# **Personal Synthesis Workstation**

OptiMax 1001





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#### 1 Introduction

The METTLER TOLEDO OptiMax™ 1001 is a reactor system for performing synthesis with a 250-mL, a 500-mL, or a 1000-mL glass reactor. The instrument is operated via the touchscreen.

- The reactor can be heated or cooled and its content stirred and refluxed.
- The temperature of the reactor content can be measured using a Pt100 sensor.
- The integrated pH measurement system, when equipped with the appropriate electrode allows you to measure the pH value of the reactor content.
- You can export the acquired data to another program for further processing.

Please also read the Operating Instructions for the full scope of functionalities of the device. The Operating Instructions can be found on the USB stick.

#### 1.1 Scope of Delivery

The following items are included in the OptiMax 1001™ thermostat set:

Order number		Description	Quantity
		OptiMax 1001 thermostat	1
51161883		TFT touchscreen 7", 1 m cable	1
11132570		Protective cover for touchscreen	1
30260369		Emergency button	1
51191125		PVC hose, soft, for reflux condenser	1
51161187	0	PVC industrial hose for coolant, 15 bar	2
51192239	0	PVC industrial hose for purge gas, 18 bar	1
51161186		PVC hose for purge gas	1
51191373	1	Y-piece for gas tubing	4

51191916	Count Course	Reducing connector for purge gas tubing	3
51190324	Ton	Quick connect coupling for purge gas inlet	5
51192126		Hose clamp for PVC tube	4
51191915		Flow indicator for coolant	1
51191914		Knurled screw, M6 x 10 mm	4
51191235		Identification clips for adhesive labels	10
51162860		Reactor block plug for bottom drain valve opening	1
51192209		O-ring for 51162860 plug, Ø 50.39 mm x 3.53 mm	1
51161782		Bubble counter	1

51161603	Magnetic bubble counter holder	1
51162886	Accessories holder set	1
51192208	Glass adapter ST19/26-GL14	2
51190317	Screw cap GL14, with aperture	2
51103947	Silicone rubber sealing ring for screw cap GL14, aperture 6 mm	2
51191945	Purge gas regulation valve	1
51161099	Lab bar, 600 mm x 14 mm	4
51162690	Overhead stirrer drive complete	1
30356209	USB Stick RXE/CSS with documents	1
	User Manual	1

If an item is missing, please contact your local support.

#### 1.2 Check on arrival

Check the following conditions once the package has arrived:

- The package is in good condition.
- The content shows no signs of damage (e.g. broken covers, scratches etc.)
- The content is complete (see [Scope of Delivery ▶ Page 3]).

If one condition is not fulfilled, please contact your local support.

#### 2 Safety Information

This thermostat has been tested for the intended purposes described in this document. However, this does not absolve you from the responsibility of performing your own tests of the product supplied by us regarding its suitability for the methods and purposes you intend to use it for. You should therefore observe the following safety measures.

We, Mettler-Toledo GmbH, accept no liability whatsoever if you do not observe the following rules and safety notes for safe operation of the thermostat.

#### 2.1 Definition of signal warnings and symbols

Safety notes are marked with signal words and warning symbols. These show safety issues and warnings. Ignoring the safety notes may lead to personal injury, damage to the instrument, malfunctions and false results.

**WARNING** A hazardous situation with medium risk, possibly resulting in death or severe injury if

not avoided.

**CAUTION** A hazardous situation with low risk, resulting in minor or moderate injury if not avoided.

**NOTICE** A hazardous situation with low risk, resulting in damage to the instrument, other

material damage, malfunctions and erroneous results, or loss of data.

Note (no symbol)

for useful information about the product.

#### Meaning of safety symbols

4	Electrical Hazard	Explosion	Burns / Hot Surface
	Rotating parts	Heavy load	General note

#### 2.2 Intended use

The METTLER TOLEDO OptiMax<sup>™</sup> 1001 is a reactor system for performing synthesis with reactor volumes up to 1000 mL.

Always operate and use your device in accordance with the instructions contained in this manual, only use it together with equipment specified in this documentation.

Any other type of use and operation beyond the limits of technical specifications without the written consent from Mettler-Toledo GmbH, is considered as not intended.

