User Manual: Calculation №85
«Natural gas. Determination of sulfur compounds»

«CHROMOS Engineering», LLC
Dzerzhinsk, Russia

Release date: 2025-05-05
Latest software version: 1.1.1
Internet: kb.has.ru

Contents

1. Introduction

The «Natural gas: Determination sulfur compounds» program is designed to calculate the calibration factors and component concentrations in accordance with GOST 34723-2021 «Natural gas: Determination of sulfur compounds using gas chromatography».

Before getting started, it is recommended to study the foregoing document.

This software works as an extension and can only be launched on a registered copy of «Chromos» software. To run the program you need a key.

The plug-in installation file and documentation are available on the Internet at: kb.has.ru/soft:dop_raschjot_85.

E-mail your suggestions and comments on the software to: soft@has.ru

2. Installing the Software

You need 5 Mb of free space on your local drive. To install the software, do the following:

1. Run the installation file.
2. Choose your language.
3. In the installer (Fig. 1), specify the components to be installed and click **Install**.

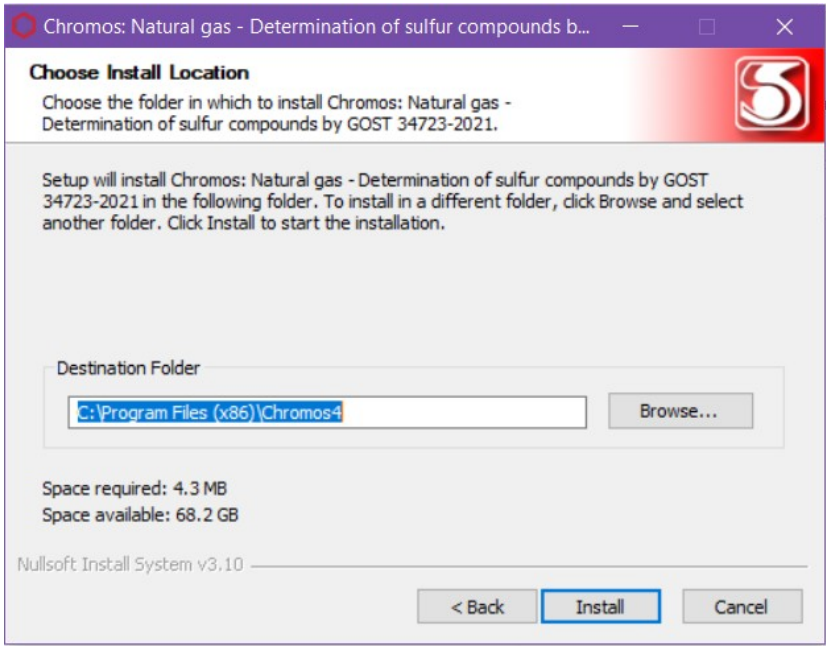

Fig. 1: Installation

4. When installed, click **Finish**.

After the software is successfully installed you can run it from «Chromos» software.

3. Running the Plug-in

This software works as an extension for «Chromos» software. To run the extension, do the following:

1. Connect the key to a USB port.
2. Run «Chromos» software.
3. In the *Data* menu, navigate to **Calculations > Chromos: Natural gas – Determination of sulfur compounds**. The main program window opens (Fig. 2).

