User manual (calc 106)

Introduction

This manual describes the interface of the **calc 106** program and describes the key points of using this software.

The program is designed for the analysis of chromatograms obtained using **Chromos4**. When analyzing chromatograms, the composition of LPG (liquefied petroleum gases) and the concentration of components are determined according to GOST R 54484-2011, GOST 33012-2014 or GOST 10679-76 (optional). Based on the concentrations and composition obtained, the pressure and density of LPG are calculated according to GOST 28656-90, and the octane number is calculated according to STB EN 589-2014.

To get started, you need to read the following documents:

- GOST R 54484-2011, GOST 33012-2014, GOST 10679-76

- GOST 28656-90

- STB EN 589-2014.

Install

The installation file can be downloaded at: <u>http://kb.has.ru/soft:dop_raschjot_106</u>

After launching the installation file, it is enough to follow the instructions of the installation wizard (Picture 1).

😽 Calc 106 1.0.0.0 Setup		—		×
Choose Components Choose which features of Calc 10	06 1.0.0.0 you want to install.			5
Check the components you want install. Click Install to start the install		onents you don't	t want to	
Select components to install:	Clean install			
Space required: 4.8 MB				
Nullsoft Install System v3.08	[Install	Cance	el

(picture 1)

The "Clean install" mark will clear all user data set by them in the previous version of the program (coefficients, aliases, settings) and set them to default values.

Upon completion of the installation, to start the calculation, open the main **Chromos4** application. The calculation will be available in the tab:

Menu->Data->Calculations->Calculation name (picture 2)

🏰 Chromos								
Chromatogram	Method	Devices	Data	Database	Window	Help		
: 🚅 🖬 🎒 🤋			E La	'olume/Mass xtension Mar anguage xternal Tools	nager	•		
			C	alculations		۰	LPG composition	

(picture 2)

Common interface

The common	interface	of the	program	is shov	vn in	picture 3.
		01 111	P-08-000	10 0110 1		p100010 00

roma	atograms Mixture										
	Add	New graduation		Del	Del all	Open in Ch	romos	Graduation mixture	:		
#	Filename			Sample		Method	Mi	xture	Release time,	Calc type	
rm in	nfo Mixture info	Calc of concentrations	Calc of grad	duations Ch	eck of graduations	Calc density, pressur	re, octane nu	imber System me	ssages		
rm in #	nfo Mixture info Peak	Calc of concentrations	Calc of grad	duations Ch	eck of graduations C		1	umber System me		time, min	
		Calc of concentrations	Calc of grac	duations Ch	eck of graduations C		e, octane nu el Square			time, min	
		Calc of concentrations	Calc of grad	duations Ch	eck of graduations C		1			time, min	
		Calc of concentrations	Calc of grac	duations Ch	eck of graduations C		1			time, min	
		Calc of concentrations	Calc of grac	duations Ch	eck of graduations C		1			time, min	
		Calc of concentrations	Calc of grac	duations Ch	eck of graduations C		1			time, min	

(picture 3)

To add chromatogram files, 2 buttons are used (picture 3) **Add** and **New Calibration**. Using the "Add" button, files are opened for calculations, and the "New calibration" button adds chromatograms to check the graduations (see GOST R 54484-2011).

Pressing these buttons opens the chromatogram window (picture 4). To work, 2 types of chromatograms are needed: "Calibration" and "Analyses" (Calculated). Using the **ctrl** and **shift** keyboard buttons, you can select multiple files at the same time. Click **OK** after selecting the desired chromatograms.

