User Manual: Calculation №107
«Simulated distillation of oil and petroleum products»

«CHROMOS Engineering», LLC
Dzerzhinsk

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2. Introduction

The “Simulated Distillation of Oil and Petroleum Products” program is designed to analyze chromatograms obtained using the Chromos software to determine the fractional composition using gas chromatography in accordance with one of the following regulatory documents: GOST R 56720-2015, GOST R 54291-2010, ASTM D2887 -2013, GOST ISO 3924-2017, ASTM D7169 (combining ASTM D7900-13). The distribution of components over the boiling point range is determined.

To get started, you need to familiarize yourself with these regulatory documents.

This program works as an extension for the Chromos software (version 4.x).

The program installation file and accompanying documentation are available on the Internet at: kb.has.ru/soft:dop_raschjot_107.

Send suggestions and wishes regarding the program to e-mail: soft@has.ru

3. Installing the Software

To install the «Simulated Distillation of Oil and Petroleum Products» program, we recommend 15 MB of free space on your hard drive.

1. Run the installation file.
2. Select the installer language (Russian or English)
3. Select components to install Fig. 1
   3.1. For initial installation you should select «Msxml6».
   3.2. For subsequent installations, you can select "Perform a clean install" if you want to clean out the folder first.
4. Click Install.
5. When installation is complete, click Finish.

The program is installed as an extension for Chromos software.

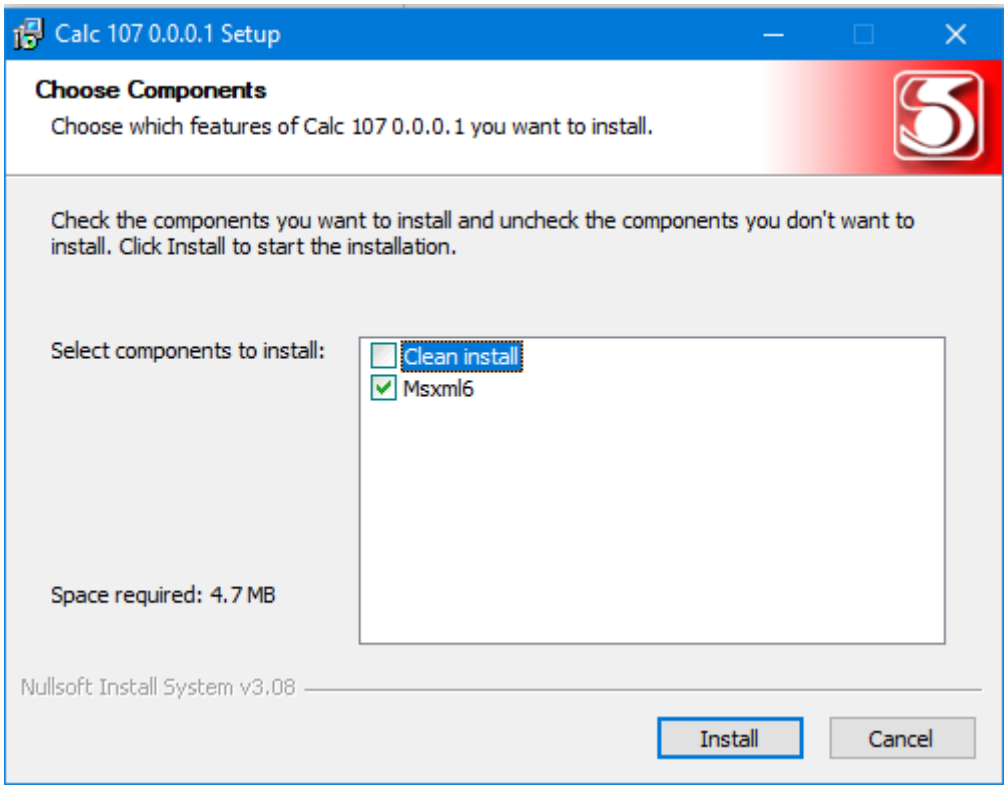

Fig. 1 Installing the software

4. Program overview

Main program window Fig. 2 consists of the following elements:

1. Chromatogram control elements;
2. Field for entering the device number;
3. Program settings elements;
4. Report controls;
5. List of open chromatograms;
6. A set of tabs and calculation workspaces.

