

SOFTWARE

CHROMATEC ANALYTIC

BUILD 4.0

USER MANUAL

214.00045-51I

APPLICATION CALCS. PLUGINS

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1 INTRODUCTION

Application calculations are added to the report sections formed in accordance with the requirements of the selected regulatory document.

The following special calculations are implemented in Chromatec Analytic:

ASTM D2421-21e1	EN 15199-2-2020	GOST 34723-2021 (change №1)
ASTM D2598-2016	EN 15199-3-2021	GOST 34858-2020
ASTM D2887-2022	EN 15199-4-2015 (0°C)	GOST 35228-2024
ASTM D2887-2024	EN 15199-4-2015 (35°C)	GOST 35228-2024 Appendix D
ASTM D3588-98 (2017)	EN 27941-1994	GOST 50802-2021
ASTM D5134-2013	EN 589:2009	GOST 50802-95
ASTM D5307-1997	ISO 15403-1:2006	GOST EN 13132-2012
ASTM D5442-2017	ISO 6974:2000-2002	GOST EN 589-2014
ASTM D6352-2019	ISO 6976:1995	GOST ISO 8973:2013
ASTM D6352-2024	ISO 7941:1988	GOST P 52087-2018
ASTM D6729-2020	ISO 8973:1997	GOST P 53367-2009
ASTM D6730-2019	ISO/TR 22302:2014	GOST P 54484-2011
ASTM D6733-2001	GOST 10679-2019	GOST P 57851.1-2017
ASTM D7096-2019	GOST 10679-2019 (change №1)	GOST P 57851.2-2017
ASTM D7096-2025	GOST 27577-2000	GOST P 57851.3-2017
ASTM D7169-2011	GOST 28656-2019	GOST P 57975.1-2017
ASTM D7169-2018	GOST 31369-2008	MI FR 1.21.2014.18560
ASTM D7169-2023	GOST 31369-2021	М-МВИ-263-12
ASTM D7213-15 (2019)	GOST 313717-2020	P Gasprom 5.9:2010
ASTM D7213-2023	GOST 313717-2020 (change №1)	ST KR ASTM D 2598-2015
ASTM D7500-2015	GOST 32507-2013 Method A	СТ РК ИСО 8973:2004
ASTM D7500-2024	GOST 32507-2013 Method B (0°C)	STB EN 589-2008
ASTM D7900-2023 (0°C)	GOST 32507-2013 Method B (35°C)	STO 03-7.76-2016
ASTM D7900-2023 (35°C)	GOST 32918-2014	STO Gasprom 5.5 Method A
ASTM D7900-2025 (0°C)	GOST 33012-2014 Method V	STO Gasprom 5.5 Method B
ASTM D7900-2025 (35°C)	GOST 33690-2015	STO Gasprom 5.6
BS EN ISO 8973:1999	GOST 34704-2020	FR 1.31.2020.37947
DIN EN 27941-1993	GOST 34723-2021	FR 1.31.2024.47968
DIN EN ISO 8973:2000	GOST 34723-2021	

... etc., the list will be updated.

In addition, Chromatec Analytic can perform repeatability calculations, display input data and a chromatogram graph. Calculations are added to the queue and performed sequentially, forming a single report that can be created in formats:

- HTML
- PDF
- XLSX
- TXT
- CSV

If necessary, reports can be created in all these formats at the same time.

2 OBTAINING A LICENSE

Most of the calculations included in the "Application Calculations" application are protected from unauthorized distribution by a software key.

To use these calculations, you need to get a license file.

If you have previously used "Chromatec Analytic 3.1" software and received a license for application calculations, this fact will not prevent you from obtaining a license for " Chromatec Analytic 4".

The license files for versions 3 and 4 are different. Licenses for version 3 are tied to a certain computer identifier (calculated based on the processor serial number). The license for version 4 is linked to the chromatograph serial number.

This means that for version 3 you need as many licenses as you use computers to work with the chromatograph, and for version 4 you get one license per chromatograph and can work with it from any computer.

Obtaining a license:


On the Chromatec Navigator desktop, click on the Licenses button. The license request page opens.

To create a license request, enter:

- Password. It is in a box with a USB drive. If it is not there, make sure that you have purchased a package of special calculations. You can clarify this issue in the commercial department of SDO "Chromatec" by phone +7(8362) 68-59-69 and 7 (8362) 68-59-70.
- Your email. A license file will be sent to it.
- List the serial numbers of your devices separated by commas.


