time, as mixing and possibly the reaction itself require a certain time. The response time of an electrode can also increase with time, i.e. reaching a constant measured value takes longer and longer. In such a case **drift-controlled measured value acceptance** is particularly advisable, as the measured values are only accepted when equilibrium has almost been achieved.

- **Waiting time min. (d):** The minimum waiting period is only important for drift-controlled measurements. Measured value acceptance only takes place when the minimum waiting time has elapsed, even when the measured value drift has already been achieved.
- **Waiting time max. (d):** If measured value drift is switched off or has not yet been achieved then the measured value will be accepted after the maximum waiting time has elapsed. If the waiting time has not been newly entered then a waiting time that is suitable for the drift will be calculated automatically according to the following equation:

$$\text{Waiting time} = 150 / \sqrt{\text{Drift} + 0.01} + 5$$


Note!

Select **titration rate optimal** when you are developing a **new titration method**. This parameter is suitable for virtually all titrations and only needs adaptation in special cases.

Parameters for predefined titration rates for DET and MET

	Titration rate	slow	optimal	quick
DET	Meas. point density	2	4	6
	Min. vol. increment	10.00 μL	10.00 μL	30.00 μL
	Max. vol. increment	off	off	off
MET	Volume increment	0.05000 mL	0.10000 mL	0.20000 mL
DET and MET	Dosing rate	maximum	maximum	maximum
	Measured value drift	20.0 mV/min 20.0 $\mu\text{A}/\text{min}$	50.0 mV/min 50.0 $\mu\text{A}/\text{min}$	80.0 mV/min 80.0 $\mu\text{A}/\text{min}$
	Waiting time min.	0 s	0 s	0 s
	Waiting time max.	38 s	26 s	21 s

Stop conditions

The conditions for terminating the titration are defined under **Stop conditions**:

- **Stop volume** (d): Stops when the preset volume (including start volume) has been added since the start of the titration. The stop volume should be adapted to suit the sample weight or the titration vessel size.
- **Stop measured value** (d): Stops when the preset value for a measuring point has been exceeded or undercut since the start of the titration.
- **Stop EP** (d): Stops when the preset number of equivalence points has been found.
- **Volume after EP** (d): When the number of equivalence points defined under Stop EP has been found this volume will be added. In this way the curve can be continued after the endpoint has been reached.
- **Stop time** (d): Stops when the preset time (including start conditions) has elapsed since the start of the titration.

If several stop conditions have been set then the first criterion to be fulfilled will stop the titration.

- **Filling rate** (d): Speed with which the buret is to be refilled after the titration. The maximum filling rate depends on the cylinder volume of the buret used (see Section 3.8.6).

Pot. evaluation

Under **Potentiometric evaluation** the parameters for the evaluation of the titration curve, i.e. for automatic equivalence point recognition, are edited:

- **EP criterion** (d): The set equivalence point criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) which has been found. Equivalence points whose ERC is smaller than the set EP criterion will not be recognized (see *p. 179* and *p. 180*). The default value is suitable for most titrations.
- **EP recognition** (d): This parameter allows you to filter out the end-points you are looking for. Either all the equivalence points can be recognized, or only those which meet particular criteria: the first (only the first EP to be found), the greatest (only the EP with the largest ERC, i.e. the steepest jump), the last (only the last EP to be found), ascending (only EPs with a positive titration curve slope), descending (only EPs with a negative titration curve slope).
- **Set windows**: Up to nine regions (windows) can be defined on both the measured value axis as well as on the volume axis. Only equivalence points in the preset windows will be recognized and numbered according to the window (e.g. EP2 in window 2).

A window defines a region in which an equivalence point is expected. Equivalence points outside this region will not be recognized. Setting windows is advisable when interference and unnecessary equivalence points are to be suppressed. The list of windows is opened with **[Set windows]**.

No.	Lower limit	Upper limit
1	pH 2.000	pH 3.000
2	pH 5.000	pH 6.000

New Delete Edit

When the list is opened for the first time you will see that it already contains a window which covers the whole measured value or volume range. You can add and edit new windows with **[New]**. The selected window can be removed from the list with **[Delete]**. You can use **[Edit]** to adapt the upper and lower limits for the selected window. Windows must not overlap but may touch one another. Equivalence point recognition criteria can be defined for each window. Please note that no direct parameters can be defined for setting windows.

- **Lower limit**: Measured value or volume for the lower limit of the window.

- **Upper limit:** Measured value or volume for the upper limit of the window.
- **EP criterion:** The set equivalence point criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) which has been found. Equivalence points whose ERC is smaller than the set EP criterion will not be recognized (see below). The default value is suitable for most titrations.
- **EP recognition:** Only equivalence points which fulfill particular criteria will be recognized: the first (only the first EP to be found), the greatest (only the EP with the largest ERC, i.e. the steepest jump), the last (only the last EP to be found), ascending (only EPs with a positive titration curve slope), descending (only EPs with a negative titration curve slope).

Only one equivalence point will be recognized per window. The numbering of the equivalence point (EP) is determined by the numbering of the window (e.g. EP2 in window 2), so that even if EPs are missing the calculations will still be carried out with the correctly assigned EP volumes.

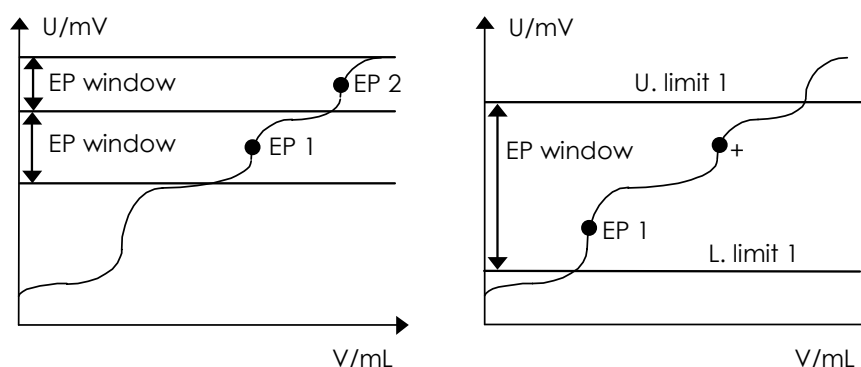


Fig. 18: Equivalence point recognition and numbering in windows

In the first example in Fig. 18 two equivalence points have been recognized in two different windows (EP1 in window 1 and EP2 in window 2). In the second example two equivalence points have been recognized in a single window, but only the first one will be recognized and the second jump will not. In order that the user can recognize that more than one equivalence point has been found in the set window, EP1 is marked with a '+' in the result display (see Section 3.18). In addition, the message **Several EPs in the window** will be entered in the list of messages.

The **evaluation of the titration curve** and therefore the EP criterion for the recognition of the equivalence points is different for dynamic equivalence point titrations (DET) and monotonic equivalence point titrations (MET).

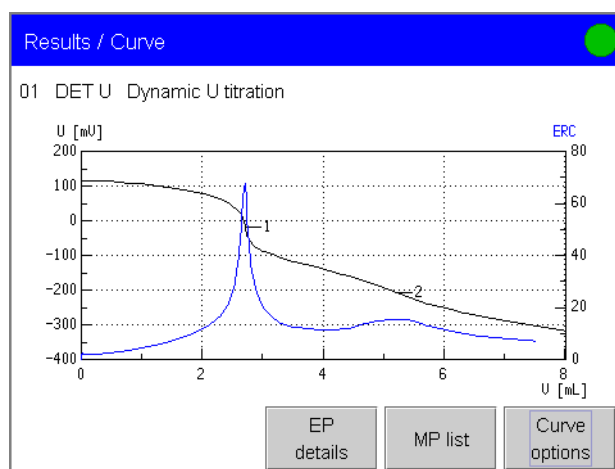
Evaluation and equivalence point criterion in the DET mode

The **equivalence points** (EPs) are calculated from the second derivative of the titration curve ($d^2\text{Meas. value}/dV^2$) according to a special Metrohm algorithm; overlapping jumps are also evaluated correctly.

For the recognition of the EPs found the set EP criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) found. The ERC is the first derivative of the titration curve combined with a mathematical function which is more sensitive for flat jumps than for steeper ones. EPs whose ERC is smaller than the set EP criterion will not be recognized. The ERC for each found and recognized EP will be shown under **Results/Curve/EP Details** (see Section 3.18.1 and Section 3.18.7). If you subsequently adapt the EP criterion so that more or fewer EPs are recognized, you can trigger the **re-evaluation** under **Results** with **[Re-calculate]** (see Section 3.18.8).

Curve / EP details				
01 DET U Dynamic U titration				
Endpoint 1				
Volume	2.7098 mL	EP1		
Measured value	-19.7 mV	EM1		
ERC	67.5	EF1		
Time	41.7 s	ED1		
Temperature	25.0 °C	ET1		
Endpoint 2				
Volume	5.2237 mL	EP2		
Measured value	-207.9 mV	EM2		
ERC	15.4	EF2		
Time	83.1 s	ED2		
Temperature	25.0 °C	ET2		

For dynamic equivalence point titrations you can also show the ERC in addition to the titration curve. If the difference between the ERCs of the endpoints is large enough you will also be able to read off a sensible value for the EP criterion from the curve.



In the example shown an EP criterion of 20 would make sense if only the first equivalence point is to be recognized.

Evaluation and equivalence point criterion in the MET mode

The **equivalence points** (EPs) are localized by a procedure based on the Fortuin method which has been adapted by Metrohm for numerical methods. A search is made for the largest measured value alteration (Δ_n). The exact EP is determined by using an interpolation factor ρ ; this depends on the Δ -values before and after Δ_n :

$$V_{EP} = V_0 + \rho \Delta V$$

V_{EP} = EP volume, V_0 = total volume added before Δ_n , ΔV = volume increment, ρ = interpolation factor according to Fortuin

For the recognition of the EPs found the set EP criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) found. The ERC is the sum of the measured value alterations before and after the jump:

$$|\Delta_{n-2}| + |\Delta_{n-1}| + |\Delta_n| + |\Delta_{n+1}| + |\Delta_{n+2}|$$

(In certain cases only three or only a single summand are taken into account.)

EPs whose ERC is smaller than the set EP criterion will not be recognized. The ERC for each found and recognized EP will be shown under **Results/Curve/EP Details** (see *Section 3.18.1* and *Section 3.18.7*). If you subsequently adapt the EP criterion so that more or fewer EPs are recognized, you can trigger the **re-evaluation** under **Results** with **[Re-calculate]** (see *Section 3.18.8*).

Curve / EP details			
01 MET U Monotonic U-Titration			
Endpoint 1			
Volume	2.7103 mL	EP1	
Measured value	-13.3 mV	EM1	
ERC	129.4 mV	EF1	
Time	57.9 s	ED1	
Temperature	25.0 °C	ET1	
Endpoint 2			
Volume	5.2320 mL	EP2	
Measured value	-208.4 mV	EM2	
ERC	19.6 mV	EF2	
Time	110.9 s	ED2	
Temperature	25.0 °C	ET2	

The parameters for **Titrand**, **Sensor**, **Dosing device** and **Stirrer** are described in *Section 4.1.3*.

Titration sequence for DET and MET

Start of titration command	
(Switch on stirrer)	The stirrer is switched on after the start.
Measure initial measured value	The initial measured value is measured.
(Start conditions: start volume start meas. value start slope pause)	The start volume is added with the start conditions being processed in succession. No measuring points are entered in the measuring point list. The pause interval is allowed to elapse.
Titration: add increments accept measured values	Volume increments are added during the titration and a measuring point is entered on the measuring point list after each increment. Measured value acceptance is either drift-controlled (equilibrium titration) or a fixed waiting time is allowed to elapse. The first criterion to be fulfilled applies.
Stop conditions	The first criterion to be fulfilled applies for stopping the titration.
(Switch off stirrer)	The stirrer is switched off.
Fill buret	After the end of the titration the buret is refilled automatically.

Optional steps are shown in brackets.

4.1.2 Endpoint titrations (SET)

Start conditions

Under **Start conditions** the parameters for the start volume of titrant and for the measurement of the initial measured value are edited:

- **Pause 1** (d): Waiting time, e.g. for electrode equilibration, before a start volume is added.
- **Start volume** (d): Volume that is added before the start of the titration. Under **Dosing rate** (d) you can enter the speed with which the start volume is to be added.
- **Pause 2** (d): Waiting time which is allowed to elapse before the start of the titration after the start volume has been added.

Parameters for the **Initial measured value**:

- **Signal drift** (d): Drift, i.e. alteration in the measured value per minute, which has to be undercut before the measured value will be accepted.
- **Waiting time min.** (d): The minimum waiting period is only important for drift-controlled measurements. Measured value acceptance only takes place when the minimum waiting time has elapsed, even when the measured value drift has already been achieved. The drift continues to be checked while the waiting time is elapsing.
- **Waiting time max.** (d): If measured value drift is switched off or has not yet been achieved then the measured value will be accepted after the maximum waiting time has elapsed.

Control parameters

Editing the **Control parameters** for Endpoint 1 and Endpoint 2:

- **EP1 at** (d): Measured value for the first endpoint.
- **Titration rate** (d): Three predefined sets of parameters can be selected for the titration rate (see Table on *p.* 183). If individual titration parameters need to be adapted you should select the **user** setting and edit the individual titration parameters under **User defined Parameters**.

User defined Parameters

Editing the **User defined Parameters**:

- **Dynamics** (d) : The control range defines the measured value range before the preset endpoint. In the control range addition is controlled by the **Minimum rate**. The closer the endpoint, the slower the titrant addition until the **Minimum rate** has been reached. The larger the control range, the slower the titration. Outside the control range addition is carried out continuously at the **Maximum rate**.
- **Maximum rate** (d): Speed at which addition is carried out outside the control range. The maximum dosing rate depends on the cylinder volume of the buret used (see *Section 3.8.6*).
- **Minimum rate** (d): This parameter determines the addition rate right at the start of the titration and in the **Dynamic** range at the end of the titration. It has a decisive influence on the titration speed and there-

fore on the accuracy. The smaller the minimum rate which is selected, the slower the titration.

Parameters for the predefined titration rates for SET

	Titration rate	slow	optimal	quick
SET	Control range	2.000 pH 300.0 mV 40.0 μ A	2.000 pH 100.0 mV 10.0 μ A	0.500 pH 30.0 mV 5.0 μ A
	Max. rate	1.00 mL/min	10.00 mL/min	maximum
	Min. rate	5.00 μ L/min	25.00 μ L/min	50.00 μ L/min

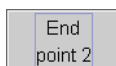
Stop criterion

Editing the parameters for the **Stop criterion**:

- **Stop criterion** (d): The titration stops when the endpoint has been reached and the stop criterion has been fulfilled. The titration can be stopped when a particular (volume) **drift** has been achieved or after a preset **time**. If no stop criterion has been selected the titration will not be stopped. The **Stop conditions** (see below) will always stop the titration even if the stop criterion has not been fulfilled.
- **Stop drift** (d): If the EP and the stop drift have been reached the titration will be stopped.
- **Delay time** (d): After the endpoint has been reached the preset time will be allowed to elapse after the last addition before the titration is stopped.

In older instructions the switch-off time was usually defined as the **Stop criterion**. The stop criterion **time** means that the endpoint must be exceeded for a certain time; this is the switch-off time. The same switch-off time with different very small volume increments (depending on the volume of the exchange or dosing unit, see below) means different switch-off points. In contrast, if **drift** is used as the stop criterion then the switch-off point will always have the same curve slope dV/dt .

You can use the switch-off time in the following way to calculate the maximum stop drift to be used: the size of the last increment to be added depends on the volume of the attached exchange unit. With a 20 mL exchange unit (10000 impulses per cylinder volume) the smallest possible increment is 2 μ L. With a switch-off time of 5 s this means that the last 2 μ L of reagent to be added must be sufficient for 5 s or longer. This results in a drift of $\leq 2 \mu\text{L}/5 \text{ s} = 24 \mu\text{L}/\text{min}$. The drift can be smaller than 24 $\mu\text{L}/\text{min}$ as we do not know whether the last increment would also have been sufficient for 10 s. This means that if you have previously worked with a 20 mL exchange unit (10000 impulses per cylinder volume) and 5 s switch-off delay then you should set a value of $\leq 24 \mu\text{L}/\text{min}$ as the stop drift.



The control parameters for Endpoint 2 are the same as for Endpoint 1.

Optimizing the control parameters

Reagent addition takes place in three phases during the titration:

- **Initial addition:** during this phase the dosing rate increases continuously. It starts with the **Minimum rate** and increases to the **Maximum rate**.
- **Continuous addition:** addition is carried out at the **Maximum rate** until the control range is reached.
- **Control range:** in this range addition is finely controlled. Shortly before the endpoint is reached addition is only carried out at the **Minimum rate**.

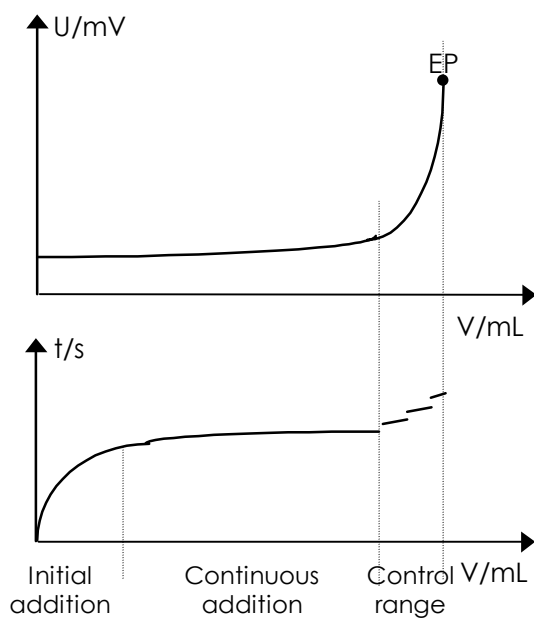


Fig. 19: Reagent addition during endpoint titrations with SET

Set a large **Control range** for steep curves and a small control range for flat ones. A good approximation for the start of the control range is given by the point where the tangents intersect:

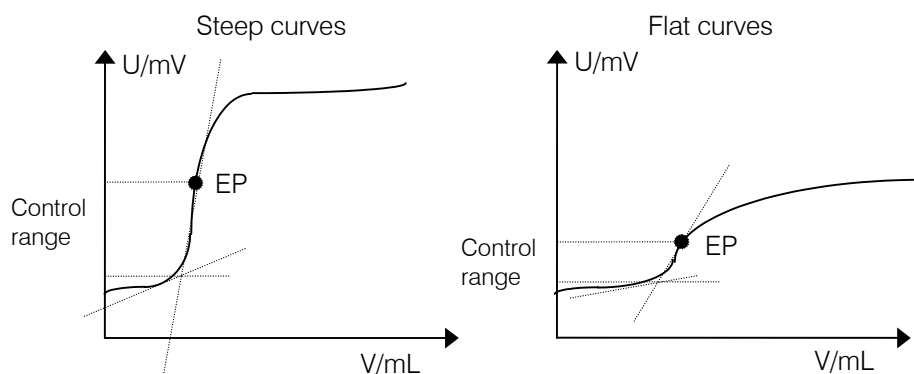


Fig. 20: Control range size

Titration parameters

The parameters for the titration sequence are edited under **Titration parameters**:

- **Titration direction** (d): The titration direction is normally determined automatically from the initial measured value and the set endpoint. We recommend that, whenever possible, a positive or negative measured value alteration is entered. If two endpoints have been set then the titration direction will be defined automatically. In this case the setting will be ignored.
- **Extraction time** (d): The titration takes place during this time. The titration will not be stopped until the extraction time has elapsed (even if the EP has already been reached). The entry of an extraction time may be advisable, e.g. for the titration of sparingly soluble samples.
- **Temperature** (d): Manually set titration temperature. If a temperature sensor is connected and temperature measurement has been set under **Sensor** to **automatic** or **continuous** (see Section 4.1.3) then the temperature will be measured continuously. The value is used for temperature compensation in pH measurements.
- **Time interval MP** (d): Time interval for entering a measuring point in the measuring point list.