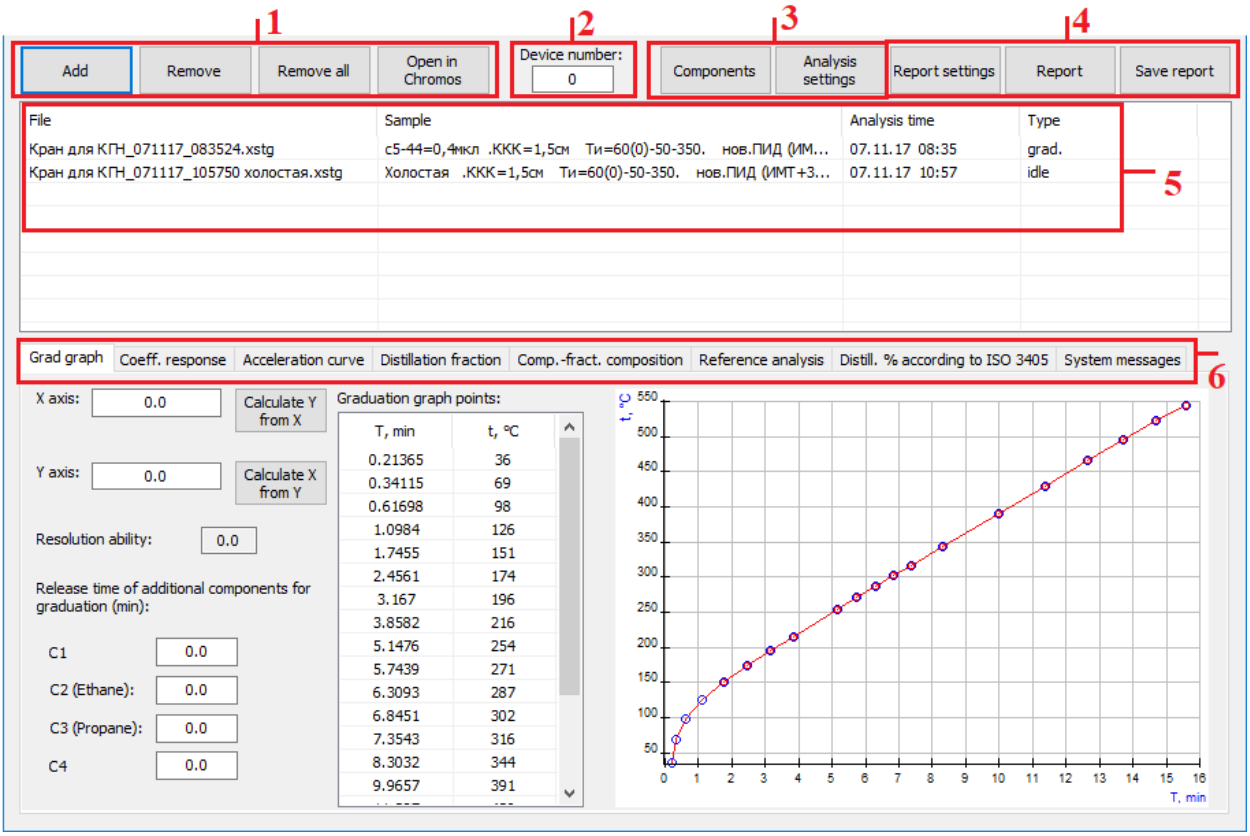

Fig. 2 Main program window

The main program window includes workspace tabs:

- Grad. Graph — displays information about the calibration graph and additional settings for the calibration graph in the form of input fields for component release times (for working with graphs, see 7.1);
- Coeff. response - contains the results of calculating response coefficients (ASTM B2887-2013):

- #—line number;
- Component—name of the sample component;
- Peak area - peak area;
- Weight in the mixture, mg - mass of the component in the mixture (in mg);
- Response - relative response rate;
- accept. — compliance with the standard;

- Acceleration curves – displays a graph depending on the fraction of acceleration from the temperature of the currency and the group of settings for the corresponding analysis graphs (for working with graphs, see 7.2);

- Distillation fraction—contains the results of calculating the sample distillation fraction:
  - Mass fraction%—mass fraction of distillate;
  - T1 (2.3), °C - boiling point of analysis 1 (2.3);
  - Tavg, °C - average boiling point;
  - ±Δ, °C — absolute error limits at P = 0.95 (GOST 56720-2015, Table 7);
  - |T1-T2|, °C—difference in measured temperatures in samples 1 and 2;
  - Norm, °C - standard;
  - acceptance - compliance with the standard;

- Comp.-fraction. composition—contains information about the component-fractional composition of the sample:
  - Fraction—fraction by boiling point;
  - Conc. 1 (2.3), % mass - mass concentration 1 (2.3);
  - Conc. avg, % mass - average mass concentration;
  - ±δ, % - relative error limits (GOST 56720-2015, Table 8-9);
  - Divergence, % - discrepancy between two consecutive measurements;
  - Norm, % - standard for discrepancy;
  - Accept. — compliance with the standard;

