

SOFTWARE

CHROMATEC ANALYTIC

BUILD 4.0

USER MANUAL

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INSTRUMENT CONTROL,
ANALYSIS AUTOMATION

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1 INTRODUCTION


"Control Panel" software is used to control chromatographs and other analytical SDO "Chromatec" equipment.

"Control Panel" program functions:

- Instruments configuration.
- Setting the instrumen methods and methods of sample injection.
- Monitoring of the instrument status.
- Malfunction detection.
- Maintenance planning
- Maintenance planning
- Performing a sequence of analyses with flexible settings of the time and conditions for performing each analysis with automatic processing and output of results, both with and without the participation of the operator.

1.1 User Interface

The interface of the "Control Panel" changes dynamically depending on the devices included in it and their interconnections. For different models of chromatographs and other analytical equipment, the lists of internal and external devices included in the complex are different.

However, despite the differences in configuration, the basic elements of the user interface are the same for all devices.


Connection. On this page, connection with the chromatograph is configured, the project is selected (the folder for saving chromatograms), and the automation parameters are configured


Status. This page displays a variety of information about the current state of the chromatograph. Maintenance log sets up


Method. This page sets the mode of the chromatograph and mass spectrometric detector (if available) – instrument method.


Configuration. On this page, the parameters defining the individual characteristics of each chromatograph are adjusted.


Scheduler. On this page, the user can configure the sequence of analysis in automatic or semi-automatic mode.

1.2 Operation stages of chromatographs

Initialization. Comes immediately after turning on the power of the chromatograph. At this stage, testing of memory, chromatograph firmware and preparation for operation is performed. The stage is used only for chromatographs with a PM2 processor module.

Standby. The initial stage of work comes immediately after initialization. All devices are turned off. The instrument is ready to receive commands from the keyboard or computer.

Not ready. The stage at which the installation of the specified parameters of the chromatograph mode occurs.

If the **Preprun** mode is activated, the values of some parameters may not be equal to the specified ones (for example, the gas flow rate through the sample discharge channel in the mode without flow splitting).

Ignition. At this stage, the flame detectors are ignited.

Waiting. This stage comes after the "**Not ready**" stage, if any of the **Preprun** conditions are met. In addition, this stage occurs if a non-zero waiting time is set in the instrument method.

Ready. The stage at which all parameters of the chromatograph mode correspond to those specified for the Preprun state. Chromatograph is ready for analysis.

Analysis. The stage occurs when you start any of the channels of the chromatograph. At this stage, the chromatograph mode and its programs (programming of temperatures, gas flow rates, etc.) are processed in accordance with a given method.

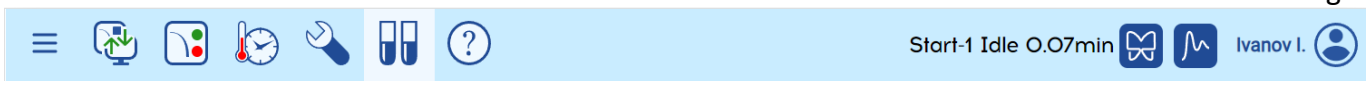
The analysis can be stopped forcibly (also using the START/STOP button).

Blowing. Programming the temperature of the oven after analysis.

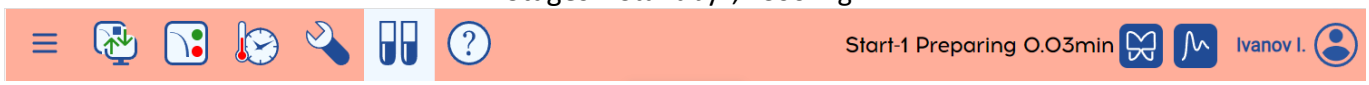
Cooling. Completion of work.

Sleep The instrument is switched to the low-power mode. It “awakens” at the time specified by the operator and starts with the mode set for autoloading.

The background color of the Control Panel dialog pages selector is used for the visual indication of the current stage:



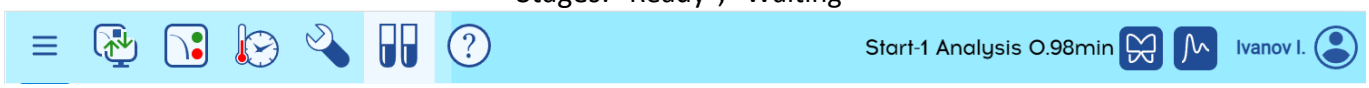
Stages: "Standby", "Cooling"



Stages: "Not ready", "Ignition", "Blowing"



Stages: "Ready", "Waiting"



Stage: "Analysis"

Preprun

Preprun is used when the value of the mode parameter (gas flow through the sample discharge channel) or the state of the internal instrument (tap-switch or valve) at the "Not ready" stage and immediately before the start of the analysis are different.

Preprun is performed when the chromatograph is at the "Waiting" stage.

- When using an automatic sampler, preprun performs Scheduler.
- With manual injection, to perform a preprun, you need to press the **START** button on the chromatograph at the "**Waiting**" stage, without **injection** a sample.

Preprun by gases

Preprun is used if more than one flow programming stage is set for discharge gas for inlets and valve-samples.

Preprun by valve (solenoid valve)

In the **Method** dialog, tick **Preprun** for the corresponding instrument.

When all parameters of the chromatograph are acceptable, it goes to the "Waiting" stage.

When a preprun is performed by the operator or an automatic dosing device, the device goes to the “Not ready” stage.

Further, as soon as all process stabilize, the instrument moves to the “Ready” stage.

Now you can inject the sample and perform "Analysis start".

Preprun by column thermostat

This type of Preprun is relevant only for chromatographs with a PM3 processor module and is used when working with **Lowox** columns.

In the Configuration dialog, tick Preprun for the corresponding instrument

When applying the mode to the chromatograph, it starts with the last stage of the temperature program.

Ignition of FID, NPD, FPD flame detectors

The transition from "Not ready" stage to "Ignition" stage occurs when the following conditions are met:

- At least one of the flame detectors (FID, NPD, FPD) is present in the channel.
- The background signal of at least one of the flame detectors is below the specified threshold for 10 seconds.
- The channel has NPD. The temperature of all the channel detectors has reached the level set in the instrument method.
- The channel has no NPD. The temperature of all channel detectors reached 150°C (incl.).
- At the moment of the method applying, the lowest detectors temperature of the channel was above 80°C (incl.).
- At the moment of the instrument method transfer, the lowest detectors temperature of the channel was below 80°C (incl.), but 10 minutes had passed since the lowest temperature reached 80°C (incl.).

Traditional FID and NPD methods of background measurement and flame detection are not applied due to the possible alternating dark background of the photomultiplier of FPD, which makes it difficult to determine the presence of a flame.

Flame firing algorithm for FID and NPD:

- Measure detector output.
- Form the configuration of air and hydrogen flow rate for each detector of the channel.
- Heat the ignition coils of the detectors of this channel for 8 seconds.
- Ignition coils are turns off.
- The presence of flame is monitored by an increased detector background.
- In case of success of ignition, the gas flow rates for the detectors set in the instrument method are formed.

The ignition is done if the increment of the output signal of the detector is greater than the increment of the threshold value set in the menu. If not, another attempt is made with the hydrogen consumption larger than hydrogen increment. Thus, the chromatograph makes seven ignition attempts, after that, in the absence of the flame, the "Standby" stage is set up and the message "Cannot ignite" is displayed.

The "Standby" stage is set for the PM2 processor module. The "Preparation" stage is set for the processor module PM3 and PM31.

Ignition algorithm for FPD:

In contrast to the ignition algorithm for FID and NPD, here the chromatograph does not constantly monitor the flame but performs a periodic check of its presence. The software believes that the flame is not ignited and the ignition must be performed in any case when moving from the stage "Standby" to the stage "Not ready". The background measurement at this moment is not performed.

- The air and hydrogen flows specified in the configuration are formed.
- The ignition coils of the detectors of this channel heats up for 8 seconds.
- Ignition coils are turns off.
- Gas flow rates for detectors are set
- Ten seconds after setting of air and hydrogen flow rates to the specified method, the detector output signal is measured.
- The air flow rate increases by 20 ml/min relative to the value set in the method (for example, at a given flow rate of 40 ml/min, the value will be set to 60 ml/min).
- The air flow rate increases by 20 ml/min relative to the value set in the mode (for example, at a given flow rate of 40 ml/min, the value will be set to 60 ml/min).
- If the signal exceeds the threshold set in the configuration, the flame is considered to be set. Gas flow rates are set according to the values specified in the method.
- Otherwise, the air flow is increased by the amount set in the configuration and the attempt to ignite is repeated.

Seven ignition attempts can be made, after that, in the absence of a flame, the "Standby" step is set up and the message "Cannot ignite" is displayed.



The chromatograph can be switched to the stage of ignition forcibly. To do this, click on the **Manual ignition** button.

2 CONNECTION

2.1 Installation of a local instrument server

Local instrument server - a program that provides direct control of the instruments. It is installed on a local computer (your workplace) outside the container, in which all other parts for the "Chromatec Analytic" work. This location allows the local server to survey the entire network and ensure the search for devices. In addition, the local server ensures the reliability of the recording of the tests, since it continues to work if for any reason the connection with the main server is lost.

The local instrument server is loaded from the main server. The Internet is not required, because the main server is usually located inside your enterprise (it can be located on the same computer).

The instrument device server is installed in cases:

- The "Chromatec Analytic" is installed on the current local (autonomous) computer with Linux OS.
- The "Chromatec Analytic" is installed on a separate server with Linux OS, and Linux was also installed on the current local computer.
- The "Chromatec Analytic" is installed on a separate server with Linux OS, and Windows is installed on the current local computer.

The local instrument server is not required if the "Chromatec Analytic" is installed on the current local (autonomous) computer with Windows OS.

To install a local server, you must download the necessary files specific for Windows and Linux from the main server, and perform actions shown in the video below:

Installation of a local device server on Linux

{video local_panel_linux local devices server, installation of a local server}

Installation of a local device server on Windows

{video local_panel_windows Local server on Windows}

2.2 Network configuration

To ensure communication with the chromatograph, the IP address of the chromatograph and the computer must be configured.

The procedures for configuring IP addresses in various operating systems are described in the corresponding manual.

2.3 Creating connection

A connection is a set of settings that tells the instrument server how it should communicate with a device or a set of devices.

On the Chromatec Navigator desktop, click on the "Setup Connection" button.

A new browser tab will open with the Control Panel application on the Connection settings page.

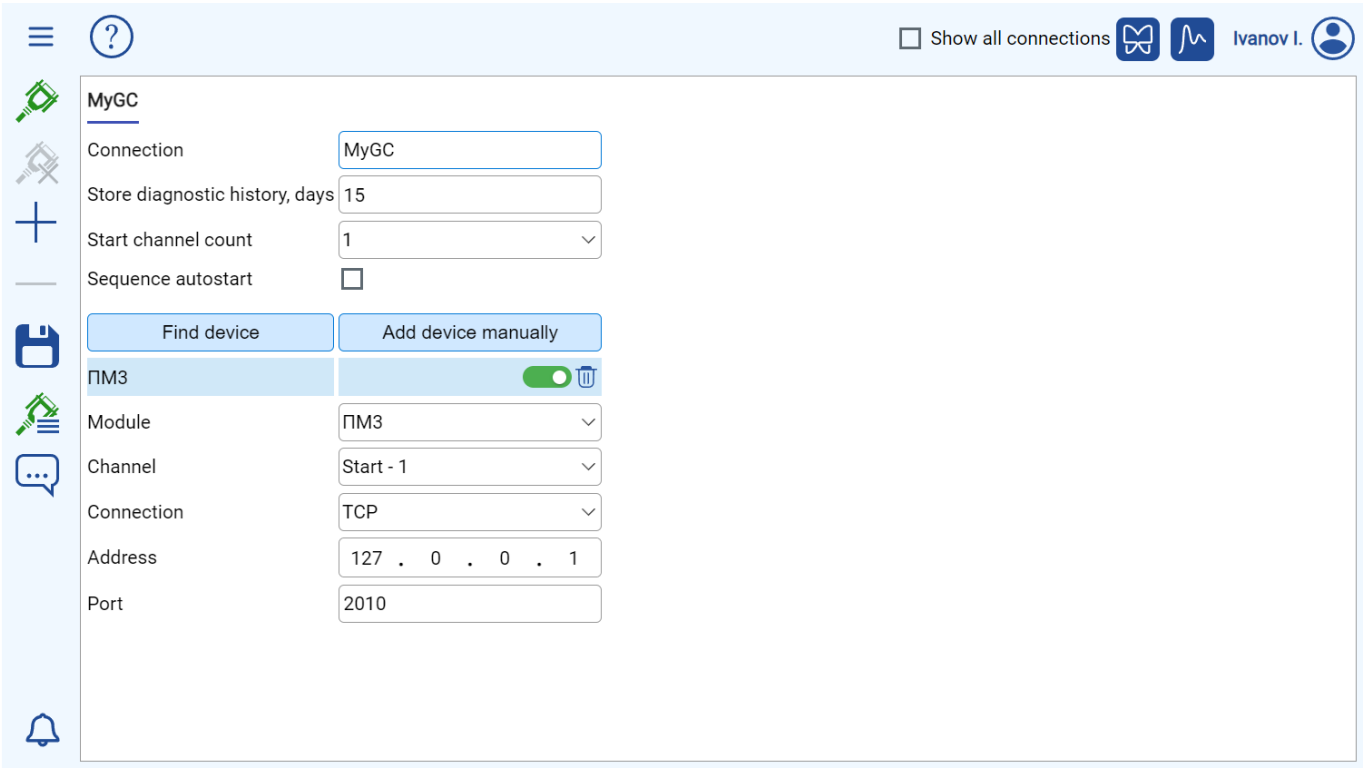


Fig 2.1 – Connection Settings

- Specify the name of the connection.
- Specify how many days to keep the diagnostic history. By default – 15.
- Specify the number of start channels.

Channel is a feature by which all chromatograph devices (inlets, columns, detectors, etc.) are grouped. Such grouping is necessary to ensure the possibility of simultaneous and independent analyses on one chromatograph. In fact, a chromatograph with two channels is two chromatographs in one.

The figure below shows an example of the organization of start channels. There are three detectors in the chromatograph. When performing Start-1, a chromatogram is recorded from one detector, and when performing Start-2, a chromatogram is recorded from two other detectors.

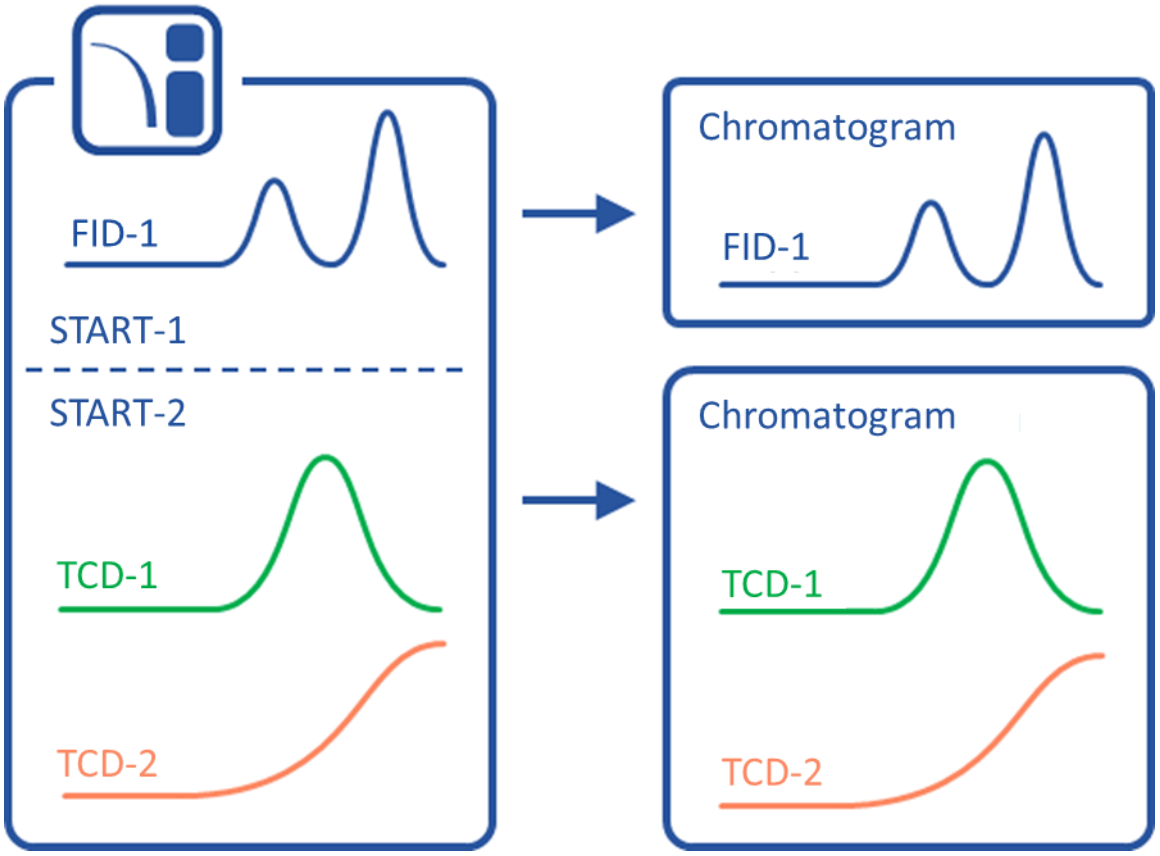


Fig 2.2 – Sessions

- You can enable the "Sequence Autostart" option. In this case, when you open the "Control Panel" tab, a pre-configured sequence of analyses will be automatically launched.

Next, connect the devices. You can add them using the “Find device” function or manually.

- Click the "Find Device" button.
- After updating the list of detected devices, select the necessary one, focusing on its type and serial number.

The connection can include several different devices. For example, a gas chromatograph, a mass spectrometric detector and an automatic thermal desorber can form one compound. At the same time, each of these devices has its own network settings – IP address and port.

If the device could not be detected, add it manually. You will need to choose:

- module (device type),
- connection type (TCP or COM),
- IP address and port (for TCP connection).

Save the connection settings.

{video panel_create_connection Connection, create connection}

2.4 Connection run

The created connections are displayed as widgets on the Chromatec Navigator desktop.

To start the connection, click on the widget. The first time you do this (on a given computer and browser), you will be prompted to configure the option to launch the Control Panel.

Connection widgets can be sorted using the mouse. The sorting is remembered for a given computer and browser.

{video navigator_connections Connections}

The widget menu displays information about which client and local server opened this connection:

- Local server IP.
- Client IP.
- Client version (build date).
- The port occupied by the connected client.

A user with administrative rights can forcefully close a connection opened by another user, as well as delete it.

3 CONFIGURATION

3.1 General information

The instrument configuration is set up at the factory and, as a rule, is not changed in the future.

Only experienced users, who are aware of what they are going to change and why, can edit configuration parameters.

Novice users can change the instrument configuration only under the guidance of SDO "Chromatec" specialist (for example, by telephone counseling), if necessary.

Expert configuration settings can be changed only by an SDO "Chromatec" employee or a certified service engineer.

 Click the Configuration button in the "Control Panel" to go to the corresponding page

Configuration parameters depend on the chromatograph model:

GC with PM3 processor module

GC with PM2 processor module

 After setting, save the configuration.

If the configuration of the chromatograph with the PM3 processor module is not saved, the most likely cause is damaged memory card.

3.2 GC Configuration (PM3)

3.2.1 Chromatograph Parameters

Expand the group of **Chromatograph** parameters.

IP-address. It can be changed in this dialog. After that, you will need to change the appropriate connection settings. Typically, the IP address is configured before connecting to the instrument..

Ambient pressure sensor reliable value. To confirm the data of the built-in atmospheric pressure sensor, enter the current data of the verified barometer in this field. The chromatograph will take into account this value and correct the reading of its sensor.

Ambient temperature sensor reliable value. To confirm the data of the built-in temperature sensor, enter the current data of the verified thermometer in this field. The chromatograph will take into account this value and correct the reading of its sensor. This parameter may be absent since the sensor is installed optionally.

Post initial. Blowing method. If you select a method that is previously stored in the chromatograph, it will be launched after switching on the instrument. The chromatograph will process it for a given analysis time.

Post initial. Default method. If a method set in the chromatograph previously is selected, then after switching on the instrument (or testing the purge method), this method will be launched.

These parameters allow you to automate the process of exit of the chromatograph at the "Ready" stage. They take into account the characteristics of the instrument, such as the need for pre-purge before performing a sequence of analyzes. They also provide an autonomous launch of the chromatograph instrument method after switching on without a personal computer or remote control panel.

Purging after switching on is not required for all chromatographs.

Sound key pressing. If this option is enabled, a beep sounds when the chromatograph key is pressed.

Sound when ready. If this option is enabled, a beep sounds when the chromatograph goes to the “Ready” stage.

Sound after initial. If this option is enabled, a beep sounds after turning on the chromatograph and loading its internal control program.

The above chromatograph parameters are always present. The list of other parameters is built dynamically, depending on the presence of a particular chromatograph node. Some parameters may be missing if their presence is not provided by the gas chromatograph scheme.

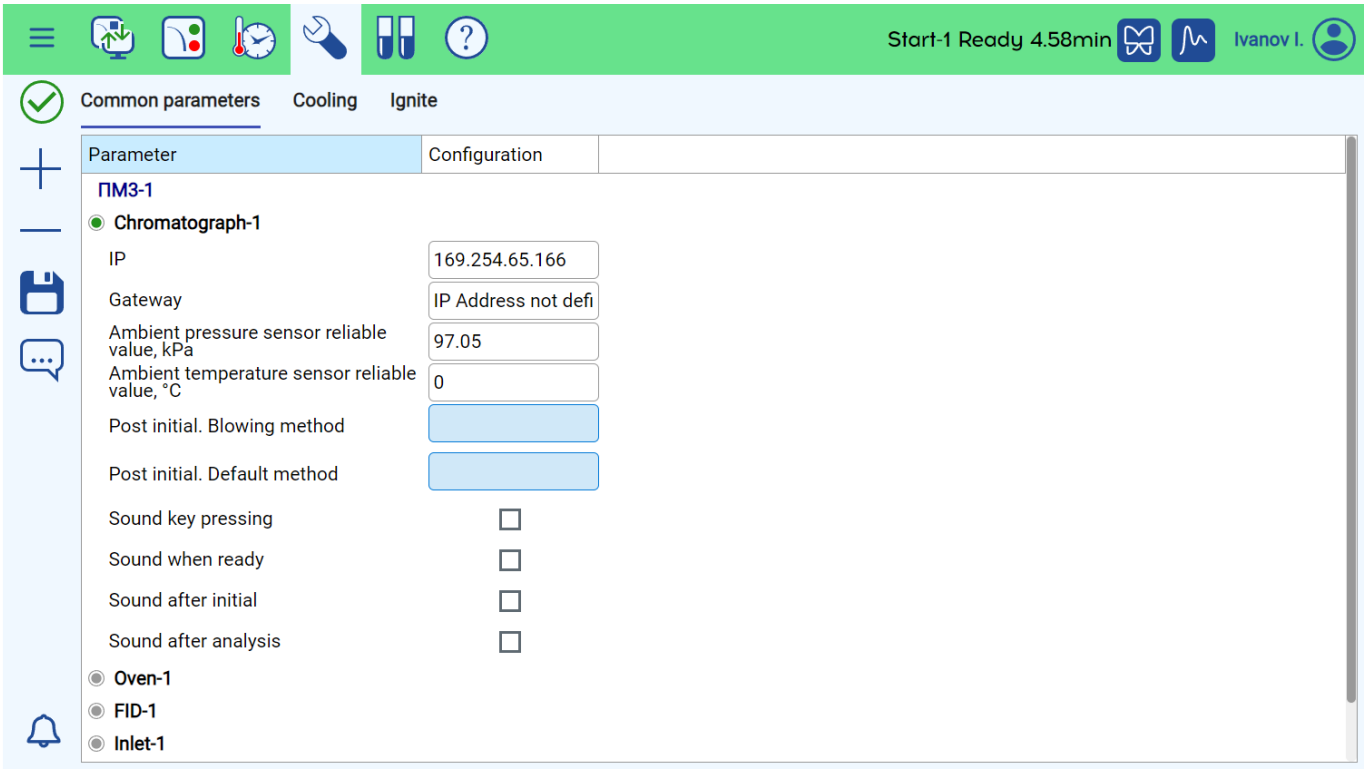


Fig 3.1 – Chromatograph parameters with PM3 Processor Module

3.2.2 Adding and Removing Devices

The following devices cannot be detected automatically by the controller; therefore, they must be added manually to configure the parameters:

- External device.
- Manual valve.
- DFC-indicator.
- DFPC.
- Column.

To add an instrument, click the corresponding button on the toolbar and select the type of instrument. A sequence number will be automatically assigned when adding a new instrument.

Removing instruments – click on the instrument header and click the appropriate button.

After removing the instrument, click the **Apply** button

"Column" and "Inlet" instruments are paired. When adding a column, the inlet is added automatically.