Stop conditions

The conditions for terminating the titration are defined under **Stop conditions** if this does not occur automatically because either the set endpoint has not been reached or the stop criteria have not been fulfilled:

- **Stop volume** (d): Stops when the preset volume has been added since the start of the titration. You should adapt the stop volume to suit the size of your titration vessel in order to prevent it from overflowing.

- **Stop time** (d): Stops when the preset time has elapsed since the start of the titration.

If several stop conditions have been set then the first criterion to be fulfilled will stop the titration.

- **Filling rate** (d): Speed with which the buret is to be refilled after the titration. The maximum filling rate depends on the cylinder volume of the buret used (see *Section 3.8.6*).

The parameters for **Titrand**, **Sensor**, **Dosing device** and **Stirrer** are described in *Section 4.1.3*.

Titration sequence for SET

Start of titration command	
(Switch on stirrer)	The stirrer is switched on after the start.
Measure initial measured value	The initial measured value is measured.
(Start conditions: Pause 1 Start volume Pause 2)	Pause interval 1 is allowed to elapse. The start volume is added. No measuring points are entered in the measuring point list. Pause interval 2 is allowed to elapse.
(Extraction time) Titration with test up to stop when stop criterion or the stop condition is reached	Titration is carried out to the first and then the second endpoint. If the extraction time has not elapsed when the (first) endpoint has been reached then it will be allowed to elapse and the titration (to the first endpoint) will only be concluded when the extraction time has elapsed.
(Switch off stirrer)	The stirrer is switched off.
Fill buret	After the end of the titration the buret is refilled automatically.

Optional steps are shown in brackets.

4.1.3 Titrand, sensor, dosing device and stirrer

The parameters for the Titrand, sensor, dosing device and the stirrer are the same for the DET, MET and SET titration modes.

Titrand

Under **Titrand** you can select the Titrand with which the titration (or measurement or calibration) is to be carried out. This button will only appear when several Titrands have been configured under **System/Device manager** (see Section 3.10.1). The instrument names are always shown in the selection list.

Sensor

The parameters for the electrode connection are edited under **Sensor**:

- **Measuring input** (d): Selects the measuring input to which the sensor is connected. The choice is not dependent on whether the Titrand has one or two measuring inputs.
- **Sensor** (d): Selects the sensor from the sensor list defined under **System/Sensors**. The selection depends on the quantity to be measured (see **online help**). The calibration data for the sensor will be adopted for pH and ISE electrodes. You can also enter a sensor name which is not contained in the sensor list. However, the sensor must be present in the sensor list when the titration is carried out.
- **I(pol)** (d): The polarization current is the current applied to the polarized electrode during a voltammetric measurement. This parameter is only available for titrations in the I(pol) mode.
- **U(pol)** (d): The polarization voltage is the potential applied to the polarized electrode during an amperometric measurement. This parameter is only available for titrations in the U(pol) mode.
- **Electrode test** (d): The electrode test for polarized electrodes is carried out during the transition from an inactive condition to a measuring condition. A check is made that the electrode is properly connected and that no short-circuit is present.
- **Temperature measurement** (d): The temperature is normally measured **automatically** if a temperature sensor is connected. Otherwise the temperature entered manually under **Temperature (Measuring parameters, Titration parameters)** will be used. With **continuous** you can ensure that a temperature sensor must be connected. With **off** the temperature entered manually under **Temperature (Measuring parameters, Titration parameters)** will always be used.

Dosing device

The parameters for the dosing device are edited under **Dosing device**:

- **Dosing device** (d): Selects the dosing device to be used for the titration. All the dosing device connections (MSB) are always shown.
- **Titrant** (d): Titrant to be used for the titration (or dosing). The titrant can be selected from the list of titrants which have been defined under **System/Titrants**. If intelligent exchange or dosing units are used then a check will be made in the method sequence that the correct titrant is present in the connected dosing device and whether the type of dosing device is correct. With non-intelligent exchange or dosing units the cylinder volume is checked. At the start of the titration the validity of the titer and the expiry date of the selected titrant will be checked as well as the GLP test interval for the buret. The titer (Variable TITER) and the concentration (Variable CONC) are also available for calculation (CALC command, see Section 4.4.1).

Stirrer

The parameters for the stirrer are edited under **Stirrer**:

- **Stirrer** (d): Selects the stirrer to be used in the titration. All the stirrer connections (MSB) will always be shown.
- **Stirring rate** (d) : You can check the optimal stirring rate manually (see Section 3.24.3). The stirring direction changes as the sign changes. The default setting **8** corresponds to 1000 min^{-1} (see Fig. 21).
- **Switch off automatically** (d): This function is used to switch off the stirrer automatically at the end of the titration.

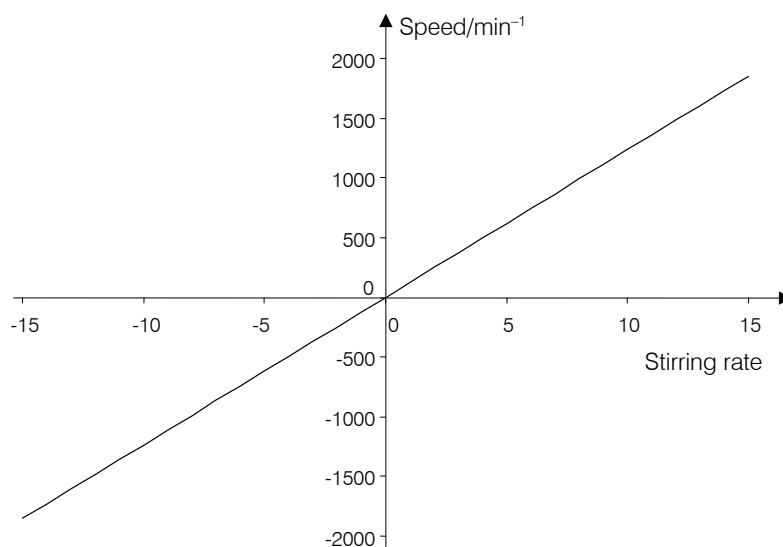


Fig. 21: Setting the stirring rate and speed

4.1.4 Direct parameters

Direct parameters can be defined for all titration commands; these are then shown in a table when the parameter dialog is opened and can be edited directly (see *Section 3.16.5*). Direct access ("**Quick Access**") to the edit dialog for selected method parameters simplifies the editing of parameters which need frequent alteration.

Direct parameters

You can define the parameters to be shown in the list of direct parameters under **Direct parameters**. For titrations these are all the parameters except those used for setting windows.

Parameters

Current method: New method

01	DET pH	Titration rate	optimal
01	DET pH	Stop volume	100.000 mL
01	DET pH	Stirring rate	8

Save method

Sequence

Edit parameter

4.2 Measurements (MEAS)

The **measured quantities or modes** pH (potentiometric pH measurement), U (potentiometric voltage measurement), Ipol (voltammetric measurement with selectable polarization current), Upol (amperometric measurement with selectable polarization voltage) and Conc (concentration measurement) can be selected for all measurements.

Measuring parameters

The parameters for the measurement sequence are edited under **Measuring parameters**.

- **Signal drift** (d): Drift, i.e. the alteration in the measured value per minute that has to be undercut for measured value acceptance. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the electrode has a very slow response.



Note!

A **constant measured value** is often only achieved after a certain time, as mixing and possibly the reaction itself require a certain time. The response time of an electrode can also increase with time, i.e. reaching a constant measured value takes longer and longer. In such a case **drift-controlled measured value acceptance** is particularly advisable, as the measured values are only accepted when equilibrium has almost been achieved.

- **Waiting time min.** (d): The minimum waiting period is only important for drift-controlled measurements. Measured value acceptance only takes place when the minimum waiting time has elapsed, even when the measured value drift has already been achieved.
- **Waiting time max.** (d): If measured value drift is switched off or has not yet been achieved then the measured value will be accepted after the maximum waiting time has elapsed. If the waiting time has not been newly entered then a waiting time that is suitable for the drift will be calculated automatically according to the following equation:

$$\text{Waiting time} = 150 / \sqrt{\text{Drift} + 0.01} + 5$$

- **Stop measured value** (d): Stops when the preset measured value has been reached since the start of the measurement.
- **Temperature** (d): Manually set titration temperature. If a temperature sensor is connected and temperature measurement has been set under **Sensor** to **automatic** or **continuous** (see Section 4.1.3) then the temperature will be measured continuously. The value is used for temperature compensation in pH measurements.
- **Time interval MP** (d): Time interval for entering a measuring point in the measuring point list. The measuring point list can contain max. 1000 measuring points.

The parameters for **Titrand**, **Sensor** and **Stirrer** are described in *Section 4.1.3*. The selection of the **Direct parameters** is carried out as described in *Section 4.1.4* .

4.3 Evaluation

A list of measuring points can have various **additional evaluations** applied to it. The evaluation (**EVAL command**) always refers to the last titration or measurement in the method sequence. Which evaluations can be used for which titrations and measurements is given in the following table:

<i>Evaluation Titration Measur.</i>	<i>EVAL Fix EP Fixed end- points</i>	<i>EVAL pK/HNP pK value Half neutraliza- tion potential</i>	<i>EVAL MIN/MAX Minimum/ Maximum</i>	<i>EVAL BREAK Breakpoints</i>
DET pH	V, MV, t	pK value	yes	yes
DET U	V, MV, t	HNP	yes	yes
DET Ipol	V, MV, t	–	yes	yes
DET Upol	V, MV, t	–	yes	yes
MET pH	V, MV, t	pK value	yes	yes
MET U	V, MV, t	HNP	yes	yes
MET Ipol	V, MV, t	–	yes	yes
MET Upol	V, MV, t	–	yes	yes
SET pH	V, MV, t	–	yes	–
SET U	V, MV, t	–	yes	–
SET Ipol	V, MV, t	–	yes	–
SET Upol	V, MV, t	–	yes	–
MEAS pH	MV, t	–	yes	yes
MEAS U	MV, t	–	yes	yes
MEAS T	MV, t	–	yes	yes
MEAS Ipol	MV, t	–	yes	yes
MEAS Upol	MV, t	–	yes	yes
MEAS Conc	–	–	–	–

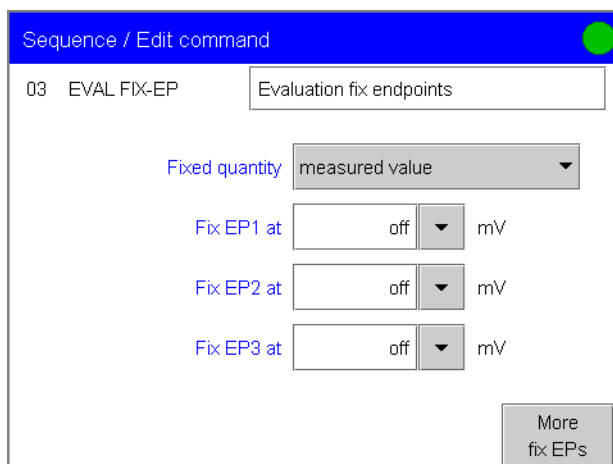
Only those evaluations which are available for the last titration or measurement before the EVAL command can be inserted in the list of commands. If a titration or measurement is deleted before the EVAL command then it will be shown in red in the list of commands, as the reference is missing.

You can also insert EVAL commands in the method sequence at a later date and trigger the **re-evaluation** under **Results** with **[Recalculate]** (see Section 3.18.8). The data for each evaluation can be shown under **Results/More determination data/View data** (see Section 3.18.1

and Section 3.18.7) and can be calculated in CALC commands (see Section 4.4.1).

4.3.1 Fixed endpoints (EVAL FIX EP)

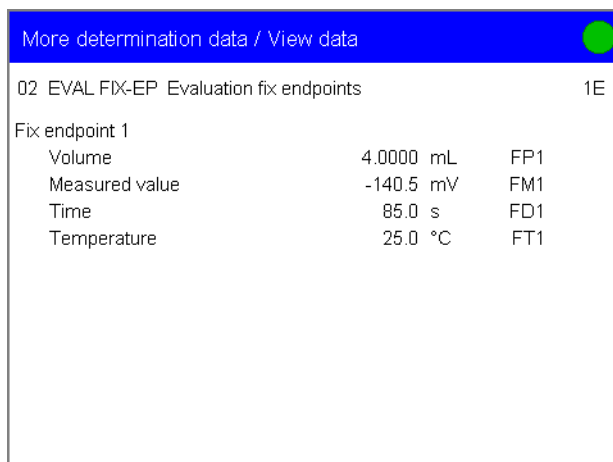
Fixed endpoints can be determined for all titrations (DET, MET and SET) and measurements (MEAS, without MEAS Conc). For a fixed quantity (measured value, volume or time) the associated values are interpolated from the list of measuring points.



- **Fixed quantity:** Selection of the fixed quantity.
- **Fix EP1 at to Fix EP9 at:** For the entered measured value, volume or time the associated values for the other quantities are interpolated from the list of measuring points. The fixed EP must lie between the first and last entries in the list of measuring points.

Up to nine fixed endpoints can be evaluated for each **EVAL FIX EP**.

The data for each fixed endpoint can be shown under **Results/More determination data/View data** (see Section 3.18.1 and Section 3.18.7).



Fix endpoint 1		
Volume	4.0000 mL	FP1
Measured value	-140.5 mV	FM1
Time	85.0 s	FD1
Temperature	25.0 °C	FT1

4.3.2 pK value and half neutralization potential (EVAL pK/HNP)

The pK value can be determined for pH titrations (DET and MET) and the half neutralization potential can be determined for U titrations.

The activities of conjugated acid-base pairs are linked by the following equation (Henderson-Hasselbalch equation):

$$\text{pH} = \text{pK}_a + \log (a_B/a_A)$$

If the activities of the acid and the conjugated base are equal ($a_A = a_B$), then $\text{pH} = \text{pK}_a$. This is the value at the half neutralization point and can be extrapolated from the titration curve. A careful pH calibration is necessary for pK evaluations and even then the determined pK value is only an approximation, as the ionic strengths are not taken into account. In order to obtain more accurate value, titrations must be carried out with decreasing ionic strengths and the results extrapolated to the ionic strength zero. pK evaluation in aqueous solution is limited to the range $3.5 < \text{pK} < 10.5$ because of the leveling effect of strong acids and the lack of jumps with very weak acids. pK values of mixtures of acids and polyvalent acids can also be determined.

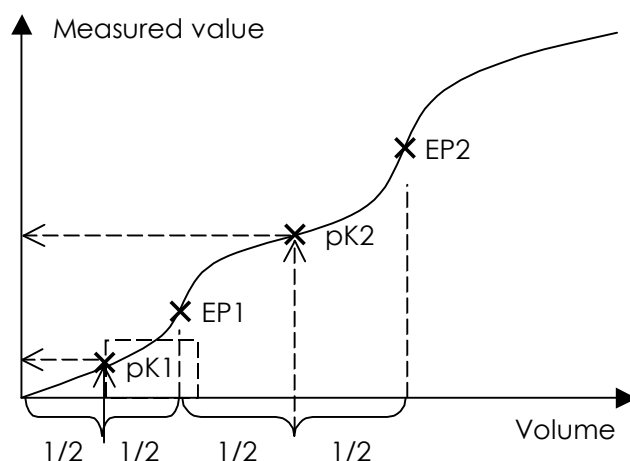


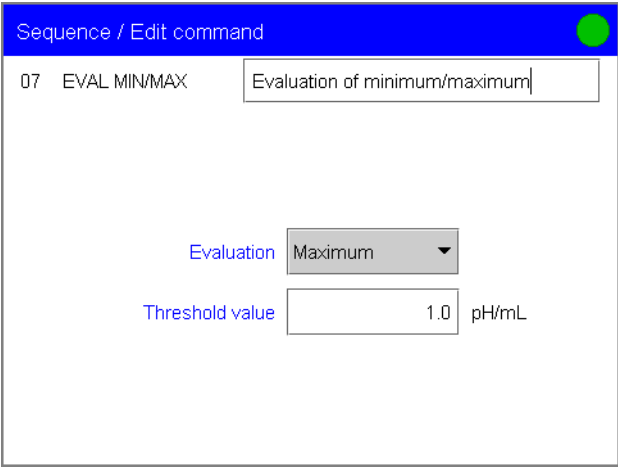
Fig. 22: Determining the pK value from the titration curve

In non-aqueous solutions the half neutralization potential (HNP) is frequently used instead of the pK value. The HNP is evaluated in the same way as the pK value.

No parameters can be edited for the command EVAL pK/HNP. If a start volume is to be added then it must be smaller than $1/2 V_{EP1}$.

4.3.3 Minimum and maximum (EVAL MIN/MAX)

For the minimum or maximum measured value the associated volume, time and temperature are interpolated from the list of measuring points. The evaluation begins as soon as the slope of the curve exceeds a particular threshold value.



Sequence / Edit command

07 EVAL MIN/MAX Evaluation of minimum/maximum

Evaluation Maximum

Threshold value 1.0 pH/mL

- **Evaluation:** In an EVAL MIN/MAX command either the minimum or the maximum can be evaluated. If you require both values then you must define a second EVAL MIN/MAX command in the method sequence.
- **Threshold value:** The evaluation begins as soon as the slope of the curve exceeds the set threshold value. Use a lower threshold value if the minimum or maximum is not found.