- Standard analysis - contains information on comparison of these fractions of distillation of a typical reference sample of batch No. 2 and a verification sample:

- Mass fraction% - share of distillate;
- Sample, batch No. 2, °C - boiling point according to the sample;
- Measuring, °C - measured boiling point;
- Divergence, °C — measurement discrepancy;
- Norm R, °C - standard;
- Accept. R - compliance with the standard;

- Portion of distillation according to ISO 3405 - contains the results of calculating the proportion of distillation according to the ISO 3405 standard:
  - Fraction, volume% - share of distillate;
  - T (ISO 3405), °C - boiling point equivalent to the temperature according to ISO 3405 (GOST 3924-2017, Form A1);
  - R, °C (Table A4) - reproducibility indicator (GOST 3924-2017, Table A4);

- System messages - displays error information, warning messages about any inconsistency or the impossibility of performing calculations due to missing data.

5. Measurement procedure

To carry out the calculation, chromatograms are added to the program.

Depending on the method selected in the settings and the results obtained, a different number of chromatograms may be required for work. Information about the lack of chromatograms is displayed in the System messages tab.

To correctly calculate the fractional composition of chromatograms, depending on their type, they must contain in the passport an additional parameter Chrm_Type:

- #graduation – chromatogram of the analysis of the calibration mixture of hydrocarbons C5-C44;
- #idle – a chromatogram obtained without sample injection under the same conditions as the analysis;
- #reference– chromatogram of analysis of a standard gas oil sample with a distillation fraction passport;
- #analysis – chromatogram of sample analysis without adding an internal standard;
- #standard – chromatogram of sample analysis with the addition of an internal standard;
- #verification – chromatogram with known hydrocarbon content from C5 to C44.

The following can be open at the same time:

- Graduation chromatogram – 1 pc.;
- Idle chromatogram – 1 pc.;
- Chromatogram of reference sample – 1 pc.;
- Verification chromatogram – 1 pc.;
- Chromatogram analysis – 3 pc.;
- Analysis chromatogram with internal standard – 3 pc.

For a minimum calculation, it is necessary to open the **graduation**, **idle** and at least one **analyzed** chromatogram.

You can view open chromatograms in Chromos software by selecting the desired chromatograms in the list of open files and clicking the «Open in Chromos» button or by double-clicking on the desired chromatogram.

If the calculation contains a component with a mass sensitivity coefficient other than 1, or if any peak needs to be excluded from the calculation, you must also add the corresponding component to the component table and adjust its parameters.

The data obtained during the calculation process is displayed in the tabs of the main program window.

The calculation results can be saved to a report file in HTML format.

6. Adding Data

To carry out the calculation, you need to add chromatograms.

To add and work with chromatograms, use the following steps:

1. Click Add. The Select Analysis window will open Fig. 3.
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 Delete.
4. To clear the list of chromatograms, click Delete All. The paths to the graduation, idle and reference (i.e. standard sample) chromatograms are saved.
5. To open the chromatogram in Chromos SW, double-click it or select it and click Open in Chromos.