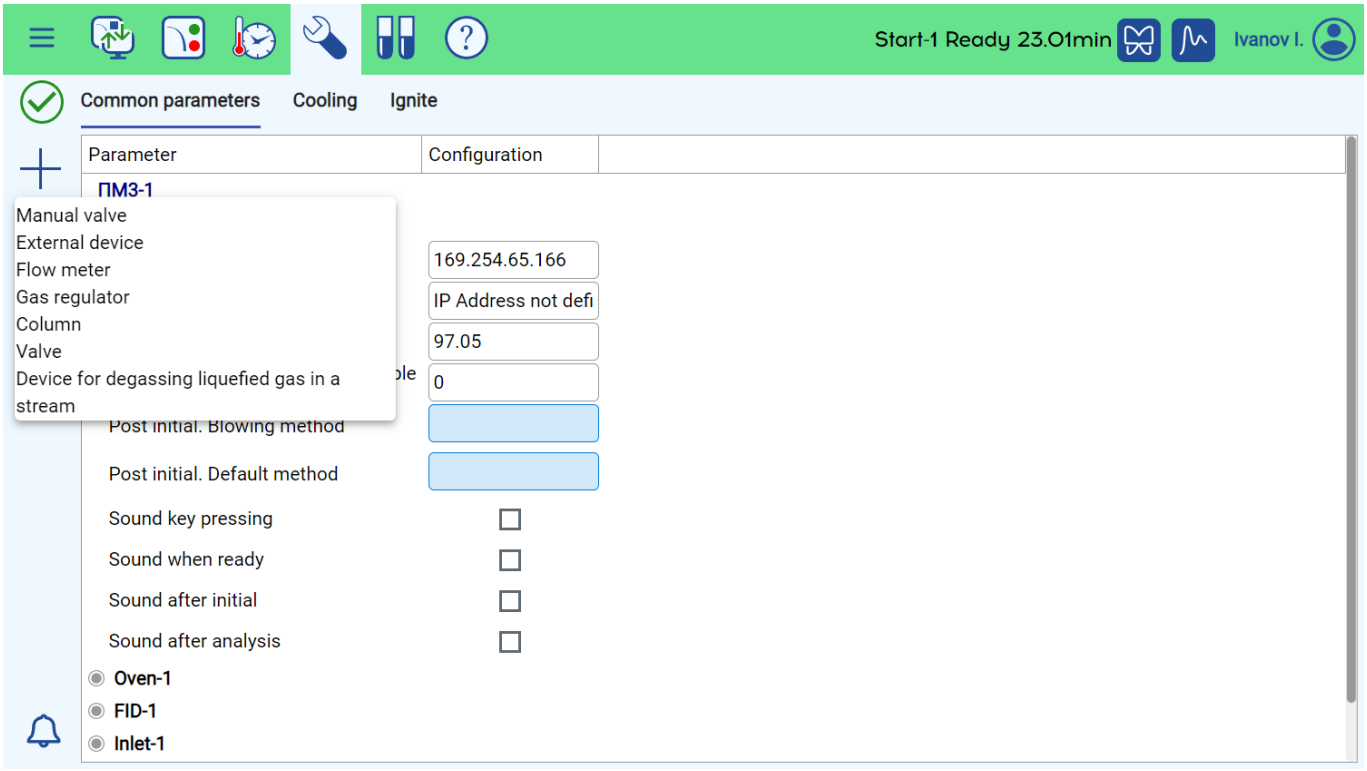


Fig 3.2 – Adding instruments

3.2.3 Start Channel

All internal devices of the chromatograph and all peripheral devices have one common configuration parameter – the channel.

Activity is a characteristic by which all chromatograph instruments are grouped (detectors, evaporators, etc.). Such a grouping is necessary to ensure the possibility of simultaneous and independent analyzes on a single chromatograph. In fact, a two-channel chromatograph is two chromatographs in one.

Often, the term "2-, 3-channel chromatograph" means that such a chromatograph has 2 or 3 detectors. In a chromatograph with a PM3 controller, this concept is broader. Here, a two-channel chromatograph can have, for example, 3-4 detectors, as well as a single-channel one.

Property "Activity" can have meanings:

Start-1, Start-2 means that this instrument will participate in the analysis when the corresponding start button is pressed.

None – this instrument does not belong to any channel, and the chromatograph will not monitor its condition and control its parameters.

The column oven is almost always only one, common to all channels, so the start channel is not specified for it.

There are few chromatographs configured for dual-channel operation. Thus, most instruments have only one channel. The number of channels is set in the expert settings of the chromatograph.

Besides, you will need to create two sessions of recording chromatograms to work with two independent channels.

3.2.4 Valves

Max. temperature. It is recommended to set max. temperature to 400°C. If the temperature exceeds this value (due to an incorrect setting or some kind of accident), the chromatograph starts emergency cooling.

Initial position. Determines the initial position of the valve according to the gas chromatograph scheme. Hand valves do not have this parameter.

Thermostat. Indicates which heater is installed on the valve. Several valves can be located in one thermostat. If the valve is not heated, the parameter is set to "No".

Heater control off. If this option is enabled, the chromatograph program does not control the heating of the valves and does not control the temperature.

Valco valve multiposition must be added to the configuration when chromatograph is shipped with an **automatic gas flow switch**. This instrument is added in the expert settings of the chromatograph. After adding, the **Valco valve multiposition** instrument appears on the **Common** tab:

Initial position is the position of the Valco valve multiposition, installed when the chromatograph is switched on. In total, this valve has eight positions and any of them can be set as the initial one.

The gas chromatograph scheme determines the specific position.

3.2.5 Inlets

The "Inlet" instrument appears when adding a column.

Inlet type. Column injection can be connected to one of the following devices:

- Packed inlet.
- Split-splitless inlet 7.2.
- PTV 8.1.
- Vaporized inlet.
- Piston injector.

"Vaporized inlet" is selected if the sample is injected into the column by a sample valve.

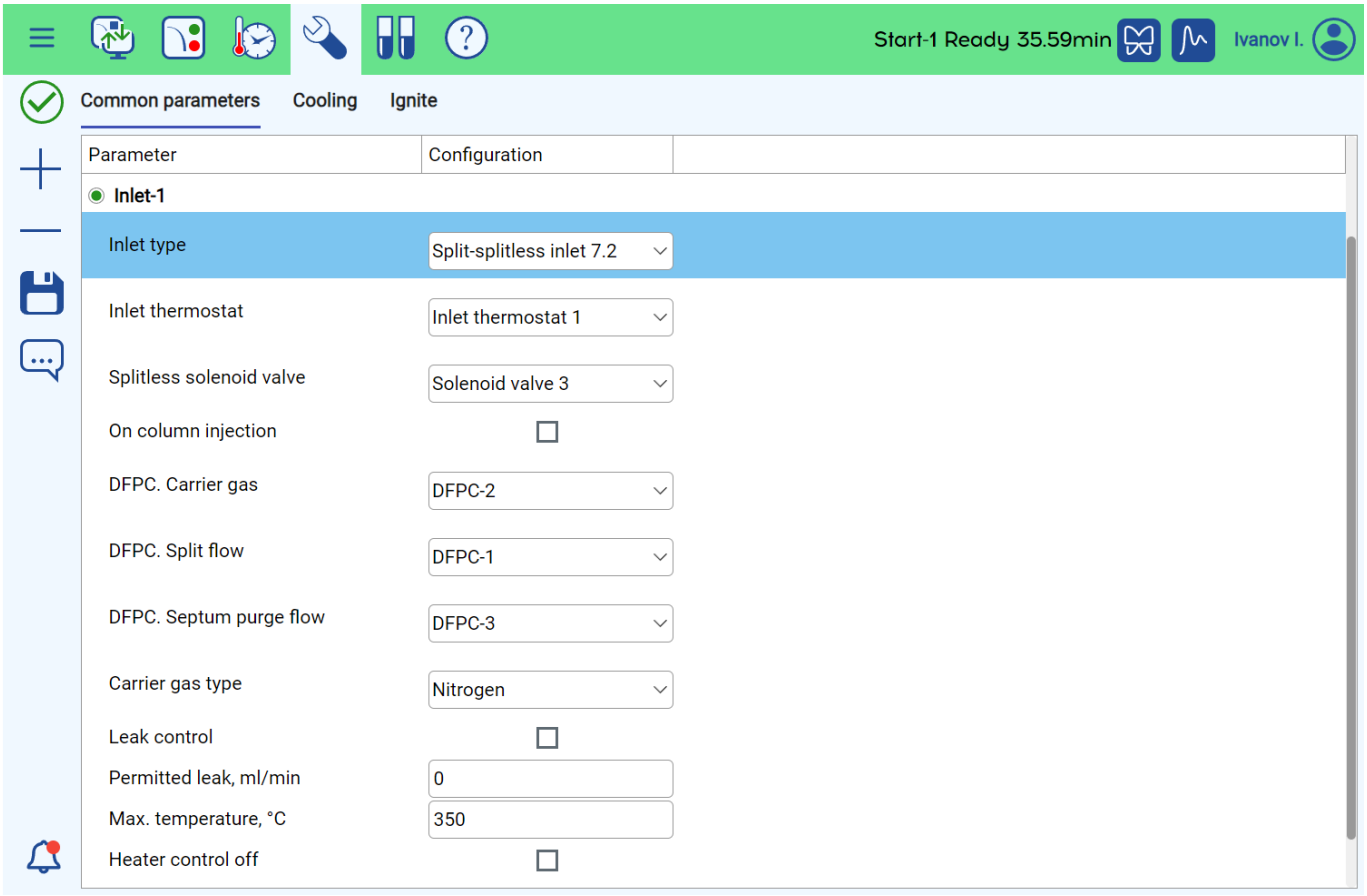


Fig 3.3 –Inlet settings

Inlet designation. Here you can specify an additional designation of the inlet. For example, if the inlet type is " Vaporized inlet ", it is convenient to designate it in accordance with the gas scheme by specifying the number of the corresponding dose (metering loop of the crane) – "Ds–1", "Ds-2", etc.

Inlet thermostat. Here you should indicate a heater on which the evaporator is installed. The nearest to the operator inlet has number 1, and the next one has number 2, etc. For the " Vaporized inlet t" port this parameter is not configured.

Heater control off. If this option is enabled, the chromatograph program does not control the heating of the inlet and does not control its temperature.

Splitless valve. When working with a capillary column in the mode without flow splitting, specify the number of the valve that performs additional locking of the vent channel (ventilation).

On column injection. If this option is enabled, then the evaporator temperature will be synchronized with the temperature of the oven.

Large volume injection. The option is available for PTV 8.1 inlet. If this option is enabled, the button for calling the solvent's blowout calculator appears in the instrument method settings.

Use universal DFPC. The option should be enabled if single-channel DFPCs are connected to the inlet and disabled when using functional (multi-channel) DFPCs.

DFPC multichannel. If functional (multi-channel) DFPC is connected to the inlet, here it is necessary to indicate its number according to the gas scheme.

DFPC. Carrier gas. If single-channel DFPCs are connected to the inlet, here you should indicate the regulator number from which carrier gas is fed to the column.

DFPC. Split flow. If single-channel DFPCs are connected to the inlet, the number of the regulator controlling the sample discharge (flow splitting) should be indicated here.

DFPC. Septum purge flow. If single-channel DFPCs are connected to the inlet, here you should indicate the number of the regulator that controls the flow through the membrane blowing channel.

Electronic DFPC "Split flow" and "Septum purge" may be absent in the gas scheme or may be replaced by mechanical ones. In this case, "None" meaning remains in these areas.

Max. temperature. It is recommended to set max. temperature to 350-450°C. If the temperature exceeds this value (due to an incorrect setting or some kind of accident), the chromatograph starts emergency cooling.

Carrier gas type. Here you should select the type of carrier-gas fed to the column.

Leak control. If this option is enabled, the chromatograph software monitors the specified acceptable leakage at the inlet.

If hydrogen is used as carrier gas, permeability control SHOULD BE TURNED ON. When leakage is detected (if the capillary column breaks near the inlet), not only a message appears, but also explosion protection is activated: the column thermostat valve opens, and the heating of all thermostats is turned off.

On the **Ignition** and **Cooling** tabs, set the inlet parameters that the chromatograph will apply at the appropriate stages of operation.

3.2.6 Columns

The chromatograph cannot detect the columns by itself so operator should add them manually. Related devices, for example, sample inlet, are added at the same time.

Two columns can be connected to one sample inlet if such a configuration is incorporated in the gas chromatograph scheme.

Some column parameters do not appear in this dialog immediately, but after other parameters (on which column parameters depend) are set.

Inlet is selected automatically. Usually, there is no need to change the value of this parameter.

Column type. Specify the type, packed or capillary, according to the gas scheme. When you select the type of column, the type of sample inlet is set automatically.

Column name. In this field, you can enter the designation of the column. Optional parameter.

Length. Specify the length of the column in meters. The parameter is available only for capillary columns.

Diameter. Specify the column diameter in millimeters. The parameter is available only for capillary columns.

Outlet pressure. Possible values:

- From ambient pressure sensor.
- Vacuum. Selected when working with a mass spectrometry detector.
- User-defined. Operator can set the outlet pressure himself. When calculating the flow through the column, the value of atmospheric pressure is not taken into account.
- User-defined + ambient. The operator can set the outlet pressure himself. When calculating the flow through the column, the value of atmospheric pressure is taken into account (from the sensor).

On the Ignition and Cooling tabs, set the column parameters that the chromatograph will apply at the appropriate stages of operation.

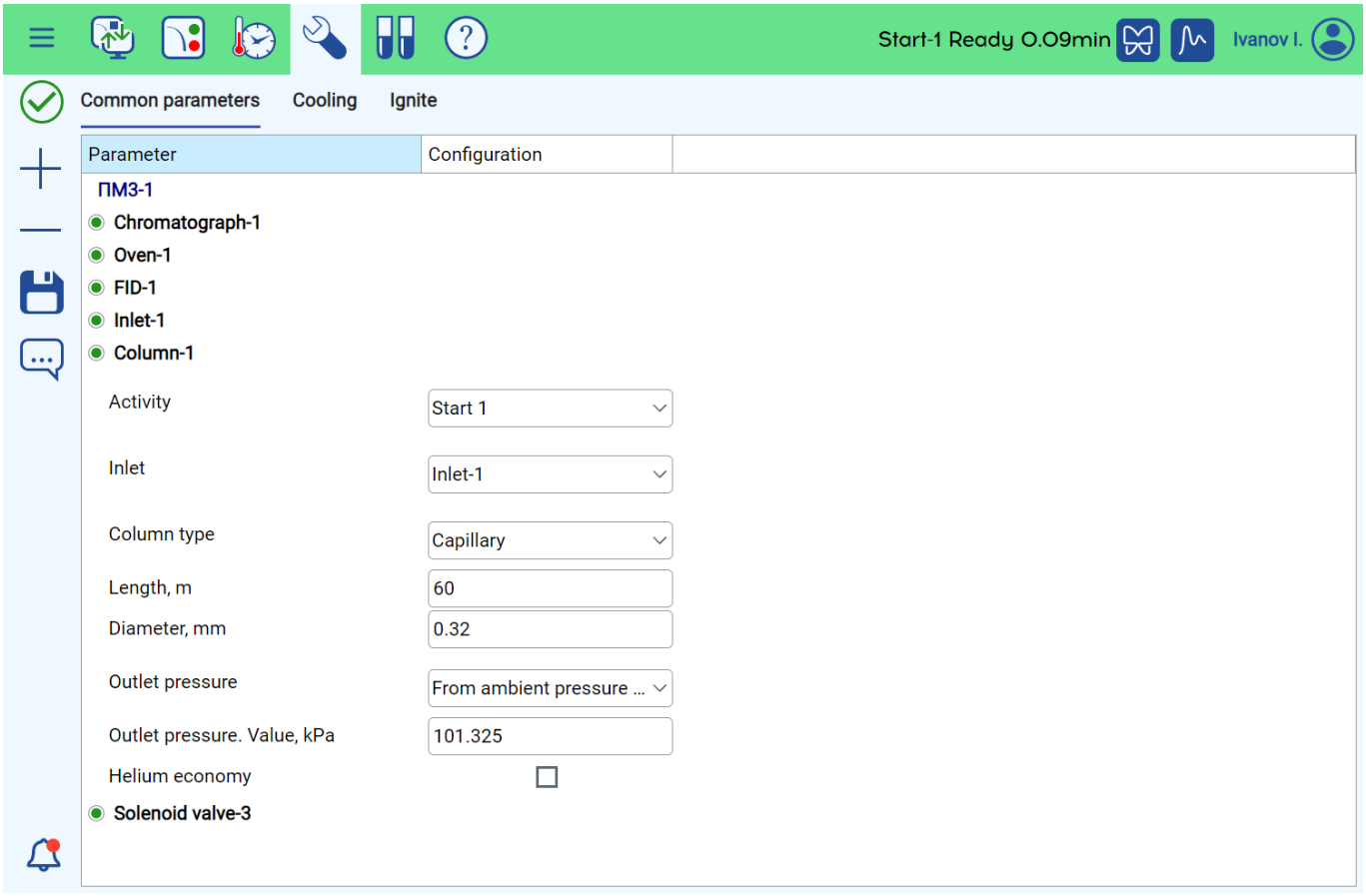


Fig 3.4 – Column parameters

3.2.7 Solenoid valves

Initial position. Determines the initial position of the valve according to the gas chromatograph scheme.

DFPC. If an additional DFPC (pressure regulator) is involved in the gas flow switching scheme, you should indicate its number here. Also indicate the type of gas.

3.2.8 Column Oven

Preprun. The option should be enabled if the recommended working temperature of the column exceeds the temperature of the first isotherm during the analysis. This parameter is used when working with Lowox columns.

When applying this mode, the chromatograph processes the last stage of oven temperature programming. When all parameters of the chromatograph are within the acceptable range, the chromatograph will proceed to the "Waiting" stage. At this stage, the operator must perform Preprun — press the START button without sample injection (when working with the autosampler, “Scheduler” will perform the Preprun).

When Preprun is executed, the chromatograph processes the first step of a predetermined temperature program and proceeds to the “Ready” stage.

Max. temperature. It is necessary to set the temperature of the column according to sample info (it is recommended to set the temperature 10-20°C below the temperature described in the sample info). If the temperature exceeds this value (due to an incorrect setting or some kind of accident), the chromatograph starts emergency cooling.

If several columns are installed in the oven, then minimal temperatures described in the sample info is set.

T column <T detector. If this option is enabled, the program does not allow the column temperature to exceed the temperature of the detectors. This is done in order to avoid moving the sample from a hot area to a colder one.

T column <T inlet. If this option is enabled, the program does not allow the column temperature to exceed the temperature of the inlets.

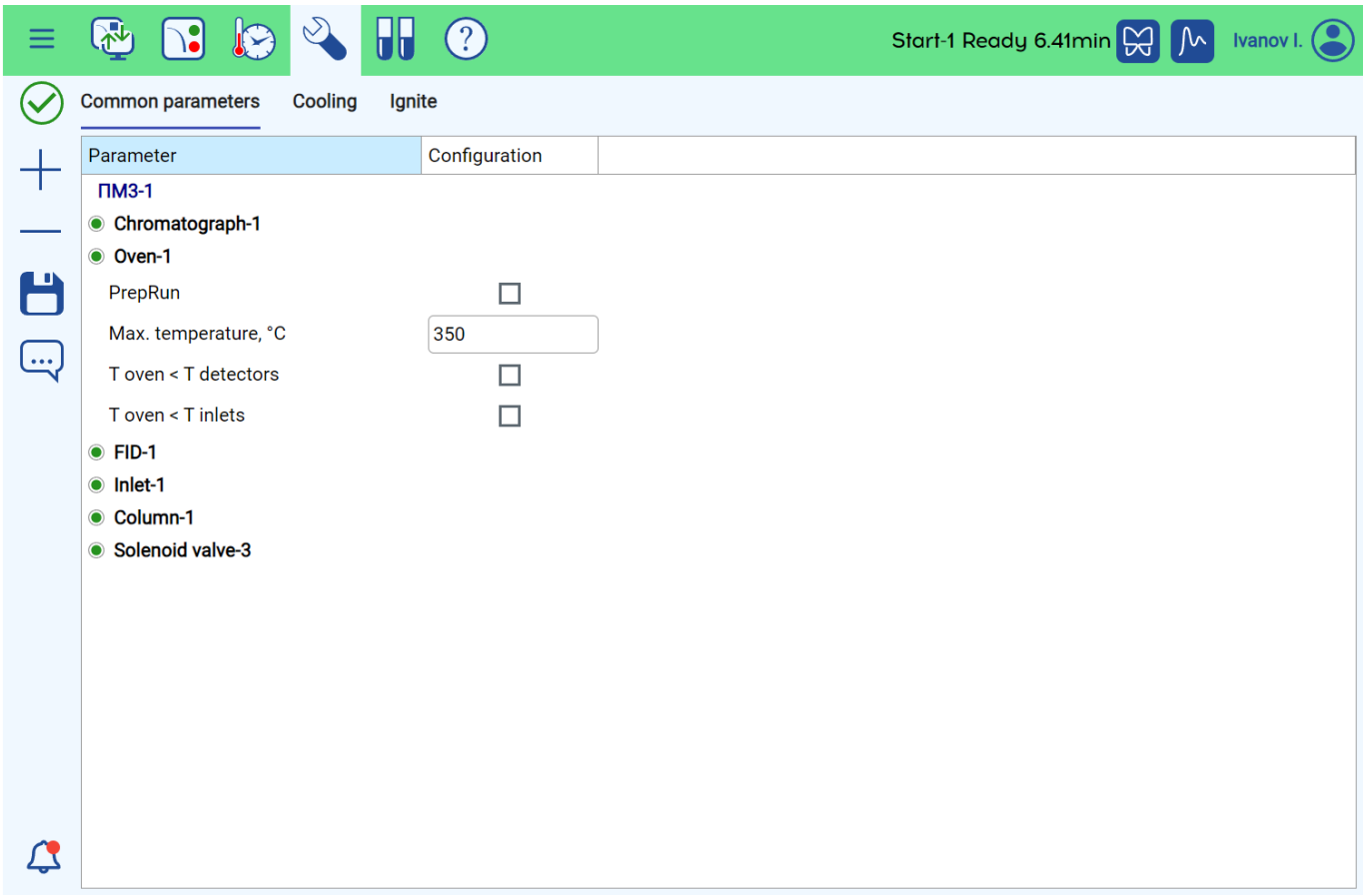


Fig 3.5 – Oven Parameters

3.2.9 Methanizer

Max. temperature should be set to 450°C.

DFPC. Hydrogen. Select a gas flow regulator that controls the flow of hydrogen to the methanizer.

In the presence of the methanizer, hydrogen enters the FID through the pipeline but not through the corresponding detector channel. In this case, hydrogen can be specified either at the detector or at the methanizer (but not simultaneously in both devices) in the DFPC configuration.

3.2.10 Detectors

Acquisition rate, Hz. The frequency of data acquisition has an impact on the information content of the chromatogram. The higher is the frequency, the narrower is the peaks that can be detected, and the higher is the noise level. The default value of 25 Hz is optimal.

Thermostat. The detector thermostat is selected. Here, the detectors thermostat 1 means that the detector is installed on the near heating platform, and the detectors thermostat 2 means that the detector is installed on the far heating platform. Several detectors can be located in the same thermostat, for example, three TCD detectors.

Max. temperature. When the maximum temperature is exceeded (due to an incorrect setting or some kind of accident), the chromatograph starts emergency cooling. Recommended values:

- FID, NPD, ECD – 450°C;
- FPD, PID – 250°C;
- TCD, CCD – 300°C.

Use universal DFPC. The option should be enabled if single-channel DFPCs are connected to the detector. The option should be turned off when functional (multi-channel) DFPCs are used.

DFPC multichannel. If a functional (multi-channel) DFPC is connected to the detector, here it is necessary to indicate its number according to the gas scheme.

DFPC. Hydrogen. For FID, NPD, FPD detectors. If single-channel DFPCs are connected to the detector, here you should indicate the number of the regulator from which hydrogen is fed to the detector.

DFPC. Air. For FID, NPD, FPD detectors. If single-channel DFPCs are connected to the detector, here you should indicate the number of the regulator from which air is fed to the detector.

DFPC. Makeup. For FID, NPD, ECD, PID, TCD, CCD detectors. If single-channel DFPCs are connected to the detector, here you should indicate the regulator number from which makeup gas is fed to the detector.

Makeup gas type. Here you should choose the type of makeup gas.

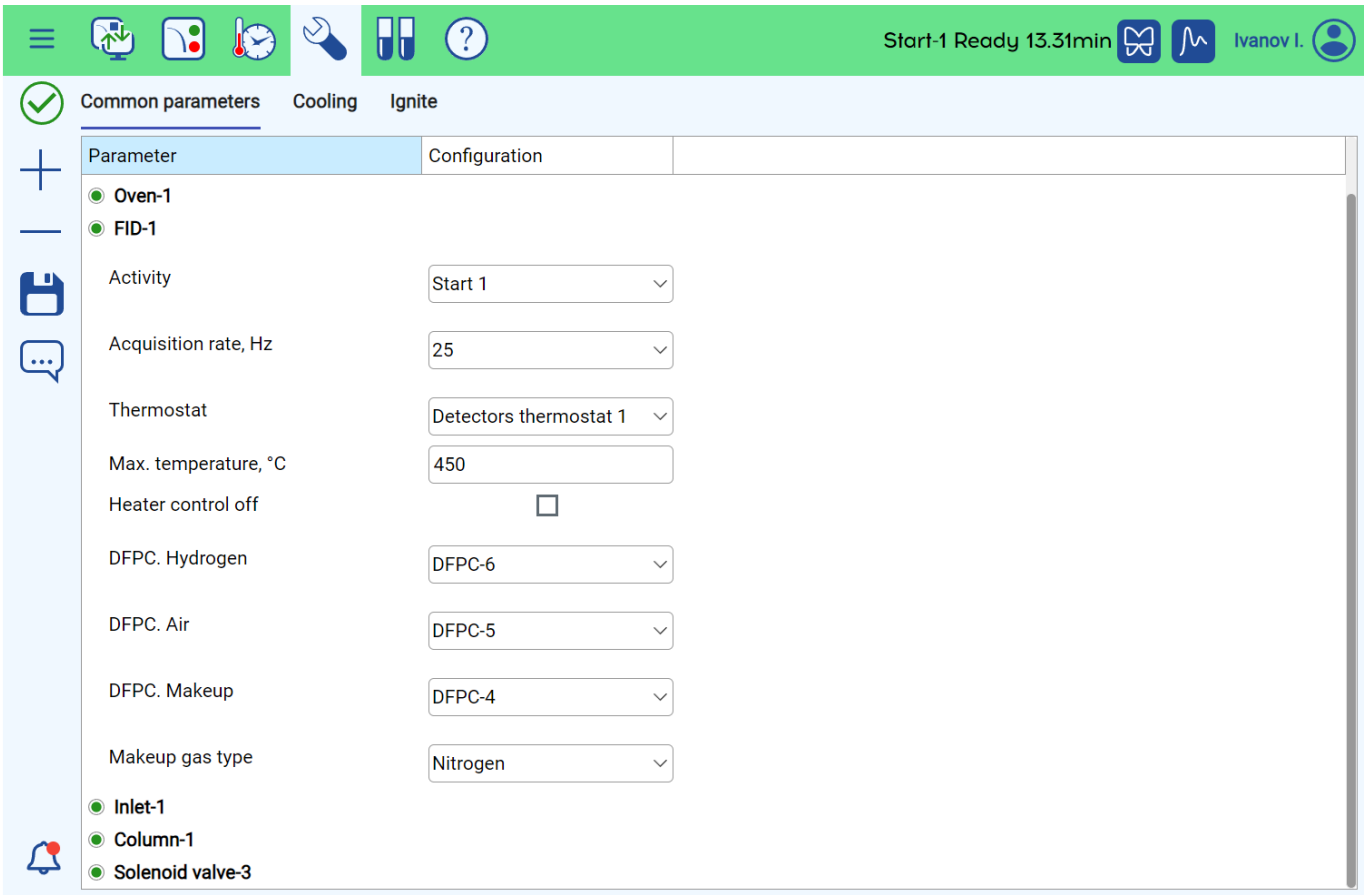


Fig 3.6 – Detector Parameters. FID Example

Additional FPD Detector Parameters

PMT. Voltage. FPD detector photomultiplier power supply on/off.