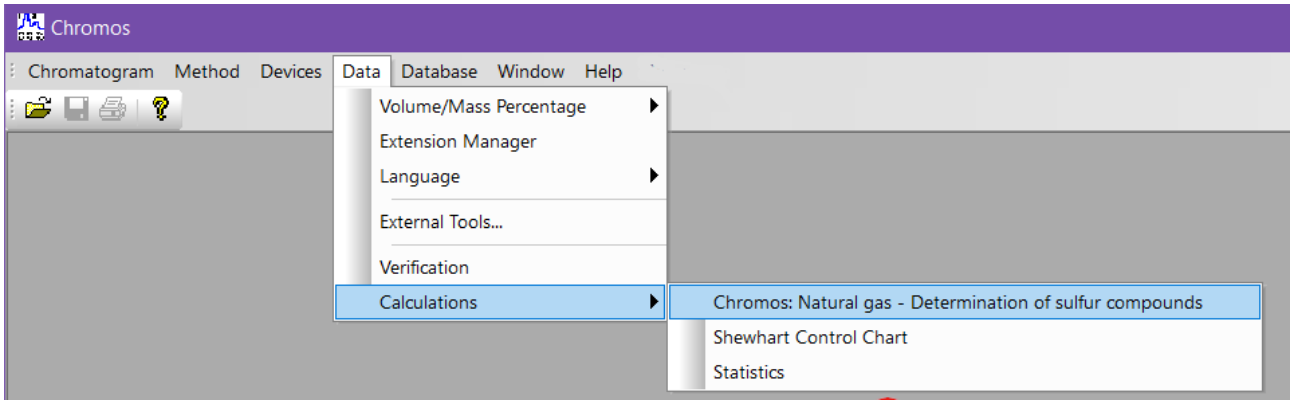

Fig. 2: Running the plug-in

4. Program Overview

The main program window (Fig. 3) contains the following elements:

1. Chromatograms/Mixtures tabs;
2. Chromatogram controls;
3. Refresh button;
4. Program settings;
5. Report controls;
6. List of opened chromatograms/mixtures;
7. Operation tabs.

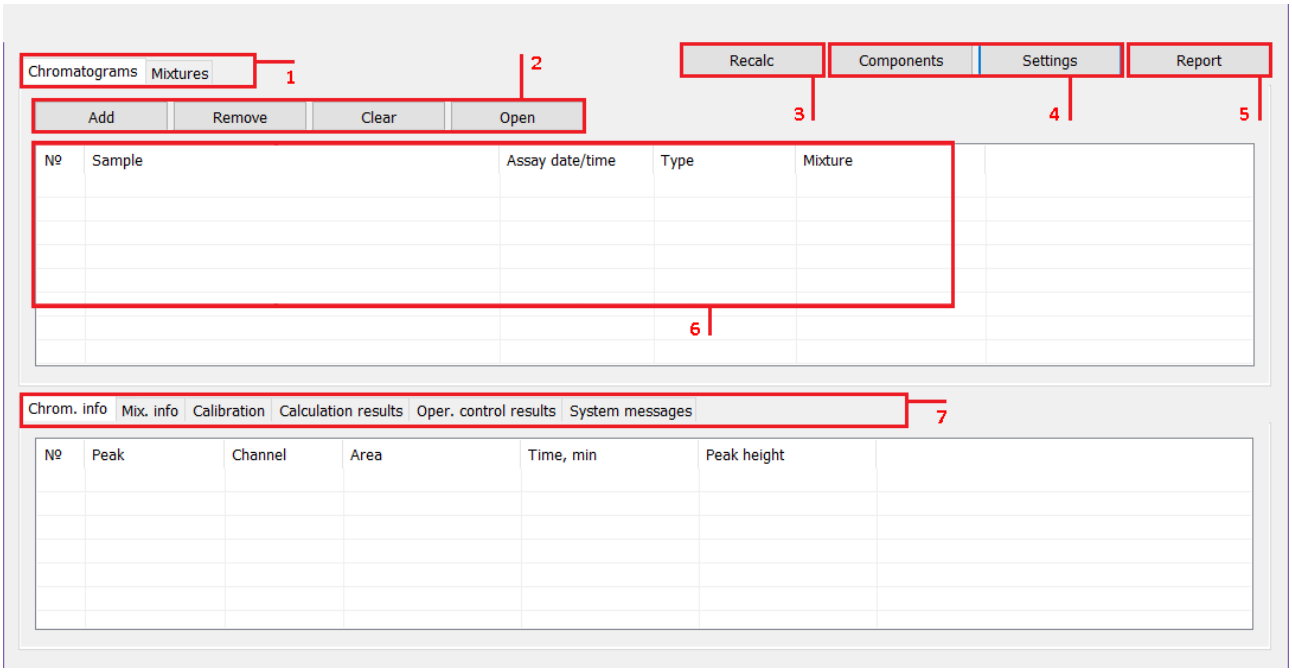

Fig. 3: Main program window

The source data block contains chromatogram control elements, displays loaded chromatograms and mixtures, and also workspaces with calculation information.