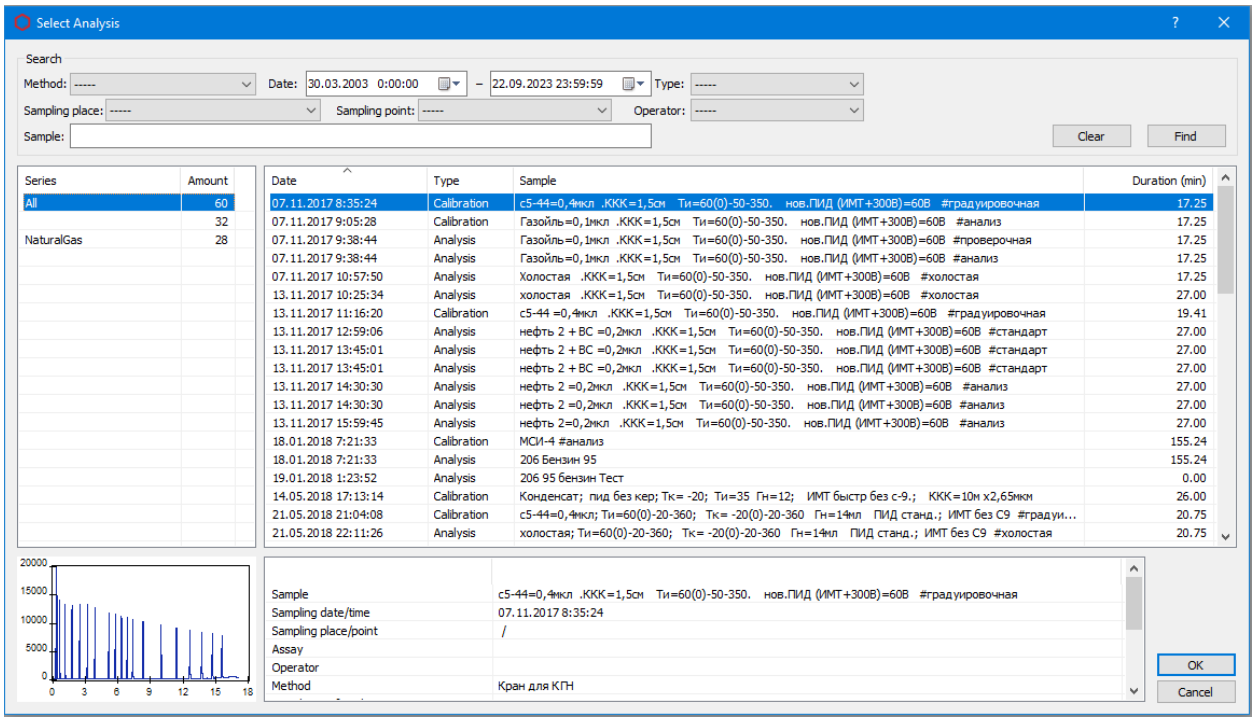

Fig. 3 Select Analysis

In the main program window, in the Device number field, enter the device number. Configure additional components (see 9.1)

7. Working with charts

7.1. Graduation chart

Information about the calibration graph is presented in the Grad tab. graph Fig. 4. Below is a description of the fields and actions for working with the chart.

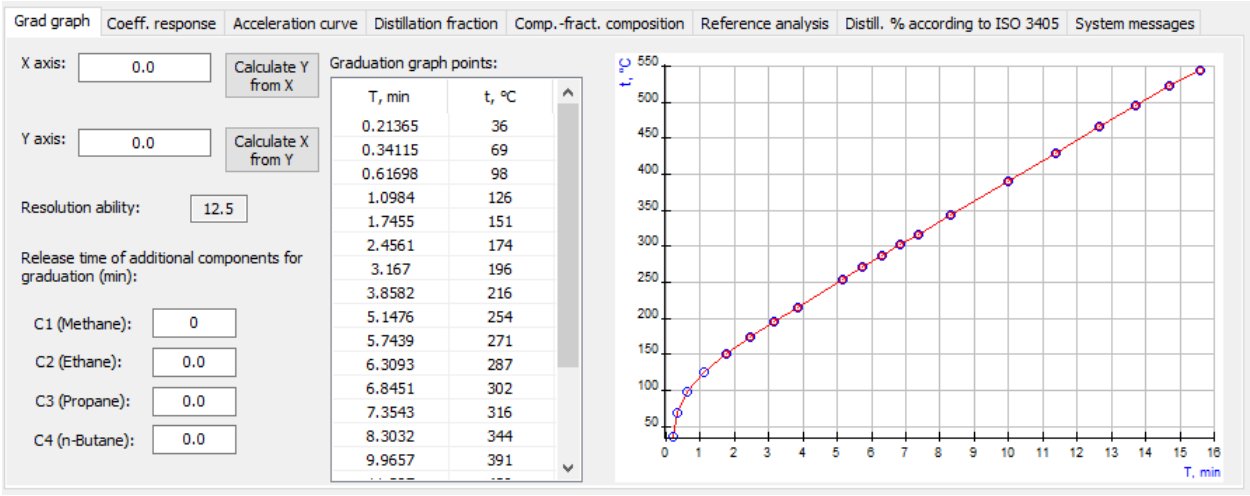

Fig. 4 Graduation graph tab

The X Axis and Y Axis input fields are intended for manual calculation of values using a calibration graph.

• To get data for one of the axes, enter a value in the X Axis or Y Axis field and click Calculate Y from X or Calculate X from Y, respectively.

Permission field ability displays the resolution value of the capillary column according to GOST R 56720-2015 clause 8.3. If this GOST value does not comply, an error message appears in the System messages tab.

Input fields Output time of additional components for calibration (min) serve to expand the range of the calibration graph. According to GOST R 56720-2015 clause 9.3, a mixture of components from C5 to C44 is used for the calibration curve, and the analyzed chromatograms often contain components with a boiling point lower than that of C5. This does not allow for some calculations, so the program has added the ability to manually enter the release times of additional components. The release times of the corresponding components can be taken from the analyzed chromatogram, pre-processed in the Chromos software.

• To expand the range of the calibration graph, enter the values of their release times in the fields of additional components.