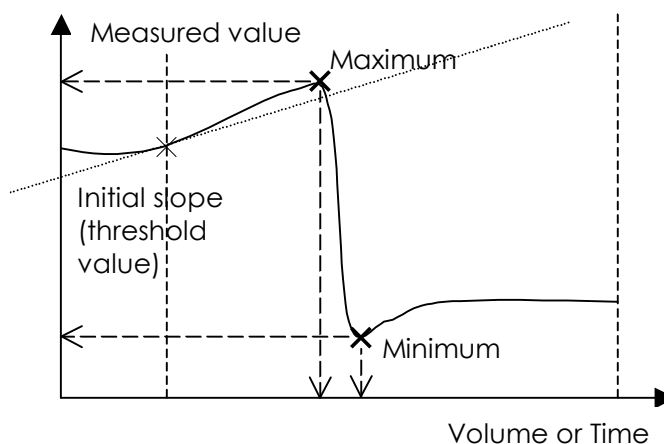
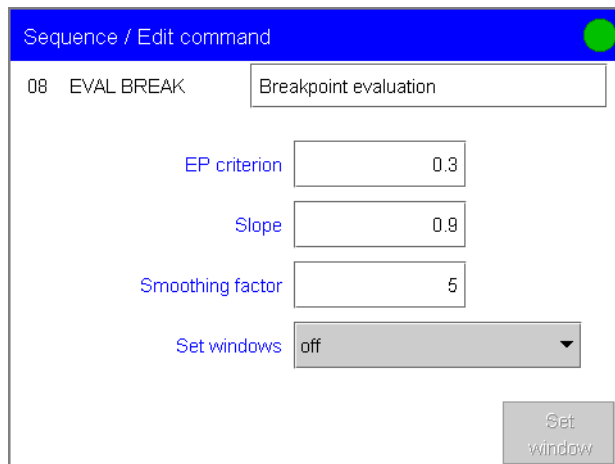


Fig. 23: Evaluation of minimum and maximum

4.3.4 Breakpoints (EVAL BREAK)

A breakpoint evaluation is used to determine sharp change of direction in the titration curve. This evaluation is primarily used for photometric and conductivity titrations. The method is based on the search for extremes in the second derivative of the curve.



Sequence / Edit command

08 EVAL BREAK Breakpoint evaluation

EP criterion 0.3

Slope 0.9

Smoothing factor 5

Set windows off

Set window

- **EP criterion:** Measure for the minimum sharpness of the break. The smaller the EP criterion set, the more breakpoints will be found. As this is a relative value related to the total measured value alteration, for a small measured value range even small changes in the measured value can be evaluated as a breakpoint.
- **Slope:** Minimum difference between the slope before and after the breakpoint. The smaller the difference, the more breakpoints will be found.
- **Smoothing factor:** The higher the smoothing factor, the fewer breakpoints will be found.
- **Set windows:** A range (window) can be defined on the measured value axis, on the volume axis or on the time axis. The breakpoint evaluation will only be carried out in the defined window. Only the first breakpoint in the defined window will be recognized.

[Set window] opens the dialog for entering the upper and lower limits.

- **Lower limit:** Measured value, time, or volume for the lower limit of the window.
- **Upper limit:** Measured value, time, or volume for the upper limit of the window.

It is also possible to evaluate several breakpoints in a single window.

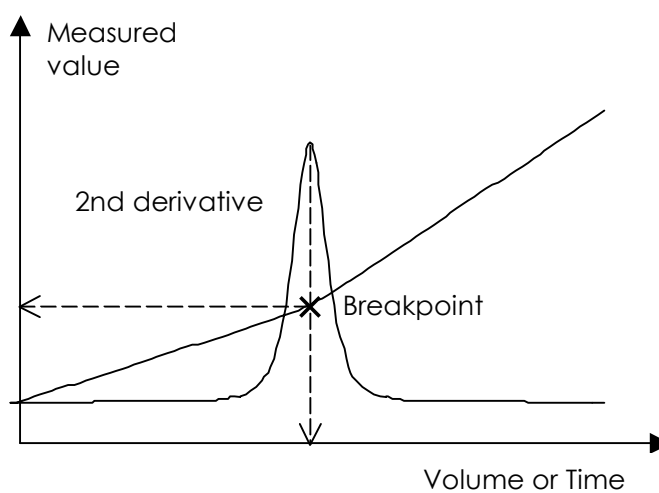


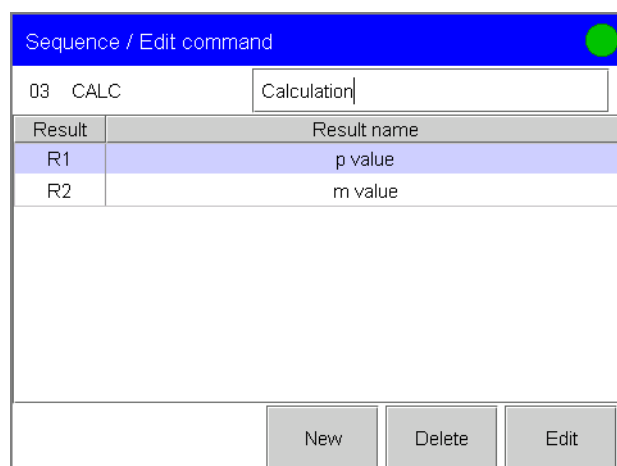
Fig. 24: Evaluating a breakpoint

4.4 Calculations

In the method sequence **result calculations** can be defined with the CALC command. A method can contain a maximum of nine CALC commands each with nine result calculations. The CALC commands also contain instructions for statistical calculations, titer assignments, storing common variables and storing results in the result silo. Limits can also be defined for the results. A range of calculable **variables** (raw data from the determination, previously calculated results and system-specific variables) are available for the calculations. Results which are calculated in the method sequence can be entered as variables for parameters.

4.4.1 CALC command

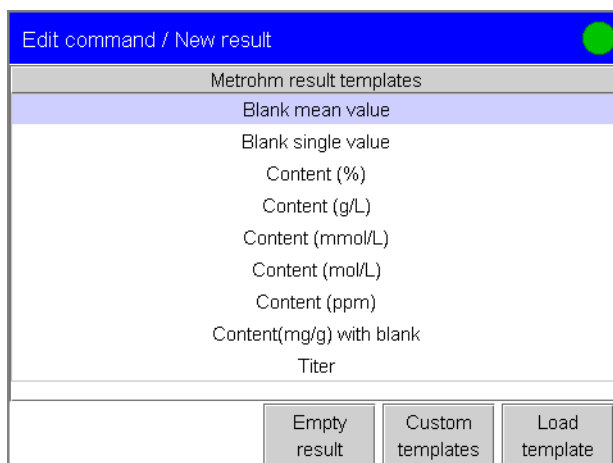
Up to nine result calculations can be defined in a CALC command. The results will be calculated in the sequence which is defined by the numbering of the result variables: R1...R9.



Result	Result name
R1	p value
R2	m value

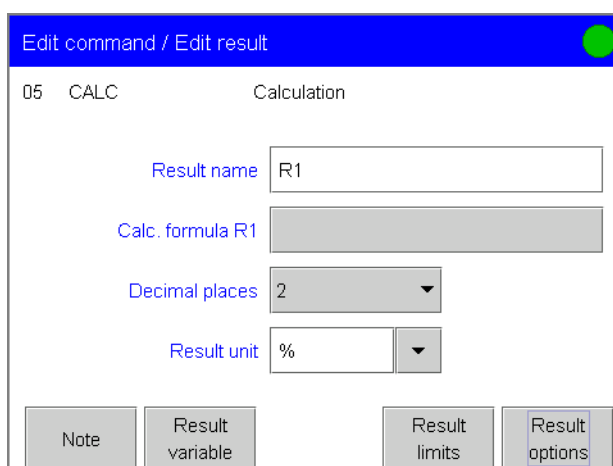
In the list of results you can use **[Edit]** to enter the equations and parameters for the result calculation and delete the selected result with **[Delete]**.

☞ You can insert a new result calculation in the list with **[New]**. The list with Metrohm result templates is opened.



The result template chosen in the selection list is loaded with **[Load template]** and a note concerning the template is shown. With **[Custom templates]** you can open the list of your own result templates (see [Section 3.14.3](#), [Section 4.4.3](#) and [Section 4.4.4](#)).

☞ Use **[Empty result]** to open the edit dialog directly.



- **Result name:** The standard result name corresponds to the result variable. The result name is the text which will be shown in the result display and in the report. It can be altered at any time.
- **Calculation formula:** The result variable is shown before the calculation formula. In subsequent calculations the calculated results can be accessed via the **[result variable]**. It can be altered later under result variable. A special editor is opened for the calculation formula if you touch the input field or click on it (see [Section 4.4.2](#)).
- **Decimal places:** Number of decimals to be shown in the result.
- **Result unit:** The result unit is shown and saved together with the result.

 Result options

Under **Result options** various parameters for the result calculation can be edited:

- **Variable for mean:** If **statistical calculations** has been switched on for the method under **Sequence/ Method options** then the mean value of the individual results will be stored as the variable **SMNx** ($x = 1$ to 9). Statistical calculations can be carried out for up to nine results in one determination. The first free statistics variable will always be shown as the default value. If no mean value is to be calculated for a result this variable should be set to **off**. The mean value for the result can be accessed via the statistics variable for further calculations.
- **Save result as titer:** In the determination sequence the result can be saved as the titer for the titrant selected in the last titration command before the calculation. If the **titer determination** is a single determination then you should select **Single value**. If a multiple determination is carried out then select **Mean value**. When the titer is assigned it will also be entered in the **History** (see *Section 3.8.4*). If a mean value is assigned then the last history entry will always be overwritten by the current mean value until all the determinations in the statistics series have been carried out. This means that there is only one history entry for a multiple determination. If single values are assigned then, when a determination is recalculated, the last entry will only be overwritten when it is the same determination that is being recalculated.
- **Save result as common variable:** The calculated result can be saved as an **instrument-specific common variable** (see *Section 3.13*). It is then also available in other methods for calculations.
- **Variable:** Selection of the common variables to be assigned to the result. Result name, value and unit are entered in the list of common variables.
- **Display result:** The **intermediate results** display can be switched off. The result will then no longer be shown in the result dialog, nor will it be printed out in the result report.
- **Save result in result silo:** In the **result silo** you can save results which have been obtained by using different methods (see *Section 3.22*). This may be advisable when, for instance, the results of all determinations carried out on a particular day are to be shown clearly. Nine results from a single determination can be stored in the result silo.
- **Precision:** Setting which determines the **accuracy** with which the result is to be further calculated. The result can be rounded off to the number of **decimal places** defined under **Edit result**, cut off after this number of decimal places or calculated with the full accuracy of the floating point number ("double precision" to Standard IEEE 754).

Result limits

Limits can be defined for each result to be calculated. These **Result limits** are monitored in the determination sequence when the calculation is carried out. If the result limits are monitored and remain within the limits then the result will be shown **green** in the result display (see *Section 3.18*); if the limits have been infringed then it will be shown in **red**.

☞ Open the dialog **Edit result/Result limits** and activate the **Monitoring result limits** checkbox.

☞ Enter an **Upper limit** and a **Lower limit** for the result. If a result is invalid then it will be treated as if the limits had been infringed.

The following **actions** are available if the result limits are infringed:

- **Display message:** The run is halted and a message is shown. You can choose whether you want to terminate the run or continue with it. The message will be documented under **Results/More determination data/Messages** (see *Section 3.18.2*).
- **Document message:** The run is not halted. A message that the result limits have been infringed will be documented under **Results/More determination data/Messages** (see *Section 3.18.2*).
- **Cancel determination:** The run is terminated and a corresponding message will be displayed and documented under **Results/More determination data/Messages** (see *Section 3.18.2*).

Result variable

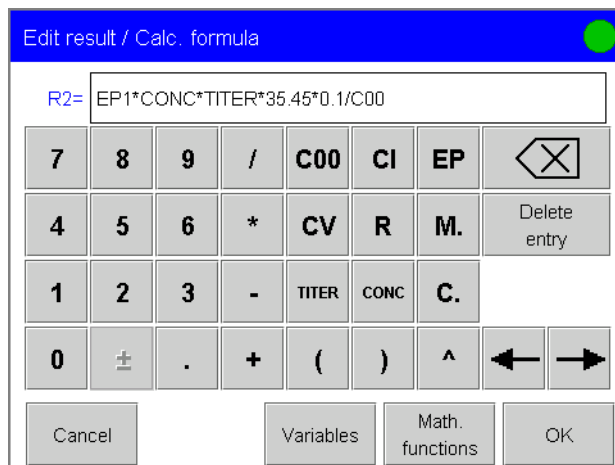
The **Result variable** is assigned automatically when a new result calculation is created. However, it can still be altered later. Only the result variables Rx (x = 1 to 9), which have not yet been assigned in this CALC command, can be selected. The value of the result can be accessed via the result variable. This means that a result can be used for further calculations.


Note

Under **Note** you can enter a short text, e.g. to describe the calculation variables used.

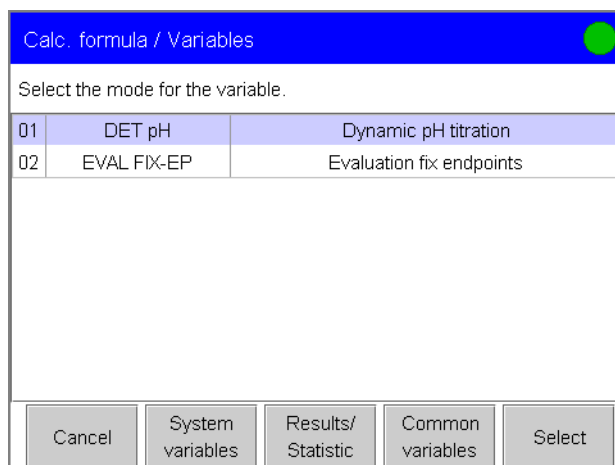
4.4.2 The formula editor

The formula editor is used to enter the **formulas for the result calculations**. The formula editor has an automatic **syntax check**, which is triggered when the formula is accepted. The priority rules which are normally valid apply to the calculation operations.



The **result variable** is shown in front of the input field. Buttons are available for entering numbers, mathematical operators and variables. The backspace key [>] deletes the character in front of the cursor. **[Delete entry]** will delete the whole formula. You can position the cursor within the formula by using the arrow keys. The maximum formula length is 100 characters.

You can use **[Variables]** to open selection lists for all the variables which are available. By selecting the variable from the list you can avoid syntax errors. If the method sequence before the calculation which you are currently editing contains several titrations, measurements or evaluations then a selection list containing the corresponding commands will first be opened.



Select the mode for the variable.		
01	DET pH	Dynamic pH titration
02	EVAL FIX-EP	Evaluation fix endpoints

You can use **[Select]** to open the list of variables for the selected titration, measurement or evaluation. For example, if you select a titration in the DET mode, the list of variables will look like this:

Calc. formula / Variables	
Variable	Description
C00	Sample size
CI1	Sample identification 1
CI2	Sample identification 2
1M.TITER	Titer of selected titrant
1M.CONC	Concentration of selected titrant
1M.EP#	Endpoint volume for EP#
1M.MCV	End volume
1M.MCD	Total duration of mode
1M.MSV	Start volume (all start conditions)
1M.MIM	Initial measured value
<div> <div>Cancel</div> <div>Insert</div> </div>	

The selected variable is entered in the formula with **[Insert]** or **[Back]**. With **[Cancel]** you can exit the list without accepting a variable. The individual variables are described in *Section 4.4.5*. The character **#** stands for a running number (usually from 1 to 9 or 10); this must be entered manually. If you want to calculate **EP1**, for example, then **EP** is inserted in the formula and you must enter the **1** in the formula editor.

If the method contains more than one data producing command then the command identification will be given before the variables (e.g. **1M.TITER** for the titrant titer used in the first titration). Data concerning the titrations, measurements and calibrations have the identification **M** for mode; evaluation data have the identification **E** for evaluation.

[System variables] opens the list of system variables:

Variables / System variables	
Variable	Description
%RN	Sample number
%SC	Start counter
%AS	Autostart status
%AC	Autostart counter
%AD	Autostart counter settings
%SS	Sample data silo status
%SL	Current silo line
%SE	Silo end reached
<div> <div>Cancel</div> <div>Insert</div> </div>	

[Results/Statistics] opens the list containing the existing results and the statistics variables:

Variables / Results, statistic	
Variable	Description
1C.R1	Blank
SMN#	Mean #
SSA#	Abs. standard deviation of SMN#
SSR#	Rel. standard dev. of SMN# in %
SNR#	Number n for mean SMN#
SSD	Statistics counter settings
SNT	Statistics status
<div> <div>Cancel</div> <div>Insert</div> </div>	

If the method contains more than one CALC command then the command identification will be given before the variable (e.g. **1C.R1** for the result variable R1 to be calculated in the first CALC command). Result variables which are to be calculated in the CALC command which is currently being edited are given without any command identification.

You can open the list of common variables with **[Common Variables]**.

In the formula editor you can use **[Math. functions]** to insert mathematical functions in the formula.

Calc. formula / Math. functions	
Function	Description
^	Power
SQRT()	Square root
ABS()	Absolute value
LN()	Natural logarithm
LOG()	Decimal logarithm
FRAC()	Fraction
INT()	Integer
TST(,)	Set replacement value
<div> <div>Cancel</div> <div>Insert</div> </div>	

The selected function is inserted in the formula with **[Insert]** or **[Back]**. With **[Cancel]** you can exit the list without accepting a function.

Examples:

- $4^2 = 4^2$ = 2nd power of 4
- $\text{SQRT}(\text{EP1}) = \sqrt{\text{EP1}}$ = square root of EP1
- $\text{ABS}(\text{CV03}) = |\text{CV03}|$ = absolute value of Common Variable 03
- $\text{LN}(5) = \ln 5$ = natural logarithm of 5
- $\text{LOG}(\text{C00}) = \lg \text{C00}$ = decimal logarithm of C00 (sample weight)
- $\text{FRAC}(123.456) = 0.456$ (fractional part)

- $\text{INT}(123.456) = 123$ (integer part)
- $\text{TST}(\text{EP1}, 0) = 0$, if EP1 is invalid.

If invalid variables (e.g. missing endpoints) could occur in a result calculation then these can be replaced with a valid value (replacement value) by using the **test function TST**. In this way invalid results can be avoided.

Syntax: TST (variable to be tested, replacement value)

4.4.3 Creating custom result templates

Under **System/Templates/Custom result templates** you can create templates for result calculations (see *Section 3.14.3*). These result templates can be used when editing a CALC command (see *Section 4.4.1* and *Section 4.4.4*).