The main program window contains the following operation tabs:

- *Chrom. info* — the tab displays chromatogram information:
  - *№* — string number;
  - *Peak* — sample component name;
  - *Channel* — chromatogram channel;
  - *Area* — peak area;
  - *Time, min* — peak exit time in minutes;
  - *Peak height* — peak height;

- *Mix. info* — the tab displays mixture information:
  - *№* — string number;
  - *Component* — component name;
  - *Concentration, mg/m^3* — component concentration in mg/m^3;

- *Uncertainty, mg/m³* — uncertainty in mg/m³;

- *Calibration* (by the absolute calibration method for detectors with a linear calibration characteristic):
  - *№* — string number;
  - *Component* — component name;
  - *Signal/noise ratio* — signal-to-noise ratio;
  - *q* — pressure and temperature area correction factor;
  - *Corr. area* — corrected area;
  - *K* — calibration factor;
  - K_{avg} — average calibration factor;
  - *R* — range;
  - *Standard* — range standard;
  - *R Compl.* — compliance to the standard;

- *Calibration* (for a detector with a nonlinear calibration characteristic):
  - *№* — string number;
  - *Component* — component name;
  - *Factor ε* — equation factor by GOST 34723-2021 p. 10.5.3.1 f. 9;
  - *Factor η* — equation factor by GOST 34723-2021 p. 10.5.3.1 f. 10;
  - *Signal/noise ratio 1 (2)* — A1 (A2) signal-to-noise ratio;
  - *q1 (q2)* — A1 (A2) pressure and temperature area correction factor;
  - *Corr. area A1 (A2)* — A1 (A2) signal corrected area;
  - $A1_{avg}$ ($A2_{avg}$) — A1 (A2) signal average calibration factor;
  - *R1 (R2)* – A1 (A2) signal range;
  - *Standard 1 (2)* — A1 (A2) signal range standard;
  - *R1 (R2) Compl.* — A1 (A2) signal range compliance;
  - *Compl.* — total compliance to the standard;

- *Calculation results*:
  - *№* — string number;
  - *Component* — component name;
  - *Avg. peak height* — average peak height;
  - *q* — area correction factor;
  - *Corr. area* — corrected area;
  - *Conc., mg/m³* — concentration (in mg/m³);
  - *Conc. avg., mg/m³* — average concentration (in mg/m³);
  - *Abs. exp. uncert., mg/m³* — absolute expanded uncertainty (in mg/m³);
  - *Avg. conc., g/m³* — average concentration (in g/m³);
  - *Avg. conc., ppm* – average concentration (in ppm);
  - *Low. detect. limit, mg/m³* — lower detection limit (in mg/m³);
  - *R* — range;
  - *Standard* — range standard;
  - *R Compl.* — compliance to the standard;

- *Oper. Control results* — operation control results:
  - *№* — string number;
  - *Component* — component name;
  - *q* — area correction factor;
  - *Area* — peak area;

- *Corr. area* — corrected area;
- *Conc., mg/m³* — concentration (in mg/m³);
- *Pass. conc., mg/m³* — concentration by passport (in mg/m³);
- *Rel. dev., %* — relative deviation between measured and passport concentrations (in %);
- *Standard* — deviation standard;
- *Compl.* — deviation compliance to the standard;
- *Pass. abs. exp. uncert., mg/m³* — passport absolute expanded uncertainty (in mg/m³);
- *Abs. exp. uncert., mg/m³* — measured absolute expanded uncertainty (in mg/m³);
- *Uncert. ratio* — passport and measured uncertainties ratio;
- *Standard* — uncertainties ratio standard (≤2);
- *Compl.* — uncertainties ratio compliance to the standard;

- *System messages* — errors, warnings, information.