PMT. Signal in the absence of flame. Due to technological variations in the PMT parameters, some FPDs have a non-zero background signal before the flame is ignited. In this case, the chromatograph can register the presence of flame in its absence. To avoid this, set the of this parameter to the value, measured at the moment of reaching the specified temperature of the detector.

Additional ECD Detector Parameter

ECD current. The value of the reference current corresponding to the magnitude of the ionization current flowing through the detector. The current ECD is set in relative units from 0 (0 nA) to 350 (4.1 nA), the default value is 100 (corresponds approximately to 1.17 nA). The specified value depends on the activity of the radioactive source located in the detector.

Additional PID Detector Parameter

Lamp initial status. Specify the state of the lamp at the start of the analysis.

The longer the lamp is in the on state, the shorter is its service life. To increase the life of the lamp, you can use its programming – turn on the lamp shortly before the peak of interest, and turn off after its ending. In this case, the initial state of the lamp is off state.

The time of the lamp switching on and off is selected experimentally when creating the method during the analysis.

Prohibit work with lamp off. If this option is enabled, the chromatograph cannot reach the “Ready” stage with the lamp turned off. If you are not currently using a PID, you can turn off this option.

Lamp on. Turn the PID lamp on and off. You can quickly turn off the lamp to remove and clean it without cooling or turning off the chromatograph.

Additional TCD Detector Parameter

Power. The parameter defines the heating power of the sensors (spirals) depending on the type of carrier gas flowing through the detector.

If the power is set to 100% (for helium or hydrogen), but nitrogen or argon flows through the detector, in reality, the sensor can be broken.

Offset. Set the offset value of the signal zero line. The amplifier is automatically balanced in such a way that the background of the detector corresponds to the specified offset. The recommended value is 1000 mV.

Filament on. When this option is enabled, the TCD switches to the automatic mode of spirals protection from overheating. During operation, the TCD spiral must be in automatic mode. When the option is turned off, the TCD spiral heating will be disabled.

Signal inversion. Set this option if all peaks on the chromatogram are negative (inverse).

Additional CCD Detector Parameter

Power. The parameter defines the heating power of the sensors depending on the type of carrier gas flowing through the detector..

If the power is set to 100% (for helium or hydrogen), but nitrogen or argon flows through the detector, in reality, the sensor can be broken.

Offset. Set the offset value of the signal zero line. The amplifier is automatically balanced in such a way that the background of the detector corresponds to the specified offset. The recommended value is 1000 mV.

Sensor on. When this option is enabled, the CCD switches to the automatic mode of spirals protection from overheating. During operation, the TCD spiral must be in automatic mode. When the option is turned off, the detectors heating will be disabled.

Signal inversion. Set this option if all peaks on the chromatogram are negative (inverse).

3.2.11 Ignition parameters for FID, NPD, FPD flame detectors

These parameters are located on the **Ignition** tab:

Flame control. If you are not currently using this detector, turn off this option so that the chromatograph program does not attempt to ignite the detector flame.

Igniter. Indicate which igniter is connected to this detector (the igniter number is written on the cable tag).

Hydrogen flow. Set the amount of hydrogen consumption in the "Ignition" stage. Recommended values:

- FID – 40 ml/min;
- NPD – 30 ml/min;
- FPD – 80 ml/min.

Air flow. Set the amount of air flow in the "Ignition" stage. Recommended values:

- FID – 250 ml/min;
- NPD – 250 ml/min;
- FPD – 180 ml/min.

Makeup flow (pressure). Set the amount of makeup gas flow in the "Ignition" phase. The recommended values for FID and NPD are 10 ml/min.

Hydrogen increment. The amount by which hydrogen consumption increases with each subsequent attempt of ignition (if the previous one was unsuccessful). The recommended value is 5-10 ml/min.

Flame threshold. When the flame is ignited, the measured background of the flame detectors increases. In order for the chromatograph to detect the presence of the flame, the background must exceed a predetermined threshold value. Recommended values:

- FID – 2 mV;
- NPD – 4 mV;
- FPD – 0.5 mV.

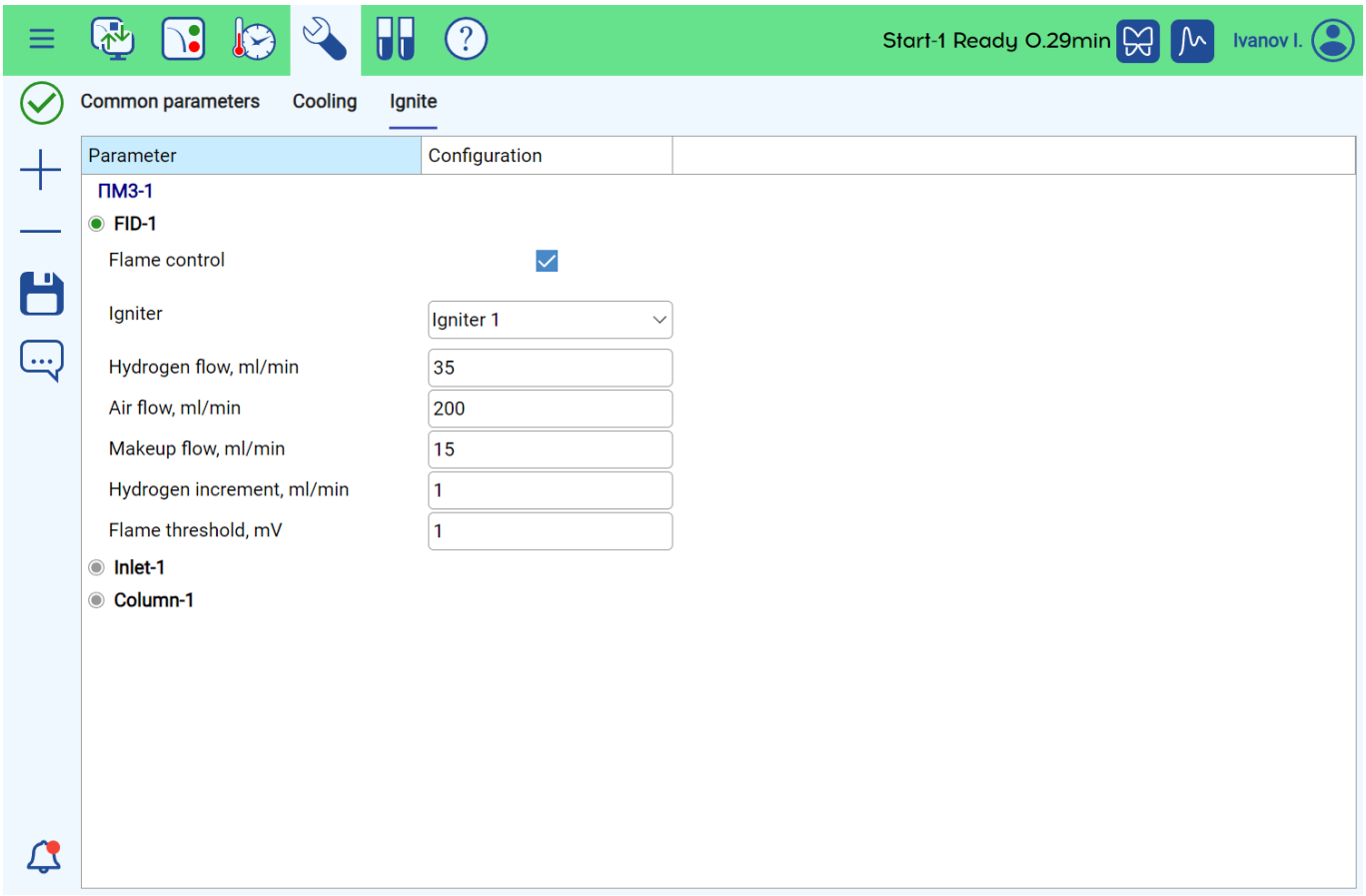


Fig 3.7 – Ignition parameters for flame detectors

3.2.12 Cooling parameters

On the **Cooling** tab, set the parameters that the chromatograph will process at the appropriate stage of operation.

At the "Cooling" stage, it is recommended to set the values of air and hydrogen flow to 15 ml/min for FPD detector, so that the condensate is removed from the detector lid when cooling by the flow of these gases occurs (the detector flame will be pre-extinguished).

For the FID and NPD detectors, there is no need to specify the flow rates of gases during the "Cooling" phase.

3.3 GC Configuration (PM2)

3.3.1 Chromatograph parameters

Expand the **Chromatograph** group of parameters.

Service mode (ignoring out of range). If this option is enabled, the chromatograph program ignores all parameters outside the acceptable range and immediately sets the "Ready" stage.

The test mode can only be used by service personnel at the stages of equipment setup and maintenance. Under normal operating conditions, this feature should always be turned off.

Reserve memory. This option should be enabled if there is a backup memory in the device.

MSD activity. The option should be enabled when operating the chromatograph with a DSQ II or ISQ mass spectrometry detector.

Sound key pressing. If this option is enabled, a beep sounds when the chromatograph key is pressed.

Sound when ready. If this option is enabled, a beep sounds when the chromatograph goes to the “Ready” stage.

Ambient pressure sensor reliable value. To confirm the data of the built-in atmospheric pressure sensor, enter in this field the current data of the verified barometer. The chromatograph will correct the reading of its sensor taking into account this value.

Detector 2 thermostate. This option should be enabled if there is the second detectors thermostat in the chromatograph (a distant heating platform).

Inlet 2 thermostate. This option should be enabled if there is the second evaporator thermostat in the chromatograph of (a distant heating platform).

T column <T detector. If this option is enabled, the program does not allow the column temperature to exceed the temperature of the detectors. This is done in order to avoid moving the sample from a hot area to a colder one.

Solenoid valve initial position:

- Opened – when the chromatograph is turned on, the valve is powered, and it opens.
- Closed – when the chromatograph is turned on, the valve is not powered, and it remains closed.
- Off – valve is not used (absent).

3.3.2 Thermostats

For devices: column oven, inlet thermostat and detector thermostat – the **Maximum temperature** parameter is set.

It is necessary to set the temperature of the column according to sample info (it is recommended to set the temperature 10-20°C below the temperature described in the sample info). When it is exceeded (due to an incorrect setting or some kind of accident) the chromatograph starts emergency cooling.

The maximum temperature of the detectors and evaporators is set in accordance with the operating manual of the chromatograph.

3.3.3 Gases

DFPC type is selected according to the gas scheme of the instrument.

Control mode:

- "Constant pressure" is used to maintain a predetermined value of the constant pressure regulator at the outlet.
- "Constant velocity" and "Constant capillary flow" (set only for the Gas 1, Gas 3 channels) can be used when working with capillary columns to maintain a given constant speed or flow through the capillary column.
- "Constant flow" is used to maintain a predetermined constant of carrier gas flow through the regulator.

Gas type. Here you should choose the type of carrier gas connected to the regulator input.

Use gas save. If this option is enabled, a reduced gas flow is set for a specified time when the "Ready" stage lasts too long.

Gas save runtime, min. Sets the idle time for the "Ready" stage. Upon expiration, gas saving is activated.

Leak control. If this option is enabled, the chromatograph software monitors the specified acceptable leakage in the inlet.

Initial blowing. Flow, ml/min. Here you set the gas flow for the "Purge before analysis" stage.

Ignore errors. Enable the option if it is not unnecessary for the chromatograph to monitor the status of the regulator (the parameter is used when operating the DFPC-11B).

3.3.4 Columns

Name. In this field, you can enter the designation of the column. Optional parameter.

Length. Specify the length of the column in meters. The parameter is available only for capillary columns.

Diameter. Specify the column diameter in millimeters. The parameter is available only for capillary columns.

3.3.5 Detectors

Start. This parameter sets the connection of the detector to one of the two channels to start the analysis. It can take the values Start 1 and Start 2

Acquisition rate, Hz. The frequency of data acquisition has an impact on the information content of the chromatogram. The higher is the frequency, the narrower is the peaks that can be detected, and the higher is the noise level. The default value of 25 Hz is optimal.

Thermostat. The detector thermostat is selected. Here, the detectors thermostat 1 means that the detector is installed on the near heating platform, and the detectors thermostat 2 means that the detector

is installed on the far heating platform. Several detectors can be located in the same thermostat, for example, three TCD detectors.

FPD Detector

PMT. Voltage. The power of the FPD detector photomultiplier is turned on and off.

PMT. Signal without flame. Due to technological variations in the PMT parameters, some FPD samples have a non-zero background signal before the flame is ignited. In this case, the chromatograph can register a flame in its absence. To avoid this, set this parameter as a value measured at the moment of reaching the specified temperature of the detector.

ECD Detector

Current. The value of the reference current corresponds to the magnitude of the ionization current flowing through the detector. The ECD current is set in relative units from 0 (0 nA) to 350 (4.1 nA), the default value is 100 (approximately corresponds to 1.17 nA). The specified value depends on the activity of the radioactive source located in the detector.

PID Detector

Lamp on. Turn the PID lamp on and off. You can quickly turn off the lamp to remove and clean it without cooling or turning off the chromatograph.

TCD Detector

Power. The parameter sets the heating power of TCD spirals depending on the type of carrier gas flowing through the detector. If helium is used as a carrier gas, set the power value to Helium 100%, if nitrogen is used, set Nitrogen 25%. In the power mode of 25%, when using helium as a carrier gas, it is possible to register peaks in the range of components concentrations up to 100 vol. % with a dose of 0.5-1.0 ml.

If the power is set to 100% (for helium or hydrogen), but in reality, nitrogen or argon flows through the detector, the sensor can break.

Offset. Set the offset value of the signal zero line. The amplifier is automatically balanced in such a way that the background of the detector corresponds to the specified offset. It is recommended to select the offset value in such a way that the background of the detector is 100-200 mV.

Filament on. When this option is enabled, the TCD switches to the automatic mode of sensor protection against overheating. During operation, the TCD spiral must be in automatic mode. When the option is turned off, the TCD spiral heating will be disabled.

Signal inversion. Set this option if all peaks on the chromatogram are negative (inverse).

CCD Detector

Power. Switchs the power level of the heating sensors detector. It can be 80% or 100%.

If the power is set to 100% (for helium or hydrogen), but in reality nitrogen or argon flows through the detector, the sensor can break.

Offset. Set the offset value of the CCD signal zero line. The CCD amplifier is automatically balanced so that the background of the detector corresponds to a given offset. It is recommended to select the offset value so that the background of the detector is 300-500 mV.

Sensor on. When this option is enabled, the CCD is switched to automatic mode of sensor protection against overheating. During operation, the sensor must be in automatic mode. When the option is turned off, the heating of the sensors will be disabled.

Signal inversion. Set this option if all peaks on the chromatogram are negative (inverse).

Ignition parameters for FID, NPD, FPD flame detectors

Located on the **Ignition** tab:

Flame threshold. When the flame is ignited, the measured background of the flame detectors increases. In order for the chromatograph to detect the presence of a flame, the background must exceed a predetermined threshold value. Recommended values:

- FID – 2 mV;
- NPD – 4 mV;
- FPD – 0.5 mV.

3.4 Expert Settings

Expert settings are intended for experienced users and service engineers and are available in the configuration when a special mode is enabled.

To enable Expert mode:


Open the main menu of the "Control Panel".


Enable the "Expert Mode" option. A red frame will appear around the window.

3.4.1 PM3 Parameters

- Enable Expert mode


Go to the Configuration page

Chromatograph Parameters

Delay before readiness. The time during which the chromatograph checks the stability of the all set parameters points. The default time is 20 seconds.

The number of independent channels. See the start channel section.

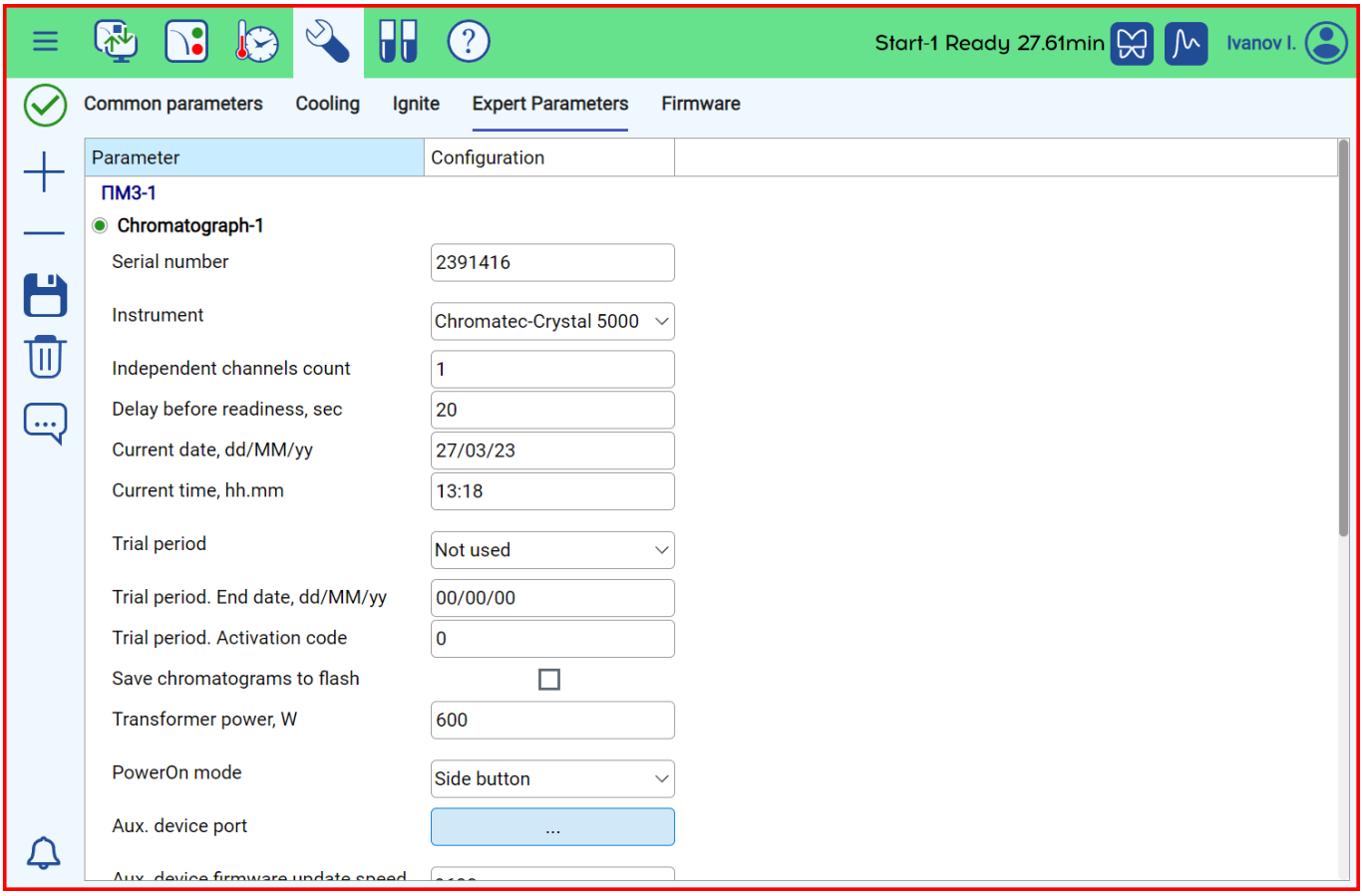


Fig 3.8 – Chromatograph expert parameters

The maximum number of connections. The default number is one. If you need to connect to chromatograph data from several computers (for example, from a desktop PC and a tablet), this number can be increased.

Save chromatogram to flash. Create backup copies of chromatograms on the controller's storage device (removable SD memory card).

Service mode (ignoring Out of Range). If this option is enabled, the chromatograph program ignores all parameters outside the tolerance and immediately sets the "Ready" stage.

Pressure units. You can choose kPa or psi.

Aux. device port. Here you can see the port number (AD-1, AD-2 or AD-3) to which the third-party auxiliary device is connected. The example in the figure below shows the connection of the Valco multi-position valve.

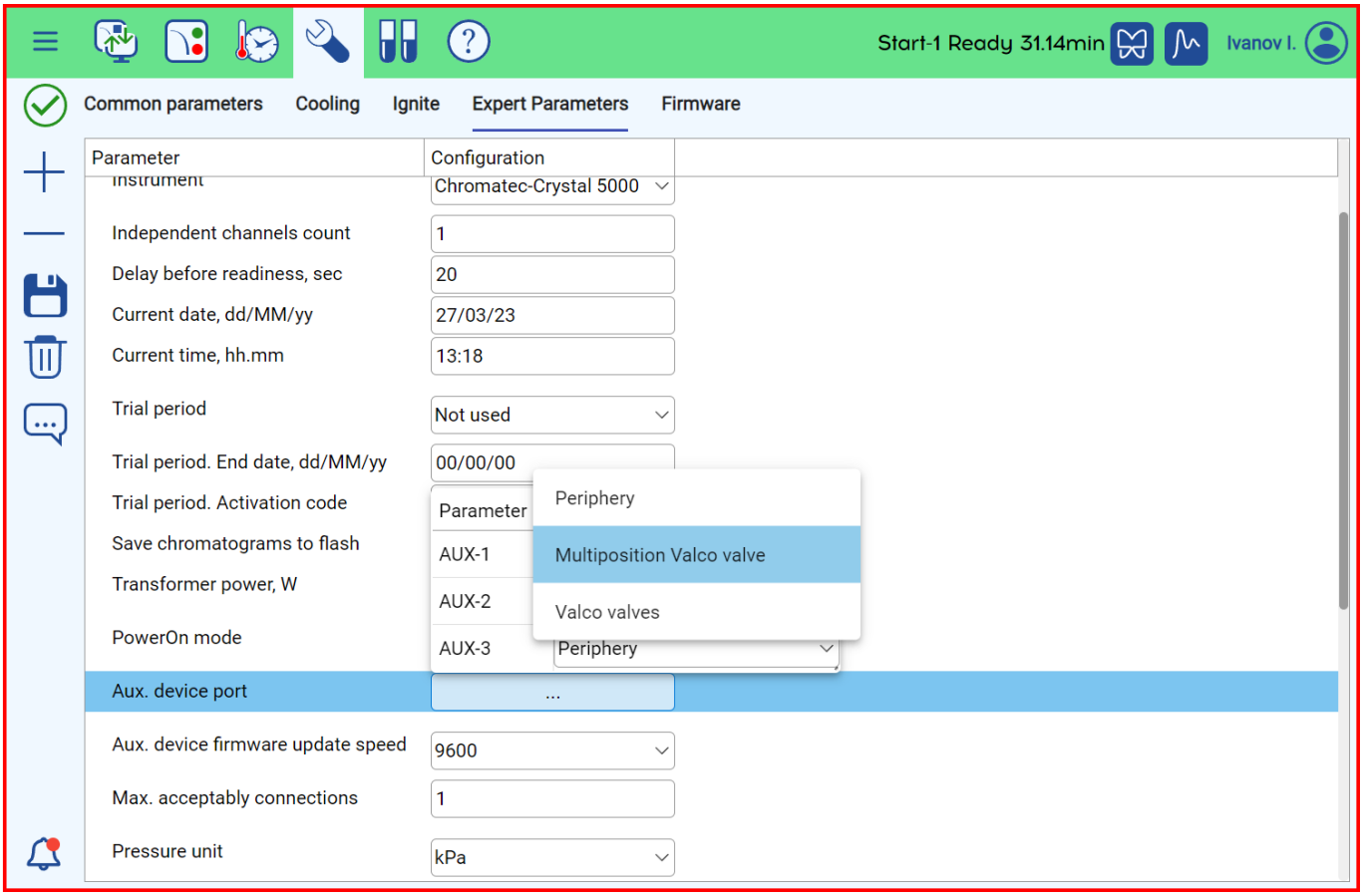


Fig 3.9 – Connection of auxiliary device (Valco multi-position valve)

Thermostat parameters

The PM3 controller can control up to fourteen thermostats:

1-12: temperature control of detectors, evaporators, valves, methanators, etc. All these thermostats are universal. Any of them can be redefined if necessary.

For example, you need to install a second methanator into the chromatograph. The first methanator occupies the thermostat No. 11. The second methanator is installed into any of the free thermostats. If the thermostat of valves 4 is absent (Thermostat No. 10), the second methanator can be installed in its place so in the thermostat table you can indicate that thermostat No.10 is a methanator 2 thermostat. For more information on thermostats connection, see the operating manual for the chromatograph.

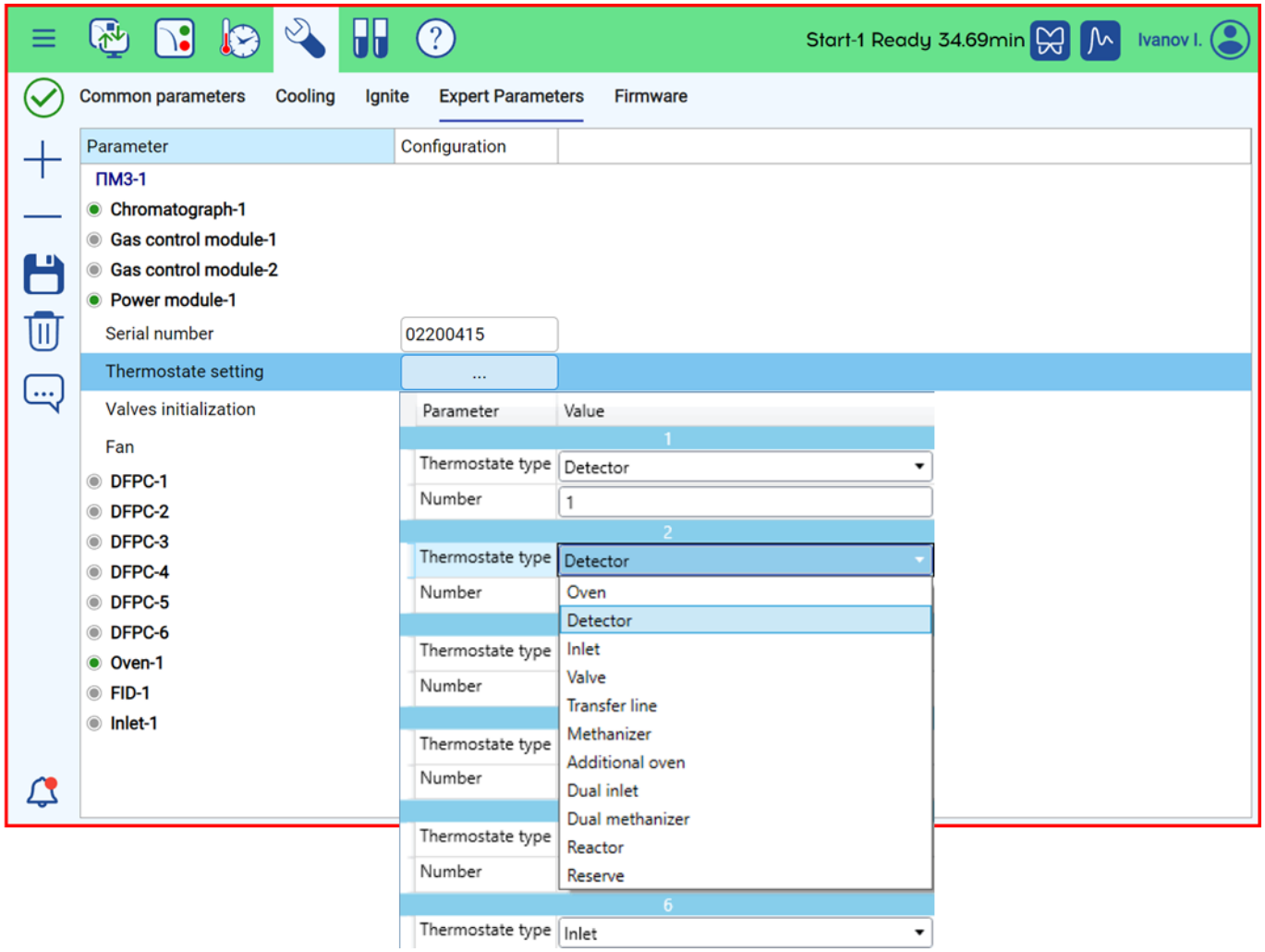


Fig 3.10 – Thermostat setting

13: an additional temperature sensor, heating channel are absent for thermostat 13 no.