The Points table of the calibration graph displays the coordinates of the points on which the graph was constructed. On the graph, table points are shown as empty blue circles.

In a separate window you can open the interactive chart Fig. 5. When you click on a point on the graph, the coordinates of that point are displayed. The chart window can be expanded to full screen.

• To open the interactive chart, in the Graduation tab chart double click on the chart.

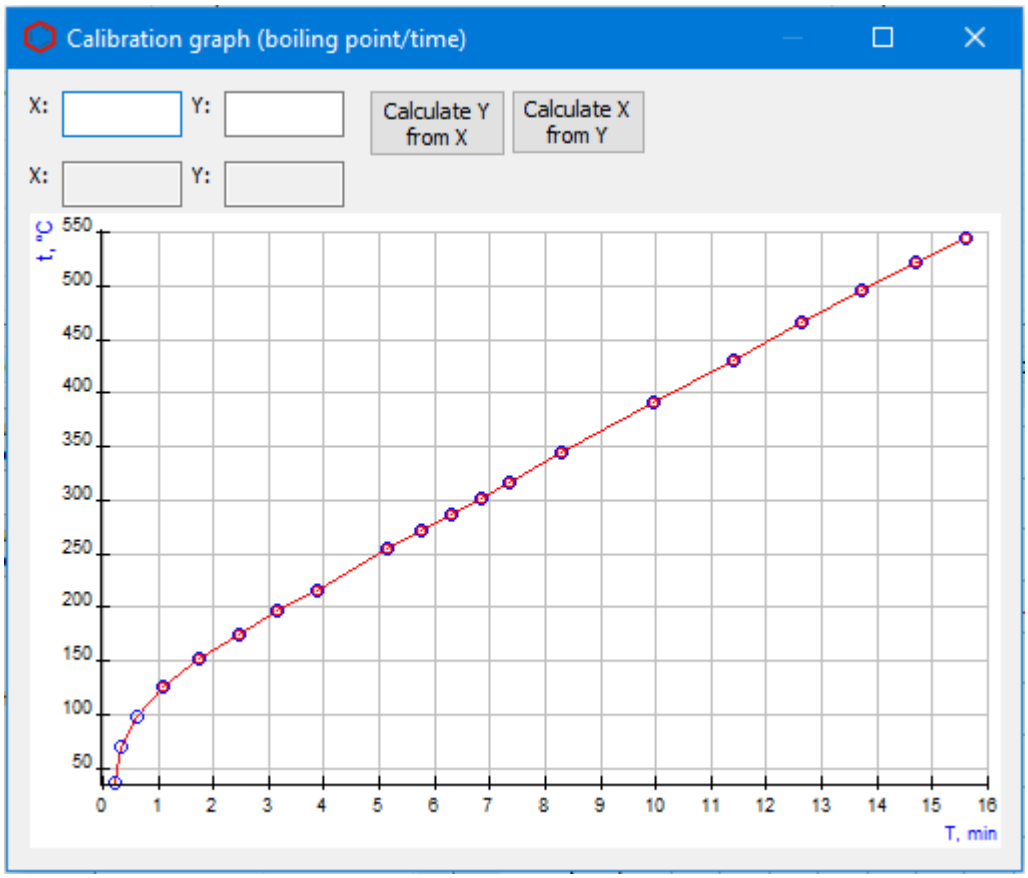

Fig. 5 Interactive graph window

7.2. Acceleration curve

Information about the acceleration curve graph is presented in the Acceleration curve tab.

Up to three analyzes can be displayed simultaneously on the ramp curve. Graphs of the corresponding analyzes are depicted by curves in red, blue and green.

• To display an analysis graph, in the relevant analysis segment, select the Display check box.

The X and Y input fields are intended for manual calculation of values according to the graph.

• To get data for one of the axes, enter a value in the X or Y field and click Calculate Y or Calculate X, respectively.

In a separate window you can open the interactive chart Fig. 6. When you click on a point on the graph, the coordinates of that point are displayed. The chart window can be expanded to full screen.

• To open the interactive graph, in the Acceleration curve tab, double-click on the graph.