#### 2.3 Product-specific safety



#### **↑** WARNING

#### Risk of electric shock

- 1 Make sure to plug the power cable supplied into a power supply outlet that is grounded. A technical fault could otherwise result in serious injury or death.
- 2 Only use the METTLER TOLEDO power supply cable and AC power adapter designed for your instrument.



#### **⚠** WARNING

#### Power failure

A power failure can lead to explosion with possibly fatal consequences.

- Implement appropriate measures like an uninterruptible power supply (UPS).

#### **⚠ WARNING**



#### Risk of explosion with critical reactions

Performing critical reactions could lead to explosions.

 Perform a safety analysis before starting an experiment with high hazardous potential for example by using a Differential Scanning Calorimeter.



#### **MARNING**

#### Electrostatic discharges through stirring the reaction mass

The following conditions can form electrostatic charge:

- High flow rates (high stirrer speed) of nonpolar liquids with a high resistivity (>10<sup>8</sup> Ohmmeter).
- Two-phase systems with suspended solids (e.g. after crystallization processes in nonconductive solvents or immiscible liquids.)
- Work under an inert gas (nitrogen or argon).



#### ♠ WARNING

#### Risk of explosion due to damaged reactors

Explosion of a reactor could cause serious injury.

- Check the reactor before each use for damage (scratches, formation of cracks).



#### 

#### Hot parts when working above 50 °C

Touching hot parts can cause burns.

Do not touch the cover plate of the device, the fixing ring, the reactor covers, attachments
of the reactor or the overhead stirrer if you work above 50 °C.



#### **CAUTION**

#### **Rotating parts of stirrer**

Touching rotating parts of a running stirrer may lead to injuries.

- Do not touch rotating parts of a stirrer.



#### **CAUTION**

#### Risk of injury due to heavy load

You can injure yourself by carrying the instrument alone.

 Never try to carry the instrument alone. At least two people are needed to carry the instrument.



#### **NOTICE**

#### Wrong connection or disconnection of cables

A wrong connection or disconnection of cables during operation could lead to instrument damage.

- 1 Before switching on the device connect the cables of stirrers and sensors to their respective inputs and outputs.
- 2 Do not disconnect the cables while the instrument is operating.



### NOTICE

#### Condensation of atmospheric moisture

The condensation of atmospheric moisture can cause corrosion of the instrument.

- To prevent this, purge the instrument with dry air, nitrogen or argon.



### NOTICE

#### Wrong coolant used

High chloride concentration in the coolant can lead to corrosion of the thermostat.

Do not use solutions of NaCl or CaCl<sub>2</sub>



### NOTICE

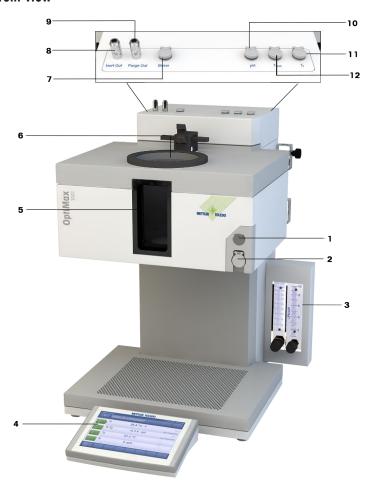
#### Thermal shock

Glass parts of the instrument or the reactor could get damaged.

- Do not fill cold liquids into hot glassware and vice versa.

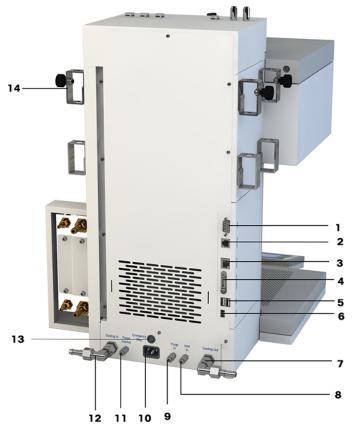
### 3 Overview

#### Front view



1	Power Button	2	USB
3	Flow indicators	4	Touchscreen
5	Reactor window (with back- and frontlight)	6	Opening for reactors
7	Stirrer connection	8	Inert out connection
9	Purge out connection	10	pH connection
11	Tr connection	12	T <sub>aux</sub> connection

#### **Back view**



1	RS232	2	CAN out
3	Ethernet	4	Control unit (Touchscreen) connection
5	USB (2x)	6	Safety relay
7	Coolant out	8	Inert in connection
9	Purge in connection	10	Power supply
11	Purge internal connection	12	Coolant in
13	Emergency Stop connection	14	Holder for lab bars

#### 4 Installation

#### 4.1 Installation requirements

- Make sure there is enough space (about 10 cm) between the ventilation slots at the back side of the instrument and any other object or the wall.
- Make sure you install the device in accordance with the [technical data ▶ Page 28].