Add the IDs of the calculations for which you want to receive a license.

When purchasing a package of special calculations, you can choose up to four of any calculations. We recommend that when requesting a lcense, immediately select all the requests that you need


If your computer is connected to the Internet, click on the "Activate license online" button. ".

If the online activation failed, you will receive a message:

"License activation denied. Most likely, you have already activated all available licenses. If this is not the case, correct the email request string soft@chromatec.ru ".

In this case, use offline activation.

Offline activation is also available when there is no internet.

A QR code will appear on the screen. You can scan it with your smartphone and get a link. Following this link, you will send a request to Chromatec". Upon successful activation, the license file will be downloaded to your smartphone. All you have to do is transfer it to your computer and activate it (see below).



If for some reason you cannot use QR codes, copy the query string to the clipboard and send it to any of the addresses:
soft@chromatec.ru
support@chromatec.ru



When the license file *.lic is sent to you by email (or you download it from your smartphone), click on the "Activate license offline" button and select this file. The license will be activated.

{video navigator_license License}

3 SETTING UP APPLICATION CALCULATIONS

The result of performing application calculations are additional sections of reports, so to apply application calculations, they need to be added to the report.

the video below shows an example of setting up calculations according to GOST 31371.7-2020 and GOST 31369-2021:

{video combine_settings App calculatios}

3.1 Error/uncertainty calculation

Some regulatory documents require attributing to the averaged result an error or uncertainty calculated from simple linear or exponential equations.

For this calculation, you can use the preset settings by selecting a regulatory document from the list, or create your own if your regulatory document is not in the list.

The procedure for configuring the report is shown in the video below.

{video method_report_uncertainty Uncertainty}

3.2 Repeatability control

This calculation makes it possible to assess the acceptability of convergence of the results of single measurements. The standard is given by a simple linear or exponential equation.

You can use the preset settings by selecting a regulatory document from the list, or create your own if your regulatory document is not in the list.

The procedure for configuring the report is shown in the video below.

{video method_report_repeatability Repeatability}

3.3 Input data

The section outputs a table of input data in the form:

Component	#7	#8	#9	Amount
methane	82.090	82.090	82.090	3
carbon dioxide	2.113	2.113	2.113	3
ethane	6.678	6.678	6.678	3
propane	9.119	9.119	9.119	3
Sum	*100.000*	*100.000*	*100.000*	
Conclusion				*Homogeneous composition*

Here #7, #8, #9 are the numbers of the selected chromatograms.

Rounding format. Choosing the output format of values.

Check the composition for homogeneity. If the option is enabled, a conclusion is issued on the homogeneity of the composition of chromatograms. The composition is considered homogeneous if a component (or a group in the case of a group composition) is present in each calculated chromatogram with a non-zero concentration or in all at the same time with a zero concentration.

From a new page. For PDF format, the section starts with a new page.

3.4 GOST 31369-2021

Natural gas. Calculation of the heat of combustion, density, relative density and Wobbe number based on the component composition.

Parameters:

- **From a new page**. For PDF format, the section starts with a new page
- Chemical handbook data.
- **Input data**. Specify the source of the input data.
- **Concentration type**. The type of input data fractions is specified: molar, mass, volume.
- **Type of concentration units**. The units of measurement of the input data fractions are specified: percentages or unit fractions.
- **Input display format**.
- **Combustion temperature, C°**. The temperature from the set is indicated: 0°C, 15 °C, 60°F, 20 ° C, 25 °C. In the Russian Federation, the standard value is 25 °C.
- **Metering temperature**. The temperature from the set is indicated: 0°C, 15 ° C, 60°F, 20 °C. In the Russian Federation, the standard value is 20 ° C.
- **Metering reference pressure, kPa (range 90..110)**. The pressure is indicated for the calculation of volumetric indicators. In the Russian Federation, the standard value is 101.325.
- **Show in report ideal gas parameters**. Displays the corresponding table of physico-chemical indicators in the report with the active feature.
- **Rounding of gas properties**. The regulatory document allows the choice of the rounding method: by uncertainty or a fixed value for each indicator.