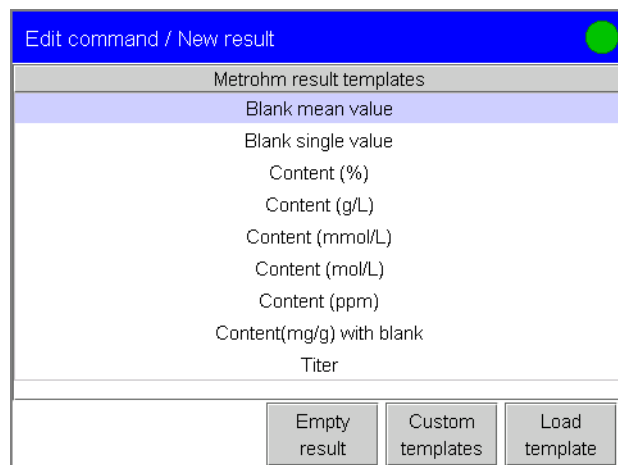
In principle, **creating result templates** works in the same way as editing a new result in the CALC command, except that no result variable can be assigned in the result template and no result limits can be defined. These are both carried out after the template has been loaded when editing the result calculation in the CALC command. The variables are also given without command identifications. If required, these must be entered in the CALC command.

In the calculation formulas for result templates you can use the **variables F1 to F9** as place holders for values which the user has to insert when using the template in a CALC command (e.g. molar mass). These F-variables are automatically requested after the display of the note when the result template is loaded.

Under **Note for wizard** you can enter a text in the result template which will be shown automatically when the result template is loaded before the F-variables are requested. If you do use F-variables in your templates then you should describe them in this note.

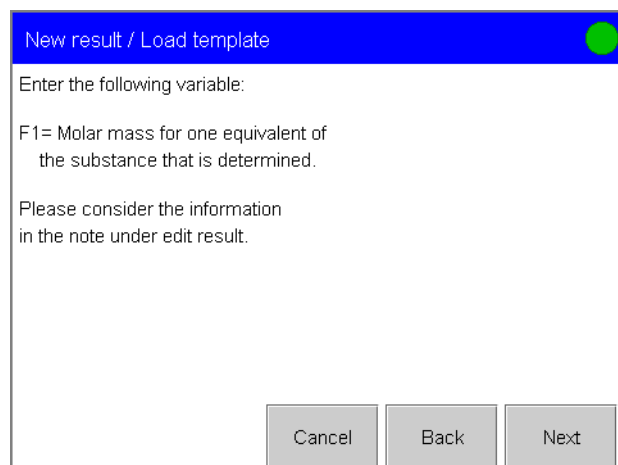
4.4.4 Loading result templates

Loading result templates takes place when new result calculations are defined in the CALC command.



With **[Load template]** the result template selected in the selection list is loaded and the note for the template is shown. With **[Custom templates]** you can show the list of your own result templates (see Section 3.14.3).

☞ Select a result template from the list and load it with **[Load template]**.



The **F-variables** used in the result template are automatically requested when the template is loaded if the display of the note is closed by pressing **[Next]**.

New result / Load template
●

F1=

F2=

F3=

F4=

F5=

F6=

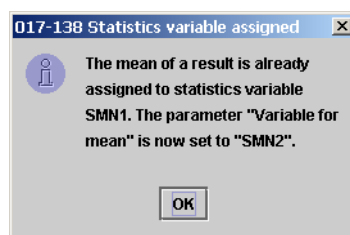
F7=

F8=

F9=

The only input fields which are active are those for the variables used in the result template. The entered values will be inserted automatically in the calculation formula in place of the variables.

If the mean value of a result is assigned to a variable SMNx (x = 1 to 9) in the result template and this has already been used in a different result calculation, then a message will appear to inform you that the next free variable will be used for the mean value assignment:



4.4.5 Calculable variables

The following table lists all those variables which can be used in calculations. When editing the formula you can either enter the variables directly or select them from the list of variables under **Calc. formula/Variables** and then insert them in the formula. For variables which contain an index (e.g. EP1) the index must be entered manually. The index is always given in the selection list as **#**.

If the method sequence contains more than one data producing command (titrations DET, MET or SET, measurements MEAS, calibrations CAL, evaluations EVAL, calculations CALC) before the calculation which you are currently editing then you can insert the command identification by using the following buttons in the formula editor: 'M.' (titration or measuring mode), 'E.' (EVAL) and 'C.' (CALC). You must enter the index for the command in front of the letter. If the variables are entered without command identification then the variables from the last command before the CALC command to provide the corresponding variables will always be used. A safer method is to insert the variables from the list of variables, as only the variables produced in the determination are available. The variables with the necessary command identifications are shown in the list of variables.



Attention!

*If you subsequently enter commands in the list of commands, then the **command identifications** of the variables in the calculations will not be adapted automatically.*

	Variable	Description	Method command
Sample data	C00	Sample weight	all
	CI1 CI2	Sample identification 1 and sample identification 2 The sample identifications can be used in calculations if numerical values are entered.	all
Determination	DD	Duration of determination (see Section 3.18.4) Time between the START of the determination and the normal end of the run or manual termination with [STOP] . If the determination is not yet finished then the time between the start and the use of the variable in the CALC command will be used.	all

	Variable	Description	Method command
Titrant	TITER	Titer of the titrant selected in the titration command (see <i>Section 4.1.3</i>)	DET, MET, SET
	CONC	Concentration of the titrant selected in the titration command (see <i>Section 4.1.3</i>)	DET, MET, SET
Titrations, measurements, calibrations	EP#	Equivalence point (DET and MET) or end-point volume (SET) for EP#	DET, MET, SET
	EM#	Equivalence point (DET and MET) or end-point measured value(SET) for EP#	DET, MET, SET
	EF#	Equivalence point ERC (see <i>Section 4.1.1</i>) for EP#	DET, MET
	ET#	Equivalence point (DET and MET) or end-point temperature (SET) for EP#	DET, MET, SET
	ED#	Equivalence point (DET and MET) or end-point time (SET) for EP#	DET, MET, SET
	ESI#	Equivalence point marking (0 if one EP in window, 1 if more than one EP in window)	DET, MET
	MIM	Initial measured value (measured value before start conditions are processed)	DET, MET, SET, MEAS
	MIT	Initial temperature (temperature before start conditions are processed)	DET, MET, SET, MEAS
	MSA	Start volume which is added according to the start volume given in the start conditions.	DET, MET
	MSP	Start volume which is added according to the start measured value given in the start conditions.	DET, MET
	MSS	Start volume which is added according to the start slope given in the start conditions.	DET, MET
	MSV	Start volume for all start conditions (start volume, start measured value and start slope)	DET, MET, SET
	MSD	Time for processing the start conditions	DET, MET, SET
	MSM	Start measured value (measured value after processing the start conditions)	DET, MET, SET
	MST	Start temperature (temperature after processing the start conditions)	DET, MET, SET
	MCV	End volume (total volume added at end of titration)	DET, MET, SET
	MCD	Total duration of titration, measurement or calibration (including start conditions)	DET, MET, SET, MEAS, CAL

	<i>Variable</i>	<i>Description</i>	<i>Method command</i>
	MCM	Final measured value (measured value at end of the titration or measurement)	DET, MET, SET, MEAS
	MCT	Final temperature (temperature at end of the titration, measurement or calibration)	DET, MET, SET, MEAS, CAL
	MMP	Number of measuring points in the measuring point list	DET, MET, SET, MEAS
	MTS	Stop type (termination of the titration, measurement or calibration), format: text	DET, MET, SET, MEAS, CAL
Sensor	MEN	Electrode zero point pH(0) or E(0)	DET, MET, SET, MEAS, CAL
	MSL	Slope of electrode	DET, MET, SET, MEAS, CAL
Evaluation fixed endpoints	FP#	Fixed endpoint volume for FP#	EVAL FIX-EP
	FM#	Fixed endpoint measured value for FP#	EVAL FIX-EP
	FT#	Fixed endpoint temperature for FP#	EVAL FIX-EP
	FD#	Fixed endpoint time for FP#	EVAL FIX-EP
Evaluation pK value / half neutralization potential	HM#	PK value, or half neutralization potential	EVAL pK/HNP
	HP#	pK/HNP volume for HM#	EVAL pK/HNP
	HT#	pK/HNP temperature for HM#	EVAL pK/HNP
	HD#	pK/HNP time for HM#	EVAL pK/HNP
Evaluation minimum	XIP	Volume to minimum measured value	EVAL MIN/MAX
	XIM	Minimum measured value	EVAL MIN/MAX
	XIT	Temperature to minimum measured value	EVAL MIN/MAX
	XID	Time to minimum measured value	EVAL MIN/MAX
Evaluation maximum	XAP	Volume to maximum measured value	EVAL MIN/MAX
	XAM	Maximum measured value	EVAL MIN/MAX
	XAT	Temperature to maximum measured value	EVAL MIN/MAX
	XAD	Time to maximum measured value	EVAL MIN/MAX
Evaluation breakpoint	BP#	Breakpoint volume for BP#	EVAL BREAK
	BM#	Breakpoint measured value for BP#	EVAL BREAK
	BT#	Breakpoint temperature for BP#	EVAL BREAK
	BD#	Breakpoint time for BP#	EVAL BREAK
Results	R1 to R9	Results which can be calculated with a CALC command.	CALC

	<i>Variable</i>	<i>Description</i>	<i>Method command</i>
Statistics	SMN#	Mean value #, the variables for the mean value are assigned under Result options (see <i>Section 4.4.1</i>).	CALC
	SSA#	Absolute standard deviation of SMN# (see <i>Section 3.21.1</i>)	CALC
	SSR#	Relative standard deviation of SMN# (see <i>Section 3.21.1</i>)	CALC
	SNR#	Number of results n from which the mean values has been obtained (see <i>Section 3.21.1</i>)	CALC
	SSD	Number of samples, i.e. number set on the statistics counter (see <i>Section 3.16.4</i>)	CALC
	SNT	Statistics status (1 for statistics on, 0 for statistics off, see <i>Section 3.16.4</i> and <i>Section 3.17.1</i>)	CALC
Common variables	CV01 to CV25	Instrument-specific common variables (see <i>Section 3.13</i>)	
System variables	%RN	Sample number (see <i>Section 3.18.4</i>)	
	%SC	Start counter (see <i>Section 3.18.4</i>)	
	%AS	Autostart status (1 for autostart on, 0 for autostart off, see <i>Section 3.17.3</i>)	
	%AC	Autostart counter (see <i>Section 3.17.3</i>)	
	%AD	Number of autostarts, i.e. number set on autostart counter (see <i>Section 3.17.3</i>).	
	%SS	Sample data silo status (1 for sample data silo on, 0 for sample data silo off, see <i>Section 3.17.2</i>)	
	%SL	No. of sample data silo lines that have been processed (see <i>Section 3.19.3</i>).	
	%SE	End of sample data silo reached (1 for yes, 0 for no)	

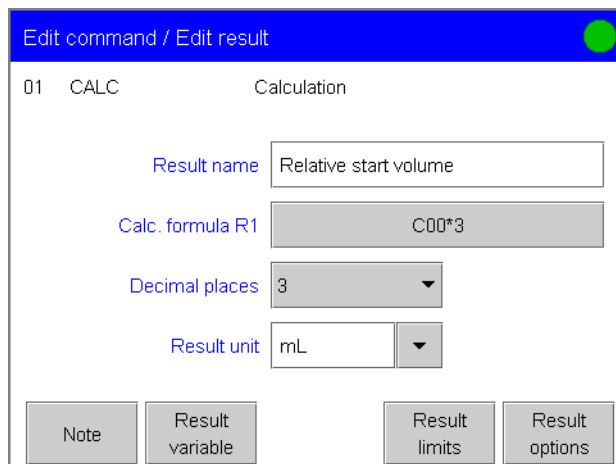
4.4.6 Result variables as parameters

In many numerical entries for **method parameters** you can also enter a **result** which has previously been calculated (e.g. **R1**) instead of a number. The result must have been calculated in a previous CALC command in the method sequence. Please note that the result must be within the input limits for the parameter, as otherwise the determination run will be halted when the parameter is accessed.

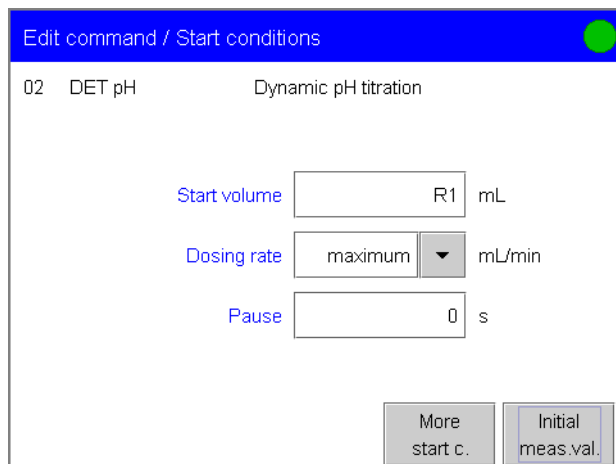
With PC Control the result variables are entered directly via the PC keyboard. With Touch Control the button **[R1]** is used to open the numerical input dialog with a selection of result variables from R1 to R9 (see Section 3.1.4).

A typical application is the use of a **relative start volume**. To define a start volume which is dependent on the **sample weight** proceed as follows:

- ☞ Before the titration command define a **CALC command** in which the relative start volume is calculated, e.g. $R1 = C00 \cdot 3$ ($C00$ = sample weight).

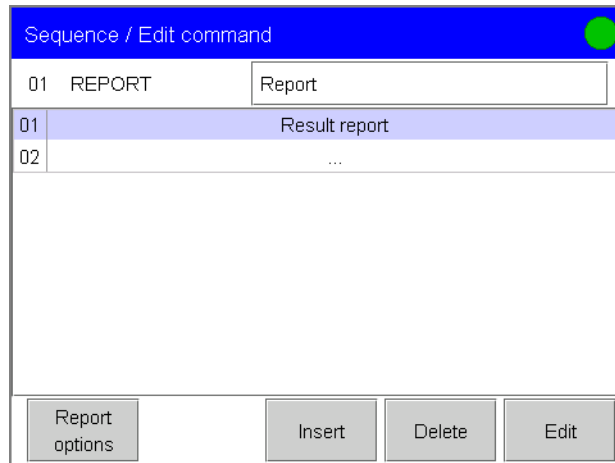


- ☞ In the **titration command** enter the variable R1 as the start volume.

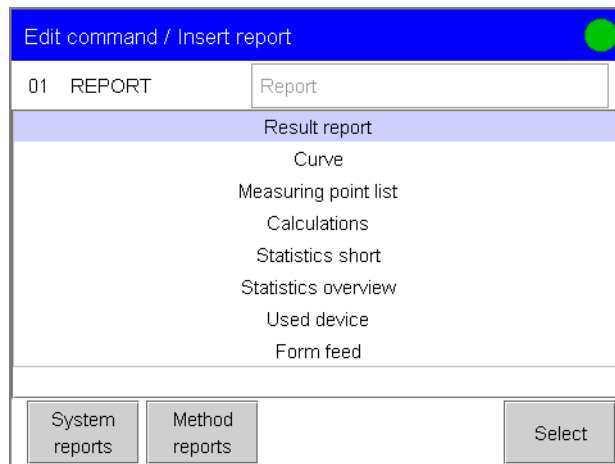


4.5 Reports

In the **REPORT command** you can define a maximum of nine reports which can be printed out in the method sequence. The reports which are defined in a report command are printed out in the sequence in which they are entered in the list.



☞ You can insert a report in the list in front of the selected line with **[Insert]**.

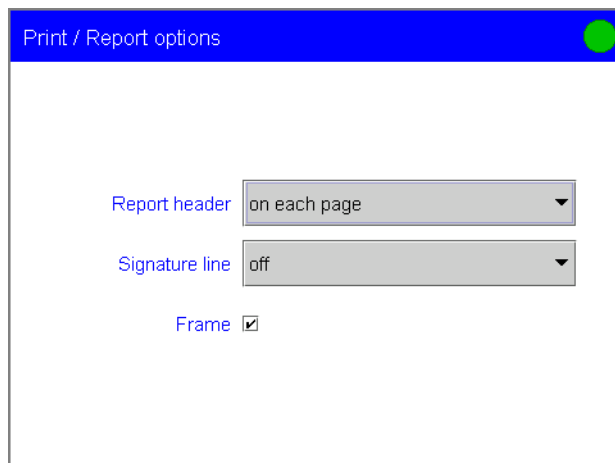


You can use **[Method reports]** to open the list of reports for the current method. **[System reports]** opens the list of reports for system-specific data.

☞ Mark the required report in the selection list and include it in the list of reports with **[Select]**.

In the list of reports you can use **[Delete]** to delete the selected report and **[Edit]** to edit the parameters for printing out the selected report.

☞ Open the dialog for the configuration of the whole report sequence with **[Report options]**.



Print / Report options

Report header on each page ▼

Signature line off ▼

Frame ☒

In the **report header** the type, serial number and program version of the software (Touch Control or PC Control), the device name which you can enter in the device manager of Touch Control or PC Control and the printout date with time zone can be printed out. You can also define your own report header under **System/Templates/Report header**; this will be printed out before the standard report header (see *Section 3.14.7*). Under **Report header** you can choose whether the report header is to be printed out on every page, on the first page of the report only or not at all. The **Signature line** gives you the possibility of signing the report together with the date. You can choose whether the **Signature line** is to appear on every page, on the last page of the report only or not at all. If you have activated the **Frame** checkbox then a frame will be printed round each page of the report.

Parameters for the following reports can be edited in the method sequence:

	Report	Parameter
Results (current determination)	Result report	<ul style="list-style-type: none"> - Determination properties (on/off) - Sample data (on/off) - Sensor data for the sensor used (on/off) - Titrant data for the titrant used (on/off) - Raw data, i.e. equivalence points (DET, MET), endpoints (SET), final measured values (MEAS), calibration data (CAL) and results of evaluations (EVAL) (on/off) - Used common variables (on/off) - Calculated results (on/off) - Statistics short (on/off) - Messages entered in the list of messages (on/off) - Lines between the sections (on/off)
	Curve	<ul style="list-style-type: none"> - Selection of the titration, measurement or calibration (mode) for which the curve is to be printed - Settings for the curve report (for a description of the settings see <i>Section 3.18.7</i>)

	<i>Report</i>	<i>Parameter</i>
	Measuring point list	- Selection of the titration or measurement (mode) for which the measuring point list is to be printed out.
	Calculations	- Determination properties (on/off) - The variables can be printed out as shown or with the full accuracy of the floating point number ("double precision" to Standard IEEE 754).
	Devices used	- Determination properties (on/off)
Statistics	Statistics short	Report printout at the end of a statistics series (statistic counter same as number of samples, i.e. samples processed = samples set) or at the end of each determination
	Statistics overview	Report printout at the end of a statistics series (statistic counter same as number of samples, i.e. samples processed = samples set) or at the end of each determination

No parameters can be edited for the system reports and the method reports. The contents of the individual reports is described in Section 3.23.


