Calculation of Volatile Compound Concentrations in Alcoholic Beverages

The calculator is designed for comparative evaluation of the metrological characteristics of various chromatographic methods for analysis of alcoholic and other alcohol-containing products

PARAMETERS OF METHODS | SS CONCENTRATIONS | SS AREAS | CALIBRATION | SAMPLES OF PRODUCTS | REPORT | FORMULA

Basic parameters of methods and standard solutions (SS)

1. The following chromatographic methods are used to analyze alcohol-containing products: external standard method using a set of standard solutions (SS), traditional internal standard method using an additional substance added to the SS and product samples at a known concentration, and new modified internal standard method (IS_Ethanol), in which ethanol contained in the SS and products is used as an internal standard.
2. All methods use multiple SS containing compounds in known concentrations. Each set of SS corresponds to several concentration levels, which are needed for determination of the calibration coefficients and verification the linearity of the detector response. It is necessary to specify the count of analyte compounds (uncluding ethanol) and the count of SS to work of the calculator.
3. Different methods of alcohol analysis may use different units of concentration measurement. To ensure accurate calculations and easy comparison of different methods, concentration values are converted from "primary" units of measurement to "final" units, which will be used in the calculations in the methods.
4. To calibrate a chromatograph using methods that use an internal standard (traditional method or IS_Ethanol), the relative response factors (*RRFs*) are determined. A single calibration level is used as a rule with an "intermediate" concentration values. The remaining levels are used to evaluate the linearity of the detector response.

Enter the count of compounds
Count of compounds:

3

Enter the count of concentration levels
Count of concentration levels:

8

Enter the number of calibration level (for *RRF* calculation)
Calibration level number:

3

Enter the primary units of concentration (µg/g = ug/g)
Primary units of concentration:

mg/L

Enter the final concentration units in which the results should be calculated.
Final units of concentration:

g/100L AA

When converting units of measurement per anhydrous alcohol, enter the SS strength value, in vol.% (from 0.5 to 100)
Strength of SS, vol.%:

40

If the units of measurement are *µg/g (µg/g = ug/g)* , enter the value of SS density at a temperature of 20 °C, in kg/m^3 = g/l (from 772 to 1000)
Density of SS, kg/m^3:

948.06

To button "Submit values" ->
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Concentrations of compounds in standard solutions (SS). Conversion of concentration units

Fill in the table:

Table 1. Concentration values of compounds in SS, expressed in primary units *mg/L*

№	Compound	Concentration level							
		1	2	3	4	5	6	7	8
1	methanol	34.914	86.85	171.585	181.7	392.4	782.8	1174.2	1565.6
2	3-pentanol	18.9	18.94	19.5	18.95	18.92	18.91	18.88	18.86
3	ethanol	0	0	0	0	0	0	0	0

To button "Submit values" ->
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Table 2. Concentration values of compounds in SS, converted into specified units of measurement *g/100L AA*

№	Compound	Concentration level							
		1	2	3	4	5	6	7	8
1	methanol	8.7285	21.7125	42.89625	45.425	98.1	195.7	293.55	391.4
2	3-pentanol	4.725	4.735	4.875	4.7375	4.73	4.7275	4.72	4.715
3	ethanol	78927	78927	78927	78927	78927	78927	78927	78927

Data from chromatograms of SS

Enter the count of repeated measurements for the concentration level 1
Count of repeated measurements

1

Concentration level 1.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area
			1
1	methanol	8.7285	4.849
2	3-pentanol	4.725	6.208
3	ethanol	78927	65492.31

To button "Submit values" ->
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Enter the count of repeated measurements for the concentration level 2
Count of repeated measurements

1

Concentration level 2.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area
			1
1	methanol	21.7125	12.2669
2	3-pentanol	4.735	6.7273
3	ethanol	78927	68473.0639

To button "Submit values" ->
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Enter the count of repeated measurements for the concentration level 3
Count of repeated measurements

2

Calibration level for *RRF*

Concentration level 3.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area	
			1	2
1	methanol	42.89625	25.564	25.645
2	3-pentanol	4.875	6.772	6.562
3	ethanol	78927	70651.736	69231.628

To button "Submit values" ->
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Enter the count of repeated measurements for the concentration level 4

Count of repeated measurements

1

Concentration level 4.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area
			1
1	methanol	45.425	26.8631
2	3-pentanol	4.7375	6.8984
3	ethanol	78927	68903.99

To button "Submit values" ->
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Enter the count of repeated measurements for the concentration level 5

Count of repeated measurements

1

Concentration level 5.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area
			1
1	methanol	98.1	54.715
2	3-pentanol	4.73	6.835
3	ethanol	78927	67722.03

To button "Submit values" ->
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Enter the count of repeated measurements for the concentration level 6