#### Site requirements

The instrument has been developed for indoor operation in a well-ventilated area. Avoid the following environmental influences:

- · Conditions outside of the ambient conditions specified in the technical data
- Powerful vibrations
- · Direct sunlight
- · Corrosive gas atmosphere
- Explosive atmosphere of gases, steam, fog, dust and flammable dust
- Powerful electric or magnetic fields

#### 4.2 Connecting power to the device



#### **⚠ WARNING**

#### Risk of electric shock

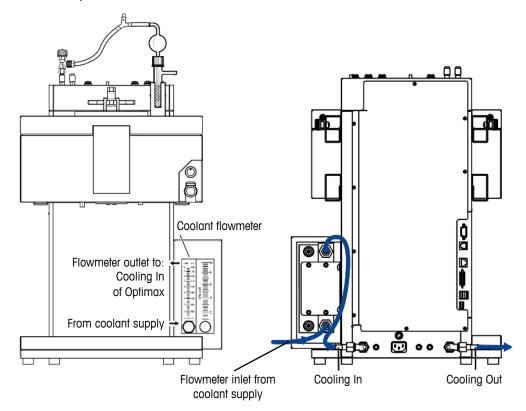
- Make sure to plug the power cable supplied into a power supply outlet that is grounded. A technical fault could otherwise result in serious injury or death.
- 2 Only use the METTLER TOLEDO power supply cable and AC power adapter designed for your instrument.
- 1 The power supply connection is on the back side of the device.



- 2 Connect the instrument to the power supply using the included country-specific cable.
- 3 Insert the plug of the power cable in a grounded power outlet that is easily accessible.

#### 4.3 Connecting water cooling

The installation via the flowmeter requires three pieces of tubing, in the box you will find two. You can cut away a piece of appropriate length (it has to cover the connection from the flowmeter to the cooling in on the back side of the instrument) from one of the two delivered tubes.



- 1 Push one piece of the PVC industrial hose (51161187) over the cooling inlet of the coolant flowmeter.
- 2 Secure it with a hose clamp.
- 3 Connect the other end to the coolant supply.
- 4 Connect the cut piece to the coolant flowmeter outlet and secure with hose clamp.
- 5 Connect the other end to the **Cooling In** of the device and secure with hose clamp.
- 6 Push the second piece of the PVC tube over the elbow coupling of the Cooling Out on the back side of the instrument.
- 7 Secure it with a hose clamp.
- 8 Connect the other end to the waste water system.

#### 4.4 Connecting cryostat cooling



#### NOTICE

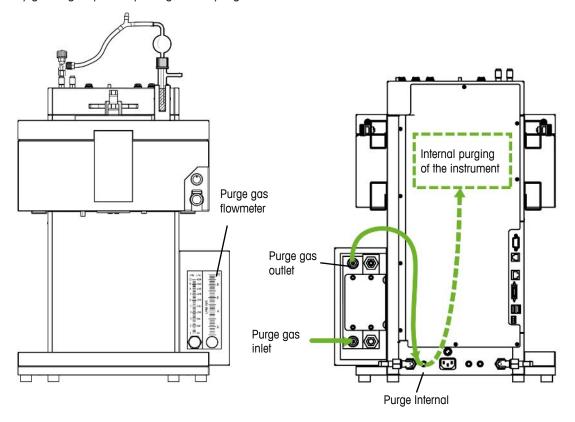
#### **Damage of Flowmeter**

The flowmeter is not resistant against any other liquids than water! Do not use it with other coolants.