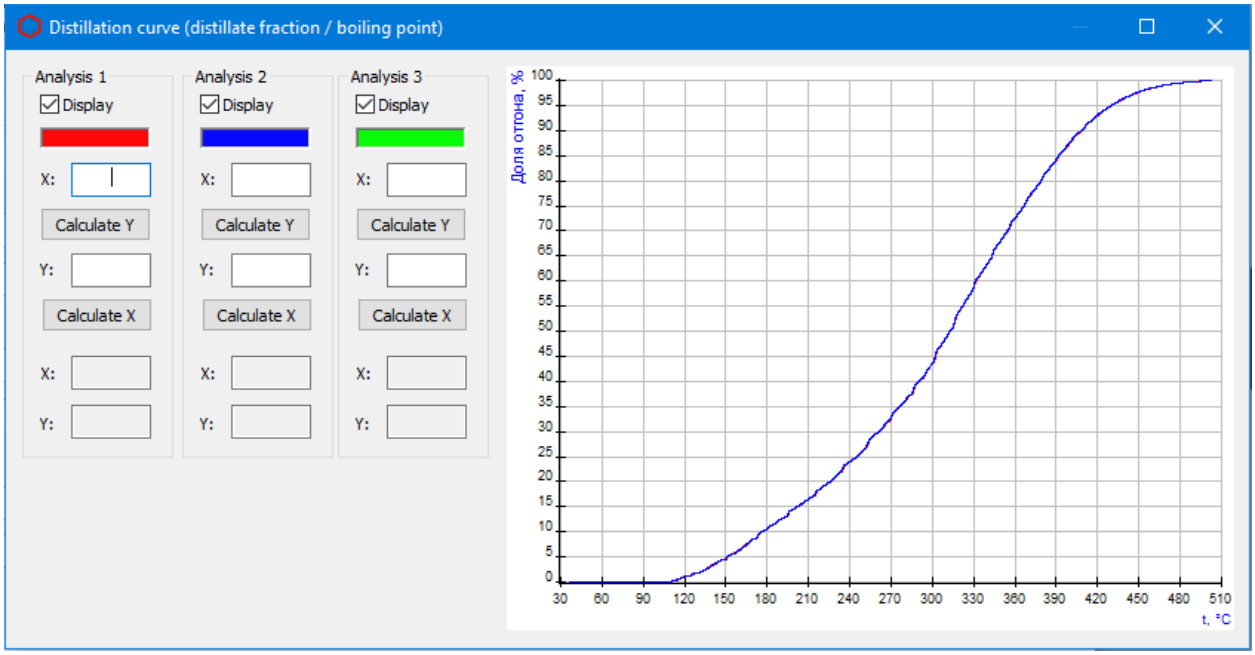

Fig. 6 Acceleration curve

8. Reporting

The resulting calculation data can be generated into a report. In the report settings (see 9.3) you select the data that will be added to the report Fig. 7.

• To generate a report, click Report. It is generated in html format and is automatically opened by the browser.

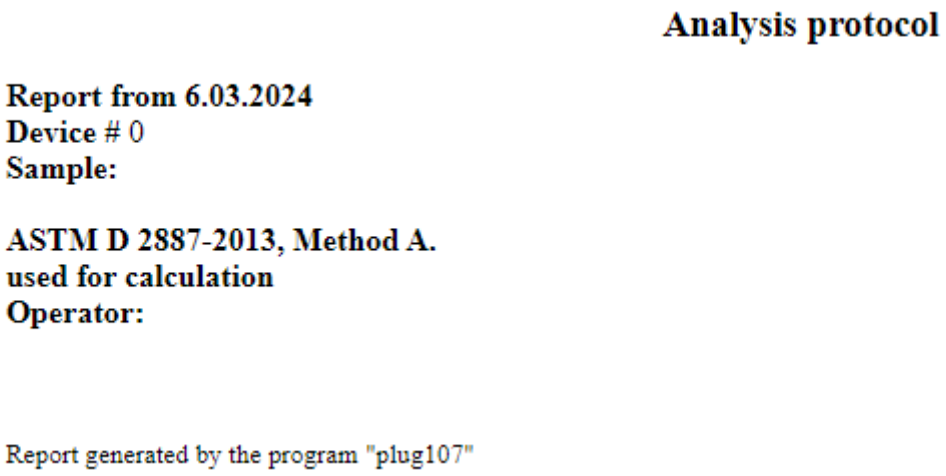

Fig. 7 Report

• To generate a report, click Report. It is generated in html format and is automatically opened by the browser.

By default, the report file name is Report107_17102023_114811.html, where:

- Report107 – program name;
- 17102023 — date in DDMMYYYY format;
- 114811 — time in HHMMSS format;
- html – file extension.

9. Configuring the Program Settings

Setting up the program includes managing components, setting analysis parameters, and setting report parameters.

