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

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. The initial stage of all methods is calibration — the determination of calibration characteristics by the analysis of SS with certified concentration values C^{cert} of volatile compounds. Then, using the established calibration parameters, the content of analyzed compounds in samples C^{meas} is determined.
3. 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 and the count of SS to work of the calculator.
4. 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. The calculator offers the following unit options (abbrevation AA - anhydrous alcohol): *mg/L (mg/L = mg/dm^3), mg/L AA, vol.%, vol.% AA, g/100L AA (g/100L AA = mg/100cm^3 AA), µg/g (µg/g = ug/g).*
5. The IS_Ethanol method calculates per *AA*, so the following can be set as "final" units of measurement for IS_Ethanol: *mg/L AA, vol.% AA, g/100L AA, mg/100cm^3 AA*. If the "primary" units of measurement are also per *AA*, then information about the strength of SS and product samples is not required.
6. 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:

3

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:

ug/g

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

vol.%

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

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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 *µg/g*

№	Compound	Concentration level		
		1	2	3
1	methanol	21.634	107.54	203.11
2	ethanol	0	0	0
3	3-pentanol	228.73	227.65	226.16

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Table 2. Concentration values of compounds in SS, converted into specified units of measurement *vol.% AA*

№	Compound	Concentration level		
		1	2	3
1	methanol	0.0064758556579944	0.032190696009093	0.060798328681485
2	ethanol	100	100	100
3	3-pentanol	0.066518332453988	0.066204251226994	0.065770935460123

Data from chromatograms of SS

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

2

Concentration level 1.
Peak area values of compounds

№	Compound	Concentration, vol.% AA	Pick area, units of area	
			1	2
1	methanol	0.0064758556579944	0.00164	0.001655
2	ethanol	100	29.0017	28.957
3	3-pentanol	0.066518332453988	0.0346	0.03461

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Enter the count of repeated measurements for the concentration level 2
Count of repeated measurements

2

Concentration level 2.
Peak area values of compounds

№	Compound	Concentration, vol.% AA	Pick area, units of area	
			1	2
1	methanol	0.032190696009093	0.00805	0.00796
2	ethanol	100	28.9454	28.94586
3	3-pentanol	0.066204251226994	0.015244	0.015139

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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, vol.% AA	Pick area, units of area	
			1	2
1	methanol	0.060798328681485	0.0151	0.01512
2	ethanol	100	28.808	29.0155
3	3-pentanol	0.065770935460123	0.0341	0.0343

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

Calibration by modified internal standard method (reference - ethanol)

Calibration $C/C_{eth} = RRF \cdot A/A_{eth}$; RRF = 1.1633041442643

Compound №1: methanol

C^{cert}, vol.% AA	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	Bias, %	Count of repeats

0.00648	0.00661	0.00005	0.00014	0.75	2.13	2
0.03219	0.03217	0.00026	0.00071	0.80	-0.06	2
0.06080	0.06080	0.00025	0.00070	0.41	-0.00	2

Calibration $C/C_{eth} = RRF \cdot A/A_{eth}$; RRF = 0.55600803184971

Compound №3: 3-pentanol

C^{cert}, vol.% AA	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	Bias, %	Count of repeats
0.06652	0.06639	0.00009	0.00024	0.13	-0.19	2
0.06620	0.02918	0.00014	0.00040	0.49	-55.92	2
0.06577	0.06577	0.00006	0.00017	0.09	-0.00	2

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	1.16	0.99984	0.99995
2	ethanol	1	-	-
3	3-pentanol	0.556	0.01212	0.99999

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 = 4.0223104001822 (vol.% AA)/(area units)

Compound №1: methanol

C^{cert}, vol.% AA	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	Bias, %	Count of repeats
0.00648	0.00663	0.00004	0.00012	0.64	2.33	2
0.03219	0.03220	0.00026	0.00071	0.79	0.02	2
0.06080	0.06078	0.00006	0.00016	0.09	-0.03	2