- 1 Screw the insulated connection tube over the **Cooling In** on the back of the instrument.
- 2 Use a wrench to tighten the connection to the instrument.
- 3 Screw the second insulated connection tube over the Cooling Out on the back of the instrument.
- 4 Use a wrench to tighten the connection to the instrument.

#### 4.5 Connecting instrument purge gas

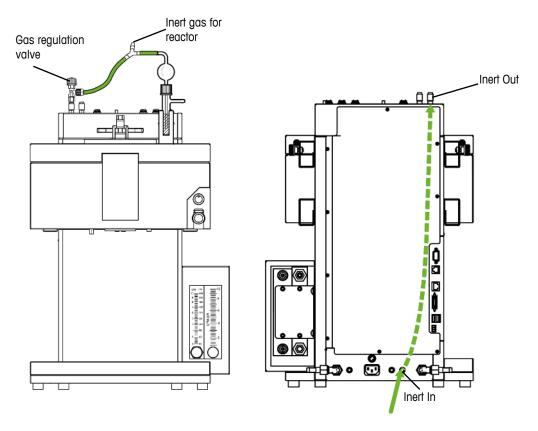
To prevent corrosion by condensed atmospheric moisture in the instrument, the instrument must be purged with a dry gas, e.g. dry air, dry nitrogen or dry argon.



- Push one piece of PVC industrial hose for purge gas (51192239, Ø 4/10 mm ) on the purge gas Inlet of the purge gas flowmeter.
- 2 Secure it with a hose clamp.
- 3 Connect the other end to the purge gas supply.
- 4 Push a second piece of PVC industrial hose for purge gas over the purge gas outlet of the flowmeter.
- 5 Secure it with a hose clamp.
- 6 Push the other end of the second piece over the **Purge Internal** quick connect coupling connection on the back side of the device.
- 7 Secure it with a hose clamp.

#### 4.6 Purging the reactor with inert gas

To perform reactions under nitrogen (or any other inert gas) you have to install the purge tubing according to the following instructions:



- 1 Install a quick connect coupling (51190324, Ø 4/6 mm, red) with the PVC tube (51161186) on the **Inert**In connector on the back side of the instrument and secure it with a hose clamp.
- 2 Connect the other end of the PVC tube to the gas supply.
- 3 Install a quick connect coupling on the **Inert Out** connector on top of the instrument and push a piece of the PVC tube over the quick connect coupling.
- 4 Integrate a bubble counter with a gas regulation valve (51161802, optional available as set) and the Y-piece (51191373) into the tubing as shown in the drawing. Proceed, depending on the type of the used reactor. (The use of the Y-piece guarantees an uncritical pressure for the reactor while the gas flow can be monitored with the bubble counter.)
- 5 Always leave a small opening in the reactor to allow a flow of the purge gas.

#### 4.7 Connecting touchscreen to OptiMax



#### **NOTICE**

#### **Touchscreen connection / disconnection**

The instrument may be seriously damaged if the touchscreen is connected or disconnected when the instrument is switched on.

Do only connect or disconnect the touchscreen when the instrument is switched off.

- 1 The touchscreen connection is on the back side of the instrument (see picture).
- 2 Connect the touchscreen cable to the socket.



### 4.8 Connecting emergency button to OptiMax

- Connect the emergency button to the **Emergency Stop** connector on the rear side of the instrument.

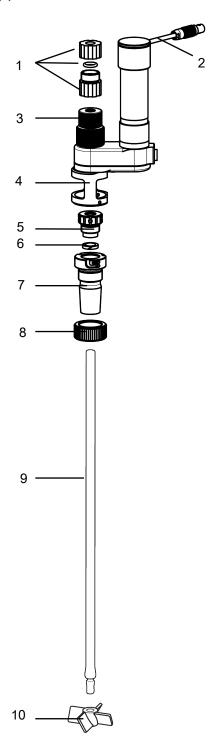


#### 4.9 Assembling the Stirrer

Step 1 and 2 are not needed when the device is installed for the first time as the adapter part comes already assembled.

The assembly of the stirrer adapter (30451755) into the stirrer housing can be a bit tight in the beginning and will improve over time.