To select the table columns to display, right click on the information table area. To display the necessary system messages, in the *System Messages* tab, check the corresponding boxes. The selected parameters are saved.

5. Measurement Procedure

The «Natural gas: Determination of sulfur compounds» software carries out calculations according to GOST 34723-2021 in the following order:

- Verification of compliance of CRM with GOST 34723-2021 Appendix Б;
- Checking the signal-to-noise ratio;
- Calculation of calibration factors;
- Calculation of concentrations;
- Calculation of mercaptan sulfur;
- Calculation of total sulfur.

The following types of chromatograms are used in the software:

- Blank run;
- Cal. – calibration;
- Assay;
- Oper. control – operation control.

The blank run chromatogram is recorded before the others. To indicate it, in the chromatogram passport, in the *Sample* field, enter **Blank run**.

For the control chromatogram in the passport, in the *Mixture* field, indicate the CRM name.

The list of calibration mixtures is automatically loaded with data on mixtures from the calibration chromatogram passport. To do this, in the calibration chromatogram passport, fill in the *Mixture* field.

To carry out a full calculation according to GOST 34723-2021 you need:

- 3 assay chromatograms;
- 1 blank run chromatogram to calculate signal-to-noise ratio;
- 3 or 6 calibration chromatograms — depending on the detector type used.

The program allows you to perform a preliminary calculation with a smaller number of chromatograms, but the system messages display a warning that the calculation does not comply with GOST.

6. Adding Data

To carry out the calculation, you need to add chromatograms. To add data, do the following:

1. Click **Add**. The *Select Analysis* window opens.
2. In the *Select Analysis* window, select the chromatograms and click **OK**. The added files are displayed in the list of chromatograms in the main program window.

> To select chromatograms, you can use filters by method, date, type, sampling place and sampling point, operator and sample. You can also select multiple files at once using combinations Ctrl + Mouse and Shift + ←↑↓→

3. To delete the chromatogram, select it and click **Remove**.
4. To clear the list of chromatograms, click **Clear**.
5. To open the chromatogram in «Chromos» software, double-click it or select it and click **Open**.
6. To refresh the chromatograms list and calculation results, click **Recalc**.

The calculation data is displayed in the information table.

To eliminate the influence of changes in atmospheric pressure during measurements, in the passport of each chromatogram for the parameter *Ambient pressure (kPa)* it is necessary to indicate a value equal to the atmospheric barometric pressure in kPa (Fig. 4). If atmospheric barometric pressure is not specified for the chromatogram, then normal atmospheric pressure of 101.325 kPa is used for calculations. To measure atmospheric barometric pressure, it is necessary to use verified measuring instruments.

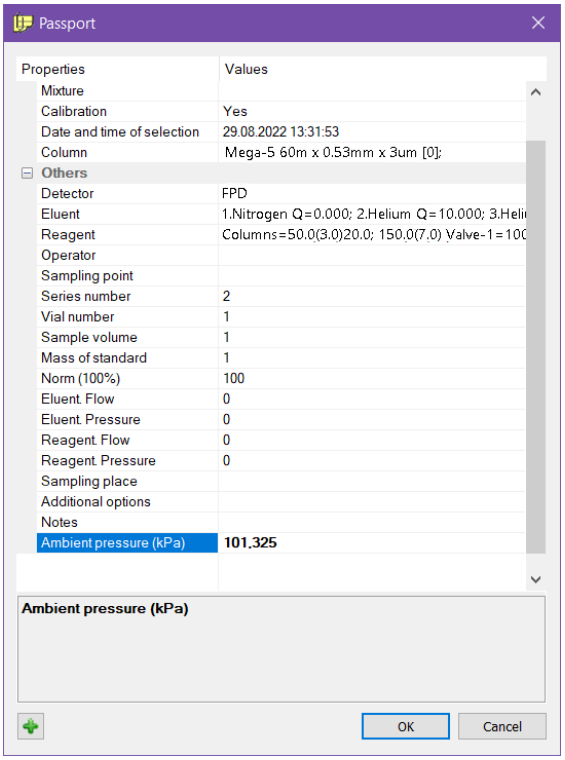

Fig. 4: Chromatogram passport

7. Operation Control

The program implements the ability to quickly check the accuracy of the measurement result of the mass concentration of sulfur-containing components. When quickly checking the accuracy of the measurement result of the mass concentration of sulfur-containing components, a certified reference material (CRM) with the mass concentration of the components to be determined in the working range is analyzed according to this method.