14: column oven. This thermostat differs in its characteristics from thermostats 1-12 and performs only one function – the temperature control of columns.

- Expand the Power module group and click on the Thermostats button.
- For each of the 12 thermostats, set the type and sequence number according to the connections on the power module board.

Connecting gas modules

The PM3 controller allows you to connect multiple gas modules to increase the number of gas regulating channels. Six DFPC can be connected to one gas module. Moreover, when using universal single-channel DFPC (compatible with PM2), the number of gas control channels will also be six. When using multi-channel DFPC, the number of gas channels can reach up to eighteen.

In case your chromatograph has more than six DFPCs, you must properly connect **the gas control modules**.

- Open the electronic compartment of the chromatograph and determine the serial number of the gas module board (the number is written on the board) to which the DFPC from the 1st to the 6th is connected. For example, the number is 930003.

- Then in the "Control Panel" in the "Configuration" dialog on the "Expert Settings" tab, select the Gas Module-1 parameter group.
- If the "Gas Module-1" serial number does not match the number of the board to which DFPC 1..6 is connected, select the "DFPC-7 ... DFPC-12" value for the DFPC parameter.
- If the "Gas Module-1" serial number matches the number of the board to which DFPC 1..6 is connected, select the "DFPC-1 ... DFPC-6" value for the DFPC parameter.

If multi-channel DFPCs are installed in the chromatograph, you can also specify a range of numbers for them.

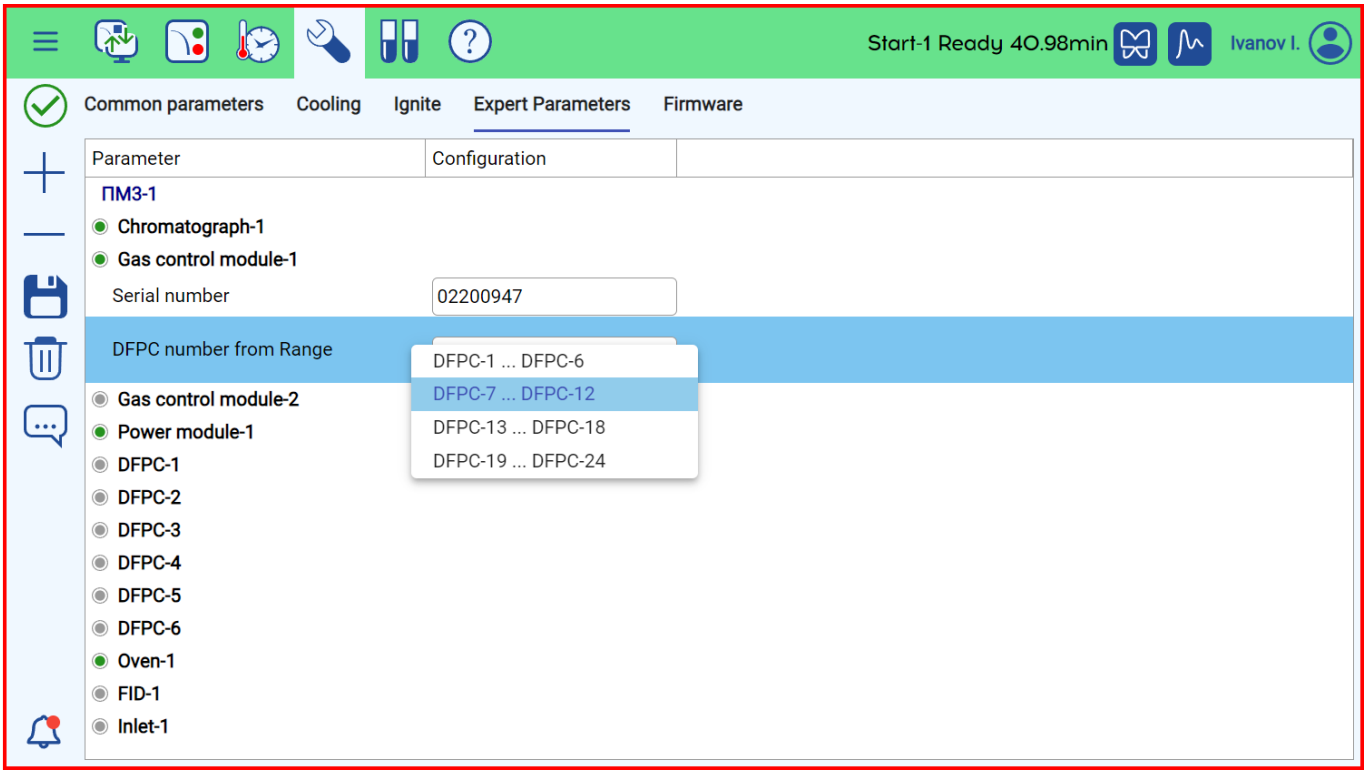


Fig 3.11 – Configure gas control modules

Setting the flow and pressure sensors

The flow and pressure values measured by the gas flow (pressure) regulator may differ from the actual values. "Control Panel" allows you to clarify the readings of the pressure and flow sensors.

Setting the flow sensor:

- Turn on the verified external flow meter in line with the adjustable DFPC..
- Set the appropriate DFPC flow to 0 ml / min.
- Measure real flow with an external meter. Record the resulting value.
- Repeat steps 2–3 for the rate of 10, 30 and 100 ml/min.
- Open the **Configuration** dialog, go to the **Expert Parameters** tab and open the section of the corresponding DFPC.
- Press the 0.0 / 10.0 / 30.0 / 100.0 button and specify the actual measured values for the given flow rates of 0, 10, 30 and 100 ml / min in the pop-up table.
- Save the configuration.

Pressure Sensor Setup:

- Connect a verified external pressure meter so that it measures pressure at the same point as the configured DFPC-11.
- Set the DFPC pressure to 0 kPa.
- Measure real pressure with an external meter.
- Open the **Configuration** dialog, go to the **Expert Parameters** tab and open the section of the corresponding DFPC.
- In the **Pressure. Zero Set** parameter set the actual pressure value obtained by an external meter.
- Set the configured DFPC to the maximum pressure that you plan to set when working with the chromatograph.
- Measure real pressure with an external meter.
- Determine the correction multiplier:

$$M = \frac{P_0}{P}$$

Where: P_0 is the pressure measured by an external verified meter, P is the pressure set for the configured regulator

- In the **Configuration** dialog on the **Expert Parameters** tab, specify the value of the **Pressure**. Correction factor parameter for the configured DFPC.
- Save the configuration.

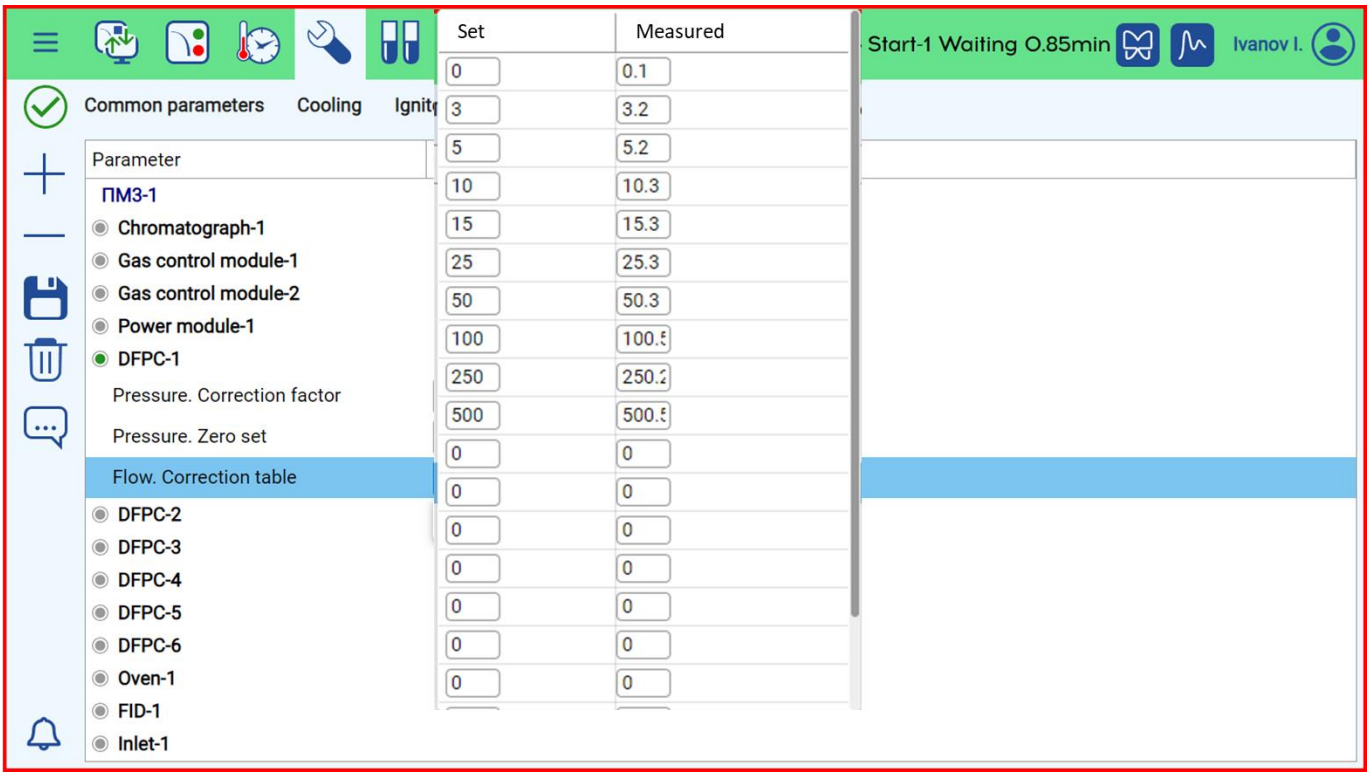


Fig 3.12 – Flow Sensor Calibration

Inlets parameters

Inlet type. Here you can choose the value – 7.x [Packed/Split-splitless] or 8.x [Programmable], corresponding to the model of the inlet.

Cryo. If the inlet is equipped with a cryo-cooling system, this option should be enabled.

Pressure regulator on the discharge channel. The option must be enabled when using the gas supply scheme of the evaporator, in which the DFPC-11B pressure regulator is connected to the sample discharge channel (it maintains the specified inlet pressure). The DFPC-10D flow controller is connected to the carrier gas channel.

When working with such a gas scheme, the splitless mode flow is not available.

Detectors settings

Allowed signal. For each detector, you can specify the signal value, above which the chromatograph will not go to the "**Ready**" stage and **Service** tab will display a message about the need to carry out a detector cleaning procedure. If this parameter is set to 0, the allowed signal control is not used.

Use signal filtering. If this option is enabled, the detector signal recorded during the analysis will be filtered in real time to reduce the noise level.

Hydrogen consumption multiplier. If one hydrogen flow regulator is connected to two detectors, this parameter should be set to 2.

Airflow multiplier. If one air flow regulator is connected to two detectors, this parameter should be set to 2.

Makeup gas flow rate multiplier. If one makeup gas flow regulator is connected to two detectors, this parameter should be set to 2.

FID, NPD and PID detectors have the same amplifiers. If NPD or PID detectors are installed in the chromatograph, and the program detects the presence of only FID detectors by default, it is necessary to change the type of amplifier for one of these detectors..

Open the electronic compartment of the chromatograph and determine the serial number of the amplifier connected to the NPD detector (PID). The number is written on the body of the amplifier.

Then select the detector of interest and change the type and sequence number of its amplifier in the "Control Panel" in the **Configuration** dialog on the **Expert Settings** tab.

Valve parameters

Do not return to the starting position. Usually, at the end of the analysis, valve returns to the initial position specified in the general configuration settings regardless of the number of settings made in the crane switching mode. However, in some gas schemes, any switching of the valve with two valve loops leads to the injection of a sample into the column from one of these loops. This option should be enabled for the operation of such a scheme.

If an automatic valve is present in the chromatograph, but the chromatograph does not detect its presence, it is necessary to set the detection parameters manually. Click the **Configure valve detection** button.

3.4.2 PM2 parameters

- Switch to Expert mode

 Go to the Configuration page

Heater Settings

The following heaters settings are available:

Type of heater. The parameter tells the chromatograph program how to control the heating of the thermostat in which the heater is installed.

Detector. The parameter appears if **Heater Type = Detector**. Here you should indicate the type of detector installed on the heater.

Valve sampler. The parameter appears if the **Heater Type = Valve sampler**. Here you should indicate the type of the valve sampler installed on the heater.

A similar parameter is added for a valve switcher.

Power, W. The parameter is determined by the design of the heater. change it to an arbitrary number is impossible. When replacing the heater, consult the developer.

Resistance, ohm. The parameter is determined by the design of the heater. Change it to an arbitrary number is impossible. When replacing the heater, consult the developer.

When the power is limited, the maximum heating rate of the thermostat decreases.

Gas Setting

Compensation, ml/min. Here you set the flow rate measured by the gas regulator at a given flow rate of 0 ml/min.

Valve parameters

Return to the starting position. If this option is enabled, the valve will return to the starting position after the analysis. In some gas schemes, any switching of a valve with two valve loops leads to the injection of a sample into the column from one of these loops. This option should be enabled for the operation of such a scheme.

3.4.3 Firmware Update

- Switch to Expert mode

Go to the **Configuration** page and then to the **Firmware** tab.

- Enable the **Allow firmware update** checkbox.

To update the firmware, you must have the appropriate privilege.

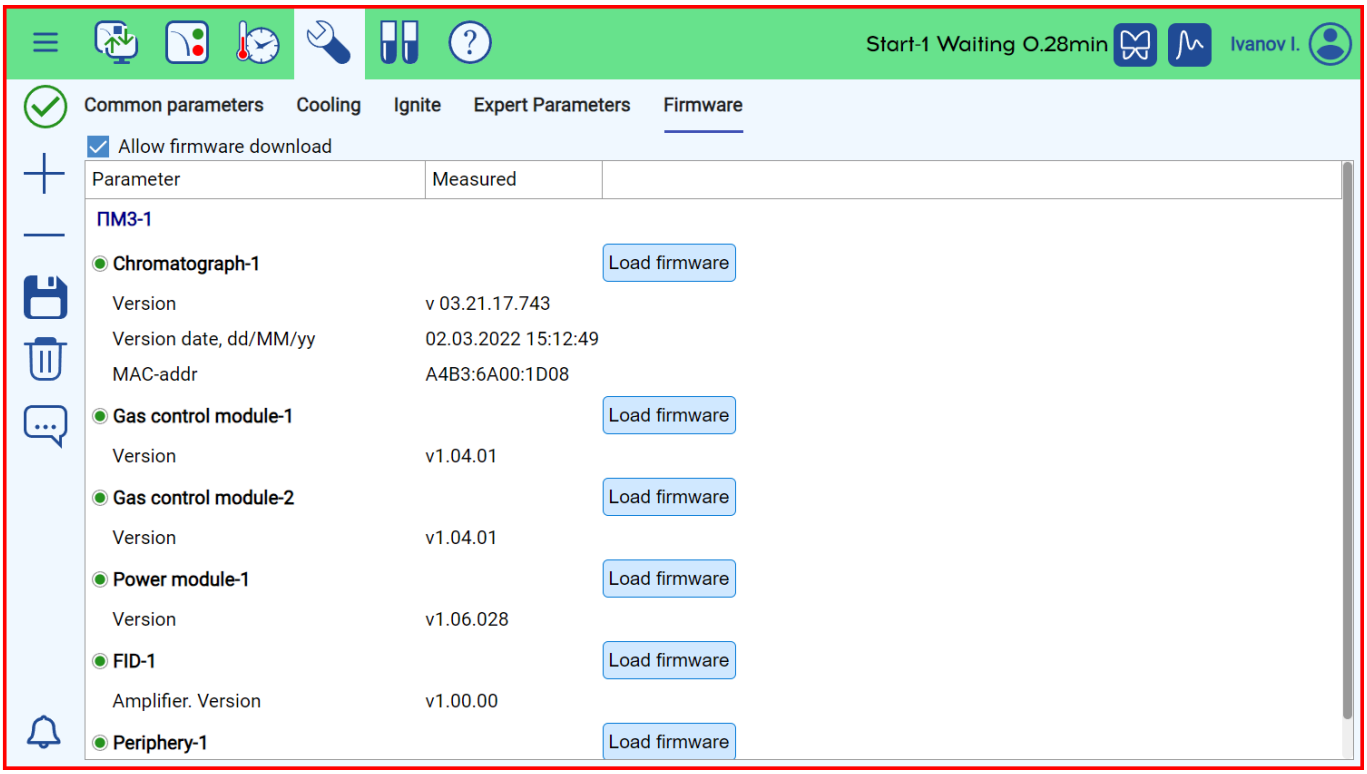


Fig 3.13 – Firmware update tab

3.4.4 Updating the main firmware of the chromatograph

The PM3 firmware is an **image.pm3** file that can be loaded into the device in two ways:

- from a computer;
- from removable USB flash drive.

Booting from a USB flash is preferable because it is faster. To prepare for a firmware update, copy the image.pm3 firmware file to the root directory of the USB flash. Install the USB flash into the appropriate socket on the back of the chromatograph.

- Click the **Load firmware** button located to the right of the name of the module in which you want to update the firmware.

The program checks the presence of a removable USB flash device connected to the chromatograph. If the USB flash device with the image.pm3 firmware file it is not connected to the chromatograph, a dialog appears asking to open the firmware file from the disk. After selecting the file, the firmware download to the chromatograph begins.

If the power supply of the chromatograph disappears at the moment of firmware download, the backup program will automatically start after its restoration. In this case, all the LEDs on the front panel of the chromatograph will blink.

After starting the backup program, the operator can try again to overwrite the firmware. The previous configuration of the chromatograph will be saved.

3.4.5 Updating the autosampler firmware

The sampler firmware file does not need to be written to the USB flash. It can be downloaded directly from the computer.

The rest of the update procedure is similar to that described for the chromatograph (see above).

The sampler firmware is located on the installation disk in the **firmware\Autosampler** folder.

When you click the **Load firmwar**e button, a dialog of file selection will appear. Select a file with *.cdp extension.

The process of uploading the firmware to the chromatograph will begin; it takes a few seconds.

Then the "Control Panel" will offer to turn off the sampler and turn it on again. After you do this, the process of the firmware update will begin.

If you are trying to download a firmware that does not correspond to the design of the sampler, the "Turn on and turn off the dispense" flashes on the "Control Panel" for some time (about 30 seconds), after that the "**The firmware is not completed**" inscription appears.

It is important to choose the correct firmware file, depending on the sampler construct. The version number consists of four digits: **A.B.C.D**.

You can load only the firmware that matches the current first three digits of the version (**A.B.C.**)

For example, the current version is AS-3D.11.3.1.03.rus.cdp. You can replace it with the AS-3D.11.3.1.05.rus.cdp version. If you try to replace it with the version AS-3D.11.3.2.05.rus.cdp, the sampler will not accept this firmware (its behavior is described above).

The table below shows the decoding of the file version:

Table 3.1 – Decoding the sampler firmware version

Version section	What does it mean	Version	Description
A	Sampler type	11	AS-2M 3D
		12	AS-2M 3D Headspace
B	Sampler construction	1	AS-2M 3D with 78-vial tray
		2	AS-2M 3D, universal platform for 150 vial (the same version is version 1 for the sampler type 12)
		3	Changing the type of drive belts (version 2 has the same construction for sampler type 12)
C	Board version	1	L6208 driver board
		2	TMC2130 driver board
D	Internal program		

4 INSTRUMENT METHOD


Click the Instrument Method button. The dialog for setting parameters of analysis mode appears on the screen.


If you have previously saved the chromatograph mode and want to open it for editing, click the **Open** button and select the desired file.

The dialog contains two tabs:

Analysis. Here, operation modes of the chromatograph nodes at the "Analysis" stage are specified. Some parameters may vary according to a given program.

PostRun. Here, operation modes of the same nodes are set at the "Blowing" stage. This stage begins after the end of the analysis (if the purge time is not zero). The parameters on this tab do not have to be set. If the value of any parameter is zero, it means that it will not change at the "Blowing" stage, the value specified for the analysis will remain.

The instrument method setting is a consistent setting of the parameters of the chromatograph instruments in accordance with the requirements of your analysis procedure. Buttons on the side toolbar allow opening the corresponding section of mode parameters for each instrument of the chromatograph.

Some instruments or their parameters described below may be missing in your chromatograph. The list of instruments and mode parameters depends on the model of the chromatograph, the type of processor module, as well as on the configuration of the chromatograph, which is formed on request.

Setting the parameters of the mode is performed in accordance with the requirements of the methodology of the analysis – GOST, ISO, ASTM, PND F, MMP, company standard, etc.

The parameters of the flame detectors depend on the detector model and are set in accordance with the recommendations of the operating manual.

An example of creating a method is shown below:

{video panel_create_imethod Instrument method}

4.1 GC and MS method (PM3)

4.1.1 Non-automatic samplers

Manual samplers, in contrast to autosampler, cannot independently perform analysis sequences. They are located outside the chromatograph and are connected to it via RS-232 interface.

Non-automatic samplers include:

- Two-stage Thermal Desorber.
- Pyrolyzer.
- Head space sampler (SDO "Chromatec" also produces automatic head space sampler).

Unlike autosamplers, the instrument method parameters for manual samplers are specified in the "Instrument Method" dialog. To set the input device mode, click the corresponding button on the side toolbar

4.1.2 Valves

To set valve method, click the corresponding button on the side toolbar.

Set the parameters in accordance with the requirements of the methodology:

Temperature. If the valve is heated, set its temperature according to the requirements of the method.

The options below are available for automatic valves only. They are not available for hand valves. A non-heated manual valve has no parameters and is absent from the list of instruments.

Preprun. If this option is enabled, at the "**Not ready**" stage the valve has a position that is different from than the one specified in the configuration of the valve.

E.g., initial position Pos.B. is set in the configuration. When transferring the mode, the valve will switch to this position. When all parameters of the chromatograph are within the acceptable range, the chromatograph will proceed to the "Waiting" stage. At this stage, the operator must perform Preprun — press the START key without introducing a sample (when working with the autosampler, Preprun will be executed by the Scheduler).

When performing Preprun, the valve will switch to position Pos.A.

Preprun is used in gas scheme with flow switchings, for example, when back flushing the precolumn.

Switching time. Sets the number and time of switchings of the valve during the analysis. Click the **[...]** button to open the switch settings dialog (in the figure below). At least one valve switch is always there, but it is inactive by default. In order for the valve to switch during analysis, set the switching time and enable the appropriate check mark.

If necessary, you can add additional switches.

Switching time is set in minutes. When working with valve samplers, the time of the first switch is set to 0 min.

If an automatic **gas flow switching device with a Valco multi-position** valve is connected to the chromatograph, adjust its parameters in accordance with the requirements of the methodology and characteristic of the gas chromatograph scheme::

1. Click the **Switch** button.
2. Add the required number of switches.
3. Set the **time** for each switch in minutes. Select the **position** to which the valve switches at the specified in the "Analysis" stage time..

4.1.3 Inlets

The name of the inlet depends on the corresponding configuration settings and can take values:

- Packed inlet.
- Split-splitless inlet.
- PTV.
- Vaporized inlet.
- Piston injector.

 To set the mode of inlet, click the corresponding button on the side toolbar

Set the parameters according to the requirements of the methodology:

Temperature.

If the inlet type is “Vaporized inlet” and the thermostat is not set in its configuration, then the “temperature” parameter is missing.

If the inlet type is “PTV”, then the temperature input field turns into a button, which should be pressed to set the temperature programming parameters during the analysis.

 To add isotherms of the temperature program, press the corresponding button.

If the **On column** option is available and enabled for the inlet configuration, the user cannot set the inlet temperature, as in this mode it is synchronized with the temperature of the oven and is set in the settings of the instrument.

The maximum number of programming steps for temperature, flow rates and gas pressures is 33.

The duration of each stage is unlimited.