- 1 Install the PTFE cord (6) in the adapter (7).
- 2 Reinstall the pressure screw (5) and lightly tighten.
- 3 Screw the pitched-blade element (10) onto the stirrer shaft (9).
- 4 Push the stirrer shaft (9) from below through the central opening of the reactor cover.
- 5 Push the adapter loosening nut (8) over the stirrer shaft (9) and screw to the adapter (7).
- 6 Insert the adapter (7) into the central opening of the cover.
- 7 Push the stirrer shaft (9) through the hole in the stirrer assembly.



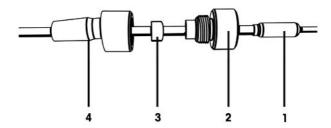
- 8 Tighten the pressure screw (**5**). Increasing the tightness will minimize solvent loss (or retention of vacuum).
- 9 Align the slits in the adapter (7) with the pins of the lower housing (4).
- 10 Turn the stirrer adapter (7) until you hear a click and the adapter is locked in the lower aluminum housing (4).
- 11 If necessary adapt the height of the stirrer shaft and the pitched-blade element with the reactor for an applicable immersion depth.
- 12 Fix the stirrer shaft by tightening the chuck (3) and secure it with the locking device (1) on top of the chuck (3). (The locking device prevents the stirrer shaft from falling into the reactor in case the chuck is loosened carelessly or by mistake.)
- 13 Connect the stirrer cable (2) to the connector on top of the instrument housing.

To change the immersion depth of the stirrer shaft:

- 1 Release the chuck (3) while holding the stirrer shaft.
- 2 Release the locking device (1) and adapt the immersion depth.
- 3 Tighten the chuck (3) and secure it with the locking device (1).

#### 4.10 Installing a Tr sensor

**Note** The Tr sensor must be immersed in the reaction solution to a depth of at least 1.5 cm to give correct measurement values.



- 1 Unscrew the pressing screw (2) from the adapter and push it over the sensor (1).
- 2 Push the sealing ring (3) over the Tr sensor with the round side pointing to the screw (2).
- 3 Push the lower part of the adapter (4) over the Tr sensor.
- 4 Screw the adapter (3 & 2) lightly together.
- 5 Install the Tr sensor (1) on the reactor cover (in an appropriate port).
- 6 Connect the Tr sensor to the Tr connection on the instrument.

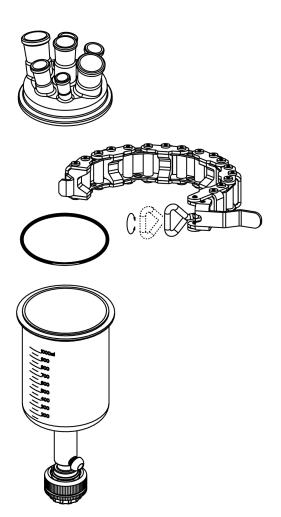
#### 4.11 Installing a 1000 mL two-piece reactor

Before you place the reactor in the thermostat, we recommend that you install the Tr sensor and other inserts in order to check their distance from the stirrer or the bottom of the reactor. We also recommend that you add the reagents and solvent for the starting volume and possibly check the fill level of the first fill.

- Push the glass stirrer or the stirrer shaft with anchor or pitched-blade element through the central opening of the reactor cover before you place the cover onto the reactor.
- 2 Connect the stirrer shaft to the stirrer motor.
- 3 Fix the reactor holder (51162782) to one of the lab bars and place the reactor in the reactor holder.



- 4 Place the O-ring on the cover rim and place the cover on the reactor.
- 5 Place the clamp chain carefully around the cover and the reactor flanges.
- 6 Screw the hook in or out so that the buckle can be easily closed (with one finger).



- 7 Remove the assembled reactor from the reactor holder and insert it into the thermostat.
- 8 Attach the drain union (51162685) to the bottom drain valve and fasten it with the pinch clamp.



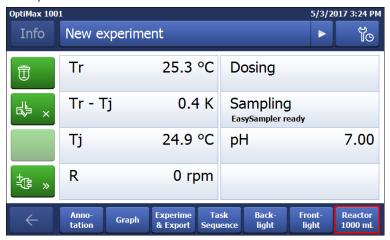
#### 4.12 Turn on Device

- Power is connected.
- Cooling is connected.
- Purging of instrument is connected.
- Touchscreen is connected
- Press the ON/OFF button on the front side of the instrument.
  - $\Rightarrow$  The touchscreen shows a splash screen during start up phase.
- $\Rightarrow$  You can use the device as soon as the reactor view appears on the screen.