Select Analysis Search Iethod: СЖ	~	Date: 30.03.2003 0:00:	00 🔲 -	12.02.2024 23:59:59	? ;
ampling place:		 Sampling poin 	t:	✓ Operator: ✓	
ample:					Clear Find
eries	Amount	Date	Туре	Sample	Duration (min
All	11	06.04.2011 9:58:08	Calibration	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	16.1
	11	06.04.2011 10:23:09	Calibration	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	20.0
		06.04.2011 10:54:04	Calibration	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	17.1
		06.04.2011 11:21:38	Calibration	1 ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	20.0
		06.04.2011 11:53:07	Calibration	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	16.1
		06.04.2011 12:18:55	Calibration	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	18.0
		06.04.2011 12:47:17	Calibration	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	20.0
		06.04.2011 13:23:25	Calibration	2 ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	20.0
		07.04.2011 7:51:45	Analysis	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	20.0
		07.04.2011 8:36:29	Analysis	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	20.0
		07.04.2011 9:06:10	Analysis	ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	16.4
0000		Sample		ПГС СЖ с пустым каппилляром 0,9кг Тк=50(1)-10-180	^
T		Sampling date/time		06.04.2011 23:00:00	
0000		Sampling place/point		1	
0000		Assay		1	
TIL		Operator			ОК
	9 12 15 18 21	Method		СЖ	V Cancel

(picture 4).

The selected chromatograms will be displayed in the main window (picture 5).

2 СЖ_060411_122138 испр.xstg 1ПГС СЖ с пустым каппилляр СЖ 06.04.11 11:2	e, Calc type 9:58 Graduation 1:21 Graduation 7:51 Calculated
1 СЖ_060411_105808rp.xstg ПГС СЖ с пустым каппилляром СЖ 06.04.11 09:5 2 СЖ_060411_122138 испр.xstg 1 ПГС СЖ с пустым каппилляром СЖ 06.04.11 11:2	9:58 Graduation 1:21 Graduation
2 СЖ_060411_122138 испр.xstg 1ПГС СЖ с пустым каппилляр СЖ 06.04.11 11:2	1:21 Graduation
3 СЖ_070411_085145.xstg ПГС СЖ с пустым каппилляром СЖ 07.04.11 07:5	7:51 Calculated
# Peak Channel Square Concentration Release t	se time, min
1 Metah 1 12,99 0,06 1,43	
2 Этан 1 246.12 0.82 1.65	
3 Пропан 1 14577,00 49,77 2,47	
3 Пропан 1 14577,00 49,77 2,47 4 изобутан 1 4409,21 15,02 4,71	
3 Пропан 1 14577,00 49,77 2,47 4 изобутан 1 4409,21 15,02 4,71 5 н-Бутан 1 9523,15 31,81 5,04	
3 Пропан 1 14577,00 49,77 2,47 4 изобутан 1 4409,21 15,02 4,71 5 н-Бутан 1 9523,15 31,81 5,04 6 изопентан 1 445,96 1,49 8,85	
3 Пропан 1 14577,00 49,77 2,47 4 изобутан 1 4409,21 15,02 4,71 5 н-Бутан 1 9523,15 31,81 5,04 6 изопентан 1 445,96 1,499 8,85 7 н-Пентан 1 157,05 0,52 9,32	
3 Пропан 1 14577,00 49,77 2,47 4 изобутан 1 4409,21 15,02 4,71 5 н-Бутан 1 9523,15 31,81 5,04 6 изопентан 1 445,96 1,499 8,85 7 н-Пентан 1 157,05 0,52 9,32	
3 Пропан 1 14577,00 49,77 2,47 4 изобутан 1 4409,21 15,02 4,71 5 н-Бутан 1 9523,15 31,81 5,04 6 изопентан 1 445,96 1,499 8,85 7 н-Пентан 1 157,05 0,52 9,32	

(picture 5)

Detailed information is available for each chromatogram (**Chrm info**), as well as information on available mixtures (**Mixture, Mixture Info**).

If suitable chromatograms are selected, a full calculation will be performed immediately, otherwise error and warning messages will be displayed in the **System Messages** window. For calculation, it is enough to add, depending on the chosen method, 1 chromatogram of the "Calibration" type and 1 chromatogram of the "Analysis" type, but in order to comply with GOST R 54484-2011, at least 3 chromatograms of the calibration type must be added (GOST R 54484-2011 paragraph 9.5.3).