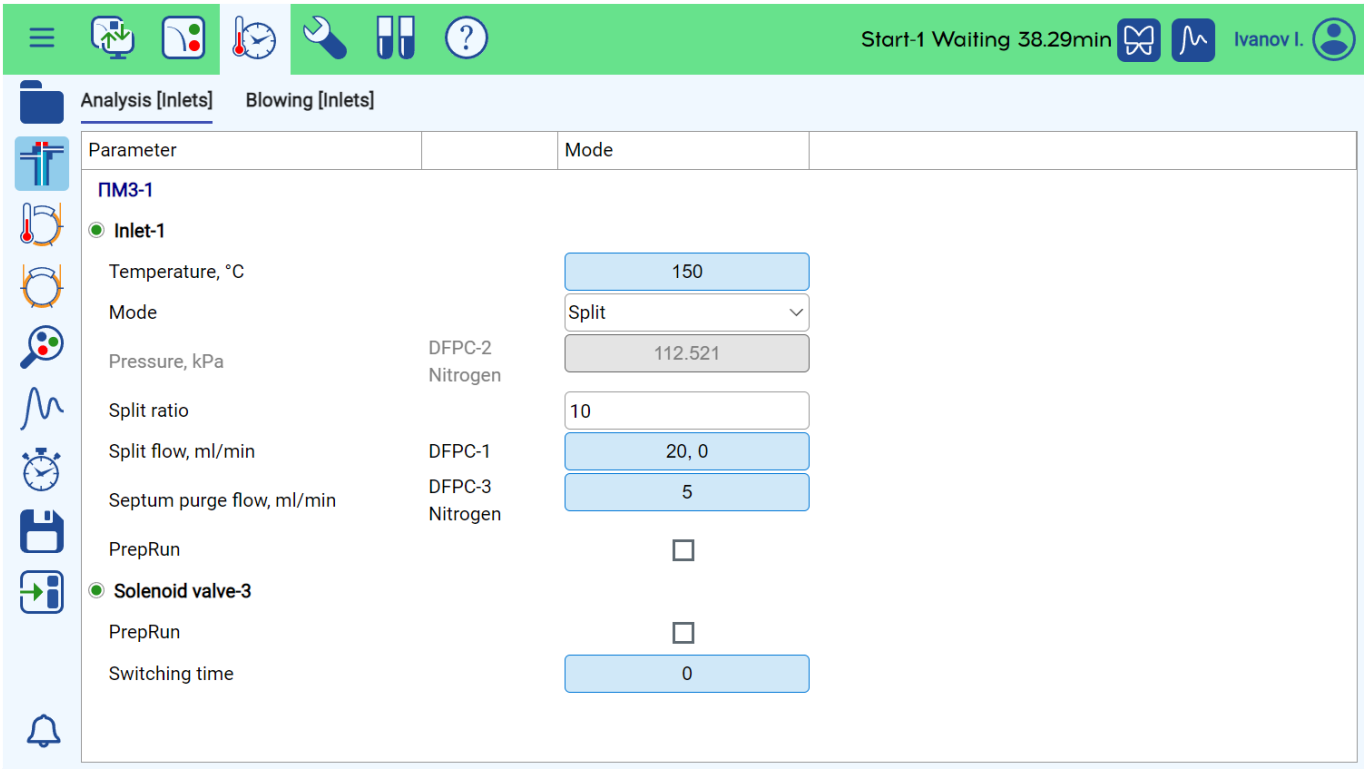


Fig 4.1 – Inlet parameters

Mode. It can take the following values:

- **Split**. The user can set the ratio of the sample. In this case, the program calculates the value of the discharge flow. The opposite is also possible: the user sets the discharge flow, and the program calculates the ratio of the sample.
- **Split with gas save**. When this mode is selected, another stage is added to the discharge flow. It equals to 10 ml/min by default. In this case, the duration of the first stage (determined by the specified splitting ratio) is set to 1 minute. The values of the added parameters are recommended, but the user can change them.

When applying such a mode, the chromatograph performs the last step of the discharge gas programming. When all parameters of the chromatograph are within the acceptable range, the chromatograph will proceed to the "Waiting" stage. At this stage, the operator must perform Preprun — press the START key without introducing a sample (when working with the autosampler, the Preprun will be executed by the Scheduler).

When Preprun is executed, the chromatograph processes the first step of the specified discharge flow program and proceeds to the “Ready” stage.

When the user enters the sample and presses START, after a specified time, an economical gas flow will be established at the analysis stage (see Figure below).

- **Splitless with gas save**. When this mode is selected, two more programming steps are added to the discharge flow. The parameter values are set as shown in the figure below.

When a sample is introduced without splitting the flow, the gas regulator valve is closed for a specified time, after which a large discharge flow is established to ventilate the sample discharge line. The reset programming cycle ends with the setting of an gas saver discharge flow.

Membrane blowing is regulated synchronously with the sample discharge.

If the inlet configuration includes synchronization with the additional valve, the time of **the first switching** of this valve is automatically synchronized with the time of the first programming stage of the discharge flow.

Pressure. The parameter duplicates (for greater convenience) the same parameter from the Columns group.

Septum purge flow. This parameter is set if DFPC is capillary or programmable connected to the corresponding gas channel of the evaporator according to the configuration settings. If pneumatic resistance or pressure regulator with mechanical control is enabled, this parameter is absent.

It is possible to save the gas flow rate by blowing the membrane if the **Split with gas save Mode** is set.

When the inlet is operating in the splitless mode, the start time of the membrane blowing is automatically synchronized with the time of the first programming step of the discharge flow.

Split flow. If the method specifies discharge flow directly, the user can set it. This will automatically calculate the splitting ratio of the flow.

Total flow. Displays the calculated total flow rate of gas flowing through the corresponding DFPC. It is impossible to change the first step of the total flow programming directly; it is calculated automatically.

This parameter appears only when using the gas supply scheme of the inlet, in which DFPC-11B pressure regulator is connected to the sample discharge channel. To work in this mode, it is necessary to enable the pressure regulator on the discharge channel option in the expert configuration settings.

Splitless mode is not available for this gas scheme.

Split ratio. It is set in accordance with the requirements of the methodology, while the program automatically calculates the discharge flow.

Large volume injection

When working with a programmable inlet, the injection of a large volume of the solvent function is available. If the corresponding option is enabled in the configuration, the mode button for calling the solvent's blowout calculator appears in the mode.

- Click the **LVI-calculator** button.
- Select a solvent.
- Set the parameters for the injection of a large sample volume.
- Click **OK**

4.1.4 Columns



To set the sample column mode, click the corresponding button on the side toolbar. In accordance with the requirements of the methodology, set the **Control mode**. It may take values:

- Constant pressure.
- Constant velocity.
- Constant capillary flow.

Next, when working with a capillary column, set the value of the selected parameter (pressure, velocity or flow). The program calculates the other two parameters and their values are displayed for reference.

When working with a packed column, set the flow rate of the carrier gas.

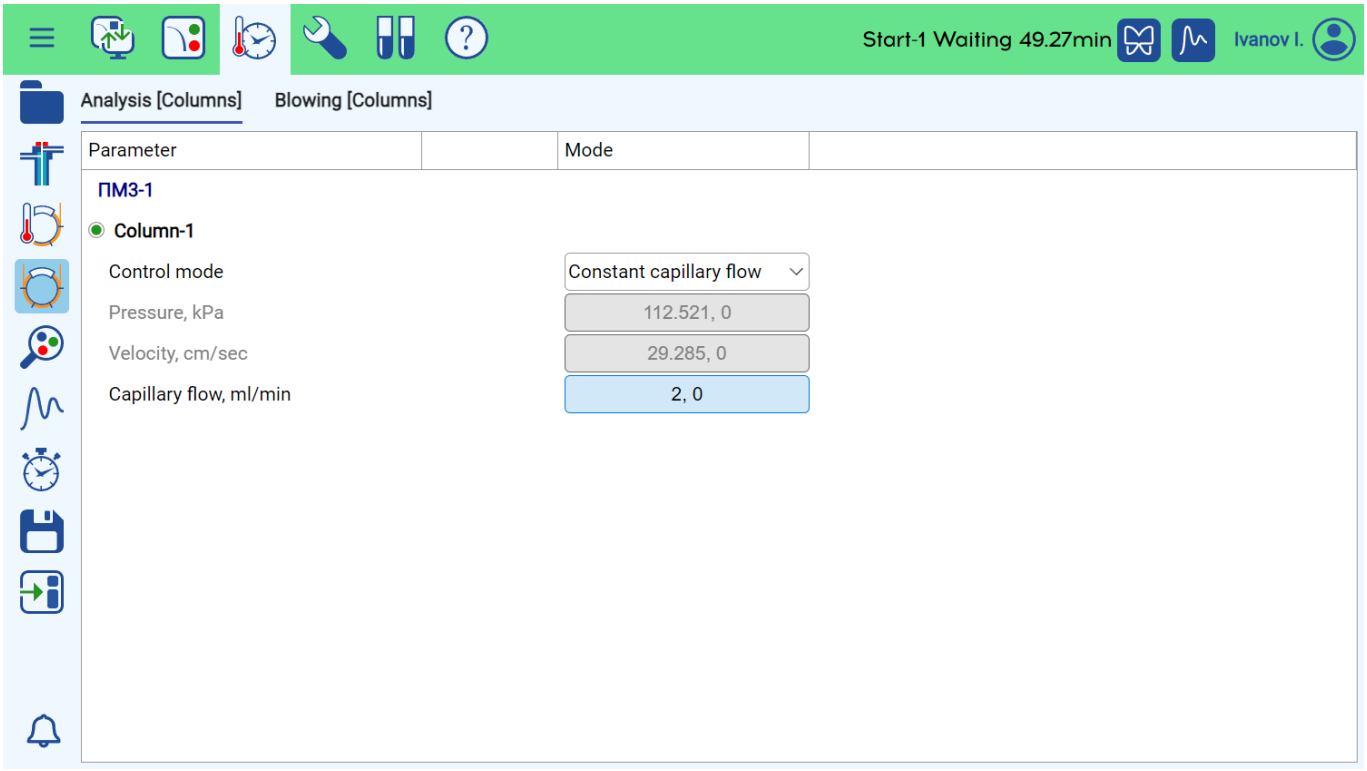


Fig 4.2 – Column parameters

4.1.5 Solenoid valves parameters

In the "Columns" section, flow switcher parameters are also set – **solenoid valves**.

The **Preprun** and **Switching tile** parameters for solenoid valves are completely identical to those of the valve.

Additionally, the pressure or gas flow can be set for the valve, if DFPC is used in the gas flow switching scheme besides the valve (specified in the configuration settings).

For example, the pressure is set for solenoid valves in the Dean switchers system.

4.1.6 Column Oven

 To set the oven mode of the sample columns, click the corresponding button on the side toolbar

Set the temperature of the oven according to the requirements of the method.

The total time of temperature programming (the time of all stages plus the time for heating) determines the duration of the analysis.

Programming can be set both with an increase and a decrease in temperature.

The maximum number of programming stages is 33. The duration of the stage is not limited.

4.1.7 Methanizer

 To set the sample methanizer mode, click the corresponding button on the side toolbar.

4.1.8 Detectors

 To set the mode for sample detectors, click the corresponding button on the side toolbar.

Set the parameters according to the requirements of the methodology:

Temperature. The parameter is present in all detectors.

Hydrogen flow. This parameter is typical for FID, NPD, FPD flame detectors.

Air flow. This parameter is typical for FID, NPD, FPD flame detectors.

Makeup flow (pressure). The parameter is available with FID, NPD, ECD, PID, TCD (when working with a capillary column), CCD detectors.

Comparative gas flow. The parameter is available for TCD detectors.

Switching lamp. This parameter is available for PID detectors. The times for turning the PID lamp on and off are set here. The lamp on/off dialog is similar to the valve switching dialog.

The time of turning on the lamp and its exit to the operational mode is no more than 5 seconds, so it is advisable to use the lamp only for target components analysis, this will significantly prolong the lamp life. The rest of the time the lamp must be switched off.

Table 4.1 – Recommended values for air and hydrogen flow rates

Parameter	FID	NPD	FPD
Hydrogen flow, ml/min	20-30	10-15	140
Air flow, ml/min	200-300	200	40

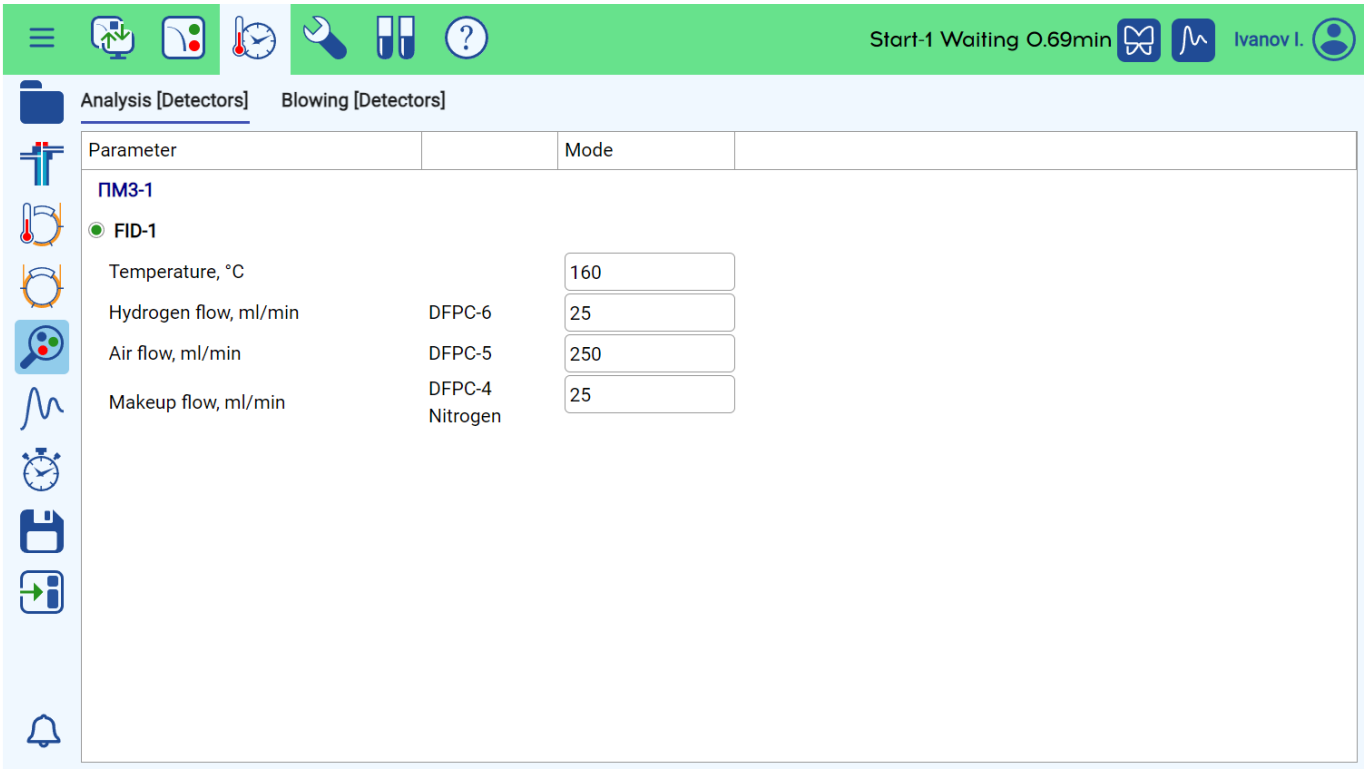


Fig 4.3 – Detector parameters

4.1.9 Mass spectrometry detector (MSD)

To set the MSD mode of a sample, click the corresponding button on the side toolbar.

The "Instrument Method" button – here is sets the parameters of the MSD operation that are not related to scanning:

Ion source temperature. Sets the temperature of the ion source to 350°C.

Transfer line temperature. Sets the transition line temperature to 400°C.

Windows width (available for SIM scan type). The range of mass scanning in SIM mode is set. Acceptable values are from 0.1 to 10.

Run time, min. Sets the analysis duration for MSD. Options:

- Set by chromatograph – the value is taken from the chromatograph instrument method.
- Set by MSD – the value is set when the direct input device is connected.
- Set by user – the value is set by the user directly in the input window on the left.

Ionization type (available if chemical ionization (CI) is set on MSD). Chooses the type of ionization: electronic or chemical.

CI gas (available if CI is set on MSD). Select the type of reagent gas from the list:

- No (in this case the gas is turned off),
- Methane,
- Isobutane,
- Carbon dioxide.

The minimum value for all types of gas is 0.05 ml/min. Maximum values:

- methane – 4,7 ml/min;
- carbon dioxide – 3,0 ml/min;
- isobutane – 6,6 ml/min.

CI gas channel (available if CI option is installed on the MSD). Selects from which input the reagent gas will be supplied. Inputs are labelled as A and B on the back of the MSD.

Scan button – sets the parameters of the MSD operation that determine the scan:

Scan type. Selects the scan type:

- Standard – scanning by segments.
- **Synchronized (t-SIM+Scan)** – organization of scanning depending on the retention time of the component, with the ability to scan the mass range. Convenience of this type of scanning: at the end of the analysis, channels and components will be created automatically in accordance with the specified parameters of the mode.

Segment information when selecting **Standard Scan type**:

A segment is a time interval of a chromatogram for which the same sequence of scans is applied. Segments are added and removed with the **Enter** and **Delete** buttons.

Start time, min. The analysis time from which the settings for this segment take effect. The first segment can start from 0 min, or from any other moment (delay on solvent), not exceeding the duration of the analysis.

Filament. Determines if the cathode is turned off or on during this segment.

Emission current. Sets the amount of emission current for this segment. Valid values are from 0 to 500 μA. When selecting "**By tune**", the value of the emission current is recorded from the settings file.

Detector gain. Sets the gain factor of the detector. Valid values are from **10,000 to 50,000,000**. When selecting "**By tune**", the gain factor is recorded from the last settings file.

Scan information when selecting **Standard Scan type**:

Scans (rows in the scan table) are added with the **Enter** key, deleted with the **Delete** key on the keyboard. A scan is a repeating process of scanning a single mass or mass range, performed under specified conditions.

Scan type. Mass range or SIM (single ion monitoring, monitoring of selected ions).

Mass range. Sets the mass range or individual masses. Specifying individual masses separated by comma implies operation in SIM mode. Valid values are from 1 to 1200.

Scan time. Sets the scan duration in seconds. The maximum value is 300 s. The minimum value depends on the scanning range and is corrected by the program if an invalid value is entered.

SIM width. Sets the mass scan range in SIM mode. The range of mass scanning in SIM mode is set. The window is available if separate masses are entered in the Mass range column. Valid values are from 0.1 to 10.

Polarity. Available for the "chemical" ionization type. The polarity of the detected ions is selected if the chemical ionization type is selected. The values of "Positive" and "Negative" are possible.

Scan rate. Reference value. The scan speed is calculated by the program, based on the specified mass range and scan duration.

Synchronized Scan type (t-SIM):

Scan the mass range: the available values are "**Yes**" and "**No**". When you select "Yes", the range scanning options become available. They are similar to the standard scanning mode. The chromatogram recorded for the mass range is intended only for qualitative analysis and cannot be used for component creation and quantitative analysis**.**

Most of the scanning parameters are similar to the parameters in Standard mode. Only the way of specifying scans and segments changes, they are set in the table through the description of components.

Rows in the table are added with the Enter key, deleted with the Delete key on the keyboard.

Name. Specifies the name of the component to be determined.

Retention time, min. Sets the retention time of the componet.

Windows width, min. Sets the length of time for which a component is expected to leave the column. For example, if you set a retention time of 2 minutes. and the width of the window is 0.5 minutes, then the output of the component is expected at 1.75 – 2.25 minutes.

Mass list. Set one or more individual masses. Valid values are from 1 to 1200. The first mass will be used to build a channel and for quantitative analysis (the so-called Quan ion). The remaining masses are used for ion confirmation when identifying the component.

The "Build by search results" button allows you to automatically fill in the component table using data from the chromatogram. For this:

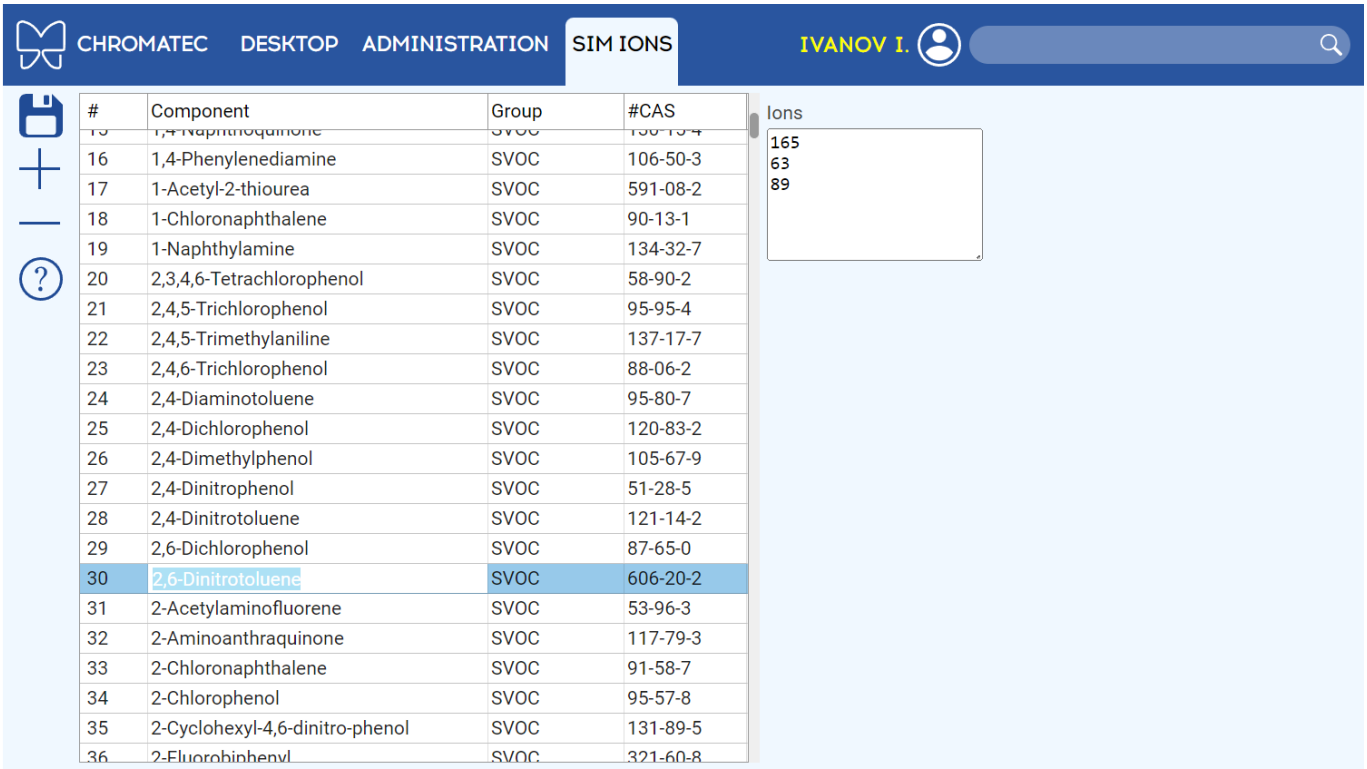
- pre-perform the analysis in Scan mode;
- in the Chromatec Analytic software, perform an automatic or manual search for the necessary components in the library of mass spectra. The data for the new method (name, retention time and component masses) will be subsequently exported from the "Search Results" table;
- in the Control Panel, click the "Build by search results" button and specify the file received in the previous step;
- the software will prompt you to specify the number of ions and the window size for the components, after which the component table will be filled in automatically;
- after autofill, the data can be adjusted manually, if necessary.

The "Direct input" button – the parameters of the operation of the direct input device are set. The description is given in the document "214.5.880.003UM. A device for direct input of MSD. Operation Manual".

For convenience and acceleration, when creating the " Synchronized (t-SIM + Scan)" method, the built-in library of optimal ions is used. When creating such a method, the operator has to analyze the spectra of the components in order to select the most suitable ions. The library already lists the main characteristic ions for each component. When accessing the library, the program searches for the necessary component by a unique CAS# and writes the ions specified for this component to the method. The library is accessed automatically, this eliminates errors and significantly speeds up the process.


To view and/or edit this library, go to the Chromatec Navigator program. Click on the button "SIM Ion Library". On the page that opens, you can add components and their optimal ions.

To edit this library, your account must have the rights – "Create and change the processing method".



#	Component	Group	#CAS
16	1,4-Phenylenediamine	SVOC	106-50-3
17	1-Acetyl-2-thiourea	SVOC	591-08-2
18	1-Chloronaphthalene	SVOC	90-13-1
19	1-Naphthylamine	SVOC	134-32-7
20	2,3,4,6-Tetrachlorophenol	SVOC	58-90-2
21	2,4,5-Trichlorophenol	SVOC	95-95-4
22	2,4,5-Trimethylaniline	SVOC	137-17-7
23	2,4,6-Trichlorophenol	SVOC	88-06-2
24	2,4-Diaminotoluene	SVOC	95-80-7
25	2,4-Dichlorophenol	SVOC	120-83-2
26	2,4-Dimethylphenol	SVOC	105-67-9
27	2,4-Dinitrophenol	SVOC	51-28-5
28	2,4-Dinitrotoluene	SVOC	121-14-2
29	2,6-Dichlorophenol	SVOC	87-65-0
30	2,6-Dinitrotoluene	SVOC	606-20-2
31	2-Acetylaminofluorene	SVOC	53-96-3
32	2-Aminoanthraquinone	SVOC	117-79-3
33	2-Chloronaphthalene	SVOC	91-58-7
34	2-Chlorophenol	SVOC	95-57-8
35	2-Cyclohexyl-4,6-dinitro-phenol	SVOC	131-89-5
36	2-Fluorobiphenyl	SVOC	321-60-8

Fig 4.4 – Saving the instrument method

4.2 GC method (PM2)

4.2.1 Thermostats


To set the thermostats mode, click the corresponding button on the side toolbar.

accordance with the requirements of the method, set the temperature of:

- thermostat detectors;
- valves thermostat (in presence of);
- inlets thermostat;
- oven.

For thermostats of inlets and columns, temperature programming can be set. For the PM2 controller, the number of programming steps is fixed and equals 5. If you need to specify a smaller number of programming steps, simply ignore the unnecessary ones (see figure below).

4.2.2 Valves


If there are automatic valves in the chromatograph, go to their settings dialog by clicking the corresponding button on the side toolbar.

Set the switching parameters in accordance with the characteristics of the analysis and gas chromatograph scheme.

4.2.3 Gases


To set the mode of gas regulators, click the appropriate button on the side toolbar.

For **DFPC-10** gas regulators, you can set up to four stages of gas flow programming (ml/min).

For **DFPC-11** gas regulators, you can set up to four steps of gas pressure programming (kPa), as well as the value of the flow in the evaporator splitting.

When working with a capillary column, two gas regulators are used. In this case, **Gas-1** and **Gas-3** regulators are used to set the pressure of the carrier gas, and the **Gas-2** and **Gas-4** regulators are used to form the flow rate of the waste gas.

When you set the pressure and the magnitude of the flow splitting for Gas-1 (Gas-3), the flow rate of Gas-2 (Gas-4) also changes.

When working with high discharge values or in the splitless mode, it is recommended to add an additional isoline for the discharge regulator with a low discharge gas flow rate.

At the same time, for correct programming of the flow rate through the sample discharge channel (Gas 2 or Gas 4), it is necessary for the chromatograph to process the first stage of the flow just before the sample is introduced into the inlet.

Thus, when setting the discharge gas flow programming at the “Not ready” stage, the **last stage** will be processed.

As soon as all parameters of the chromatograph come within tolerance, it proceeds to the “Waiting” stage.

In order to go to the "Ready" stage, press START **without sample injection**.