### 5 Operation

#### 5.1 Select Reactor type

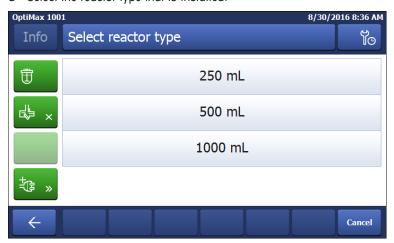
1 Tap the icon Reactor 1000 mL.



2 Tap the Reactor type field.



3 Select the reactor type that is installed.



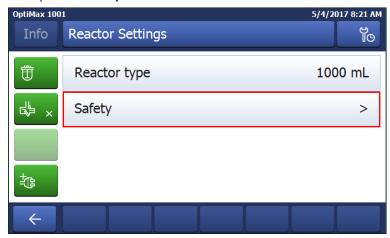
⇒ Make sure the safety settings for the reactor are still within the range.

#### **5.2 Change Safety Settings**

1 Tap the Reactor button.



2 Tap on the Safety field.



3 Change the necessary parameters according to your experiment and setup.

#### 5.2.1 Change Safety Temperature (T safe)

1 Tap on **T safe**.



2 Enter a value for **T safe** that is valid for your experiment.



3 Tap **OK**.

#### 5.2.2 Change Reaction Temperature limits (Tr)

1 Tap on **Tr max** or / and **Tr min**.



- 2 Enter a value for Tr max and Tr min that is valid for your experiment.
- 3 Tap **OK**.

#### 5.2.3 Change Range of Jacket Temperature (Tj)

1 Tap on **Tj min** or / and **Tj max**.



- 2 Enter a value for **Tj min** and **Tj max** that is valid for your experiment.
- 3 Tap **OK**.

#### 5.2.4 Change T diff max

1 Tap on **T diff max**.



2 Enter a value for **T diff max** that is valid for your experiment.



3 Tap **0K**.

#### 5.2.5 Change Rsafe

1 Tap on Rsafe.



- 2 Enter a value for **Rsafe** that is valid for your experiment.
- 3 Tap **0K**.

#### 5.2.6 Change Rmax

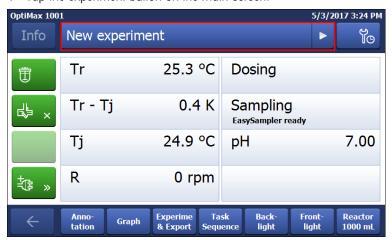
1 Tap on Rmax.



- 2 Enter a value for **Rmax** that is valid for your experiments.
- 3 Tap **0K**.

#### 5.3 Start an Experiment

1 Tap the experiment button on the main screen.

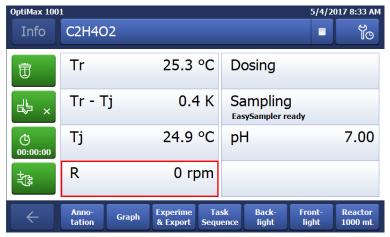


- 2 Enter an experiment name.
- 3 Tap **Start** to start the experiment.
- ⇒ All tasks that are executed will be saved under the experiment and available for export.

#### **5.4 Change Stirrer Speed**

Note The value cannot be higher than the safety limit value.

- A stirrer is connected.
- The touchscreen is connected.
- 1 Tap on the R field.

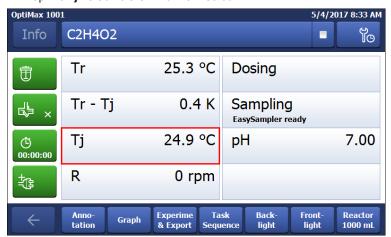


- 2 Enter the desired value.
- 3 Tap Start.
- ⇒ The stirrer will immediately start stirring.