Note!

Some tables (statistics overview and sample data silo) are always printed out in **landscape format**, as otherwise the data could not be printed out on a single page. For PC Control you must select the Windows-specific **Printer setting: portrait**, as printout in landscape format is automatic.

4.6 Calibrating pH electrodes (CAL pH) and ISE (CAL Conc)

For **pH measurements**, titrations to a preset endpoint (SET pH) and the determination of pK values and fixed endpoints the calibration of the pH electrode (command CAL pH) is essential; it is also recommended for all other pH titrations. As least two buffers should be used for the calibration; these should cover the expected measuring range. For **concentration direct measurements** with ISE electrodes the sensor must be calibrated with a series of standards (CAL Conc). During the sequence the calibration data is stored automatically together with the sensor data for the used sensor.

Calibration parameters

Under **Calibration parameters** you can edit the parameters for the calibration sequence. These are identical for pH calibrations and ISE calibrations. In the command CAL pH you must define the calibration buffers, in the command CAL Conc the concentrations of the standards.

- **Signal drift** (d): Drift, i.e. the alteration in the measured value per minute that has to be undercut for measured value acceptance. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the electrode has a very slow response.
- **Waiting time min.** (d): The minimum waiting period is only important for drift-controlled measurements. Measured value acceptance only takes place when the minimum waiting time has elapsed, even when the measured value drift has already been achieved.
- **Waiting time max.** (d): If measured value drift is switched off or has not yet been achieved then the measured value will be accepted after the maximum waiting time has elapsed. If the waiting time has not been newly entered then a waiting time that is suitable for the drift will be calculated automatically according to the following equation:

$$\text{Waiting time} = 150 / \sqrt{\text{Drift} + 0.01} + 5$$

- **Temperature** (d): Manually set calibration temperature. If a temperature sensor is connected and temperature measurement has been set under **Sensor** to **automatic** or **continuous** (see *Section 4.1.3*) then the temperature will be measured. The calibration temperature can also be entered during the run.
- **Sample changer** (d): This parameter must be activated for calibrations using a sample changer. As the buffers or standards are changed by the sample changer this means that the run is not stopped in order to request values. When the measurement of a buffer or standard has been completed the Titrand sends a signal to the sample changer via the remote connection (EOD, see *Section 6.2.2*). The sample changer then switches to the next buffer or

standard. The calibration temperature must first be entered under **Temperature**.

Buffers

CAL pH only: The type and number of buffers used for calibration are entered under **Buffers**. Alternatively the pH values for a special buffer series can be entered.

- **Buffer type** (d): Selects a predefined buffer series for the calibration. The following buffer series are available: **Metrohm**, **NIST**, **DIN**, **Fisher**, **Novartis** (Fluka Basle), **Mettler**, **Merck**, **Beckman**, **Radiometer**. The temperature tables for the buffer series can be found in *Section 6.4*. If these buffers are used then the system will recognize them automatically. If you have defined your own series of buffers under **System/Templates/Custom calibration buffers** then select **Custom** in order to use them. Automatic buffer recognition will then be active for this series of buffers. You can also use **Special** to define up to five buffers directly in the calibration command. Automatic buffer recognition will then not be active and the buffers must be used for the calibration in the given sequence.
- **Number of buffers** (d): For predefined or custom buffer series: the number of buffers to be used for the calibration. During the sequence the user will be requested to change the buffer the corresponding number of times. If you use more than two buffers for your calibration then you can use a particular buffer several times in order to give it more statistical weight. The first two buffers must always be different.
- **Buffer 1 pH to Buffer 5 pH** (d): For buffer type **Special**: pH values of the buffers. Please note that you must enter the pH values corresponding to the measuring temperature used. **off** means that the buffer and all those following will not be used. During the sequence a message will appear the corresponding number of times to indicate the next buffer to be used.

Standards

CAL Conc only: Under **Standards** the concentration unit for the concentration measurements and the concentrations of the standard solutions are entered.

- **Unit Conc.** (d): Selects the concentration unit of the standard. The concentration unit for concentration measurements always depends on the unit entered for the concentration of the standard.
- **Conc. standard 1 to Conc. standard 5** (d): Enters the concentration for 1 to 5 concentration standards. **off** means that the standard and all those following will not be used. During the sequence a message will appear the corresponding number of times to indicate the next standard to be used.

Stirrer control

Under **Stirrer Control** you can edit the parameters for controlling the stirrer during the calibration. Take care that you have selected a stirrer under **Edit command/Stirrer**.

- **Stir solution during measurement** (d): Automatic stirrer switch-on and switch-off when the measurement of a buffer is started and finished respectively.

- **Stir before measurement** (d): If the stirrer is to be switched off during the measurement you can enter a time during which stirring is to be carried out before the measurement.
- **Pause before measurement** (d): If the stirrer is to be switched off during the measurement and stirring is to be carried out before the measurement then you can enter a time during which no stirring or measurement will be carried out so that the liquid has time to come to rest.

The parameters for **Titrand**, **Sensor** and **Stirrer** are described in Section 4.1.3.



Note!

*Make sure that the sensor to be calibrated has been defined under **System/Sensors** and that this sensor has been selected under **Edit command/Sensor**. This is the only way to ensure that the **Calibration data** for this sensor is stored in the correct place under **System/Sensors**.*

The choice of the **Direct parameters** is described in Section 4.1.4 .

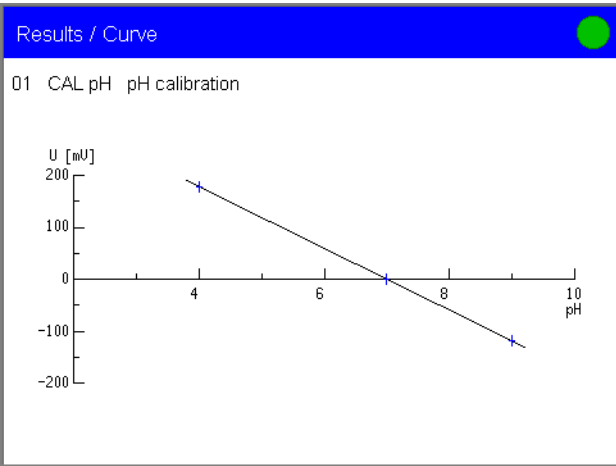
2-Point calibration with automatic buffer recognition

Immerse electrode in first buffer	With automatic buffer recognition the order of the buffers does not matter.
Start the calibration command	
Measure or enter the calibration temperature	If a temperature sensor is connected then the calibration temperature will be measured. Otherwise a query will appear and the calibration temperature must be entered manually or adopted from the calibration parameters with [Continue] .
(Stir before measurement and/or pause before measurement)	The solution is stirred before the measurement. Pause will be allowed to elapse before the measurement.
(Switch on stirrer)	The stirrer will be switched on before the measurement if Stir solution during measurement is activated.
Measure buffer 1	The potential of buffer 1 is measured.
(Switch off stirrer)	The stirrer will be switched off after the measurement if Stir solution during measurement is activated.

Message showing which buffer has been recognized.	A message will be shown with instructions for the next buffer. When the electrode has been immersed in the second buffer the second measurement is started with [OK] .
(Stir before measurement and/or pause before measurement)	<p>The solution is stirred before the measurement.</p> <p>Pause will be allowed to elapse before the measurement.</p>
(Switch on stirrer)	The stirrer will be switched on before the measurement if Stir solution during measurement is activated.
Measure buffer 2	The potential of buffer 2 is measured.
(Switch off stirrer)	The stirrer will be switched off after the measurement if Stir solution during measurement is activated.
Calculate calibration data	The calibration data, i.e. the slope and the electrode zero point pH (0) are calculated, the limits checked and, if necessary, an appropriate message displayed. The calibration data will also be added to the sensor data for the particular sensor stored under System/Sensors .

Optional steps are shown in brackets.

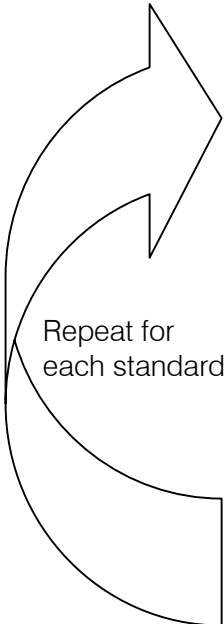
At the end of the determination sequence the calibration data is shown on the result page (see *Section 3.18*). The calibration curve is shown under **Results/Curve**:



The individual measured values for all buffers are shown under **Results/More determination data/View data**:

More determination data / View data				
01 CAL pH pH calibration				1M
Stop criterium	Regular stop			
Calibration duration	83.2 s		MCD	
Temp. measurement	manual			
Calibration temp.	25.0 °C		MCT	
	pH	U [mV]	T [°C]	t [s]
Buffer 1	9.000	-118.2	25.0	11
Buffer 2	7.000	0.1	25.0	10
Buffer 3	4.000	177.6	25.0	10

Concentration calibration with up to 5 standards

 <p>Repeat for each standard</p>	Immerse electrode in first standard	
	Start the calibration command	
	Measure or enter the calibration temperature	If a temperature sensor is connected then the calibration temperature will be measured. Otherwise a query will appear and the calibration temperature must be entered manually or adopted from the calibration parameters with [Continue] .
	Message	A message appears with instructions for the first standard. Start the measurement with [OK] .
	(Stir before measurement and/or pause before measurement)	The solution is stirred before the measurement. Pause will be allowed to elapse before the measurement.
	(Switch on stirrer)	The stirrer will be switched on before the measurement if Stir solution during measurement is activated.
	Measure standard	The potential of the standard is measured.
	(Switch off stirrer)	The stirrer will be switched off after the measurement if Stir solution during measurement is activated.
	Calculate calibration data	The calibration data, i.e. the slope, electrode zero point E (0) and the blank concentration c (blank) are calculated, the limits checked and, if necessary, an appropriate message displayed. The calibration data will also be added to the sensor data for the particular sensor stored under System/Sensors .

Optional steps are shown in brackets.

4.7 Dosing

With the dosing commands you can add a fixed volume in the method sequence; burets can also be prepared and emptied automatically.

4.7.1 Dosing (ADD)

The ADD command is used to add a preset volume of a solution.

- **Volume** (d): Volume to be added.
- **Dosing rate** (d): Rate at which the volume is to be added. The maximum dosing rate depends on the cylinder volume of the buret used (see *Section 3.8.6*).
- **Filling rate** (d): Speed with which the buret is to be refilled after addition has been carried out. The maximum filling rate depends on the cylinder volume of the buret used (see *Section 3.8.6*).

The parameters for **Titrand**, **Dosing device** and **Stirrer** are described in *Section 4.1.3*. Selection of the **Direct parameters** is described in *Section 4.1.4*.

4.7.2 Preparing (PREP) and emptying (EMPTY)

Preparation is used to rinse the cylinder and the tubing. **Empty** is used to empty the cylinder and the tubing. The empty command is only available for **Dosino**-type dosing devices.

- **Titrand**: Selects the Titrand to which the dosing device is connected and which is to be prepared or emptied. This button is only shown when several Titrands have been configured under **System/Device manager** (see *Section 3.10.1*). The device names are always shown in the selection list.
- **Dosing device**: Dosing device to be prepared or emptied. All dosing device connections (MSB) are always shown.
- **Titrant**: Titrant with which the preparation or empty command is to be carried out. The titrant can be selected from the list of titrants which have been defined under **System/Titrants**. If intelligent exchange or dosing units are used then a check will be made in the method sequence that the correct titrant is present in the connected dosing device and whether the type of dosing device is correct. With non-intelligent exchange or dosing units the cylinder volume is checked. At the start of the command the validity of the titer and the expiry date of the selected titrant will be checked as well as the GLP test interval for the buret. The tubing parameters defined under **System/Titrants** for the selected titrant will be used for preparing and emptying the buret. The parameters for the preparation are also defined under **System/Titrants**. If no titrant has been defined then the standard tubing parameters and the default parameters for the preparation will be used (see *Section 3.8.6*).

A detailed description of the preparation and emptying sequences is given in *Section 3.24.2, p. 165 and p. 166*).

4.8 Communication

With the communication commands SCAN and CTRL you can scan and set remote lines at a connected remote box. The connection of the remote box is described in the Installation Instructions for the 808 Titrandos and 809 Titrandos. The pin occupancy of the remote connection and the functions of the individual remote lines are described in *Section 6.2*.

4.8.1 Scanning lines (SCAN)

Definition of input signals which are to be waited for before the next command is carried out (SCAN).

- **Titrandos:** Selects the Titrandos to which the remote box is connected. This button is only shown when several Titrandos have been configured under **System/Device manager** (see *Section 3.10.1*). The device name is always shown in the selection list.
- **Remote box:** Remote box at which the lines are to be scanned. All the remote box connections (MSB) will always be shown.
- **Input signal:** Selects the signal from the templates which have been defined under **System/Templates/Input lines** or enters the binary pattern directly. Please consult the **online help** for the input of the binary pattern.

4.8.2 Setting lines (CTRL)

Definition of output signals which are to be transmitted (CTRL).

- **Titrandos:** Selects the Titrandos to which the remote box is connected. This button is only shown when several Titrandos have been configured under **System/Device manager** (see *Section 3.10.1*). The device name is always shown in the selection list.
- **Remote box:** Remote box at which the lines are to be set. All the remote box connections (MSB) will always be shown.
- **Output signal:** Selects the signal from the templates which have been defined under **System/Templates/Input lines** or enters the binary pattern directly. Please consult the **online help** for the input of the binary pattern. The pulse length for **p** is fixed at 200 ms. If you wish to use a pulse with a pulse length other than 200 ms then you must define a corresponding template.

4.9 Various commands

Various commands are brought together in the command group **Miscellaneous**: switching the stirrer on/off, defining a waiting period or stopping the run, requesting sample data or common variables, acoustic signal and stopping the method sequence.

4.9.1 Stirring (STIR)

The STIR command is used to switch a connected stirrer on or off.

- **Titrande**: Selects the Titrande to which the stirrer which is to be controlled is connected. This button is only shown when several Titrands have been configured under **System/Device manager** (see *Section 3.10.1*). The device name is always shown in the selection list.
- **Stirrer**: Selects the stirrer. All the stirrer connections (MSB) will always be shown.
- **Switch**: Switches the stirrer on/off. When the stirrer is switched on you can set the stirring rate.
- **Stirring rate**: You can test the optimal stirring rate manually (see *Section 3.24.3*). The stirring direction changes as the sign changes. The default setting **8** corresponds to 1000 min^{-1} (see *Section 4.1.3*, *Fig. 21*).

4.9.2 Waiting (WAIT)

This command can be used either to define a waiting period or to stop the method sequence. It must then be restarted manually with **[Continue]**.

- **Hold sequence**: When this function is activated the method sequence will be halted (HOLD) until it is restarted manually with **[Continue]**.
- **Waiting time**: If **Hold sequence** is deactivated then a waiting time can be entered. The method sequence will restart automatically when this waiting time has elapsed.
- **Message**: When this function is activated the text for the message will be shown during the waiting time.
- **Message text**: Text to be shown during the waiting time.

4.9.3 Requesting sample data and common variables (REQUEST)

With the REQUEST command you can request sample data (sample identification 1, sample identification 2 and sample size, see also *Section 3.19.2*) or a common variable (see also *Section 3.13.1*) during the method sequence. You can choose whether the run is to be stopped or whether it should continue in the background.

- **Sample identification:** Selects which sample identification(s) are to be requested in the sequence.
- **Sample size:** If this function is active then the value for the sample size will be requested.
- **Sample size unit:** If this function is active then the unit for the sample size will be requested.
- **Common variable:** Selects the common variables to be requested in the sequence.
- **Hold sequence:** If this function is switched on then the sequence will be halted for the request. If it is switched off then the method will continue to run in the background until the following titration, measurement or calibration has been completed.

4.9.4 Acoustic signal (BEEP)

The BEEP command is used to produce an acoustic signal during the method sequence.

- **Number of sounds:** Number of tones for the signal in the method sequence. For PC Control the tone selected in the Control panel under **Sounds and Audio Devices** will be used. With Touch Control the number of sounds cannot be altered.

4.9.5 End (END)

The method sequence will stop as soon as the command END is reached. This is a good idea if you only want to test the first part of a method. The END command has no parameters that can be edited.

5 Troubleshooting – Maintenance

This section contains troubleshooting information and a description of the diagnosis functions integrated in Touch Control and PC Control. For Touch Control a description is given of how to change the batteries and carry out a "RAM initialization".

5.1 Troubleshooting

This section describes several problems that could occur when operating the system together with possible causes and their remedies.

5.1.1 Editing methods

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The required command cannot be inserted with Insert command.	The use of the command has been deactivated under Dialog options/Command list .	Activate the command under Dialog options/Command list (see <i>Section 3.7.3</i>).
An evaluation (EVAL command) cannot be inserted.	A data producing command (titration or measurement) to which the evaluation could be applied is missing.	First insert a titration or measurement command and then the evaluation (see <i>Section 4.3</i>).
An evaluation (EVAL command) is shown in red in the list of commands.	A data producing command (titration or measurement) is missing, or the data producing command has been replaced by another one, (e.g. DET pH by DET U) to which the evaluation cannot be applied.	Delete the EVAL command and first insert the titration or measurement command and then the evaluation (see <i>Section 4.3</i>).

5.1.2 Sample series

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The method cannot be entered in the sample data silo.	The use of the sample assignment table is switched on under System/Templates /Sample data . The method assigned to the sample identification will be automatically loaded at the start of the determination.	Switch off the use of the sample assignment table under System/Templates/Sample data (see <i>Section 3.19.3</i>).
When using a sample changer (e.g. 730 or 824) the next titration starts before the beaker has been changed.	The Autostart function is switched on under Control .	If you use a sample changer from which the Titrand is started automatically then the number of samples is defined in the sample changer. The Autostart function of the Touch Control or PC Control cannot be used for such applications (see <i>Section 3.17.3</i>).