9.1. Managing the Components

The list of components contains preset entries for components C1 to C44, which are protected from modification and deletion. Components added during operation can be edited and deleted. To manage components, follow these steps:

1. In the main window, click Components. The Components window will open. Fig. 8.
2. To add a component, click Add Component. A new entry appears in the list of components.
3. To change data, double-click on the desired field. When editing, new components are highlighted in yellow, existing ones are highlighted in green.
   3.1. In the Name field, enter a name for the component.
   3.2. Component names should not be repeated.
   3.3. In the Mass. coefficient sensitivity. enter the mass sensitivity factor value.
   3.4. To exclude any peak from the calculation, add the appropriate component and set the sensitivity coefficient to zero.
   3.5. (Optional) In the Additional field. Name Enter an optional name for the component.
   3.6. In the Boiling temperature field, °C, enter the boiling temperature value (in °C).
   3.7. In the Comp. Weight field. in a mixture, enter the mass value of the component in the mixture.
4. To remove a component, select it and click Remove Component(s). New components (yellow) will be deleted immediately, pre-existing ones will be marked in red.
5. Save your changes by clicking OK. The color coding of entries will disappear.

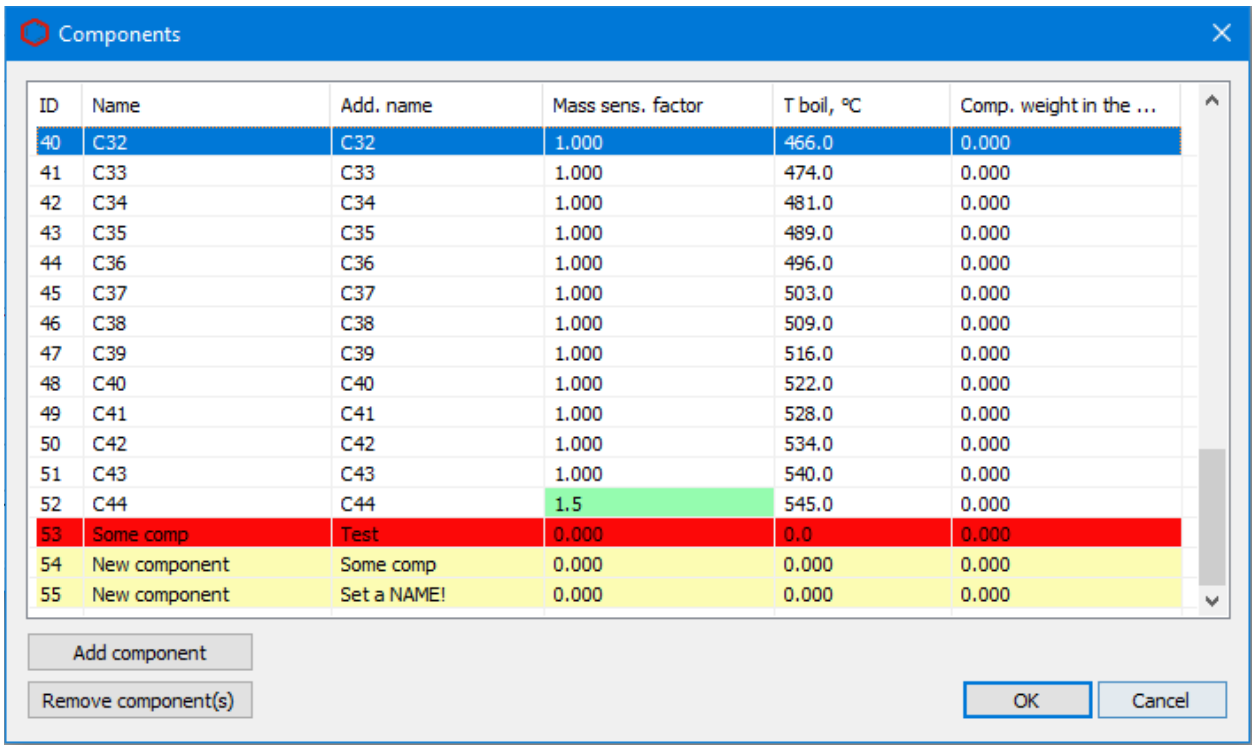

Fig. 8 Components window

9.2. Configuring the Analysis Settings

To set analysis parameters, follow these steps:

1. In the main window, click Analysis Settings. The Analysis Settings window will open. Fig. 9.
2. In the Analysis settings window, select the calculation method. Depending on the selected method, some option fields will be available.
3. In the Beginning of sample output, min field, enter the start time of sample output (in minutes).
4. In the Sample distillation step, % field, enter the value of the sample removal step (in %).
5. (Optional) To clear the Sample distillation step, % field, click Reset distillation step.
6. In the Weight internal standard, g field, Enter the mass of the internal standard (in grams).
7. In the Sample weight, g field, enter the mass of the sample (in grams)
8. In the Beginning of fraction marking, °C field, enter the initial temperature of fraction marking (in °C).
9. In the Fraction marking step, °C field, enter the temperature value of the fraction marking step (in °C).
10. In the Mass fraction of Hydrogen sulfide, % field, enter the hydrogen mass fraction (in %).
11. In the Mass fraction of mercaptan sulfur, % field, enter the mass fraction of mercaptan sulfur (in %).
12. In the Mass fraction of water, % field, enter the mass fraction of water (in %).
13. Save your changes by clicking OK.