#### 5.5 Change Tj

**Note** The value cannot be higher than the safety limit value.

1 Tap the Tj value field on the main screen.

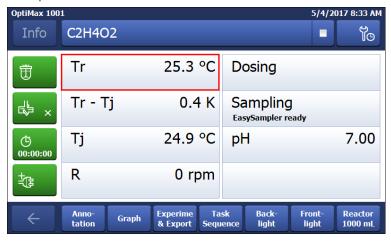


- 2 Enter the end temperature for Tj.
- 3 Tap Start to initiate the task.
- ⇒ The task will start immediately.

#### 5.6 Change Tr

Note The value cannot be higher than the safety limit value.

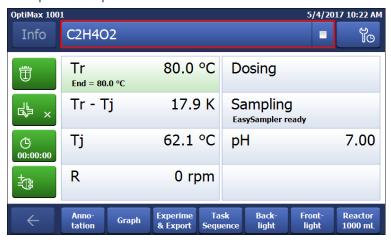
- A Tr sensor is connected to the thermostat.
- 1 Tap the **Tr** value field on the main screen.



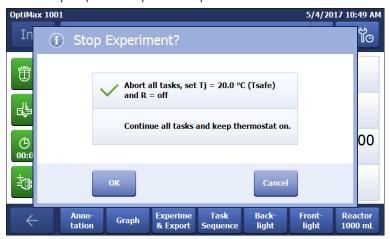
- 2 Enter the end temperature for Tr.
- 3 Tap Start to initiate the task.

#### 5.7 End an Experiment

1 Tap on the Stop button on the mainscreen.



2 Select your preferred option for experiment end conditions.



- 3 Tap **OK**.
- ⇒ Your experiment is stored on the device and can be exported.

#### 6 Maintenance

A troubleshooting chapter is available in the Operating Instructions.

Maintenance tasks have to be performed in accordance with the instructions given in this chapter. After performing any maintenance tasks it should be ensured that the device still fulfills all safety requirements.

#### 6.1 Update Firmware

The latest firmware versions and instructions for installation are available on the following website: https://community.autochem.mt.com/?q=software

#### **6.2** Checking the Reactor

To check the reactor vessel for possible damage (scratches and cracks), it must be empty, clean, dry and open. Small hairline cracks can be detected by refraction using an additional light source (focused, not dispersed light).

#### 6.3 Cleaning the Instrument



#### **CAUTION**

#### Hot instrument parts

Touching hot parts of the instrument can result in burnings.

- Do not clean the instrument before all parts have reached room temperature.



#### **NOTICE**

#### Damage to the device due to incompatible cleaning agents

Inappropriate cleaning agents could damage the housing of the device.

- 1 Use the described cleaning agent.
- 2 Should you use other cleaning agents, ensure that they are compatible with the housing material.

The housing of the instrument is not watertight (i.e. splash proof). We therefore recommend that you clean it with a damp cloth using ethanol.

If you have questions about the compatibility of cleaning agents, contact your authorized METTLER TOLEDO dealer or service representative.

#### 6.4 Disposal

In conformance with the European Directive 2012/19/EU on Waste Electrical and Electronic Equipment (WEEE) this device may not be disposed of in domestic waste. This also applies to countries outside the EU, per their specific requirements.



Please dispose of this product in accordance with local regulations at the collecting point specified for electrical and electronic equipment. If you have any questions, please contact the responsible authority or the distributor from which you purchased this device. Should this device be passed on to other parties, the content of this regulation must also be related.

### 7 Technical Data

Certifications regarding the product can be found under: https://www.mt.com/us/en/home/search/compliance.html/

The model number is identical to the product name of your device.

#### **Power supply**

AC power adapter rating	Line voltage	100240 VAC
	Input frequency	50/60 Hz
	Mains supply voltage fluctuations	Up to $\pm$ 10 % of the nominal voltage
Instrument rating	Power consumption	Max. 1290 W

#### **Ambient Conditions**

Humidity	Max. relative humidity 80 % for temperatures up to 31 °C decreasing linearly to 50 % relative humidity at 40 °C
Altitude	Up to 2000 m
Overvoltage category	II
Pollution degree	2
Ambient temperature	5 °C40 °C
Usage	For indoor use only