4.3 Selection of recorded signals

Specify which signals to record when performing the analysis

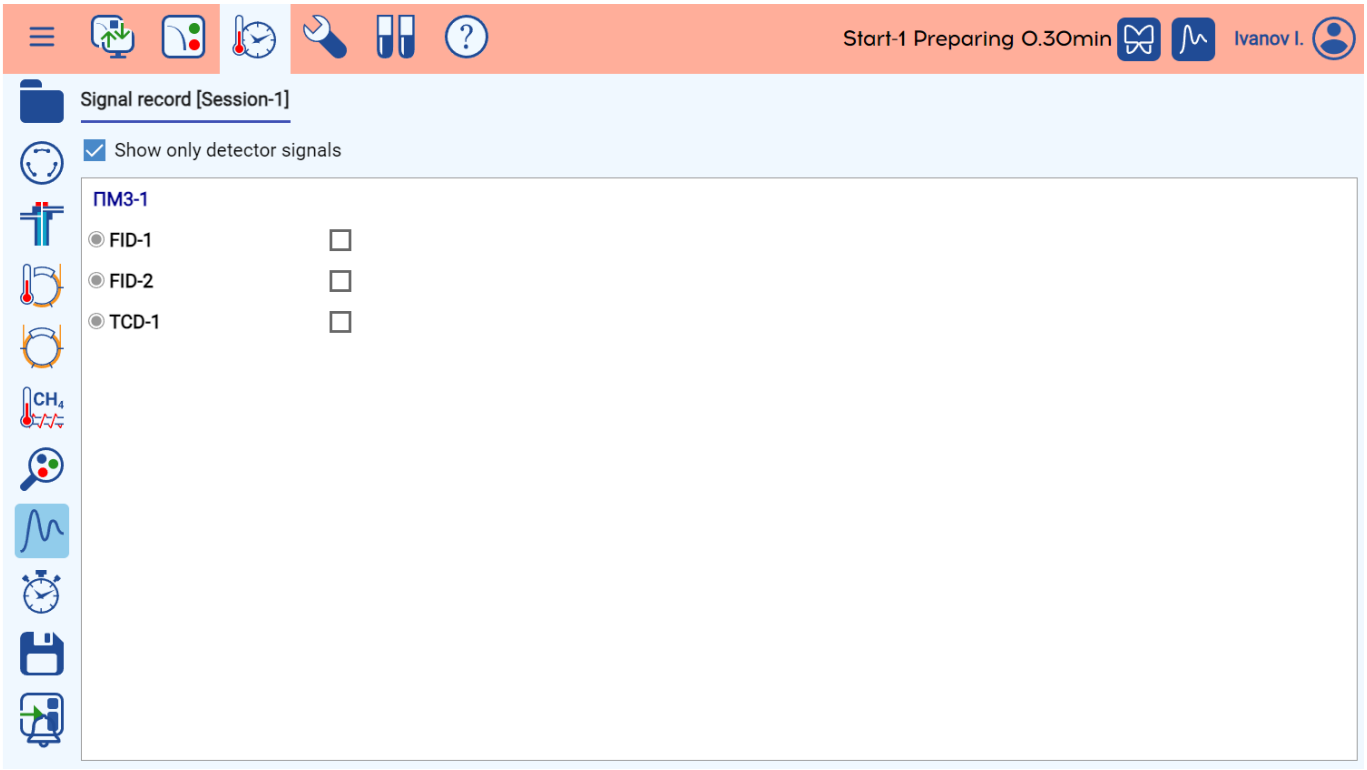


Fig 4.5 – Selection of recorded signals

In addition to the detector signal, you can record a diagnostic signal – a change in any parameter of the chromatograph over time. For this:

- **Turn off the** "Show detector signals only" option.
- Specify which diagnostic signal you want to record.

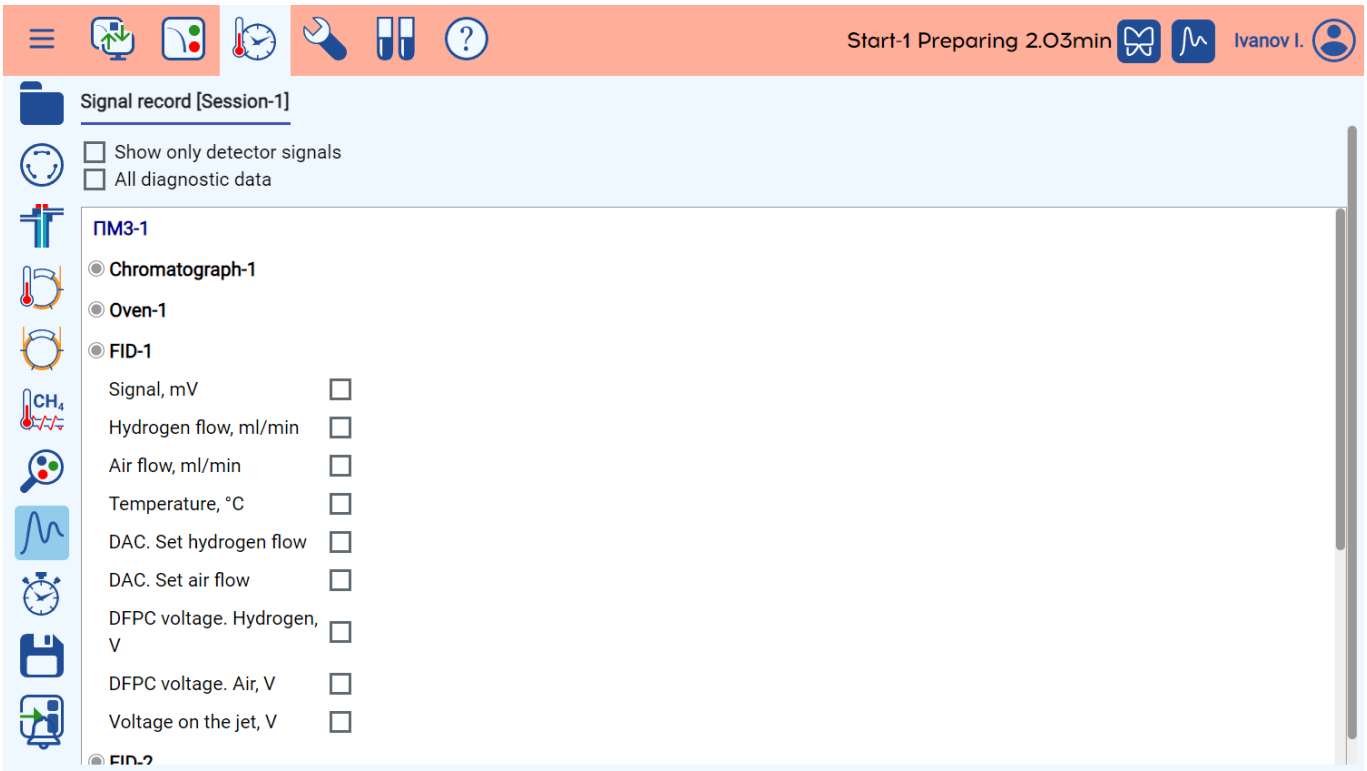


Fig 4.6 – Selection of diagnostic signals

4.4 Runtime Events

Go to the Runtime events section to control and, if necessary, to change the programmable parameters of the mode. Set the **runtime** according to the requirements of the methodology.

In this dialog, the analysis time is set when working with a gas chromatograph equipped with a PM2 processor module or a liquid chromatograph. If the PM3 processor module is installed in your chromatograph, the analysis time will be calculated automatically when you set the temperature program of the oven. In this dialog, the analysis time can be set only if you use the isothermal mode of operation of the thermostat columns.

If necessary, specify the duration of additional time intervals:

Blowing time. The time the chromatograph spends at the "Blowing" stage, which comes immediately after the end of the analysis. By default, the blowing time is 0 (blowing is not used).

Equilibration time. The countdown of this time begins after all the parameters come within tolerance. The stage is used as a delay when the chromatograph goes to the "Ready" stage so that the zero line has time to stabilize.

It is useful to set the stabilization time if an invalid zero-line drift remains after the chromatograph has reached the "Ready" stage. The stabilization time is determined experimentally.

If you hover the mouse cursor over the parameter programming diagram, a hint appears, indicating the duration of the part of the graph over which the cursor is currently located.

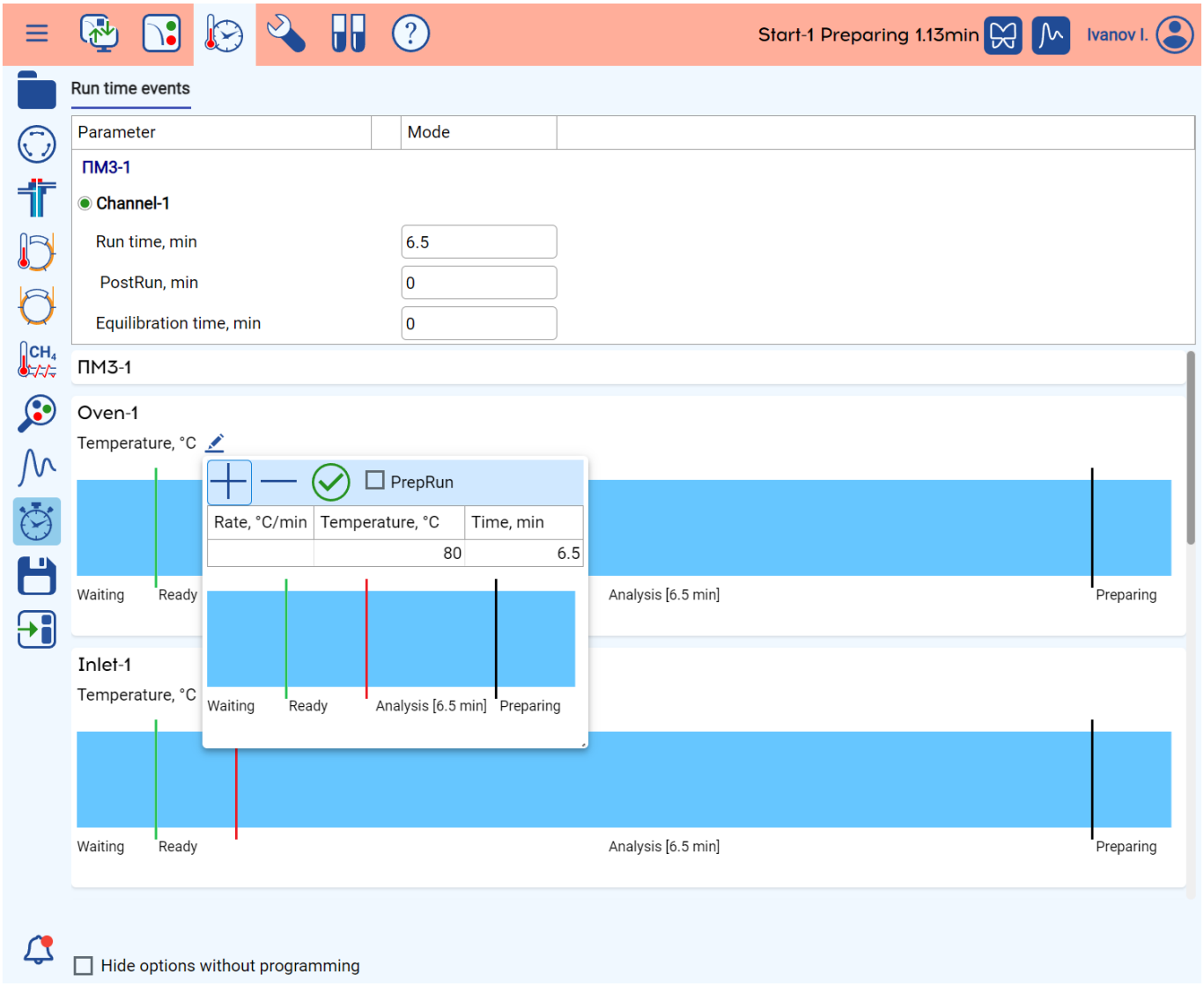


Fig 4.7 – Runtime events

4.5 Save method

When the mode settings are configured, click on the Save button

- Enter the name of the mode file (instrument method).
- Click Save.

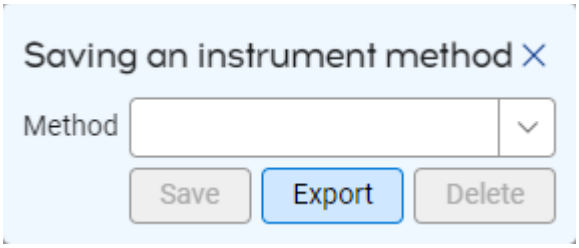


Fig 4.8 – Saving an instrumental method

You can also export the method to a file to download it to your computer. If all computers are on the same network and work with the same server, this operation is not necessary, the method will be available for this connection on any computer.

4.6 Applying of the instrumental method

You can transfer the instrumental method to the chromatograph using the "**Apply**" button. The chromatograph will immediately begin to perform it.

The immediate applying of the instrumental method makes sense when carrying out diagnostic work. In normal work, you do not need to apply the method immediately –when you run a sequence of analyses, the program will apply the instrumental method selected for the first analysis in the queue.

4.7 Load method

You can load methods saved in the connection settings or on your local computer. To do this, click the "Download" button on the sidebar.

- Select a method from the list.
- Click "Download".

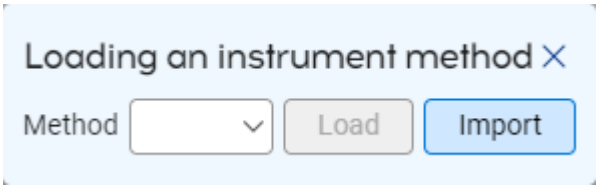


Fig 4.9 – Loading an instrument method

You can also import a tool method from your local computer. File formats supported:

- **mthx** – method of the Chromatek Analyst 3 tool.
- **imthx** – method of the Chromatek Analyst 4 tool.

When the chromatograph is delivered on a USB drive with a software installation package, some instrumental methods may be recorded. In this case, when you click on the "Import" button, a menu appears:

- **Locally**. When you select this option, you will be prompted to open the tool method file from your local computer.
- **From the server**. Selecting this item will open a submenu with a list of methods supplied with the device.

5 STATE MONITORING

To oversee the chromatograph status, go to the **State** page of the main window.

The right side of the toolbar displays the name and time of the current stage.

Legend (see figure below):

All parameters of the instrument are within tolerance.

One or more parameters of the instrument are outside the tolerance.

The instrument is not active (not involved in the configuration or the value of the parameter **Activity = None**).

The parameter whose value is outside the tolerance limits is highlighted in **red** .

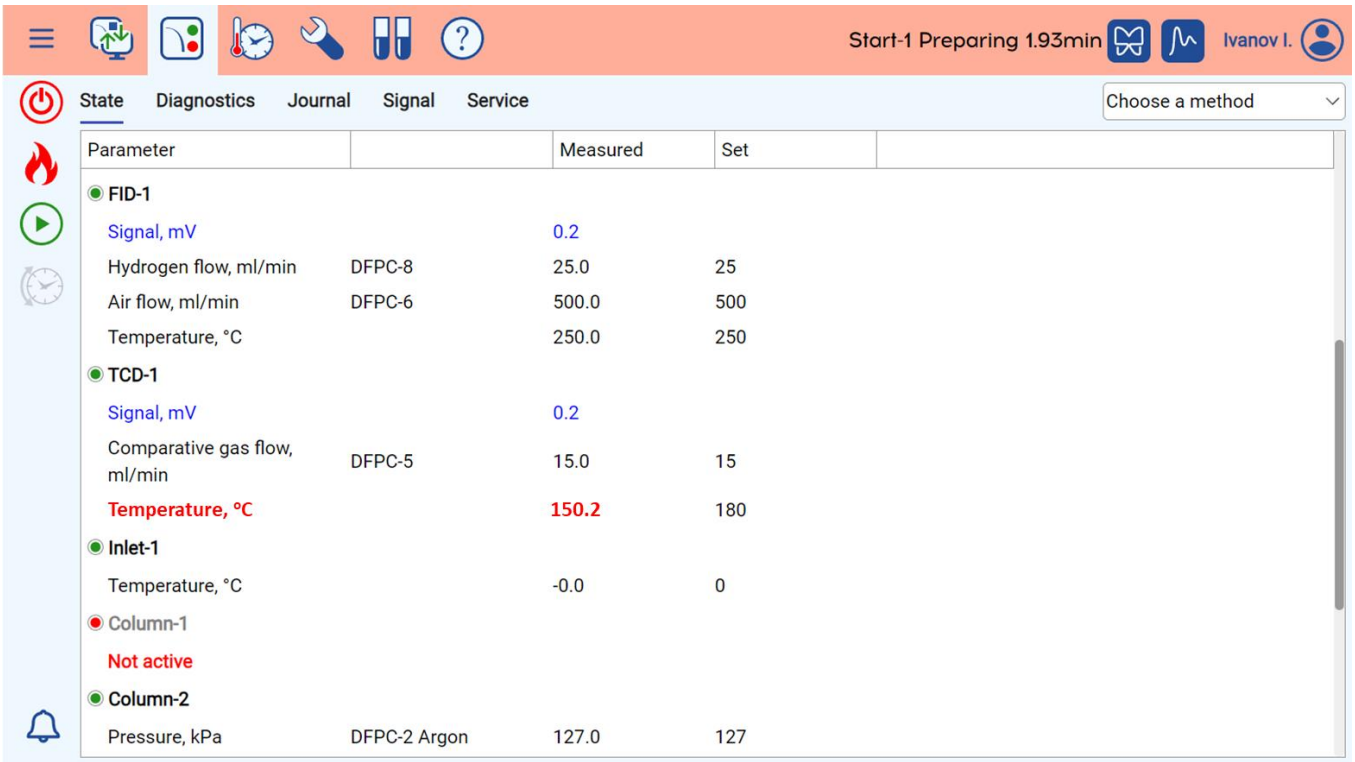


Fig 5.1 – Status of the gas chromatograph with PM3 processor module

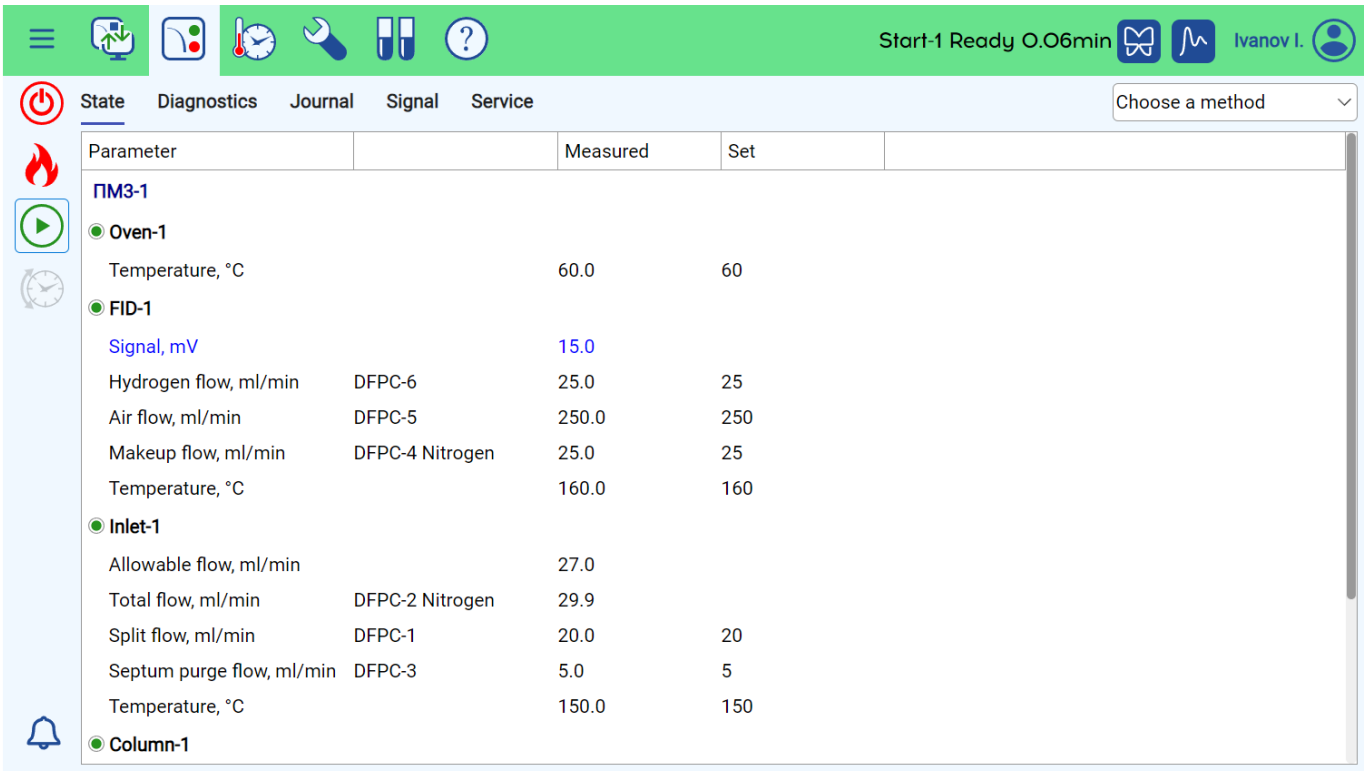


Fig 5.2 – Status of the gas chromatograph with PM3 processor module. Ready state

If you have a mass spectrometric detector, a button is available on the side panel that opens the MSD operations menu:

- **Diagnostics**.
- **Automatic configuration**.
- **Open MS Tune**. The above operations launch automatic procedures, and this command opens the MS Tune application in a new tab. It is used by service engineers for deeper diagnostics and configuration of the MSD.

5.1 Viewing of detector signal

The detector signal can be evaluated on the State page in the table. It is displayed in the header of each detector in blue font.

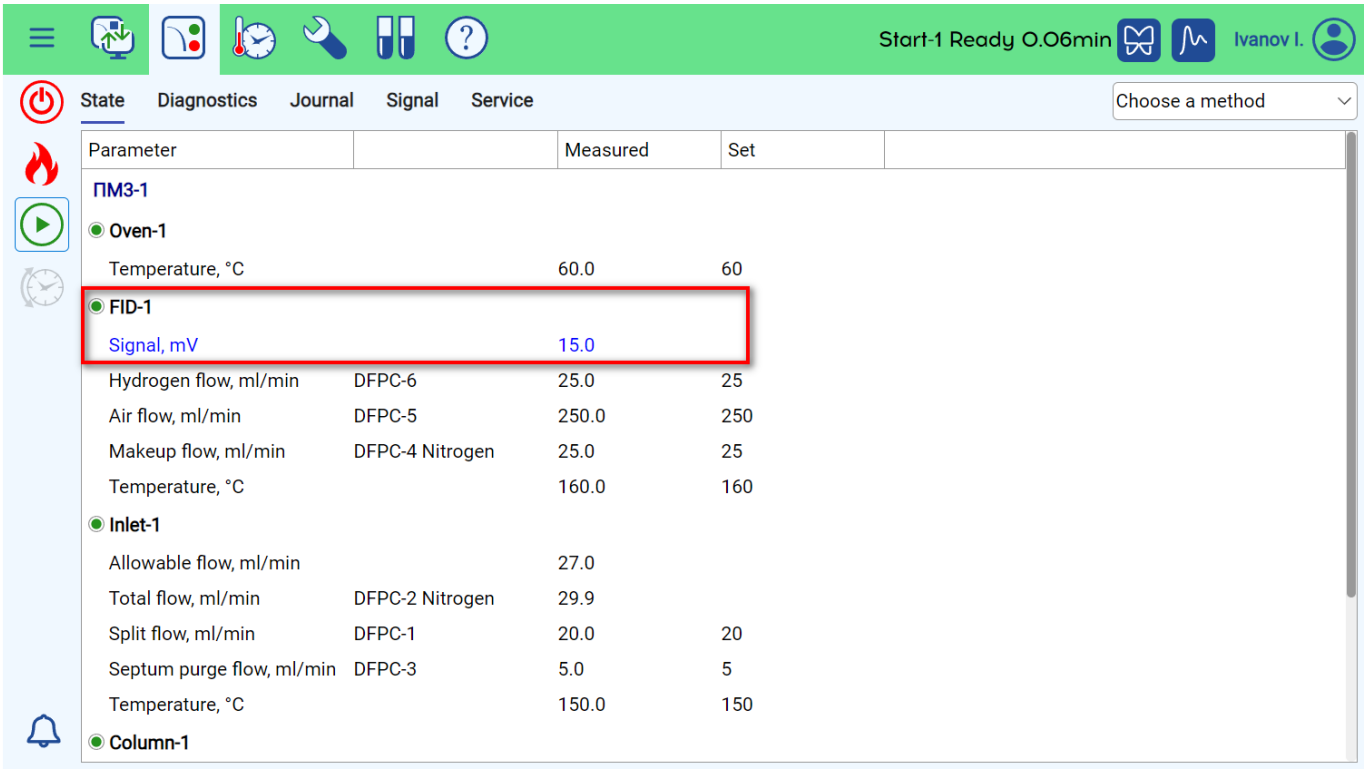


Fig 5.3 – Detector signal

"Control Panel" allows you to view the signals of the detectors and some diagnostic parameters in the form of dynamic graphs. Viewing signals is possible at any time, at any stage of the chromatograph operation.

- For the operational control of a signal, go to the **Signal** tab.
- Select the instrument for which you want to view the signal.
- Select the parameter of interest.

The signal is displayed with a frequency of 1 Hz (i.e., if the data acquisition rate is set to 25 Hz for the detector, then this graph will be shown in a simplified way, with distortions). The frequency is reduced to reduce the consumption of RAM.

The signal can be scaled in the same way as a chromatogram in the "Chromatec Analytic" processing program.