- **Coverage ratio**. The choice of the coefficient value corresponding to the confidence probability for calculating the extended uncertainty of the ideal gas: 2 (P≈95%); 1,960 (P=95%); 2,576 (P=99%).
- **Additional calculations in units other than SI**. Allows you to display indicators in non-system units: calories (for energy indicators), kWh (for energy indicators), the English system of measures (for all indicators).
- **Correlation matrix of the molar fraction r(xi, xj)**. The regulatory document allows for a choice when calculating the uncertainty of the ideal gas: single, complete. In the case of a complete matrix, the determination of the method of calculating the main component (by the difference relative to the others or by graduation) occurs automatically according to the settings of the first among the calculated chromatograms.

3.5 GOST 31371.7-2020

Natural gas. Determination of the composition by gas chromatography with uncertainty estimation. Part 7. Method of measuring the molar fraction of components.

Parameters:

- **From a new page. For PDF format, the section starts with a new page**.
- Chemical handbook data.
- **Calculation**. Selection of the calculation type: determination of the sample composition or verification of the acceptability of calibration. If the **Composition** is selected, but the chromatograms of the sample calculation are not specified, then the acceptability of the calibration will be checked.
- Analysis method. Values to select: Automatically, Method B.

The normative document implies the determination of the composition of the sample by three methods: A, B, V. Each component can be determined by any of the methods.

Method B is established if the component has more than one calibration level (different calibration molar fractions).

Method B is set if Method B is selected in the settings and the component has no more than one calibration level. For a component with the name "C6+" and one calibration level, method B is always set. For hydrocarbons with a number of carbon atoms greater than 6, method B cannot be set.

For hydrocarbons with more than 6 carbon atoms and one calibration level, method A is always established . In other cases, the component is set to method A.

- **Calibration chromatograms**. Specify the list of calibration chromatograms. These should be chromatograms with the designation "Calibration" in the passport, the concentration and uncertainty of the graduated components should be set.
- **Calibration control chromatograms for method V.** When working with method V, specify a list of control chromatograms. These should be chromatograms with specified concentrations and uncertainties, the type of destination does not matter.
- **Linearity test chromatograms for Method V.** When working with method V, specify a list of chromatograms. These should be chromatograms with specified concentrations and uncertainties, the type of destination does not matter**.**

- **Calculate additionally C_{6+} and C_{6+} higher for non-backflush methods**. Analytical method for determining the total proportion of components. The component "C6+" is determined through the calibration coefficient of n-hexane and the total area of all hydrocarbon components with a number of carbon atoms of 6 or more. The component "C6+higher" is simply the summation of all the individual components of group C6 and higher, which were calculated by their calibration coefficients.
- **Uncertainty out of range**. It can be used to output the composition table in the organization format. The choice of values: do not calculate, approximation, by the nearest limit.
- Rounding format.
- **Output of the composition in the format of the organization.** Setting up the method for displaying rounded values: no (the table is not output), you can specify a fixed number of decimal places, or round by uncertainty.

4 CHEMICAL HANDBOOK

Many application calculations of Chromatec Analytic contain physico-chemical reference data. For each type of calculation, the set of reference data is individual.

If you need to change the reference data, you can do it using a special editor.


The editor is called using the button on the desktop "Chromatec Navigator" or directly from the settings of a special calculation.

{video handbook Handbook}

The built-in handbooks are available for viewing only. To edit the handbook, click on the "Allow editing" button. In this case, you will be prompted to set a new handbook name. The program will not allow you to use existing names.


In the user handbook, you can add components.

… or delete them.


You can delete the user directory if you have the privilege to delete data.


Any handbook can be downloaded to your computer.


… or upload from the computer to the server.

5 MEASUREMENT HISTORY

5.1 Consistent data saving

Some calculations allow you to save the measurement history, which can be viewed in tabular and graphical form.

The corresponding option is present in the sections of the report:

- **Components**. The result of calculating peak areas and component concentrations is saved.
- **GOST 31369-2021**. The result of calculating the physico-chemical parameters of natural gas is saved.
- **GOST 31371.7-2020**. The result of calculating the component composition of natural gas is saved.

{video trend_start Trend init}

When saving option is enabled, the program saves its results when performing each analysis, for each of the above sections its own.

The data is stored in files on the server with relative paths:

Sampling location / group of calculated indicators / year-month

For example:

Gas 1 / Concentration / 2023-05

Here is:

- "Gas 1" – sampling location (for example, the name of the sampling line),
- "Concentrations" – a group of parameters.
- 2023-05" is the file name corresponding to the year and month of the analysis.