5.1.3 Results, calculations and statistics

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
No statistics are carried out for a result.	The Statistics function has not been activated in the method under Sequence/ Method options .	Activate the statistics function under Sequence/Method options (see <i>Section 3.16.4</i>).
	No Variable for mean has been selected in the method for the result calculation.	Select a Variable for mean in the CALC command under Edit result/Result options for the result (see <i>Section 4.4.1</i>).
	The Statistics function is switched off under Control .	Activate the Statistics function under Control (see <i>Section 3.17.1</i>).
Results have been deleted in the statistics, but the variables (e.g. titer or common variable) have not been reassigned.	If the statistics results are subsequently altered then the assignment is not automatic.	Trigger the assignment of the current statistics results with [Recalculate] under Results (see <i>Section 3.18.8</i>).

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The result is not shown in the result silo.	The numbering of the results corresponds to the sequence in which the results are calculated in the determination sequence and stored in the result silo and not to the result variables.	Under Results/Result silo/Properties alter the settings for the result silo display so that the required result is shown (see <i>Section 3.22.1</i>).
	The function Save result in result silo has not been switched on for the result.	Activate this function for the required result in the CALC command under Result options/More options (see <i>Section 4.4.1</i>).

5.1.4 SET titrations

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Dosing at the end takes too long and the increments are too small.	Max. rate too low.	Increase the max. rate under Control parameters .
	Unfavorable Stop criterion .	Try increasing the Stop drift or select a shorter Delay time .
"Overshoot"	The titration is not properly controlled, i.e. individual increments are not added at the end.	<ul style="list-style-type: none"> - Select a larger control range (dynamics) under Control parameters. - Reduce the max. rate under Control parameters. - Reduce the min. rate under Control parameters. - Ensure that the solution is better mixed and that the arrangement of electrode and buret tip is optimal (see Installation Instructions for 808 Titrando and 809 Titrando).
Titration time too long.	Unfavorable control parameters.	<ul style="list-style-type: none"> - Select a smaller control range under Control parameters. - Increase the max. rate under Control parameters. - Increase the min. rate under Control parameters.
Results widely scattered.		Reduce the min. rate under Control parameters .

5.1.5 Sensor data

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
After calibration the calibration data is not stored together with the sensor data.	In the method the correct Sensor has not been selected in the CAL command.	Take care that the sensor to be calibrated has been selected under Edit command/Sensor (see Section 4.6).

5.1.6 Print

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The [Print] fixed key is inactive.	The [Print] fixed key is deactivated.	Activate the [Print] fixed key under Dialog options/Fixed keys (see Section 3.7.3).
	The system is in the BUSY status, i.e. a determination is running.	Wait until the determination is finished.
PC Control: empty pages are produced when printing out the result silo report or the statistics overview.	Landscape format has been selected under orientation in the Windows-specific printer settings .	in the Windows-specific printer settings select portrait format as the printout is automatically made in landscape format.

5.1.7 Manual Operation

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The [Manual] fixed key is inactive.	The [Manual] fixed key is deactivated.	Activate the [Manual] fixed key under Dialog options/Fixed keys (see Section 3.7.3).
Manual operation buttons are inactive.	The corresponding hardware is either not connected or not properly connected.	Connect the hardware correctly (see Installation Instructions for 808 Titrand and 809 Titrand).
	The appropriate hardware has not been recognized correctly.	Switch off the system and then switch it on again.
	The corresponding hardware is occupied with a determination run.	Wait until the determination is finished.

5.1.8 File manager

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Files, e.g. methods, which have been saved on a data card by a PC, cannot be read by Touch Control.	Windows Explorer has been used for copying and the correct folder structure has not been maintained (see <i>Section 3.11</i>).	Use PC Control to copy the files.

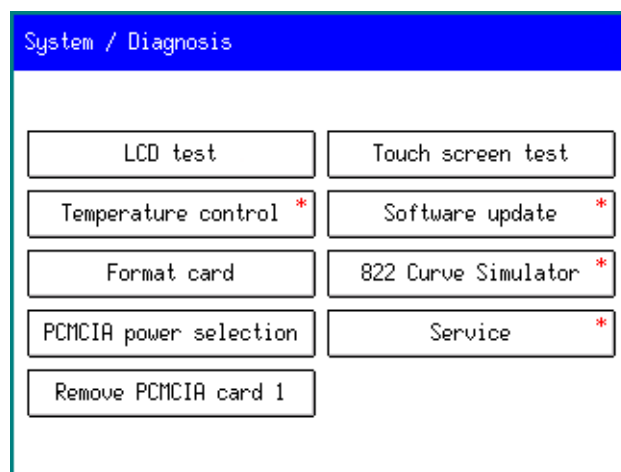
5.1.9 Miscellaneous

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Touch Control cannot be switched on.	Touch Control is connected to an MSB socket of the Titrando.	Connect the Touch Control to the Controller socket (see Installation Instructions for 808 Titrando and 809 Titrando).
PC Control does not recognize the Titrando.	The PC is connected to an MSB socket of the Titrando.	Connect the PC to the Controller socket (see Installation Instructions for 808 Titrando and 809 Titrando).
	The suitable USB driver has not been found.	Remove the USB plug from the PC and reinsert it. Please note that the PC Control software must be installed before the Titrando is connected to the PC (see Installation Instructions for 808 Titrando and 809 Titrando).

5.2 Diagnosis

You can carry out selective tests on the Titrando system or trigger special functions.

☞ Select **Diagnosis** in the **System** menu:



All the diagnosis functions are available for Touch Control. With PC Control the selection is limited to those functions marked with an *.

5.2.1 LCD test

- ☞ Select **[LCD test]** in order to check the functions of the Touch Control display. The whole screen appears in white.
- ☞ Continue with **[START]** to show further colors and patterns. You can use **[Back]** to switch back step by step.
- ☞ Check whether the display has any pixel errors or other irregularities. If this is the case please contact your local Metrohm agency.
- ☞ You can exit the LCD test automatically by switching through to the end with **[START]**. It can also be exited at any time with **[Home]**.

5.2.2 Temperature monitoring (Temperature control)

The operating temperature of the Titrando **Temperature TI** and the Touch Control **Temperature TC** are both measured inside the housing and monitored automatically. If a limit is infringed then a corresponding message will first be produced; when the second limit is reached the system will be switched off automatically.

Information about the limits can be found in the Installation Instructions for the 808 Titrando and 809 Titrando and in *Section 6.1.6* of these Instructions (Touch Control).

5.2.3 Formatting a memory card (Format card)

- ☞ Select **[Format card]** in order to format a PCMCIA or CompactFlash memory card inserted in the Touch Control.
- ☞ Select the memory card to be formatted (**Card 1 / Card 2**) and the formatting mode. With **normal** the memory card will be completely cleared; with **quick** only the "main folder" of the card will be overwritten with zero so that the whole capacity is again available.
- ☞ Start formatting with **[Format]** and answer the safety query with **[Yes]**.

5.2.4 PCMCIA specification (PCMCIA power selection)

Two different voltages (3.3 V and 5.0 V) are normal for the power supply of the PCMCIA or CompactFlash cards. These are automatically set on the Touch Control with the option **auto VS1/VS2**. This setting should be retained if possible. You should only set one of the two voltages if the automatic setting does not work and you know the exact specifications of your memory card.

5.2.5 Remove PCMCIA card 1/2

As long as the Touch Control is not accessing the data on the inserted memory card for loading or storing you can remove and insert the memory card without any problems with the Touch Control switched on.

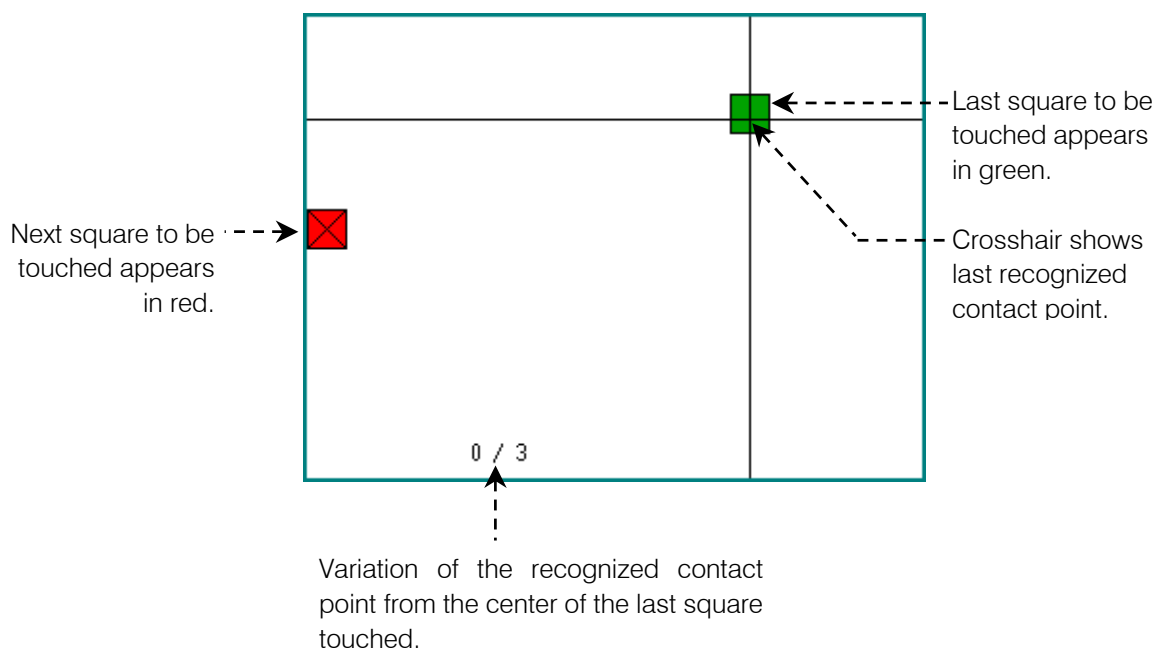
This option offers additional data protection as it ensures that the data to be stored is completely written onto the card before the power supply to the card is switched off.

Remove the card as soon as the appropriate message appears:

The PCMCIA card can be removed now

5.2.6 Touch screen test

- ☞ Select **[Touch screen test]** to check the functions of the Touch screen.
- ☞ A red square now appears at various locations on the display in succession. You should try to touch the center of this square as exactly as possible in a suitable way (see *Section 3.1.3*). The contact point which is actually recognized is indicated by a crosshair:



- ☞ You can use **[Back]** to switch back again step by step.
- ☞ When you have checked all the display areas a list of **fixed keys** appears; you should touch them in any sequence. If they function correctly the request will always change to an appropriate message (e.g. **PRINT ok**).
- ☞ You can use **[Home]** to end the Touch screen test at any time or to conclude it.

5.2.7 Software update

The instrument program (firmware) of the Titrandos can be updated with both the Touch Control and the PC Control. With the Touch Control you can carry out an update of the instrument program or load a new dialog language.

Program version

Information about the existing program version is given under **System/Device manager**. Select the corresponding device and open the **Edit** dialog with **[Edit]**.

Data source

If **PC Control** is used then the Titrandos program file is available on one of the data carriers of the computer. This could be a hard disk, CD-ROM or a PCMCIA or CompactFlash card connected by a card reader.

The **Touch Control** requires the program files on a memory card in **Card slot 1** (Card 1).

Loading a new dialog language (Load new language) (Touch Control only)

- ☞ Use **[Load new language]** under **System/Diagnosis/Software update** to open the selection of the language files stored on Card 1. These have the following file names:

Touch Control- 580xz1yy.BIN

Dialog language x = 8 / 9 (Touch Control versions 808 / 809)

yy = 10 or higher (program version)

z = 1 (German), 2 (French), 5 (Spanish)

- ☞ Take care that the device and version numbers are correctly assigned.
- ☞ Confirm the selected file directly with **[Continue]** or first select a different language file.
- ☞ Start loading the language with **[Start]**. Further steps are shown in the dialog.
- ☞ When the loading process has finished switch off the Touch Control, wait a few seconds, and then switch it on again.

Update Touch Control (Touch Control only)

- ☞ Use **[Update Touch Control]** under **System/Diagnosis/Software update** to open the selection of the program files stored on Card 1. These have the following file names:

Touch Control 580x01yy.BIN

Program x = 8 / 9 (Touch Control versions 808 / 809)

yy = 10 or higher (program version)

- ☞ Take care that the device and version numbers are correctly assigned.
- ☞ Confirm the selected file directly with **[Continue]** or first select a different program file.
- ☞ Start the update with **[Start]**. Further steps are shown in the dialog.
- ☞ When the update has finished switch off the Touch Control, wait a few seconds, and then switch it on again.

Update Titrando (Touch Control and PC Control)

- ☞ Use **[Update Titrando]** under **System/Diagnosis/Software update** to open the update dialog. You can access the selection of the program files with **[File]**. These have the following file names:

Titrando 580x00yy.BIN

x = 8 / 9 (Titrando versions 808 / 809)

yy = 10 or higher (program version)

- ☞ Take care that the device and version numbers are correctly assigned.
- ☞ Start the update with **[Start]**. Further steps are shown in the dialog.

Touch Control:

- ☞ When the update has finished switch off the Touch Control, wait a few seconds, and then switch it on again.

PC Control:

- ☞ When the update has finished start the Titrando again by pulling out the Titrando mains plug or removing the USB plug from the PC; re-insert it after waiting a few seconds. The PC Control program is automatically ended when you activate **[Back]** or **[Home]** and then confirm the message which appears with **[OK]**.
- ☞ Restart PC Control.

5.2.8 822 Curve Simulator

The 822 Curve Simulator can be used as a diagnosis tool for checking the recording of the titration curves and their evaluation. Titration methods can be carried out and simulated measuring curves recorded without the actual presence of a measuring solution.

Details about the connection and operation of this instrument are given in the appropriate Instructions for Use.

Please note that such a simulation requires that a correctly configured Dosimat or Dosino must be connected. A normal titration method is started. This means that the exchange or dosing unit should be emptied or the corresponding buret tip should be placed in a sufficiently large collection vessel.

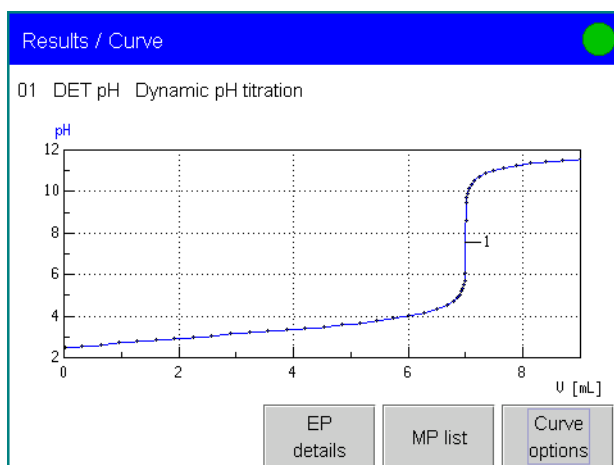
Connection

- ☞ Switch off the Touch Control or pull out the Titrando mains cable or the USB plug at the PC (PC Control).
- ☞ First connect the analog output of the curve simulator with the electrode input "Ind." of the Titrando. Use the **6.2116.020** Cable with F-plugs at both ends.
- ☞ The 822 Curve Simulator is connected to the MSB port of the Dosimat or Dosino used. Take care that the Dosimat is always the last device behind the curve simulator in as short a chain of MSB devices as possible (e.g. Titrando-MSB – 801 Stirrer – 822 Curve Simulator – 805 Dosimat).

- ☞ If the internal exchange unit of the 808 Titrande is used then connect the 822 Curve Simulator to MSB port 2 of the Titrande. In this case when the 808 Titrande is switched on you must also activate the checkbox "**Send dosing signals to MSB2**" under **System/Diagnosis/822 Curve Simulator**. This copies the dosing signals to MSB port 2. Please note that this status can only be **deactivated** by a system restart.
- ☞ Switch on the Touch Control again or reinsert the mains plug and start the PC Control software.

Simulation of a titration

- ☞ For the following example of a simulation you should load the **Tutorial** method from the examples of methods stored under **Card 1/Examples**.
- ☞ Rotate the curve selection switch on the 822 Curve Simulator to curve **0** (Titration of an acid with a base).
- ☞ Start the titration with **[Start]**.
- ☞ When the titration has been carried out you will obtain the following example of a curve under **Results/Curve**:



5.2.9 Service

Access to the service functions is password-protected and only accessible to Metrohm service technicians. We recommend that you have your Titrande system serviced by **Metrohm-Service** at regular intervals. You can automatically monitor the **time interval** after which the Titrande system needs to be serviced again (see *Section 3.12.2*).

5.3 Maintenance

5.3.1 Changing the batteries (Touch Control only)

The Touch Control indicates that its batteries need changing with the message "Battery low". Please note that the current date and time will be reset to 1.1.2000 and 00:00:00 respectively.

Proceed as follows:

- ☞ Switch off the Touch Control.
- ☞ Remove the three fastening screws of the protective cover on the base of the housing:

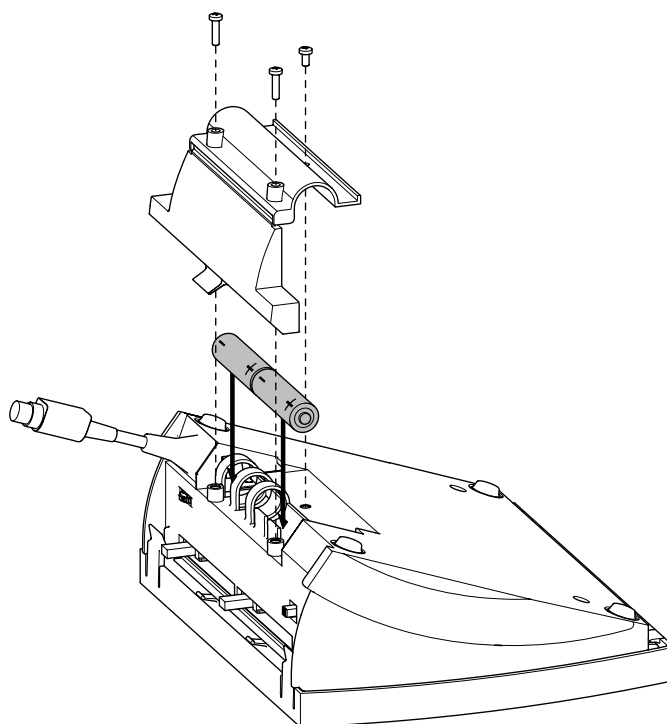


Fig. 25: Changing the batteries for Touch Control

- ☞ Exchange the existing batteries for two new 1.5 V alkaline manganese batteries, type LR6/AA/AM3 (Metrohm Order number 6.2133.010).
- ☞ Make sure that the poles of the batteries are positioned correctly! The correct arrangement is shown in the battery compartment.
- ☞ Reattach the protective cover to the rear panel with the three screws and close it.
- ☞ Switch on the Touch Control and reset the date and time (see Section 3.7.2).