Count of repeated measurements

1

Concentration level 6.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area
			1
1	methanol	195.7	111.7128
2	3-pentanol	4.7275	6.7989
3	ethanol	78927	67461.3126

To button "Submit values" ->
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Enter the count of repeated measurements for the concentration level 7

Count of repeated measurements

1

Concentration level 7.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area
			1
1	methanol	293.55	162.467
2	3-pentanol	4.72	6.57
3	ethanol	78927	64763.602

To button "Submit values" ->
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Enter the count of repeated measurements for the concentration level 8
Count of repeated measurements

1

Concentration level 8.
Peak area values of compounds

№	Compound	Concentration, g/100L AA	Pick area, units of area
			1
1	methanol	391.4	215.821
2	3-pentanol	4.715	5.803
3	ethanol	78927	64332.578

To button "Submit values" ->
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Calibration

Select calibration methods:

- modified internal standard method with ethanol
- external standard method
- internal standard method with additional reference

If you select internal standard method, please indicate reference substance
Reference substance (internal standard):

3-pentanol

To button "Submit values"->
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Calibration by modified internal standard method (reference - ethanol)

Calibration $C/C_{eth} = RRF \cdot A/A_{eth}$; RRF = 1.4842326443714

Compound №1: methanol

C^{cert}, g/100L AA	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	Bias, %	Count of repeats
8.7285	8.6734	0.0000	0.0000	0.00	-0.63	1
21.7125	20.9866	0.0000	0.0000	0.00	-3.34	1
42.8962	42.8903	0.7117	1.9715	1.66	-0.01	2
45.425	45.6709	0.0000	0.0000	0.00	0.54	1
98.1	94.6464	0.0000	0.0000	0.00	-3.52	1
195.7	193.988	0.000	0.000	0.00	-0.87	1
293.55	293.874	0.000	0.000	0.00	0.11	1
391.4	392.998	0.000	0.000	0.00	0.41	1

Calibration $C/C_{eth} = RRF \cdot A/A_{eth}$; RRF = 0.64798613422395

Compound №2: 3-pentanol

C^{cert}, g/100L AA	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	Bias, %	Count of repeats
4.725	4.84789	0.00000	0.00000	0.00	2.60	1
4.735	5.02473	0.00000	0.00000	0.00	6.12	1
4.875	4.87485	0.03859	0.10690	0.79	-0.00	2
4.7375	5.1203	0.0000	0.0000	0.00	8.08	1
4.73	5.16178	0.00000	0.00000	0.00	9.13	1
4.7275	5.15437	0.00000	0.00000	0.00	9.03	1
4.72	5.18831	0.00000	0.00000	0.00	9.92	1

4.715	4.61331	0.00000	0.00000	0.00	-2.16	1

Calibration $C/C_{eth} = RRF \cdot A/A_{eth}$

Coefficients of calibration and FID response linearity

№	Compound	Coefficient of calibration $RRF^{ethanol}$	Coefficient of determination R^2	Coefficient of correlation C_P
1	methanol	1.48	0.99986	0.99995
2	3-pentanol	0.648	0.04247	0.55446
3	ethanol	1	-	-

To button "Submit values"->
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- Calibration by modified internal standard method (reference - ethanol) ->
- Calibration by external standard method ->
- Calibration by internal standard method (reference - 3-pentanol) ->

Calibration by external standard method

Calibration $C = RF \cdot A$; RF = 1.7993573840793 (g/100L AA)/(area units)

Compound №1: methanol

C^{cert}, g/100L AA	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	Bias, %	Count of repeats
8.7285	8.72508	0.00000	0.00000	0.00	-0.04	1
21.7125	22.0725	0.0000	0.0000	0.00	1.66	1
42.8962	46.0716	0.1031	0.2855	0.22	7.40	2
45.425	48.3363	0.0000	0.0000	0.00	6.41	1
98.1	98.4518	0.0000	0.0000	0.00	0.36	1
195.7	201.011	0.000	0.000	0.00	2.71	1
293.55	292.336	0.000	0.000	0.00	-0.41	1

391.4	388.339	0.000	0.000	0.00	-0.78	1

Calibration $C = RF \cdot A$; RF = 0.7221848555932 (g/100L AA)/(area units)

Compound №2: 3-pentanol

C^{cert}, g/100L AA	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	Bias, %	Count of repeats
4.725	4.48332	0.00000	0.00000	0.00	-5.11	1
4.735	4.85835	0.00000	0.00000	0.00	2.61	1
4.875	4.81481	0.10724	0.29705	2.23	-1.23	2
4.7375	4.98192	0.00000	0.00000	0.00	5.16	1
4.73	4.93613	0.00000	0.00000	0.00	4.36	1
4.7275	4.91006	0.00000	0.00000	0.00	3.86	1
4.72	4.74475	0.00000	0.00000	0.00	0.52	1
4.715	4.19084	0.00000	0.00000	0.00	-11.12	1