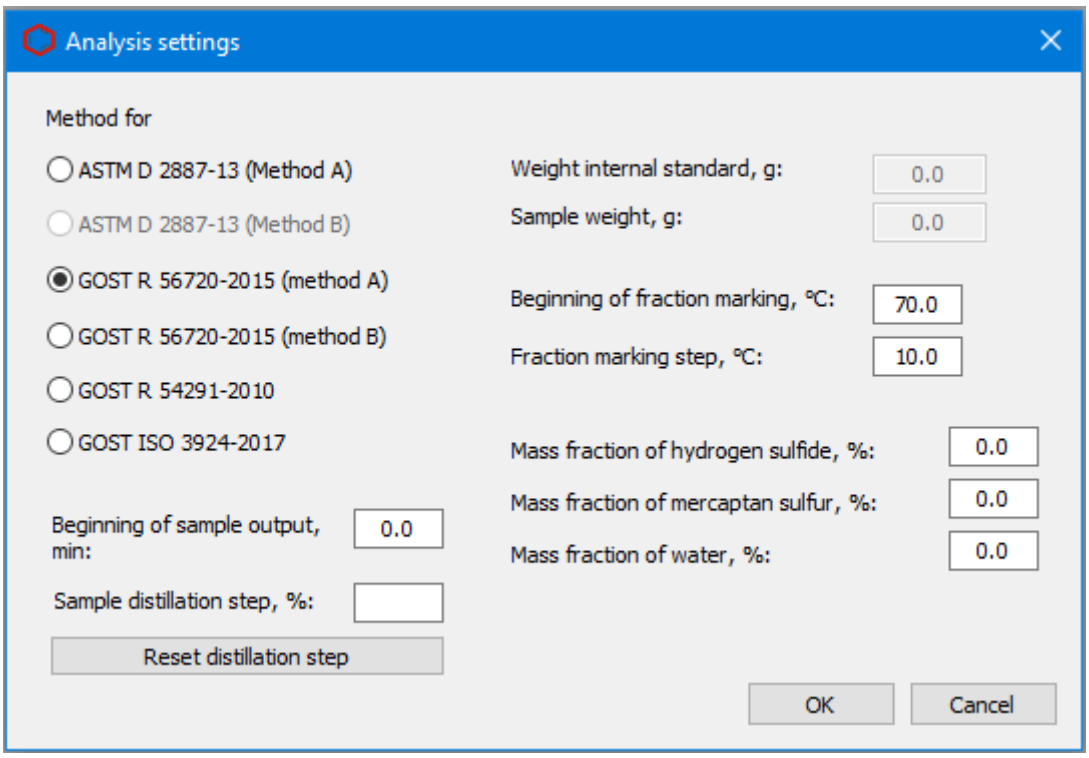

Fig. 9 Analysis Setup Window

9.3. Configuring the Report Setting

To customize the report content:

1. In the main window, click Report Settings. The Report Settings window will open. Fig. 10.
2. In the Report Settings window, check the boxes next to the elements that you want to include in the report.
3. Click OK.

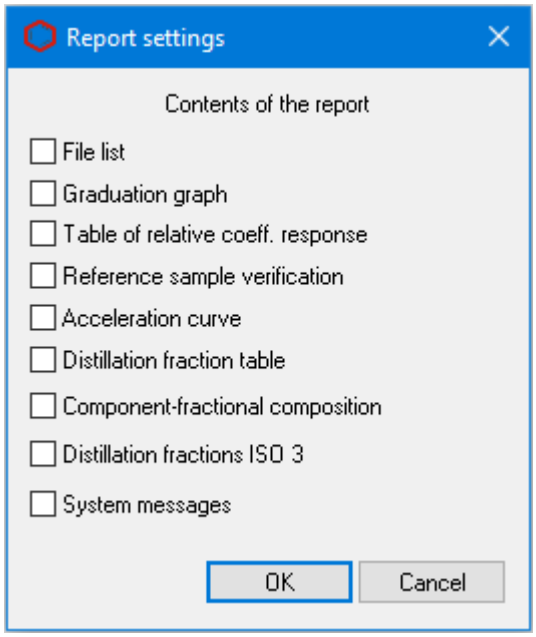

Fig. 10 Report Settings window