5.3.2 RAM initialization (RAM Init, Touch Control only)

In very rare cases excessive interference could affect the functions of the processor and cause a program crash. In this case the RAM sector must be initialized. RAM initialization is also the only way of making the system accessible again if it is impossible for a user to log in because, for example, even the Administrator has forgotten the password or no Administrator has been defined (see Section 3.7.5).



Attention!

*If you carry out a **RAM initialization** (RAM Init) then **all user data will be lost**. The contents of the internal memory will be deleted. The system will return to the "works settings".*



Note!

*You should make a **backup** at **regular intervals** in order to avoid data loss. For the Touch Control we recommend – depending on how frequently you alter methods or system settings – making a backup every week to every month. For the PC Control software the period should be in accordance with that usually used for data security backups in your company.*

For RAM initialization proceed as follows:

- ☞ Switch off Touch Control with ON/OFF switch **11**.
- ☞ Switch Touch Control on again with ON/OFF switch **11** while keeping contrast controller **14** pressed down. You can release the contrast controller when you hear an acoustic signal (beep).

The RAM will be checked and initialized.

6 Annex

In this section you will find the most important technical data for the Touch Control, a list of standard accessories and optional accessories for the Touch Control and PC Control software as well as the warranty and declarations of conformity.

6.1 Technical data

Provided that nothing to the contrary is mentioned, the published values represent typical technical data for the 808 Touch Control and 809 Touch Control.

6.1.1 Touch screen

<i>Display</i>	1/4 VGA color display, 320 pixel x 240 pixel, 12 cm x 9 cm
<i>Touch panel</i>	analog resistive

6.1.2 Interfaces

Titrand connection

<i>Cable</i>	8-pole, 70 cm, shielded, mini-DIN plug with lock
--------------	--

PCMCIA card slot

<i>Card slot</i>	PCMCIA (Personal Computer Memory Card International Association) ATA Card type I/II
<i>Cards</i>	FlashCards for storing methods, determinations, sample data silos, result silos and backups (PCMCIA cards or CompactFlash cards with CompactFlash adapter)

6.1.3 Power supply

<i>Voltage</i>	$\pm 12\text{ V}$, $+5\text{ V}$
<i>Power consumption</i>	5 W
<i>Batteries</i>	2 x 1.5 V alkaline manganese, type LR6/AA/AM3

6.1.4 Safety specifications

<i>Construction and testing</i>	To EN/IEC 61010-1, UL 3101-1 protection class 3
<i>Safety information</i>	The Instructions for Use contain safety information that must be observed by the user in order to ensure the safe operation of the instrument.

6.1.5 Electromagnetic compatibility (EMC)

<i>Emission</i>	Standards fulfilled: - EN/IEC 61326-1 - EN 55022 / CISPR 22 - EN/IEC 61000-3-2 - EN/IEC 61000-3-3
<i>Immunity</i>	Standards fulfilled: - EN/IEC 61326-1 - EN/IEC 61000-4-2 - EN/IEC 61000-4-3 - EN/IEC 61000-4-4 - EN/IEC 61000-4-5 - EN/IEC 61000-4-6 - EN/IEC 61000-4-11

6.1.6 Ambient temperature

<i>Nominal working range</i>	+5 °C...+40 °C (at max. 85% rel. humidity)
<i>Automatic inner temperature monitoring</i>	> 50 °C pre-alarm > 55 °C alarm
<i>Storage</i>	–20 °C...+60 °C
<i>Transport</i>	–40 °C...+60 °C

6.1.7 Dimensions

<i>Housing material</i>	Polybutylene terephthalate (PBT)
<i>Film material</i>	Polyester
<i>Width</i>	210 mm
<i>Height</i>	83 mm
<i>Depth</i>	approx. 198 mm
<i>Weight</i>	1437 g

6.2 Remote box

The 6.2148.010 Remote box allows devices to be controlled which cannot be connected directly to the MSB interface of the Titrando, e.g. sample changers. The connection of the Remote box is described in the Installation Instructions for the 808 and 809 Titrando.

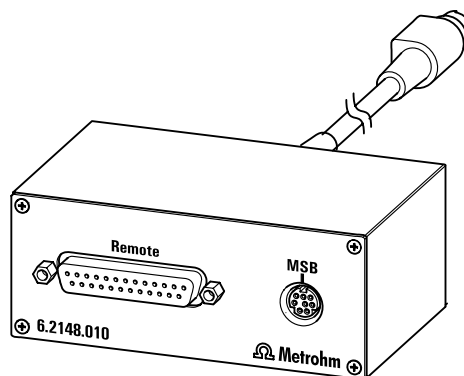


Fig. 26: View of the connections of the optional 6.2148.010 Remote box

6.2.1 Pin occupancy of the remote connection at the Remote box

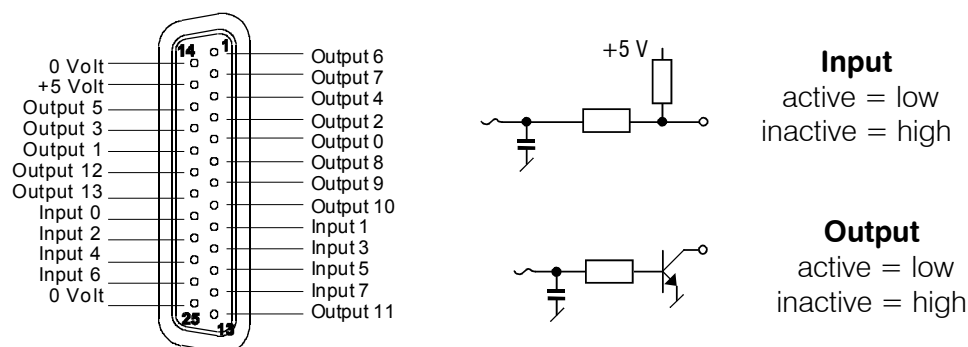


Fig. 27: Pin occupancy at remote interface

The following applies for all outputs:

$$\begin{aligned} V_{CE0} &= 40 \text{ V} \\ I_C &= 20 \text{ mA} \\ t_{\text{pulse}} &> 100 \text{ ms} \end{aligned}$$

6.2.2 Functions of the individual remote lines

Name	Pin.	Function
Input 0	21	START On activation the current method is started. $t_{\text{pulse}} > 100 \text{ ms}$
Input 1	9	STOP On activation the current determination is halted (Stop). $t_{\text{pulse}} > 100 \text{ ms}$
Input 3	10	CANCEL On activation the current command in the determination run will be halted. $t_{\text{pulse}} > 100 \text{ ms}$
Input 4	23	- Not occupied, can be used for scanning the sample changer (sample in work position).
Input 5	11	- Not occupied, can be used for scanning the sample changer (sample in work position).
Output 0	5	READY The Titrand is ready to receive a start signal.
Output 1	18	- Not occupied.
Output 2	4	TITRATION The Titrand is carrying out a data producing sequence.
Output 3	17	EOD End of Determination Pulse ($t_{\text{pulse}} = 200 \text{ ms}$) after a determination or after a buffer/standard during calibration using a sample changer.
Output 4	3	- Not occupied.
Output 5	16	ERROR Line is set for error message display.
Output 6	1	- Not occupied.
Output 7	2	- Not occupied.
Voltage:		
+5 V	15	$I \leq 40 \text{ mA}$ 0 V: active (low), 5 V: inactive
0 V	14 / 25	

6.3 USB-RS 232 box

If Touch Control is used then the 6.2148.020 USB-RS 232 box allows devices with a serial RS 232 interface to be directly connected to the Titrando. Such a device could be a balance or computer for data transmission.

The connection of devices via the USB-RS 232 box is described in the Installation Instructions for the Titrando.

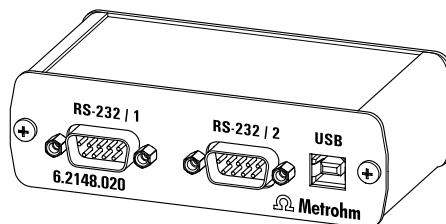


Fig. 28: View of the connections of the optional 6.2148.020 USB-RS 232 box

6.3.1 RS 232 parameters

The USB-RS 232 box makes the **RS 232 interfaces 1 and 2 (RS-232 1 and RS-232 2)** available to the Titrando. The configuration of these interfaces can be carried out in the device manager in the settings for the device which is connected (see *Section 3.10.6* and *Section 3.10.7*). The following list shows the default parameters for Touch Control and PC Control in bold type:

Baud rate:	1200, 2400, 4800, 9600 , 19200, 38400, 57600, 115200
Data bits:	7, 8 Bits
Parity:	even, odd, none
Stop bits	1 , 2 bits
Handshake:	none, software(XOn/XOff), hardware(DTR/CTS)

6.3.2 RS 232 pin occupancy

RS 232 connection: D-sub 9-pole, male, full

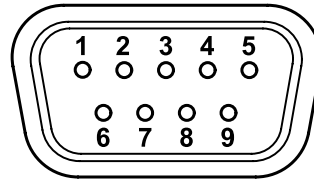


Fig. 29: View of the RS 232 connections on the USB-RS 232 box

Pin 1: -

Pin 2: RxD ← Data reception (Receive Data)

Pin 3: TxD → Data transmission (Transmit Data)

Pin 4: DTR → Ready to receive (Data Terminal Ready)

Pin 5: GND ⊥ Zero voltage, reference potential (ground)

Pin 6: DSR ← Only used for diagnosis (Data Set Ready)

Pin 7: RTS → Transmitter to send (Request To Send)

Pin 8: CTS ← Receiver ready to receive (Clear To Send)

Pin 9: -

6.4 Stored buffer series for CAL pH

For automatic buffer recognition during pH calibration the temperature-dependent pH values of several common pH buffers are stored in the system. As well as the Metrohm 6.2307.1X0 Buffer solutions the tables also contain other reference and technical buffers.

The following tables provide an overview of the stored pH(T) series:

Temp. (°C)	Metrohm			NIST				
	Met4 pH 4.00	Met7 pH 7.00	Met9 pH 9.00	NIST1 pH 1	NIST4 pH 4	NIST7 pH 7	NIST9 pH 9	NIST13 pH 13
0	3.99	7.11	9.27	-	4.01	6.98	9.46	13.42
5	3.99	7.08	9.18	1.67	4.00	6.95	9.39	13.21
10	3.99	7.06	9.13	1.67	4.00	6.92	9.33	13.00
15	3.99	7.04	9.08	1.67	4.00	6.90	9.28	12.81
20	3.99	7.02	9.04	1.68	4.00	6.88	9.23	12.63
25	4.00	7.00	9.00	1.68	4.01	6.87	9.18	12.45
30	4.00	6.99	8.96	1.69	4.02	6.85	9.14	12.29
35	4.01	6.98	8.93	1.69	4.03	6.84	9.11	12.13
40	4.02	6.98	8.90	1.70	4.04	6.84	9.08	11.98
45	4.03	6.97	8.87	1.70	4.05	6.83	9.05	11.84
50	4.04	6.97	8.84	1.71	4.06	6.83	9.02	11.71
55	4.06	6.97	8.81	1.72	4.08	6.83	8.99	11.57
60	4.07	6.97	8.79	1.72	4.09	6.84	8.96	11.45
65	4.09	6.98	8.76	1.73	4.11	6.84	8.94	-
70	4.11	6.98	8.74	1.74	4.13	6.85	8.92	-
75	4.13	6.99	8.73	1.75	4.15	6.85	8.90	-
80	4.15	7.00	8.71	1.77	4.16	6.86	8.89	-
85	4.18	7.00	8.70	1.78	4.19	6.87	8.87	-
90	4.20	7.01	8.68	1.79	4.21	6.88	8.85	-
95	4.23	7.02	8.67	1.81	4.23	6.89	8.83	-

Temp. (°C)	DIN						Fisher		
	DIN1 pH 1	DIN3 pH 3	DIN4 pH 4	DIN7 pH 7	DIN9 pH 9	DIN12 pH 12	Fis4 pH 4	Fis7 pH 7	Fis10 pH 10
0	1.08	-	4.67	6.89	9.48	-	4.01	7.13	10.34
5	1.08	-	4.66	6.86	9.43	-	3.99	7.10	10.26
10	1.09	3.10	4.66	6.84	9.37	13.37	4.00	7.07	10.19
15	1.09	3.08	4.65	6.82	9.32	13.15	3.99	7.05	10.12
20	1.09	3.07	4.65	6.80	9.27	12.96	4.00	7.02	10.06
25	1.09	3.06	4.65	6.79	9.23	12.75	4.00	7.00	10.00
30	1.10	3.05	4.65	6.78	9.18	12.61	4.01	6.99	9.94
35	1.10	3.05	4.66	6.77	9.13	12.44	4.02	6.98	9.90
40	1.10	3.04	4.66	6.76	9.09	12.29	4.03	6.97	9.85
45	1.10	3.04	4.67	6.76	9.04	12.13	4.04	6.97	9.81
50	1.11	3.04	4.68	6.76	9.00	11.98	4.06	6.97	9.78
55	1.11	3.04	4.69	6.76	8.97	11.84	4.07	6.97	9.74
60	1.11	3.04	4.70	6.76	8.92	11.69	4.09	6.98	9.70
65	1.11	3.04	4.71	6.76	8.90	11.56	4.11	6.99	9.68
70	1.11	3.04	4.72	6.76	8.88	11.43	4.13	7.00	9.65
75	1.12	3.04	4.74	6.77	8.86	11.30	4.14	7.02	9.63
80	1.12	3.05	4.75	6.78	8.85	11.19	4.16	7.03	9.62
85	1.12	3.06	4.77	6.79	8.83	11.08	4.18	7.06	9.61
90	1.13	3.07	4.79	6.80	8.82	10.99	4.21	7.08	9.60
95	-	-	-	-	-	-	4.23	7.11	9.60

Temp. (°C)	Novartis (Fluka Basle)			Mettler Toledo				
	FBS4 pH 4	FBS7 pH 7	FBS9 pH 9	MT2 pH 1	MT4 pH 4	MT7 pH 7	MT9 pH 9	MT11 pH 11
0	4.01	7.11	9.20	2.03	4.01	7.12	9.52	11.90
5	4.00	7.08	9.15	2.02	4.01	7.09	9.45	11.72
10	4.00	7.05	9.10	2.01	4.00	7.06	9.38	11.54
15	4.00	7.02	9.05	2.00	4.00	7.04	9.32	11.36
20	4.00	7.00	9.00	2.00	4.00	7.02	9.26	11.18
25	4.01	6.98	8.96	2.00	4.01	7.00	9.21	11.00
30	4.01	6.97	8.91	1.99	4.01	6.99	9.16	10.82
35	4.02	6.96	8.88	1.99	4.02	6.98	9.11	10.64
40	4.03	6.95	8.84	1.98	4.03	6.97	9.06	10.46
45	4.04	6.94	8.80	1.98	4.04	6.97	9.03	10.28
50	4.06	6.94	8.77	1.98	4.06	6.97	8.99	10.10
55	4.07	6.93	8.74	1.98	4.08	6.98	8.96	-
60	4.09	6.93	8.71	1.98	4.10	6.98	8.93	-
65	4.11	6.93	8.69	1.98	4.13	6.99	8.90	-
70	4.13	6.94	8.67	1.99	4.16	7.00	8.88	-
75	4.14	6.94	8.65	1.99	4.19	7.02	8.85	-
80	4.16	6.95	8.63	2.00	4.22	7.04	8.83	-
85	4.18	6.96	8.61	2.00	4.26	7.06	8.81	-
90	4.21	6.97	8.60	2.00	4.30	7.09	8.79	-
95	4.23	6.98	8.59	-	4.35	7.12	8.77	-

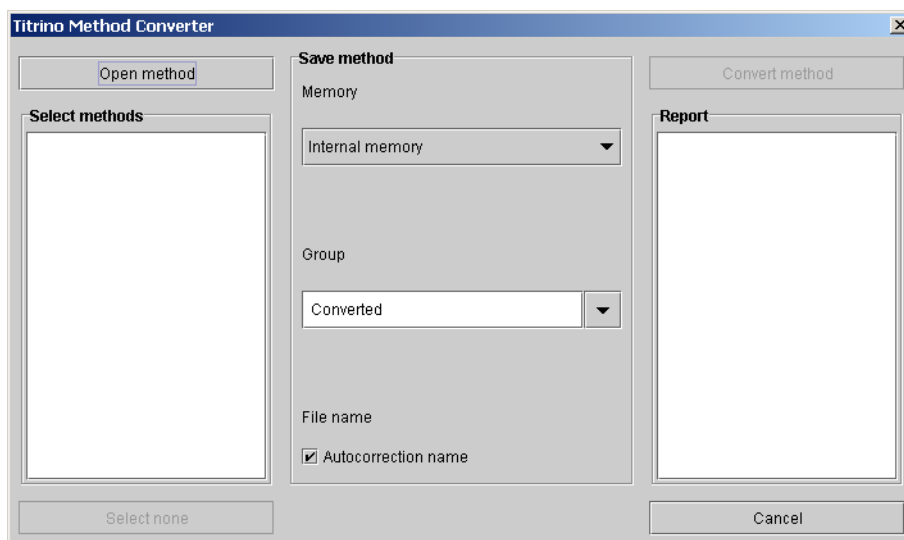
Temp. (°C)	Merck					Beckman		
	Mer2 pH 2	Mer4 pH 4	Mer7 pH 7	Mer9 pH 9	Mer12 pH 12	Bec4 pH 4	Bec7 pH 7	Bec10 pH 10
0	2.01	4.05	7.13	9.24	12.58	4.00	7.12	10.32
5	2.01	4.04	7.07	9.16	12.41	4.00	7.09	10.25
10	2.01	4.02	7.05	9.11	12.26	4.00	7.06	10.18
15	2.00	4.01	7.02	9.05	12.10	4.00	7.04	10.12
20	2.00	4.00	7.00	9.00	12.00	4.00	7.02	10.06
25	2.00	4.01	6.98	8.95	11.88	4.00	7.00	10.01
30	2.00	4.01	6.98	8.91	11.72	4.01	6.99	9.97
35	2.00	4.01	6.96	8.88	11.67	4.02	6.99	9.93
40	2.00	4.01	6.95	8.85	11.54	4.03	6.98	9.89
45	2.00	4.00	6.95	8.82	11.44	4.05	6.98	9.86
50	2.00	4.00	6.95	8.79	11.33	4.06	6.97	9.83
55	2.00	4.00	6.95	8.76	11.19	4.08	6.98	-
60	2.00	4.00	6.96	8.73	11.04	4.09	6.98	-
65	2.00	4.00	6.96	8.72	10.97	4.11	6.99	-
70	2.01	4.00	6.96	8.70	10.90	4.12	6.99	-
75	2.01	4.00	6.96	8.68	10.80	4.14	7.00	-
80	2.01	4.00	6.97	8.66	10.70	4.16	7.00	-
85	2.01	4.00	6.98	8.65	10.59	4.18	7.01	-
90	2.01	4.00	7.00	8.64	10.48	4.19	7.02	-
95	-	4.00	7.02	-	-	4.21	7.03	-