Calibration $C = RF \cdot A$

Coefficients of calibration and FID response linearity

№	Compound	Coefficient of calibration RF, (g/100L AA)/(area un.)	Coefficient of determination R^2	Coefficient of correlation C_P
1	methanol	1.8	0.99954	0.99986
2	3-pentanol	0.722	0.05180	0.22899
3	ethanol	0	-	-

To button "Submit values"->
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- Calibration by modified internal standard method (reference - ethanol) ->
- Calibration by external standard method ->
- Calibration by internal standard method (reference - 3-pentanol) ->

Calibration by internal standard method (reference - 3-pentanol)

Calibration $C/C_{st} = RRF \cdot A/A_{st}$; RRF = 2.2898650589124

Compound №1: methanol

C^{cert}, g/100L AA	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	Bias, %	Count of repeats
8.7285	8.45108	0.00000	0.00000	0.00	-3.18	1
21.7125	19.7708	0.0000	0.0000	0.00	-8.94	1
42.8962	42.8834	1.0510	2.9114	2.45	-0.03	2
45.425	42.2442	0.0000	0.0000	0.00	-7.00	1
98.1	86.704	0.000	0.000	0.00	-11.62	1
195.7	177.871	0.000	0.000	0.00	-9.11	1
293.55	267.271	0.000	0.000	0.00	-8.95	1
391.4	401.544	0.000	0.000	0.00	2.59	1

Calibration $C/C_{st} = RRF \cdot A/A_{st}$

Coefficients of calibration and FID response linearity

№	Compound	Coefficient of calibration $RRF^{3\text{-pentanol}}$	Coefficient of determination R^2	Coefficient of correlation C_P
1	methanol	2.29	0.99230	0.99662
2	3-pentanol	1	-	-
3	ethanol	1.54	-	-

To button "Submit values"->
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- Calibration by modified internal standard method (reference - ethanol) ->
- Calibration by external standard method ->
- Calibration by internal standard method (reference - 3-pentanol) ->

Parameters of the samples of the products

Enter the count of the samples of the alcoholic beverages

Count of samples: 1

To button "Submit values" ->
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Enter a name of the product sample and the count of its repeated measurements

Sample's name: Head, 1

Count of repeated measurements: 2

To perform calculations per anhydrous alcohol by external standard method, indicate the strength value of the product sample

Strength of the product sample, vol.% (from 0.5 to 100): 40

If you use units µg/g and external standard method, provide the density value of the product sample

Density of the product sample at temperature of 20 °C, in kg/m^3 = g/l (from 772 to 1000): 948

If you need to perform calculation by internal standard method, then indicate the value of concentration of the internal standard substance in the product sample

Concentration of substance "3-pentanol" in the product, in mg/L: 19.5

To button "Submit values" ->
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Peak area values of compounds in sample *"Head, 1"*

№	Compound	Pick area, units of area	
		1	2
1	methanol	25.564	25.645
2	3-pentanol	6.772	6.562

3	ethanol	70652	69232

To button "Submit values" ->
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To the next product ->

Results for sample "Head, 1", obtained by modified internal standard method (reference - ethanol)

Calibration $C/C_{eth} = RRF \cdot A/A_{eth}$

№	Compound	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	$RRF^{ethanol}$
1	methanol	42.8901	0.7117	1.9713	1.66	1.48
2	3-pentanol	4.87483	0.03860	0.10692	0.79	0.648

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- Results using by the internal standard "ethanol" ->
- Results using by external standard method->
- Results using by the internal standard "3-pentanol" ->

Results for sample "Head, 1", obtained by external standard method

Calibration $C = RF \cdot A$, (g/100L AA)/(area units)

№	Compound	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	RF, (g/100L AA)/(area un.)
1	methanol	46.0716	0.1031	0.2855	0.22	1.8
2	3-pentanol	4.81481	0.10724	0.29705	2.23	0.722

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- Results using by the internal standard "ethanol" ->
- Results using by external standard method ->
- Results using by the internal standard "3-pentanol" ->

Results for sample "Head, 1", obtained by internal standard method (reference - 3-pentanol)

Calibration $C/C_{st} = RRF \cdot A/A_{st}$

№	Compound	C^{meas}, g/100L AA	SD, g/100L AA	Repeatability limit, g/100L AA	RSD, %	$RRF^{3\text{-pentanol}}$
1	methanol	42.8834	1.0510	2.9114	2.45	2.29
2	3-pentanol	4.875	0.000	0.000	0.00	1

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- Results using by the internal standard "ethanol" ->
- Results using by external standard method ->
- Results using by the internal standard "3-pentanol" ->

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