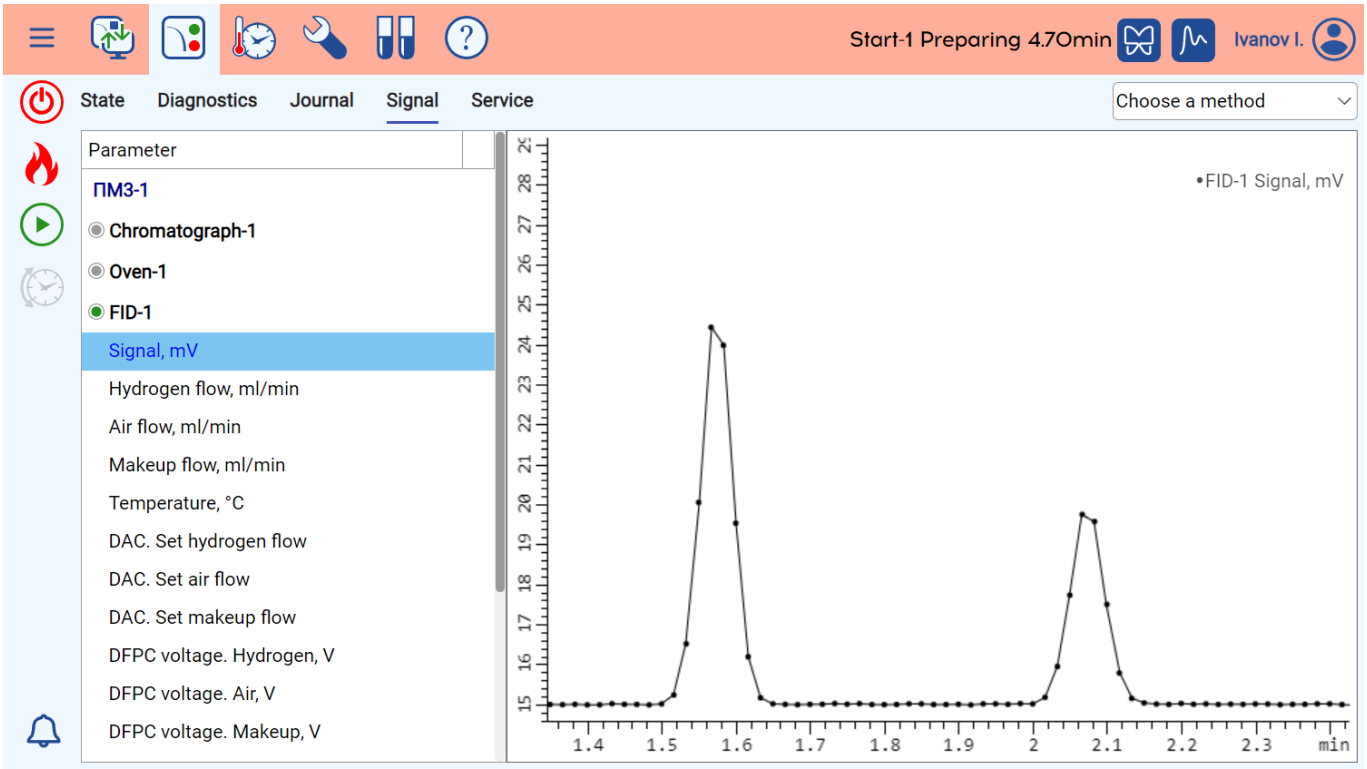


Fig 5.4 – Viewing signals

5.2 Diagnostics

To view the extended state of the chromatograph, go to the **Diagnostics** tab in the "Control Panel". Additional parameters that do not require constant monitoring in normal operation are displayed here.

GC self-diagnostic test is performed automatically all the time. Its results are displayed (depending on the importance of the message):

- On the **State** tab – the most important messages.
- On the **Journal** tab – messages of lower importance that the user can ignore without damage to the equipment.
- In the program log (extended log) – messages for analysis by the developer.

The following parameters are used to control the power supply of the chromatograph:

Voltage, V. Monitoring of the voltage in the 220V mains is available if an additional voltage meter was supplied as part of the instrument.

Low-voltage heaters total power, W. The parameter value should not exceed the transformer power.

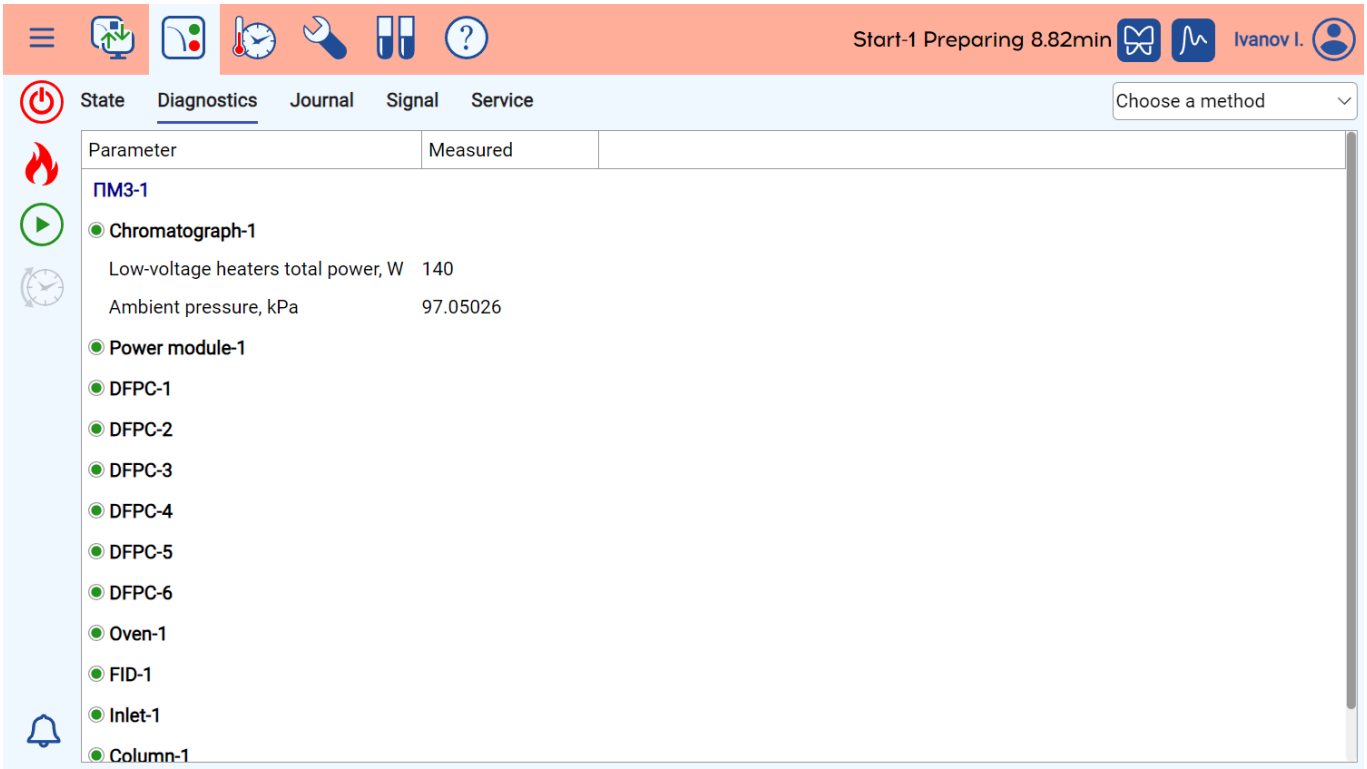


Fig 5.5 – Diagnostics

5.3 Journal

On this tab, you can view the history of chromatograph events that occurred during the current connection session.

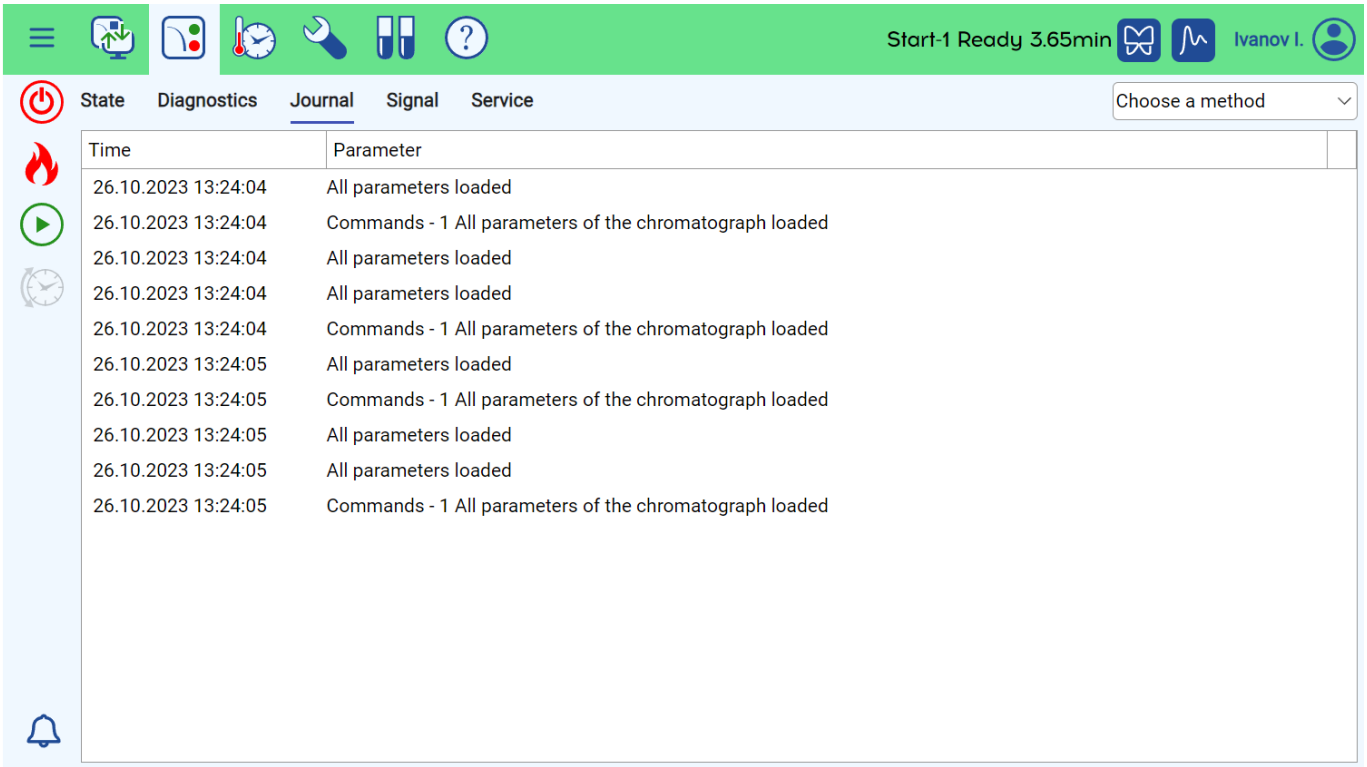


Fig 5.6 – Journal

6 AUTOMATION OF ANALYZES

To set up an analysis plan, go to the Scheduler page.

On this page, you can customize the execution of a **single analysis** or a **sequence of analyzes**.

In Chromatec Analytic 4, the setup of single analyses and analysis sequences is performed the same way. That is, if you need to perform a single analysis, you create a "sequence" from a single analysis.

The sequence is created even if you don't use any automatic samplers.

6.1 Scheduler interface

On the Scheduler page are located tabs:

- **Analyzes.** Here is the list of analyzes performed by the sampler is set – the work plan.
- **Journal**. Messages about the statuses of samplers and performed analyses are displayed here.
- **<Sampler name>**. Here the parameters of the dispenser are set. This tab is present only if there is any dispenser specified in the connection settings.

Side toolbar buttons:

Start. Clicking this button **starts the execution sequence**.

Pause. Clicking this button pauses the execution of the sequence. With this, the currently running analysis will be completed, and the next one will not start until the **Start** button is pressed again.

Stop. Stop The plan stops working, and the current analysis also stops.

Repeat sequence. Once completed, the plan will be repeated until the operator presses **Stop**. Turning off this mode will cause the plan to be finalized until the end, after which it will stop.

Add analysis. This button adds a new row to the list of analyzes. The new row is a copy of the previous one.

Delete analysis. Delete analysis.

Additional command and settings. Open auxiliary menu.

On the **Analyses** tab there is a table where the parameters of the sequence of analyses are set. The columns in the table are grouped by purpose. For the convenience of scrolling the table horizontally (if it does not fit into the screen), you can use the quick jump buttons:

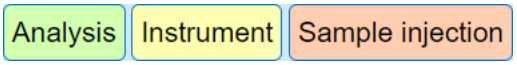


Fig 6.1 – Quick jump buttons

This button opens a drop-down list in which the operator can turn on or off the display of certain columns in the table..

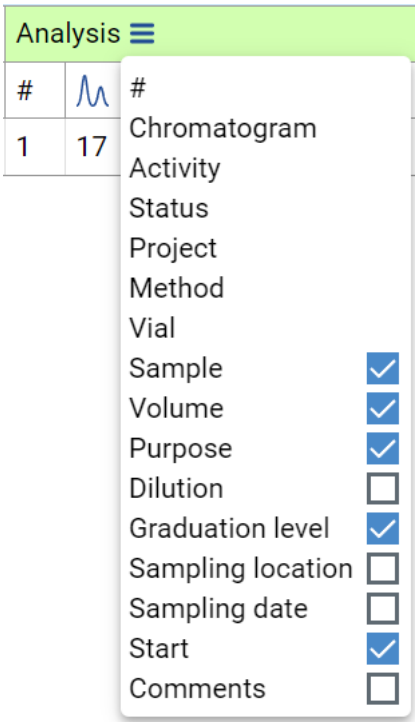


Fig 6.2 – Configuring Column Display

6.2 Sequences of analyzes

A sequence of analysis is a group of several analyses performed by the program at a certain time.

By default, the plan contains a sequence of analyses performed when the chromatograph is ready (if the plan is started for execution with the "Start" button).

The operator can add an unlimited number of analysis sequences. This is usually done in order for the "**Scheduler**" to perform some analyses at a certain time.

Click the **Settings** button ".

- Select the menu item "Add sequence".
- Select the type of series – **On readiness** or **By time**.
- For the "**by time**" sequences, specify on which days to perform it and set the start time of execution.

You can turn off the activity of the sequence if it is not needed now.

It is convenient to collapse the sequences that are not executed so that they do not take up space on the screen.

If the sequence is no longer needed, delete it.

In each series, there can be an unlimited number of analyzes.

When starting, "Control Panel" sequence checks whether the runtime of any series has come up.

- If the runtime has come up, then the analysis of this series begins. Until all of them are completed, the "Control Panel" does not move to the next series.
- If the execution time of the next series has not yet come up or the series with a fixed time is not in sequence, then the first one in the list is executed with the sign "On readiness".

For example, three sequences are created:

- On readiness
- Mondays at 08:00
- Every day at 8:00

Here, when you start the sequence, "Control Panel" checks what day of the week is it. If Monday, the current time is checked. If it is not 08:00, the "Control Panel" checks the conditions for the third sequence. Since they are not fulfilled, it proceeds to the first sequences, "On readiness " and carries it out.

When the conditions for two sequences are fulfilled simultaneously (in the example above, on Monday, at 10:00, the conditions for series 2 and 3 are satisfied), they are executed in order from top to bottom.

6.3 Analysis parameters

These parameters are configured in the "Analysis" cell group.

- Go to the "Analyses" tab.
- By default, only one sequence of analyses is set – "On readiness". If necessary, add additional series and select the desired one.

Add a new analysis. You can add analyses not only one by one, but also 5, and you can also specify any number of analyses to be added by selecting the appropriate item in the menu of this button.

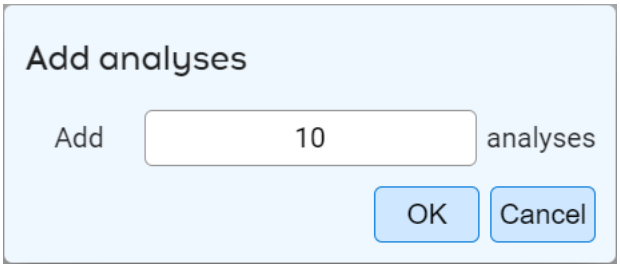


Fig 6.3 – Adding any number of analyses

- Create a project or select an existing one.
- Create a new (empty) processing method. A new method is created during the initial setup. In the future, you can choose an existing method to edit it.

{video sequence_create}

- Fill out the analysis passport.

{video sequence_sample}

If you use internal standards, or in the sample there are undetectable components, or it is necessary to assess the accuracy of the analysis, set in the passport the known concentrations of the components. See more...

6.4 Instrument parameters

These parameters are configured in the "Instrument" cell group.

- Create a instrumental method (or multiple methods if necessary).
- Select the created instrumental method.

{video sequence_imethod Sequence instrument method}

6.5 Sample injection parameters

These parameters are configured in the group of cells "Sample injection".

Sample injection into the chromatograph can be performed:

- manually by the operator,
- by device built into the chromatograph (a sampling valve, piston injector).
- by external sampler.

The external sampling device (AS-2M, TDA, etc.) is traditionally called "Chromatec" "periphery".

We will consider the first two input options as injection without peripherals.

{video sequence_sampler Sampler}

The sequence may simultaneously contain analyses with different devices – with AS-2M, TDA or without peripherals.

For example, if you are working with AS-2M if you need to perform an idle analysis from time to time, then you should add an analysis "**No peripheral**".

6.5.1 Sample injection without peripherals

If the injection will be performed manually by the operator, then you should set the injection mode = "**Waiting for start**".

When executing the plan, as soon as the queue reaches the analysis, in the settings of which "Waiting for start" is selected, the software expects the operator to manually enter the sample with a syringe or a valve and press the "Start" button on the chromatograph.

If the chromatograph contains built-in automatic sample input devices (sampling valve, piston injector), then the injection mode = "**Automatic start**" should be set.

6.5.2 Sample injection using automatic samplers

The program supports the following types of peripherals (sampler models):

- AS-2M with a rotary tray for 14 samples.
- AS-2M with the rotary tray for 18 samples.
- AS-2M with the rotary tray for 24 samples..
- AS-2M 3D with the tray for 150 samples.
- AS-2M 3D HSS (with headspace and liquid options).
- AS TDA (thermal desorber automatic).

In more detail, the methods of sample input and the algorithms of the samplers are described in the corresponding user manuals.

The operator can create an unlimited number of operating methods for each sampler, which are stored separately from the instrumental method files.

To add a new injection method:

- Go to the **<Sampler Model>** tab. For example, it can be called **AS-2D-127.0.0.1:400** (sampler IP-adress is indicated here). The default method settings will open.
- Click the "Create Method" button.
- Specify the name of the sample injection method.

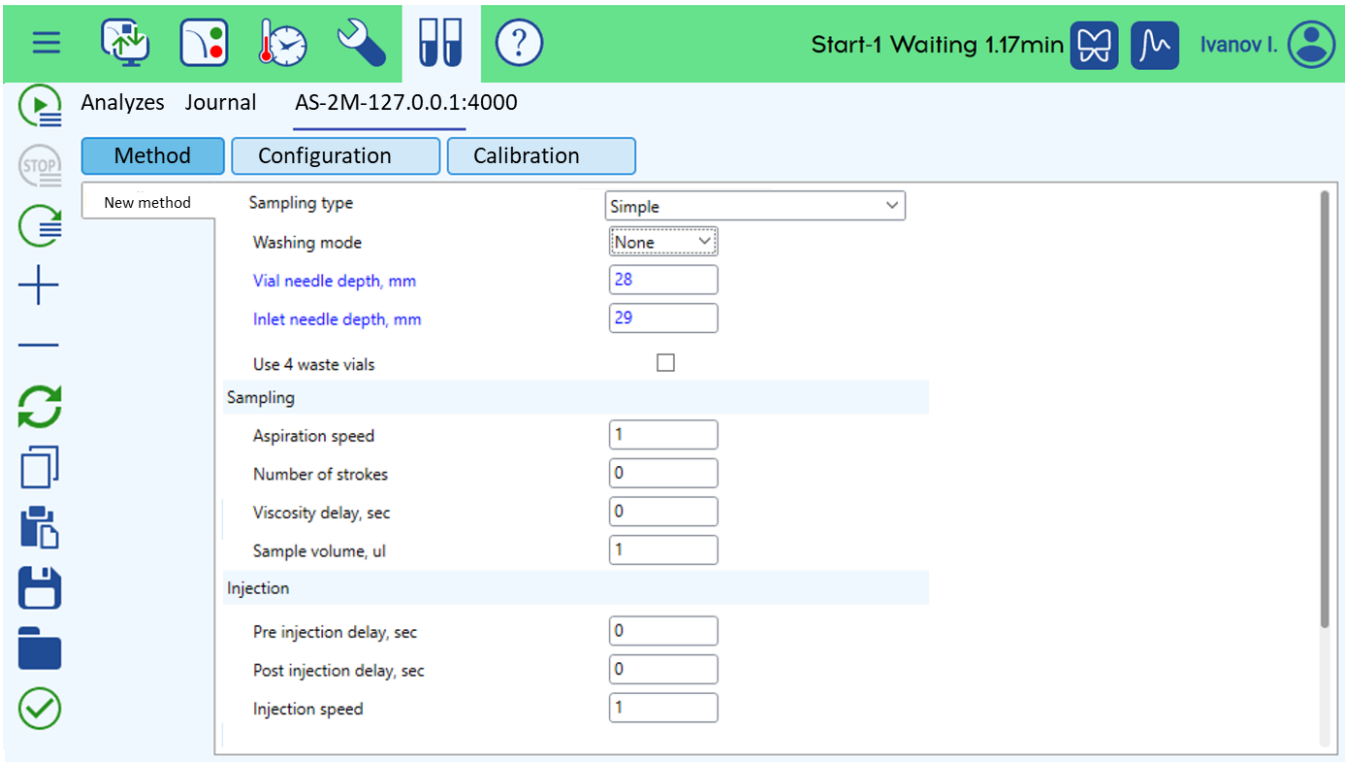


Fig 6.4 – Sample injection using automatic samplers

When working with AS-2M 3D HSS, preparation for sample injection of each next analysis begins even before the completion of the previous one. This was done to reduce the total analysis time, since such an autosampler is characterized by a long temperature control time for the vials. To make it easier to control the current stage, there is an operation diagram above the list of analyzes:

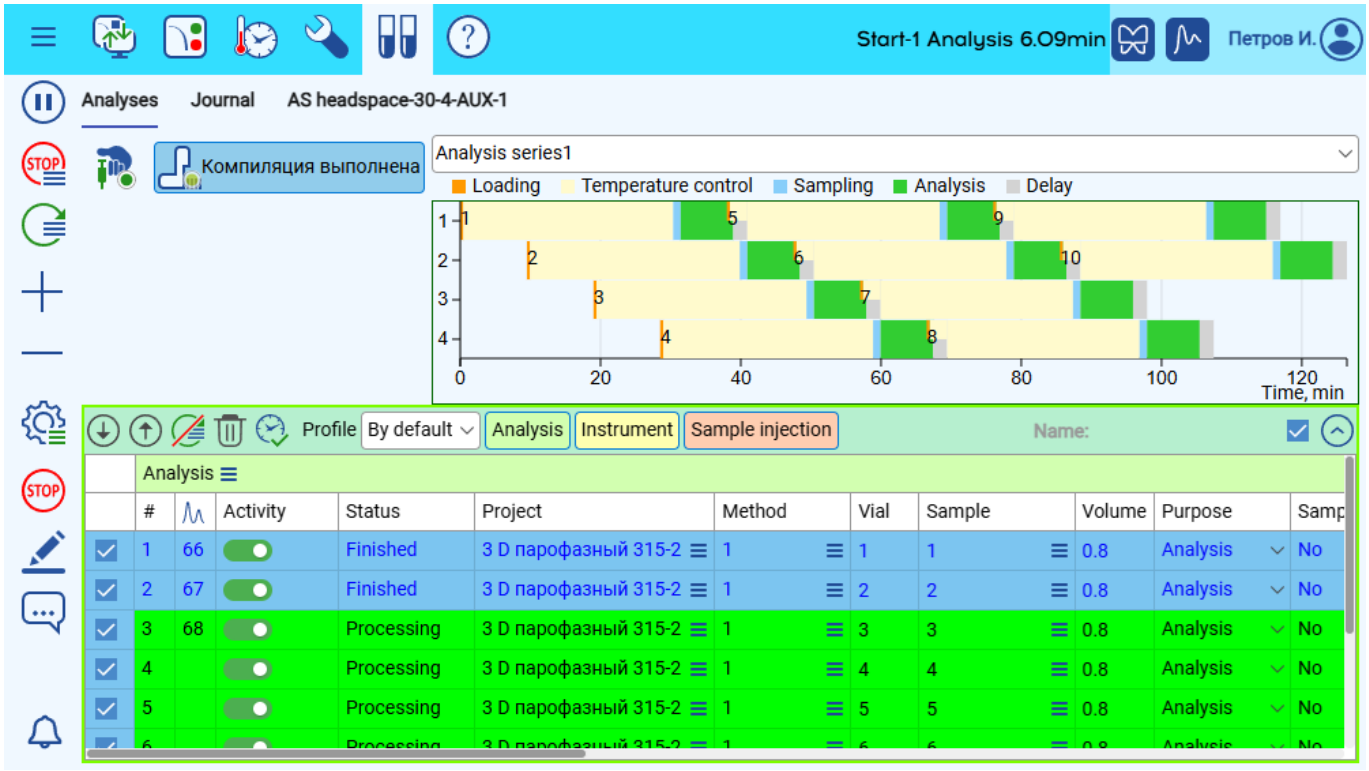


Fig 6.5 – Diagram of operations with the DAZH-2M 3D HSS

6.6 Group operations

6.6.1 Build calibration

When a group of analyzes is completed, "Schebuler" can build a new calibration method based on them and analyze its acceptability.

To do this, follow these steps:

- Select the calibration chromatograms in sequence.
- Click the right mouse button and select from the menu: **Group operations / Build calibration**.
- A new “Scheduler” tab will appear – "Build calibration". Go to it.