A standard sample of an approved type with metrological characteristics that provide an accuracy margin of at least two should be used as a control sample.

The results of operational control are displayed in the main program window on the *Oper. control results* tab.

8. Reporting

To write the calculated data to a report, do the following:

1. Click **Report**. The *Report* window opens (Fig. 5).
2. In the *Report* window, in the *Device ID* field, enter the device ID.
3. In the *Operator* field, enter the operator name.
4. Select the report format:

    - Editable, “.odt” – an Open Document file;
    - Non editable, “.html” – a web page.

5. Click **Report**.

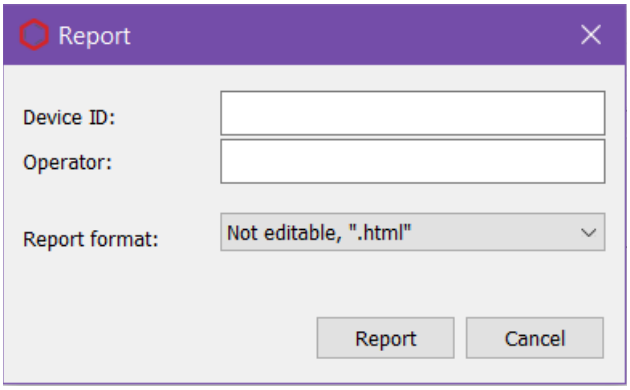

Fig. 5: Report settings

9. Configuring the Program Settings

9.1. Managing the Components

To compare components in the calculation and chromatograms, a component table is used. If other names are used in the chromatograms, the name alias for the components can be set in the program. To manage components:

1. In the main program window, click **Components**. The *Components* window opens.
2. In the corresponding cell of the *Name alias* column, double-click to edit.
3. Enter an additional name.
4. Press Enter.

9.2. Configuring the Analysis Settings

You can set up the following parameters:

- Round values — up to the required number of decimal places or, according to GOST 34723-2021, depending on the value of the absolute expanded uncertainty;
- Correction by pressure — correction of the detector signal for atmospheric pressure, according to GOST 34723-2021, p. 10.5.2.2. For this option, the *Ambient pressure (kPa)* field in the chromatogram passport must be filled in;
- Correction by temperature — correction of the detector signal based on the ambient temperature, according to GOST 34723-2021, p. 10.5.2.2. For this option, the *Ambient temperature (°C)* field in the chromatogram passport must be filled in;
- Use a nonlinear detector — performing calculations using the algorithm for a detector with a nonlinear dependence (the linear detector algorithm is used by default);
- Instrument noise value.

To set up the parameters, do the following:

1. Click **Settings**. The *Settings* window opens (Fig. 6).
2. In the *In the program* field, enter the number of digits to which the values in the program are rounded.
3. In the *In the report* field, enter the number of digits to which the values in the report are rounded.
4. To round values by GOST, check the **Round values by GOST** option.
5. To correct the area by ambient pressure, check the **Correction by pressure** option.
6. To correct the area by ambient temperature, check the **Correction by temperature** option.
7. To carry out the calculation using the algorithm for a nonlinear detector, check the **Use a nonlinear detector** option.

> Depending on the detector type selected, the columns in the *Calibration* tab will differ.

8. In the *Instrument noise value* field, enter the noise value (units depend on the detector type).

If a blank run is not specified in the calculation, the detector noise value is taken from the program settings.
Note: The procedure and frequency of checking compliance with the signal-to-noise ratio requirement should be included in the internal laboratory control plan.