In a file with the extension .csv data is entered as follows:

```
Date;Number;helium;hidrogen;methane;oxigen;carbon dioxide
2023-02-01 9:10;1;1,2852E-05;1,18668E-05;0,067221726;5,98793E-06;0,002147976
2023-02-01 9:45;2;1,16953E-05;1,07988E-05;0,06386064;5,92805E-06;0,002083537
2023-02-01 10:20;3;1,13444E-05;1,15547E-05;0,067053672;6,22446E-06;0,002041866
2023-02-01 10:55;4;1,11176E-05;1,23635E-05;0,070406355;5,7265E-06;0,001858098
2023-02-01 11:30;5;1,03393E-05;1,1869E-05;0,064773847;5,95556E-06;0,001672289
2023-02-01 12:05;6;1,06495E-05;1,10381E-05;0,069308016;5,65778E-06;0,001755903
2023-02-01 12:40;7;1,12885E-05;1,04862E-05;0,074852658;5,43147E-06;0,00180858
2023-02-01 13:15;8;1,08369E-05;9,64732E-06;0,074104131;5,86599E-06;0,001935181
```

To view the measurement history, go to the corresponding Chromatec Navigator page.

{video trend_review Trend review}

5.2 Creating a set of data by chromatograms

In addition to the sequential construction of the data set (each record in the table is formed when processing the next analysis), you can quickly create a set of data on the already recorded chromatograms for parameters:

- Component concentration.
- Peak area.
- Peak height.
- The result of the calculation according to the user formula for the component.

To do this, click on the "Create data from chromatograms" on the side panel.

The dialogue will open, select the project and chromatograms in it. You can use filters by the name of the sample, comments. Can be shown in the table of chromatograms for a certain period of time.

The data set can be created immediately for all components in selected chromatograms or listed in the corresponding line (see the figure below).

After the chromatograms of interest are selected in the table, click "OK".

If necessary, on the upper toolbar indicate the values of the minimum and the maximum of the measured value. At the same time, dashed lines corresponding to the specified boundaries will appear on the graph.