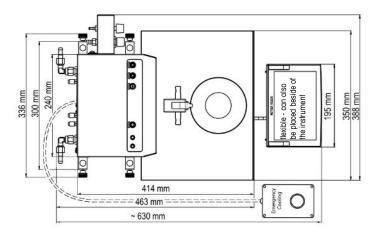
#### Materials

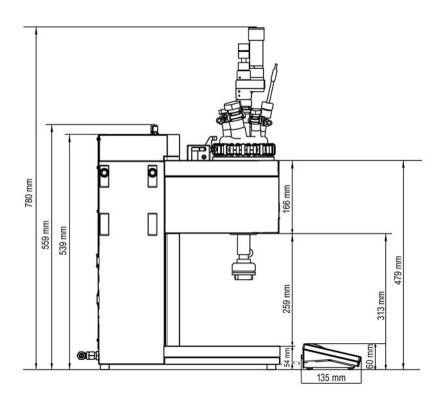
Cover plate	Stainless steel coated with PFA/FEP
Housing material	powder-coated stainless steel
Connectors for purge gas	stainless steel, nickel-plated brass
Purge gas lines	PVC, FEP, PP, PVDF, PTFE, aluminium, nickel-plated brass
Coolant tubing	PVC, PVDF, copper
Cooling connector	Nickel-plated brass
Flowmeters	Stainless steel, acrylic, HDPE
Holder for lab bars	Aluminium
LEMO connectors for Tr sensor and overhead stirrer	Chrome-plated brass with protection cap in POM
Reactor window	Borosilicate glass 3.3
Receptacles for reactors	Anodized aluminum
Fixing rings of thermostats	PTFE C25
Anti twist protection	PEEK HPV and aluminium
USB connector	Stainless steel with protection cap in POM
On/Off switch	Stainless steel
Stirrershaft, -blade	Borosilicate glass 3.3 or Hastelloy® C-22, PTFE
Overhead stirrer	PTFE, PEEK, aluminum, steel
Tr sensor	Borosilicate glass or Hastelloy® C-22
Glass reactors	Borosilicate glass 3.3
Touchscreen	PA 12, aluminum
Protective cover for Touchscreen	Barex®

#### **Device**

Walahtiaal tarrahaanaa	OF Ive	
Weight incl. touchscreen	35 kg	

#### **Dimensions**





#### 7.1 Thermostat

#### **Temperatures**

Range	Tj: -40 °C to 180 °C*
	Tr: -40 °C to 180 °C*
	Tc: -40 °C to 60 °C
	* The temperature range of Tr / Tj is depending on the temperature of the coolant and the cooling power of the used external cooling system.
Resolution	Tj: 0.1 K
	Tr: 0.1 K
Maximum permissible errors	1.0 °C for the whole range

Measured value acqui-	Every 2 seconds
sition	

### 7.2 Stirrer

Operating mode	Control to constant value or ramp		
Speed range	301200 rpm		
Torsional moment Max 153 mNm (for continuous operation)			
Lifespan	10003000 hours of continuous operation		

### 7.3 Purge gas

Purge gas housing (Purge	Max. inlet pressure	0-7 bar
Internal)	Min. gas flow	0-3 L/min
Inert gas reactor (Inert in)	Max. inlet pressure	0-7 bar
	Min. gas flow	as needed (controlled with the bubbler)
Stirrer (Purge In)		as inert

### 7.4 Reactors

	1000 mL reactor	500 mL reactor	250 mL reactor	
Pressure	0.05 bar to ambient pressure			
Nominal volume (2-piece reactors)	1310 mL	830 mL	370 mL	
Nominal volume (1-piece reactor	1150 mL	700 mL	400 mL	
Working volume (with Tr sensor)	150 - 1000 mL	80 - 500 mL	60 - 250 mL	

Min. working volumes for reactors equipped with standard Hastelloy temperature sensor and immersion depth of  $1.5\ cm$ :

Reactor type	Stirrer Blade	Min. working volume 1000 mL reactor	Min. working volume 500 mL reactor	Min. working volume 250 mL
Two piece	Pitched blade	150 mL	80 mL	60 mL
Two piece	Anchor	320 mL	140 mL	80 mL
One piece	Half-moon	320 mL	120 mL	80 mL

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Mettler-Toledo GmbH

Im Langacher 44 8606 Greifensee, Switzerland www.mt.com/contact

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