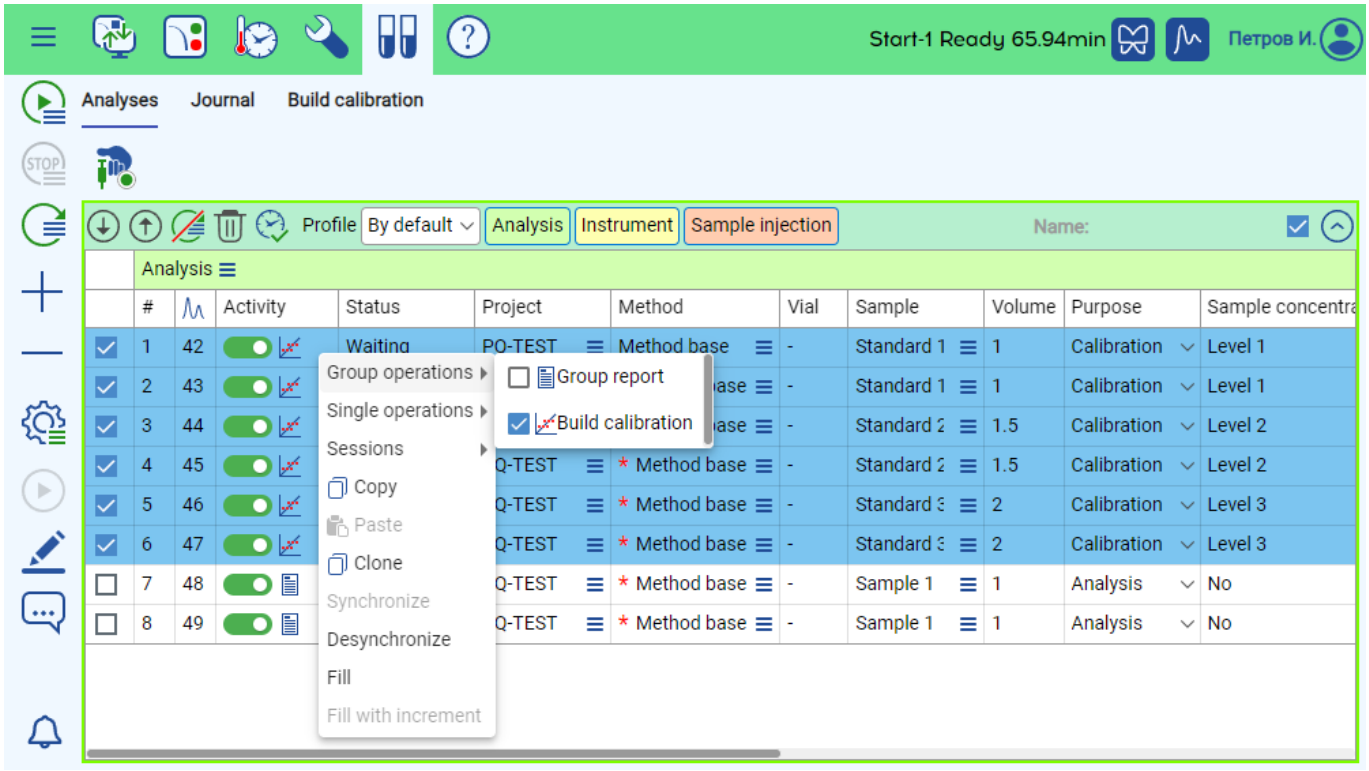


Fig 6.6 – Adding a group operation "Build calibration" for selected calibration analyzes

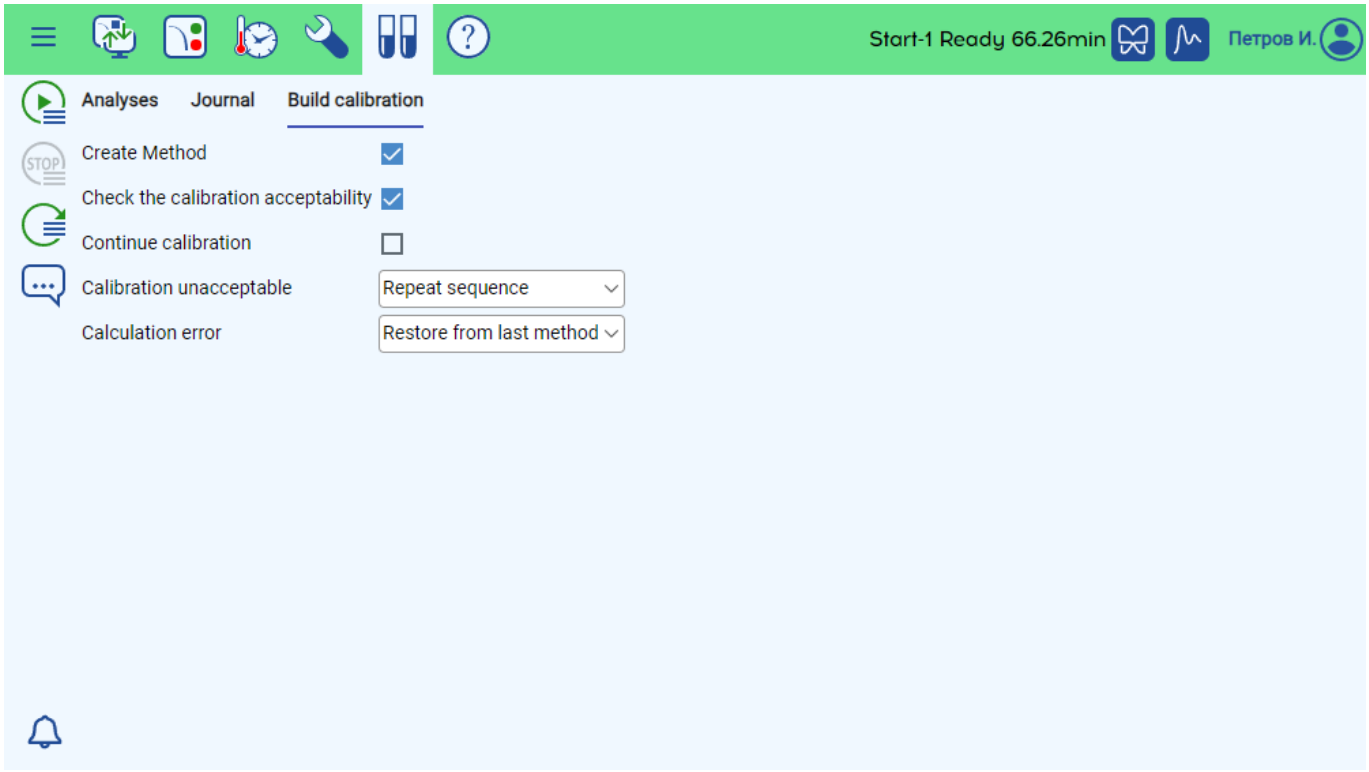


Fig 6.7 – Build calibration settings

The following options are available here:

Create a method. If the option is enabled, a new method will be created based on the base one and the calibration chromatograms recorded during the execution of this sequence will be included in it. If the

option is disabled, calibration chromatograms will be included directly in the base method, which is indicated in the corresponding lines of the plan (in this case, those calibration chromatograms that were previously there will be deleted).

It is recommended to always enable this option to avoid losing basic methods.

Check the calibration acceptability. When building a report, "Analytic" always returns an indicator of calibration acceptability. If the report does not contain specific calculations that analyze acceptability, then the result will be acceptable. If there are such calculations and this option is enabled, the "Scheduler" will react to the result obtained and perform the actions specified by the "Calibration unacceptable" option (see below).

Continue calibration. If the option is enabled, then calibration points inherited from the base method will not be cleared; new ones will be added to them.

Calibration unacceptable. This option instructs the "Scheduler" on what to do if the “Analytic” reports that the calibration is unacceptable:

- Repeat the sequence.
- Repeat the last analysis.
- Stop sequence execution.

Calculation error. If an error occurs, the "Scheduler" can:

- Restore from previous method. In this case, all new calibrations are discarded and new chromatograms will be processed using the basic method.
- Continue with the current method. Errors are ignored.

6.6.2 Group report

Once the analysis sequence is complete, you can automatically generate a report.

To do this, follow these steps:

- Select the required tests in sequence.
- Right-click and select from the menu: Group operations / Group report.
- A new “Scheduler” tab will appear – "Group report". Go to it.

Here you can select a report template.

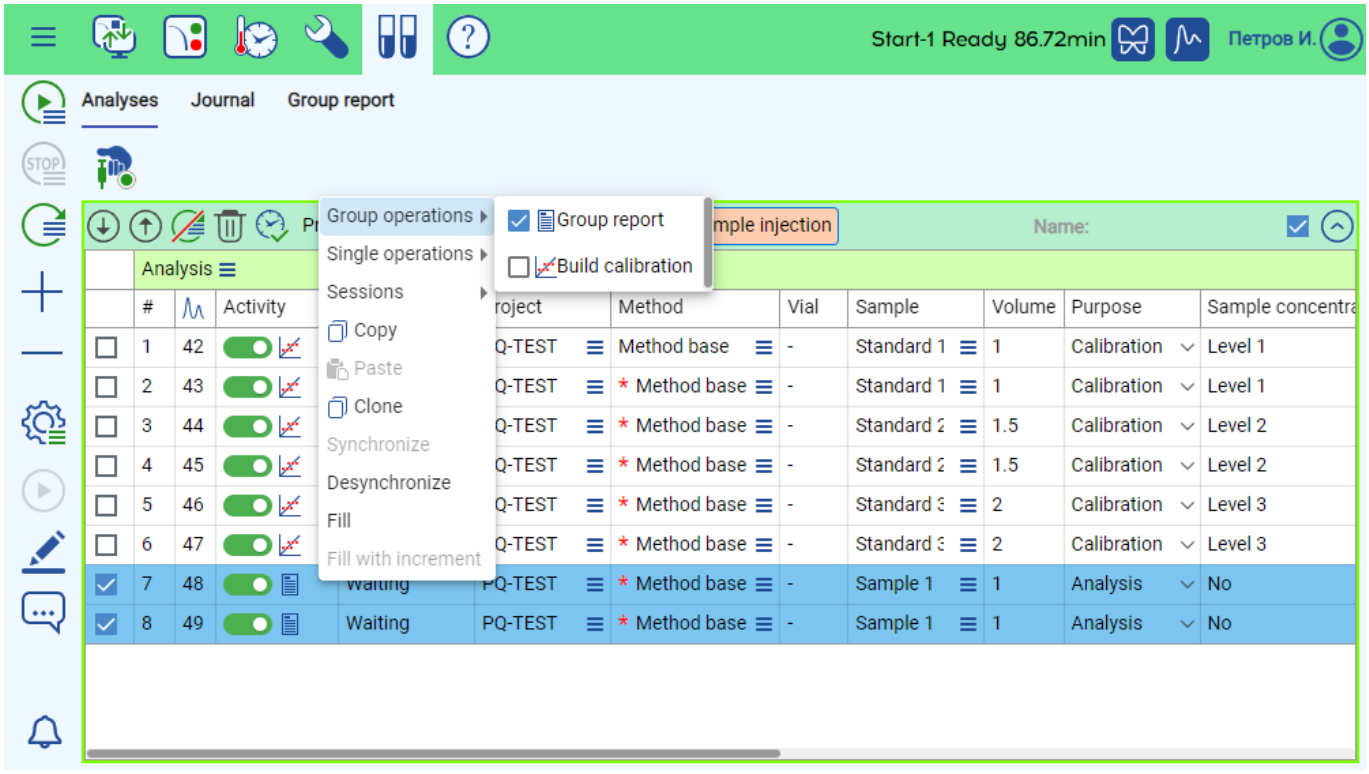


Fig 6.8 – Adding a group operation "Group report" for selected analyzes

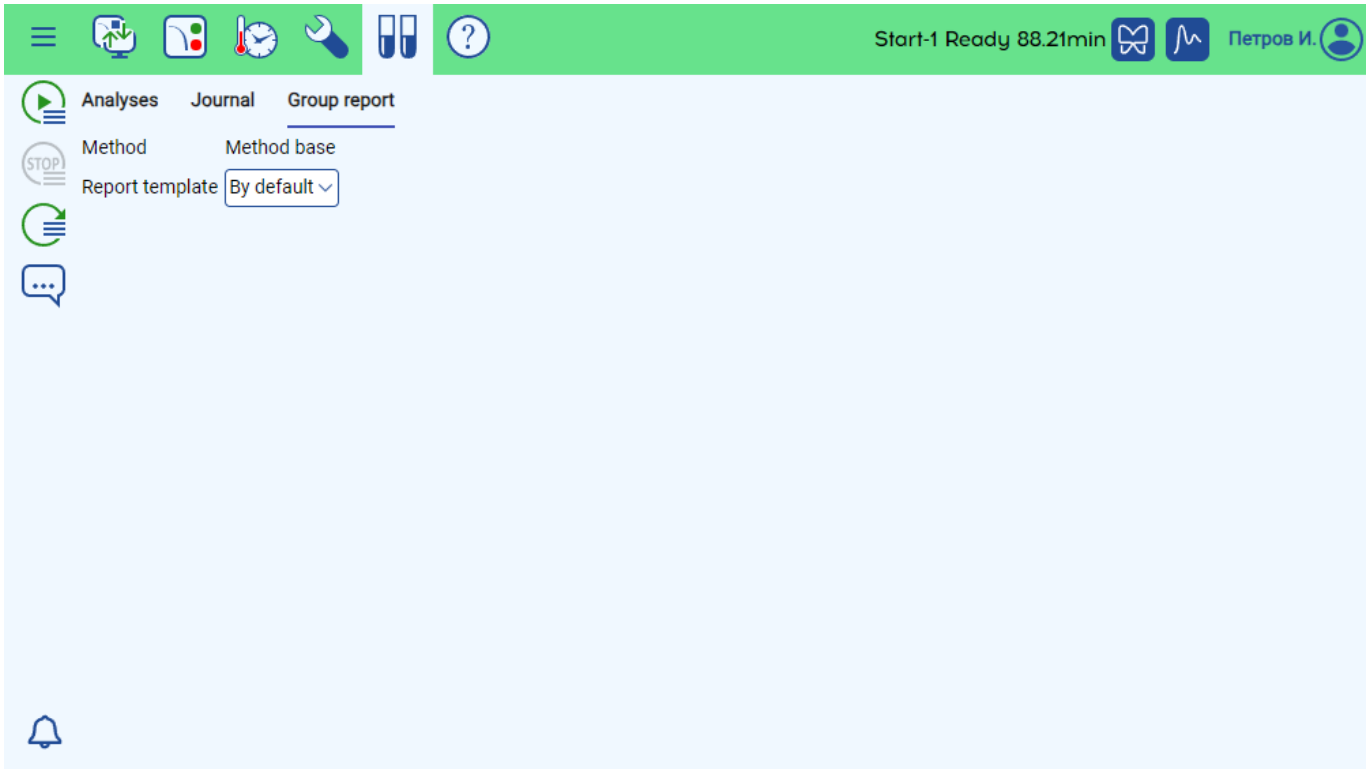


Fig 6.9 – Group report settings

7 SERVICE

7.1 Using an uninterruptible power supply

When using an uninterruptible power supply (UPS), it is necessary to enable tracking its charge.

To perform these settings, turn on the expert mode:

Open the main menu of the "Control Panel".

Enable the "Expert Mode" option. A red frame will appear around the window.

Go to the page "Status" of the "Control panel" main window and then – to the "Settings" tab

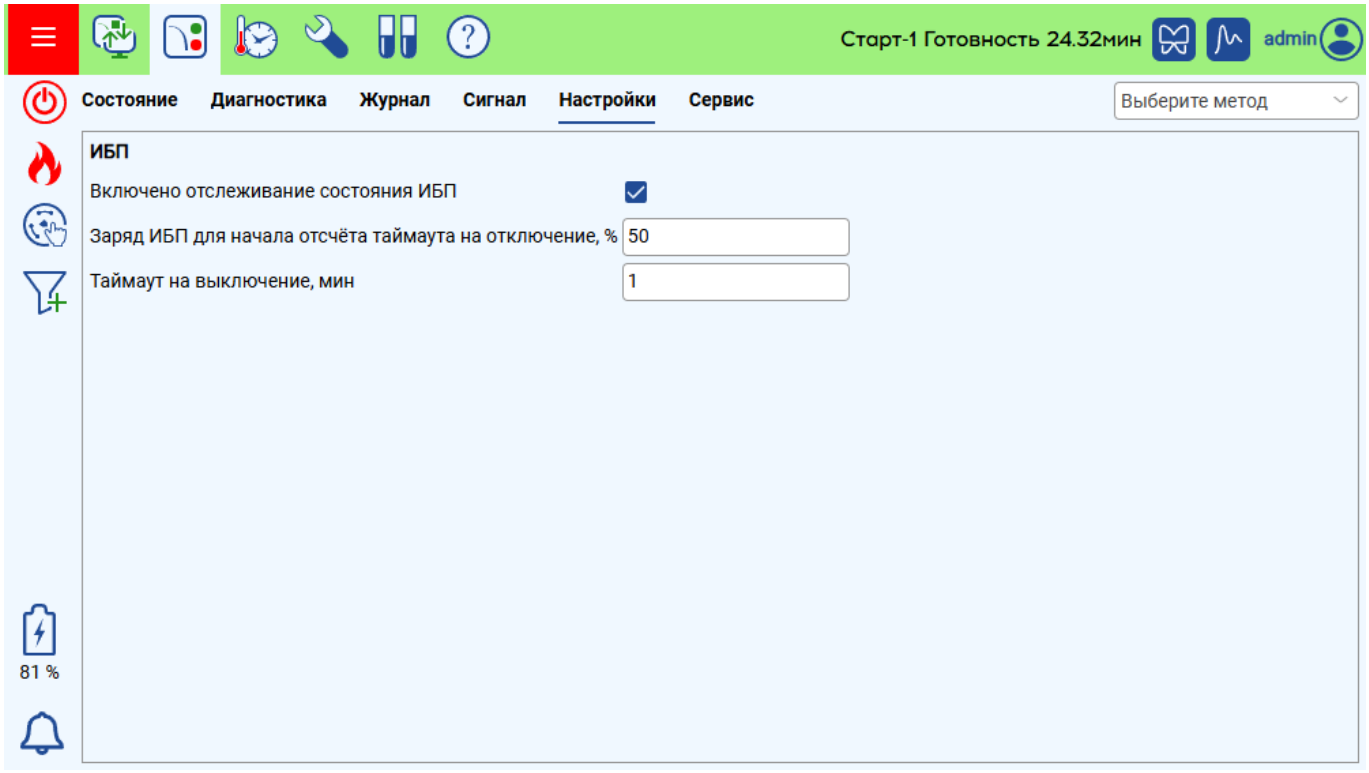


Fig. 7.1 – UPS settings

- Turn on the monitoring of the condition of the UPS.
- Wash the percentage of the UPS charge to start the countdown of the time off (100%by default).
- Set the duration of the time in minutes.

When the UPS switches to the battery from the battery and its charge percentage reaches the value set in setting up, the time is counted, after which the command is sent to safe shutdown of the chromatograph and mass spectrometric detector.

- The chromatograph starts cooling with the subsequent shutdown.
- Mass-spectrometric detector disables the pump.

Pay attention – the computer will also be turned off!

The UPS charge indicator is displayed in the lower left corner of the "Status" page.

7.2 Maintenance

"Control Panel" allows you to set up a reminder of the need for routine maintenance. To set up a memo, go to the **Maintenance** tab.

On this tab, enable the activity of maintenance operations you want to be reminded about.

For each operation, specify the period of time after which the program will offer to conduct it, or the number of samples injected.

In addition to tracking these counters, the program responds when the detector signal exceeds the permissible value, if it is set. You can set a valid signal value for each detector in the expert configuration settings.

When the limit value of a counter is reached or when the chromatograph reports that the permissible signal of the detector has been exceeded, "Control Panel" window is displayed on top of the other windows with the "Maintenance" tab active.

Perform the suggested maintenance and close the message.

The message about exceeding the permissible signal of the detector cannot be closed! It will disappear itself when the detector signal enters the limits of the allowable range.

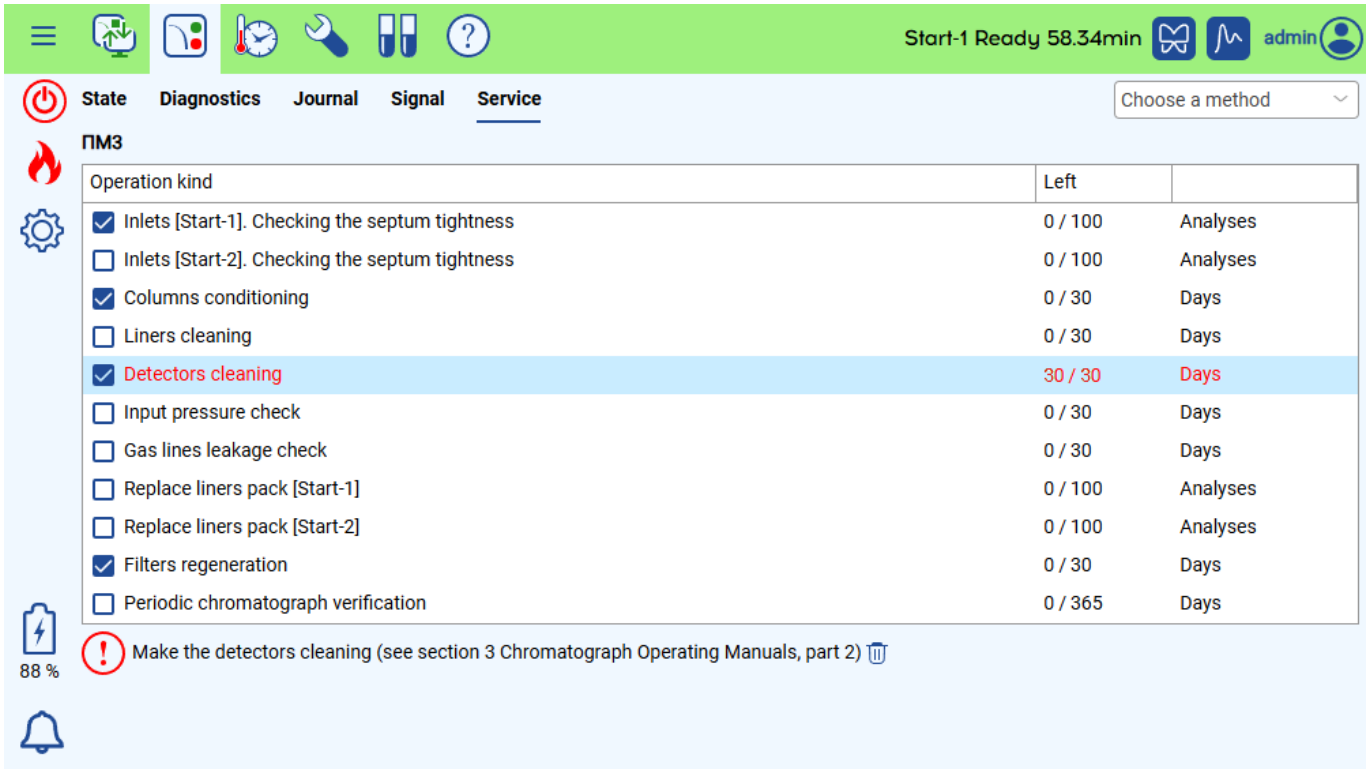


Fig. 7.2 – Messages about the need for maintenance

8 SHUTDOWN

In the "Control Panel", go to the **State**.

Click Stop in "Control Panel". The dialog shown in the figure below appears on the screen:

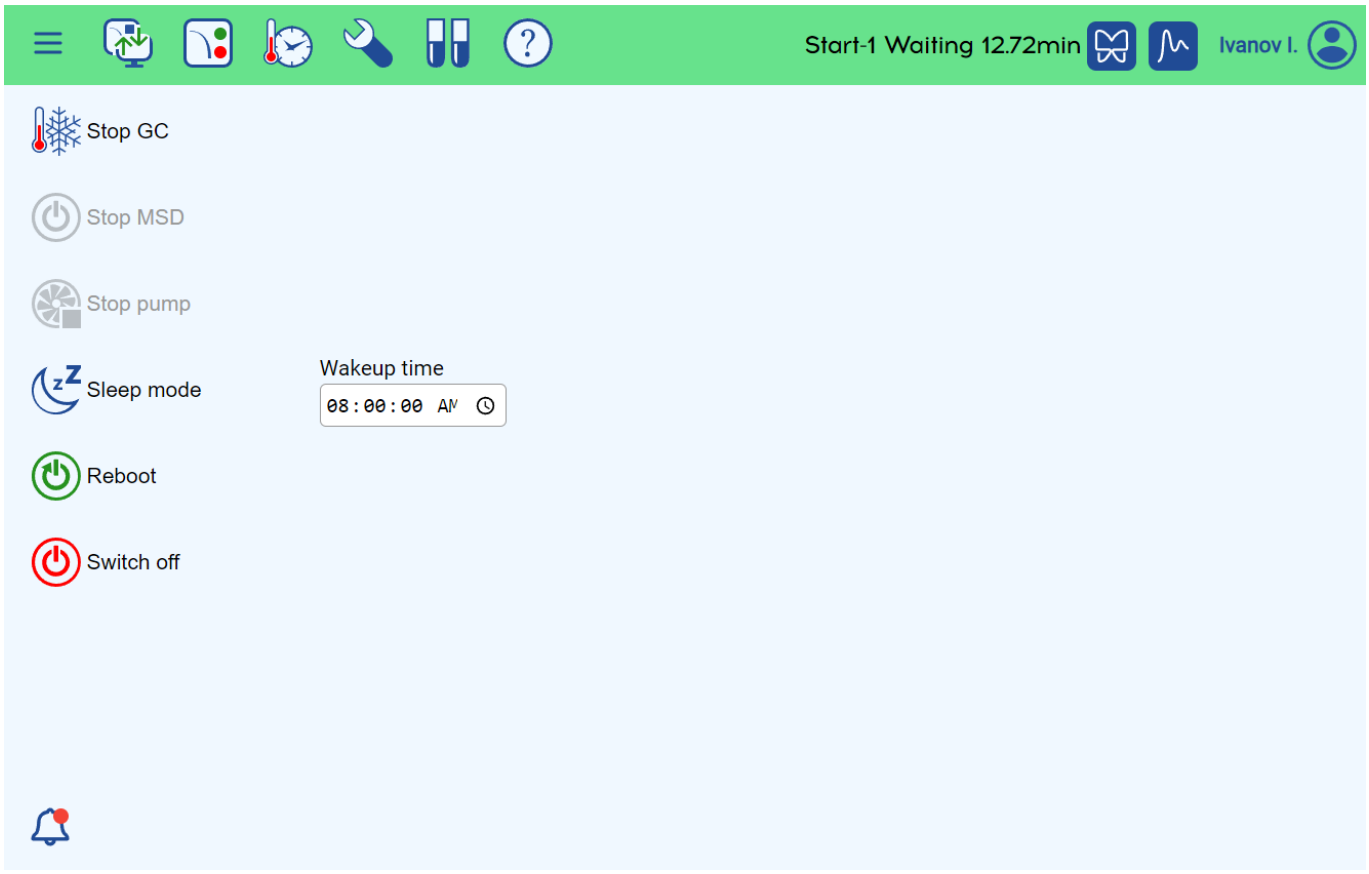


Fig 8.1 – Shutdown page

GC Cooling. To cool the gas chromatograph, click on the appropriate button. Chromatograph will go to the "Cooling" stage. Control the temperature of the oven on the **State** tab of the "Control Panel". When the temperature of the oven reaches 50°C, the chromatograph can be turned off

Stop MSD. To stop MSD, click the appropriate button. After confirmation of the command, the pump will be stopped, cooling of the ion source and the transition line will begin.

Stop pump. When working with a HPLC chromatograph, press the appropriate button to stop the pump.

Sleep mode. You can put the chromatograph in this mode for the night, so that in the morning it will automatically resume work and be ready for testing by the specified time.

In this mode, all heaters are turned off, the valves of gas regulators are closed (gas consumption is stopped). The chromatograph enters a low power state. Only timer works.

Reboot. Allows you to restart the instrument.

Upon reaching the specified time, the chromatograph is awakened. If the configuration settings indicate which methods to load during power on/wakening-up, these methods are processed.

Thus, the sleep mode allows you to bring the chromatograph to readiness and carry out the necessary preliminary purging of the system by the beginning of the working day. Of course, the power supply for the night should not be turned off.

To enter sleep mode, set the wake-up time and click the appropriate button.

In sleep mode, the connection with the chromatograph will be broken, but if the user does not close the "Control Panel" and does not turn off the computer, then upon waking up, the connection will be automatically restored.