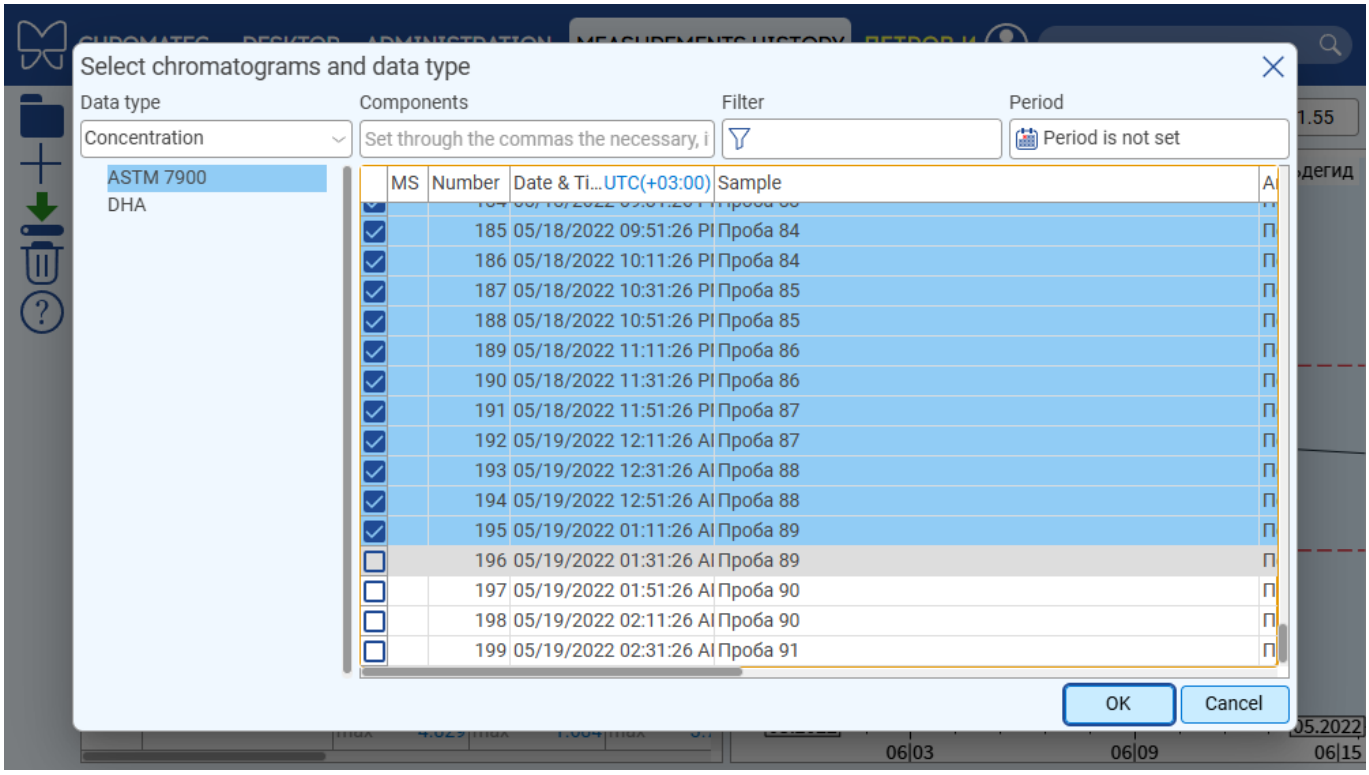


Fig. 5.1 – Chromatogram selection

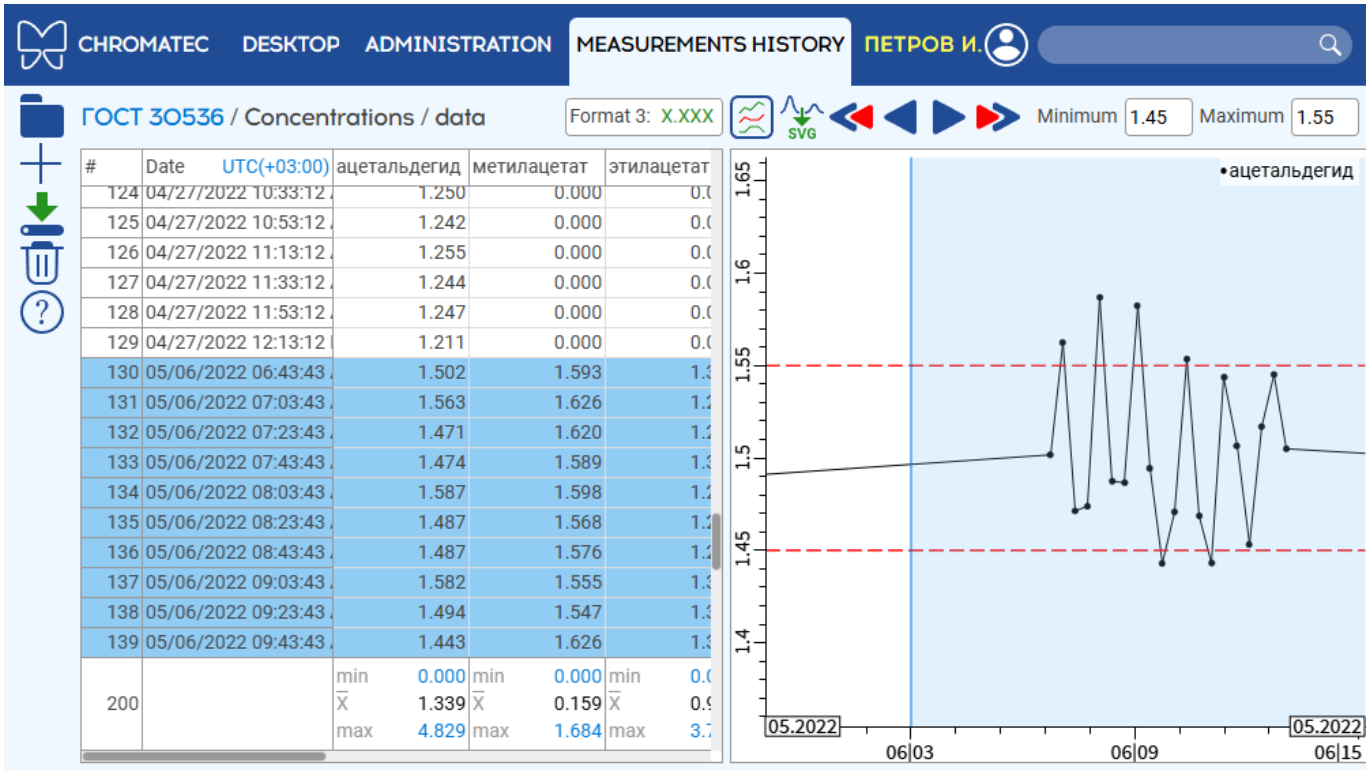


Fig. 5.2 – Change in the concentration of the selected component