9. Click **OK**.

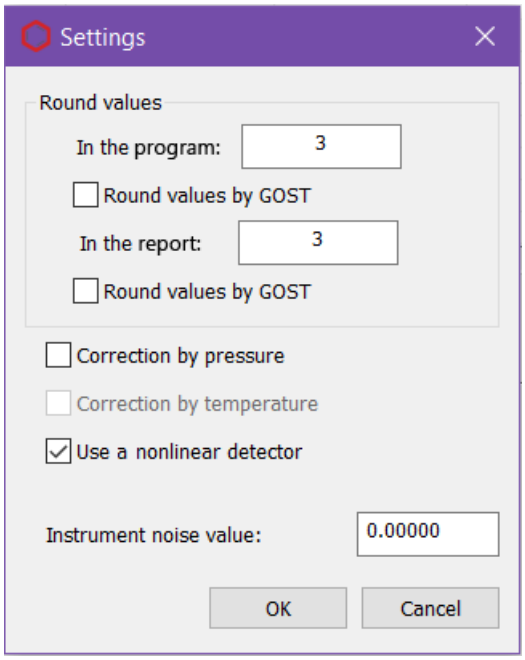

Fig. 6: Analysis settings

10. Program Identification

To view program data, click on the icon in the upper left corner of the window and select **About...** The identification window opens (Fig. 7).

The identification data of the certified calculation module are indicated in the certificate of metrological certification of the «Natural gas: Determination of sulfur compounds» software.

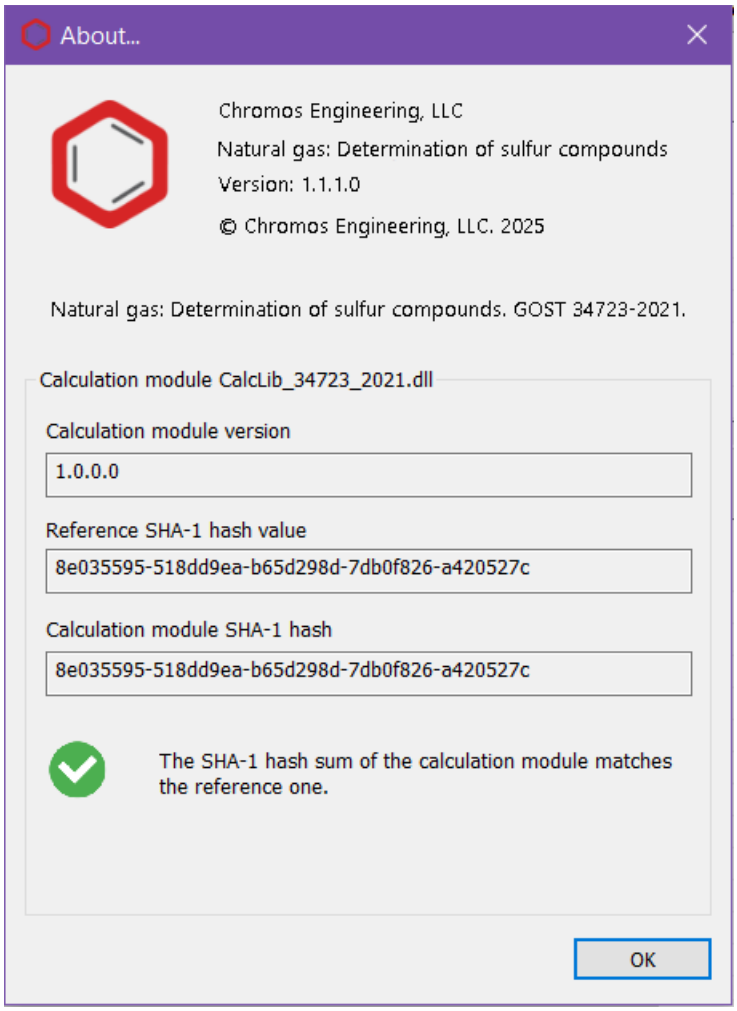

Fig. 7: Identification window