Calibration $C = RF \cdot A$; RF = 2.1389923348166 (vol.% AA)/(area units)

Compound №3: 3-pentanol

C^{cert}, vol.% AA	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	Bias, %	Count of repeats
0.06652	0.07402	0.00002	0.00004	0.02	11.28	2
0.06620	0.03249	0.00016	0.00044	0.49	-50.92	2
0.06577	0.07315	0.00030	0.00084	0.41	11.22	2

Calibration $C = RF \cdot A$

Coefficients of calibration and FID response linearity

№	Compound	Coefficient of calibration *RF*, (vol.% AA)/(area un.)	Coefficient of determination R^2	Coefficient of correlation C_P
1	methanol	4.02	0.99996	0.99999
2	ethanol	0	-	-
3	3-pentanol	2.14	-0.00231	-0.07352

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 = 2.092252852374

Compound №1: methanol

C^{cert}, vol.% AA	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	Bias, %	Count of repeats
0.00648	0.00663	0.00004	0.00011	0.62	2.32	2
0.03219	0.07299	0.00022	0.00062	0.31	126.74	2
0.06080	0.06080	0.00019	0.00054	0.32	-0.00	2

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	2.09	0.97194	0.99999
2	ethanol	1.8	-	-
3	3-pentanol	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) ->

Parameters of the samples of the products

Enter the count of the samples of the alcoholic beverages

Count of samples: 2

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: Wine

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): 18.1

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): 975.6

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 μg/g: 214.11

To button "Submit values" ->
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Peak area values of compounds in sample *"Wine"*

№	Compound	Pick area, units of area	
		1	2
1	methanol	0.01695	0.01704
2	ethanol	12.9809	13.04125
3	3-pentanol	0.03306	0.033353

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

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

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

№	Compound	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	$RRF^{ethanol}$
1	methanol	0.15195	0.00007	0.00020	0.05	1.16
2	3-pentanol	0.14190	0.00042	0.00116	0.30	0.556

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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 "Wine", obtained by external standard method

Calibration $C = RF \cdot A$, (vol.% AA)/(area units)

№	Compound	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	RF, (vol.% AA)/(area un.)
1	methanol	0.15107	0.00057	0.00157	0.37	4.02
2	3-pentanol	0.15697	0.00098	0.00271	0.62	2.14

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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 "Wine", obtained by internal standard method (reference - 3-pentanol)

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

№	Compound	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	$RRF^{3\text{-}pentanol}$
1	methanol	0.15163	0.00038	0.00105	0.25	2.09
2	3-pentanol	0.14160	0.00000	0.00000	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" ->

Enter a name of the product sample and the count of its repeated measurements

Sample's name: Whiskey

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): 41

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): 946.4

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 μg/g: 224.46

To button "Submit values" ->
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Peak area values of compounds in sample *"Whiskey"*

№	Compound	Pick area, units of area	
		1	2
1	methanol	0.002258	0.002175
2	ethanol	29.5443	29.4638
3	3-pentanol	0.03689	0.0339845

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

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

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

№	Compound	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	$RRF^{ethanol}$
1	methanol	0.00874	0.00021	0.00059	2.45	1.16
2	3-pentanol	0.06678	0.00374	0.01037	5.60	0.556

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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 "Whiskey", obtained by external standard method

Calibration $C = RF \cdot A$, (vol.% AA)/(area units)

№	Compound	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	RF, (vol.% AA)/(area un.)
1	methanol	0.00870	0.00023	0.00064	2.65	4.02
2	3-pentanol	0.07395	0.00429	0.01188	5.80	2.14

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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 "Whiskey", obtained by internal standard method (reference - 3-pentanol)

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

№	Compound	C^{meas}, vol.% AA	SD, vol.% AA	Repeatability limit, vol.% AA	RSD, %	$RRF^{3\text{-}pentanol}$
1	methanol	0.00833	0.00026	0.00073	3.15	2.09
2	3-pentanol	0.06357	0.00000	0.00000	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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