Temp. (°C)	Radiometer		
	Rad4.01 pH 4.01	Rad7.00 pH 7	Rad9.18 pH 9.18
0	4.000	7.118	9.464
5	3.998	7.087	9.395
10	3.997	7.059	9.332
15	3.998	7.036	9.276
20	4.001	7.016	9.225
25	4.005	7.000	9.180
30	4.011	6.987	9.139
35	4.018	6.977	9.102
40	4.027	6.970	9.068
45	4.038	6.965	9.038
50	4.050	6.964	9.011
55	4.064	6.965	8.985
60	4.080	6.968	8.962
65	4.097	6.974	8.941
70	4.116	6.982	8.921
75	4.137	6.992	8.900
80	4.159	7.004	8.885
85	4.183	7.018	8.867
90	4.210	7.034	8.850
95	4.240	-	-

6.5 Importing Titrino methods (PC Control only)

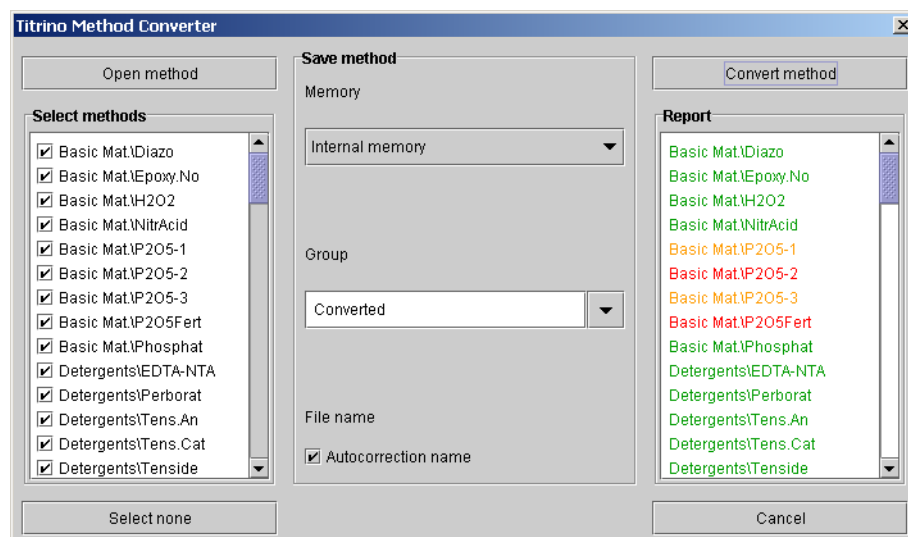
With the Titrino method converter you can import Titrino methods into the PC Control software.

- ☞ Use the Metrohm **VESUV** software to save the methods which are stored in the Titrino. The methods are stored in a .vmb file.
- ☞ In the **File** menu open the menu item **Import Methods...**



- ☞ Use **[Open method]** to open the **Vesuv backup file** dialog. Select the required .vmb file and open it. The methods are listed under **Select methods**. If the methods have been stored in folders in the Titrino then the folder will be shown in front of the method name and separated from it by "/".
- ☞ If you do not want to import all the methods in the backup file then you can deactivate the checkboxes for these methods. With **[Select none]** or **[Select all]** you can select either none or all of the methods in the list respectively.
- ☞ Under **Save method** select the **Memory** and **Group** in which the converted methods are to be stored. If the **Autocorrection name** function is switched on then invalid characters in method names will be replaced by "_".
- ☞ Start the conversion with **[Convert method]**. The conversion can be stopped at any time with **[Cancel]**.

Any messages produced during the conversion of the methods will be shown under **Report**.



The methods are shown in color. The colors have the following meanings:

- Green: conversion OK.
- Yellow: 1:1 not possible. The converted method must be checked.
- Red: conversion not possible.

If you click on the method name then all the messages referring to this method will be shown in a new dialog window. The following messages may be produced:

Conversion OK (green-marked methods)

- The method has been converted successfully.
- An old method file with the same name has been replaced.
- The method file has been renamed to: New method name

Check converted method (yellow-marked methods)

- Single commands could not be converted.
- The assignment to a temporary variable (C70 to C79) for TIP was ignored.
- The assignment of a temporary variable (C70 to C79) to a common variable is not possible.
- The assignment of a temporary variable (C70 to C79) to a statistics variable is not possible.
- A formula contains a temporary variable (C70 to C79). The variable has been replaced by -0.
- The assignment to a silo calculation variable (C24 to C27) has been ignored.
- The assignment of a silo calculation variable (C24 to C27) to a common variable is not possible.

- The assignment of a silo calculation variable (C24 to C27) to a statistics variable is not possible.
- A formula contains a silo calculation variable (C24 to C27). The variable has been replaced by -0.
- The assignment of sample identification 3 (C23) to a common variable is not possible.
- The assignment of sample identification 3 (C23) to a statistics variable is not possible.
- A formula contains the sample identification 3 (C23). The variable has been replaced by -0.
- The method contains the parameter 'activation pulse: first'. This parameter has been ignored.
- Measuring input 'diff.' has been replaced by measuring input '1'.
- The relative start volume has been replaced by 0.00 mL.
- The relative stop volume has been replaced by 100.00 mL.
- SET: The delay time for EP1 and EP2 was set to 'inf.'
- An old method file with the same name has been replaced.
- The method file has been renamed to: New method name

Conversion not possible (red-marked methods)

- The method could not be converted.
- This mode is not supported. Only DET, MET, SET and MEAS can be converted.
- Conditioning is switched on. The method cannot be converted.

6.6 Standard equipment

Immediately upon receipt of the Touch Control or PC Control software please check that the delivery is complete. Please also consult the lists of accessories in the Installation Instructions for the 808 Titrand and 809 Titrand, where the Titrand accessories are described.

6.6.1 808 Touch Control

<i>No.</i>	<i>Order no.</i>	<i>Description</i>
1	1.808.0100	808 Touch Control
1	6.6048.000	808 CompactFlash card (8 MB) with user methods and 6.2247.000 Adapter
1	A.704.00XX	PC Control CD-ROM
1	8.808.1303	Instructions for Use for 808 Touch Control, 809 Touch Control and PC Control
1	8.808.1403	Tutorial for 808 Touch Control and 809 Touch Control

6.6.2 809 Touch Control

<i>No.</i>	<i>Order no.</i>	<i>Description</i>
1	1.809.0100	809 Touch Control
1	6.6049.000	809 CompactFlash card (8 MB) with user methods and 6.2247.000 Adapter
1	A.704.00XX	PC Control Demo-CD
1	8.808.1303	Instructions for Use for 808 Touch Control, 809 Touch Control and PC Control
1	8.808.1403	Tutorial for 808 Touch Control and 809 Touch Control

6.6.3 PC Control Software with Dongle (6.6050.000)

<i>No.</i>	<i>Order no.</i>	<i>Description</i>
1	A.704.00XX	PC Control CD-ROM
1	6.2145.100	USB dongle with registration card
1	8.808.1303	Instructions for Use for 808 Touch Control, 809 Touch Control and PC Control
1	8.808.1503	Tutorial for PC Control

6.6.4 PC Control software, demo version (6.6050.005)

The demo version is fully functional for 100 days after installation. After this period has elapsed you must purchase a USB dongle.

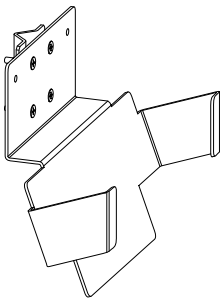
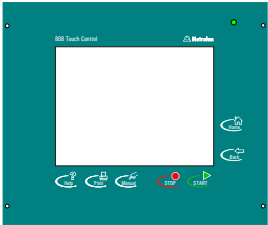
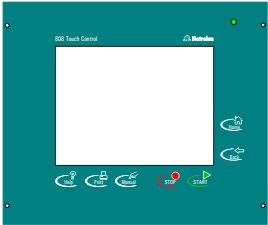
<i>No.</i>	<i>Order no.</i>	<i>Description</i>
1	A.704.00XX	PC Control CD-ROM
1	8.808.1303	Instructions for Use for 808 Touch Control, 809 Touch Control and PC Control
1	8.808.1503	Tutorial for PC Control

6.6.5 USB dongle for PC Control software

<i>No.</i>	<i>Order no.</i>	<i>Description</i>
1	6.2145.100	USB dongle with registration card

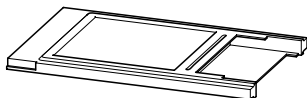

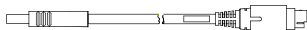
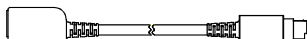
6.7 Additional devices and optional accessories

6.7.1 Miscellaneous accessories

Order no.	Description	
6.2051.030	Wall holder for attaching the Touch Control to a wall or support rod (diameter 10 mm). You can also use the wall holder to achieve a steeper display angle on the bench.	
6.2834.010	Spare film for 808 Touch Control 3 pieces The films can be exchanged when they become dirty or damaged.	
6.2834.020	Spare film for 809 Touch Control 3 pieces The films can be exchanged when they become dirty or damaged.	
6.2133.010	Batteries 1.5 V, 2 pieces Spare batteries for Touch Control, 1.5 V LR6	

6.7.2 Communication

Further cables can be found in the Installation Instructions for the 808 Titrandos and 809 Titrandos.

<i>Order no.</i>	<i>Description</i>	
6.2247.000	Adapter CompactFlash card – PC card type II Adapter for using CompactFlash cards in PCMCIA card slots	
6.2247.010	CompactFlash card 8 MB Memory card for methods, determinations, sample data silos, etc.	
6.2151.000	Cable for connecting a Titrandos to a PC (USB connection, type A) and for connecting further Titrandos USB A – Controller (1.8 m)	
6.2151.010	Extension cable for MSB connections and for Touch Control – Titrandos mini-DIN socket – mini-DIN plug (2 m)	

6.8 Warranty and conformity

6.8.1 Warranty

The warranty on our products is limited to defects that are traceable to material, construction or manufacturing error which occur within 12 months from the day of delivery. In this case the defects will be rectified in our workshops free of charge. Transport costs are to be paid by the customer.

For day and night operation the warranty is limited to 6 months.

Glass breakage in the case of electrodes or other parts is not covered by the warranty. Checks which are not a result of material or manufacturing faults are also charged during the warranty period. For parts from outside manufacturers, insofar as these constitute an appreciable part of our instrument, the warranty stipulations of the manufacturer in question apply.

With the regard to the guarantee of accuracy the technical specifications in the instruction manual are authoritative.


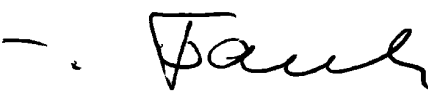

Concerning defects in materials, construction or design as well as the absence of guaranteed features the purchaser has no rights or claims except those mentioned above.

If damage of the packaging is evident on receipt of a consignment or if the goods show signs of transport damage after unpacking, the carrier must be informed immediately and a written damage report demanded. Lack of an official damage report releases Metrohm from any liability to pay compensation.



If any instruments and parts have to be returned then the original packaging should be used if at all possible. This applies above all to instruments, electrodes, buret cylinders and PTFE pistons. Before embedding in wood shavings or similar material the parts must be packed in a dustproof package (for instruments the use of a plastic bag is essential). If open assemblies are included that are sensitive to electromagnetic voltages (e.g. data interfaces, etc.) then these must be returned in the associated original protective packaging (e.g. conductive protective bag). (Exception: assemblies with a built-in voltage source belong in non-conductive protective packaging).

For damage which arises as a result of non-compliance with these instructions no warranty responsibility whatsoever will be accepted by Metrohm.




6.8.2 EU Declaration of conformity for 808 Touch Control

 EU Declaration of Conformity					
<p>The company Metrohm AG, Herisau, Switzerland, certifies herewith, that the following instrument:</p> <p style="text-align: center;">808 Touch Control</p> <p>meets the CE mark requirements of EU Directives 89/336/EEC and 73/23/EEC.</p>					
<p>Source of specifications:</p> <table style="width: 100%; border: none;"> <tr> <td style="width: 20%;">EN 61326-1</td> <td>Electrical equipment for measurement, control and laboratory use – EMC requirements</td> </tr> <tr> <td>EN 61010-1</td> <td>Safety requirements for electrical equipment for measurement, control and laboratory use</td> </tr> </table>		EN 61326-1	Electrical equipment for measurement, control and laboratory use – EMC requirements	EN 61010-1	Safety requirements for electrical equipment for measurement, control and laboratory use
EN 61326-1	Electrical equipment for measurement, control and laboratory use – EMC requirements				
EN 61010-1	Safety requirements for electrical equipment for measurement, control and laboratory use				
<p>Description of apparatus:</p> <p>Control unit with touch-sensitive screen for the 808 Titrande and 809 Titrande titrators and peripheral devices such as dosing devices, stirrers and titration stands.</p>					
<p>Herisau, April 30, 2002</p> <div style="display: flex; justify-content: space-around; align-items: flex-end; margin-top: 20px;"> <div style="text-align: center;">  Dr. J. Frank Development Manager </div> <div style="text-align: center;">  Ch. Buchmann Production and Quality Assurance Manager </div> </div>					



6.8.3 Certificate of conformity and system validation: 808 Touch Control

Certificate of Conformity and System Validation	
<p>This is to certify the conformity to the standard specifications for electrical appliances and accessories, as well as to the standard specifications for security and to system validation issued by the manufacturing company.</p>	
Name of commodity:	808 Touch Control
System software:	Stored in ROMs
Name of manufacturer:	Metrohm Ltd., Herisau, Switzerland
<p>This Metrohm instrument has been built and has undergone final type testing according to the standards:</p> <p><i>Electromagnetic compatibility: Emission</i> IEC 61326-1, EN 55022 / CISPR 22, IEC 61000-3-2, IEC 61000-3-3</p> <p><i>Electromagnetic compatibility: Immunity</i> IEC 61326-1, IEC 61000-4-2, IEC 61000-4-3, IEC 61000-4-4, IEC 61000-4-5, IEC 61000-4-6, IEC 61000-4-11</p> <p><i>Safety specifications</i> IEC 61010-1, UL 3101-1</p> <p>It has also been certified by the Swiss Electrotechnical Association (SEV), which is member of the International Certification Body (CB/IEC).</p> <p>The technical specifications are documented in the instruction manual.</p> <p>The system software, stored in Read Only Memories (ROMs) has been validated in connection with standard operating procedures in respect to functionality and performance.</p> <p>Metrohm Ltd. is holder of the SQS-certificate of the quality system ISO 9001 for quality assurance in design/development, production, installation and servicing.</p>	
<p>Herisau, April 30, 2002</p> <div style="display: flex; justify-content: space-around; align-items: flex-end;"> <div style="text-align: center;">  <p>Dr. J. Frank Development Manager</p> </div> <div style="text-align: center;">  <p>Ch. Buchmann Production and Quality Assurance Manager</p> </div> </div>	

6.8.4 EU Declaration of conformity for 809 Touch Control

 EU Declaration of Conformity					
<p>The company Metrohm AG, Herisau, Switzerland, certifies herewith, that the following instrument:</p> <p style="text-align: center;">809 Touch Control</p> <p>meets the CE mark requirements of EU Directives 89/336/EEC and 73/23/EEC.</p>					
<p>Source of specifications:</p> <table style="width: 100%; border: none;"> <tr> <td style="width: 20%;">EN 61326-1</td> <td>Electrical equipment for measurement, control and laboratory use – EMC requirements</td> </tr> <tr> <td>EN 61010-1</td> <td>Safety requirements for electrical equipment for measurement, control and laboratory use</td> </tr> </table>		EN 61326-1	Electrical equipment for measurement, control and laboratory use – EMC requirements	EN 61010-1	Safety requirements for electrical equipment for measurement, control and laboratory use
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EN 61010-1	Safety requirements for electrical equipment for measurement, control and laboratory use				
<p>Description of apparatus:</p> <p>Control unit with touch-sensitive screen for the 808 Titrande and 809 Titrande titrators and peripheral devices such as dosing devices, stirrers and titration stands.</p>					
<p>Herisau, April 30, 2002</p> <div style="display: flex; justify-content: space-around; align-items: flex-end; margin-top: 20px;"> <div style="text-align: center;">  Dr. J. Frank Development Manager </div> <div style="text-align: center;">  Ch. Buchmann Production and Quality Assurance Manager </div> </div>					

6.8.5 Certificate of conformity and system validation: 809 Touch Control

Certificate of Conformity and System Validation	
<p>This is to certify the conformity to the standard specifications for electrical appliances and accessories, as well as to the standard specifications for security and to system validation issued by the manufacturing company.</p>	
Name of commodity:	809 Touch Control
System software:	Stored in ROMs
Name of manufacturer:	Metrohm Ltd., Herisau, Switzerland
<p>This Metrohm instrument has been built and has undergone final type testing according to the standards:</p> <p><i>Electromagnetic compatibility: Emission</i> IEC 61326-1, EN 55022 / CISPR 22, IEC 61000-3-2, IEC 61000-3-3</p> <p><i>Electromagnetic compatibility: Immunity</i> IEC 61326-1, IEC 61000-4-2, IEC 61000-4-3, IEC 61000-4-4, IEC 61000-4-5, IEC 61000-4-6, IEC 61000-4-11</p> <p><i>Safety specifications</i> IEC 61010-1, UL 3101-1</p> <p>It has also been certified by the Swiss Electrotechnical Association (SEV), which is member of the International Certification Body (CB/IEC).</p> <p>The technical specifications are documented in the instruction manual.</p> <p>The system software, stored in Read Only Memories (ROMs) has been validated in connection with standard operating procedures in respect to functionality and performance.</p> <p>Metrohm Ltd. is holder of the SQS-certificate of the quality system ISO 9001 for quality assurance in design/development, production, installation and servicing.</p>	
<p>Herisau, April 30, 2002</p> <div style="display: flex; justify-content: space-around; align-items: flex-end;"> <div style="text-align: center;">  <p>Dr. J. Frank Development Manager</p> </div> <div style="text-align: center;">  <p>Ch. Buchmann Production and Quality Assurance Manager</p> </div> </div>	

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