The **Del** button excludes the selected chromatograms from the calculation.

The **Del all** button excludes all chromatograms from the calculation.

Calc settings

Calc 106 has a settings window (picture 6).

Calc settings		×
Calc method:		
GOST P 54484 Substance sta	I-2011 Relative coeff. ndard: 〜	Octane number calc method: OGOST EN 589-2014 OGOST P 52087-2018
🔾 GOST P 54484	4-2011 Graduation coeff.	0 00011 020072010
○ GOST 33012-2	2014 Method A (packed col)	Rounding values:
◯ GOST 33012-2014 Method B (capillary col)		Round to sign: 3
○ GOST 10679-7	'6	 Round by GOST 10679-2019
) GOST 10679-2	2019 (relative grad.)	Round phys and chem
○ GOST 10679-2	2019 (absolute grad.)	☐ parameters by GOST 10679-2019
Detector type:	Dimension of grad conc:	
ODTP	🔘 mass %	
PID	🔘 mol %	
		OK Cancel

(picture 6)

Depending on the selected calculation method, certain settings become available.

When changing the configuration of the settings, they must be saved with the **OK** button. To get up-to-date results corresponding to the current settings, it is necessary to recalculate by clicking the **Calculate** button (main program window, picture 5).

During recalculations, the **System Messages** tab is updated and provides detailed information about the current calculation status (warnings, errors, etc.).

The Components window (picture 7) is called by clicking the **Components** button (the main program window, picture 5). In this window, you can set alternative component names and corresponding sensitivity coefficients. To edit the alternative name or sensitivity coefficient of a component, double-click in the field opposite the desired component and enter the desired value. If there is a dash in the sensitivity coefficient field, it means that the component was not explicitly specified in the selected guest. Components with a dash instead of a sensitivity coefficient will be skipped during calculations, if the component needs to be taken into account, then the corresponding coefficient should be entered instead of a dash.

	mponents			
ŧ	Component	Alternative name	Coef. sensitivity.(PID, mass)	
	methane	methane	1,100	
2	ethane	ethane	1,030	
3	ethene	ethene	0,970	
4	propane	propane	1,010	
5	propene	propene	0,970	
6	cyclopropane	cyclopropane	0,970	
7	propadiene	propadiene	0,920	
8	methylacetylene	methylacetylene	0,970	
9	isobutane	isobutane	1,000	
10	n_butane	n_butane	1,000	
11	butene_1	butene_1	0,970	
12	isobutylene	isobutylene	0,970	
13	trans_butene_2	trans_butene_2	0,970	
14	cis_butene_2	cis_butene_2	0,970	
15	butadiene_1_3	butadiene_1_3	0,930	
16	isopentane	isopentane	0,990	
17	n_pentane	n_pentane	0,990	
18	2_2_dimethylpropane	2_2_dimethylpropane	0,990	
19	pentene_1	pentene_1	0,970	
20	3_methyl_1_butene	3_methyl_1_butene	0,970	
21	2_methyl_1_butene	2_methyl_1_butene	0,970	
22	trans_pentene_2	trans_pentene_2	0,970	
23	cis_pentene_2	cis_pentene_2	0,970	
24	2_methyl_2_butene	2_methyl_2_butene	0,970	
25	n_hexane	n_hexane		
26	2_3_dimethylpropane	2_3_dimethylpropane		
27	2_methylpentane	2_methylpentane		
28	3 mathulnantana	3 methulnentene		

(picture 7)

Generating a report

To generate a report, you must specify what content it will be filled with, as well as specify how it will be saved (picture 8).

Report settings X
Contents of the report
File list
Preliminary calc of concentrations
Calc of concentrations
Calc of graduation
Check graduation
Density tabled
Density and pressure
Octane number
Molecular mass
Erros messages
Device number:
Report:
Save to file
O Open in browser
OK Cancel

(picture 8)

The file report is generated in the format **.html**