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Application News

GC-MS GCMS-QP2020 NX

Simplifying the Calculation of TVOC Using TVOC Calculation Tool and Thermal Desorption GC-MS

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User Benefits

- TVOC Calculation Tool easily calculates quantitative values using toluene conversion.
- Thermal desorption GC-MS can perform high-throughput VOC analysis as it does not require solvent extraction.
- The TD-30R thermal desorption system uses nitrogen gas for primary desorption from the collection tube, reducing the amount of helium gas used.

■ Introduction

The amount of toxic volatile organic compounds (VOCs) in air is one index of air pollution, and is monitored in various places including factories, urban areas, and indoor environments. One method of quantitating such VOCs is by quantitating all compounds eluted, from hexane to hexadecane, using toluene conversion, and then calculating the total volatile organic compounds (TVOC) from the total. If the TVOC exceeds a criterion value, it may be necessary to quantitate each compound. For details on how to calculate TVOC and the recommended procedures, refer to the recommended procedure of ECA (EUROPEAN COLLABORATIVE ACTION).

Calculating TVOC manually is quite labor-intensive, as it requires the calculation of values using toluene conversion for each compound, calculation of the total, and calculation of precise quantitative values in some cases if required. However, the calculations are quickly and easily performed using TVOC Calculation Tool. This program can also calculate precise quantitative values for individual compounds specified by the user.

This article describes the use of TVOC Calculation Tool to easily calculate the TVOC detected in a laboratory air sample through data analysis of the results from analysis with an efficient thermal desorption gas chromatograph/mass spectrometer (TD-GC/MS) system, which does not require solvent extraction when analyzing VOCs.

■ TVOC Calculation Tool

The TVOC Calculation Tool can automatically calculate the toluene conversion values and output a report by just importing the detected compound qualitative results. Also, depending on the use, by simply switching between the following [1] and [2], the concentrations can be recalculated. For details regarding the method of use, refer to the link on the above right.

[1] Quantitate all the detected compounds using toluene conversion.

[2] Precisely quantitate only the target compounds, and use toluene conversion to quantitate the other compounds detected.

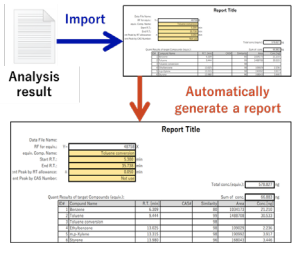

Fig. 1 TVOC Calculation Tool

■ Experiment

In this example, mixed standard samples of benzene, ethylbenzene, m,p,o-xylene, 1,4- dichlorobenzene, and tetradecane, diluted with methanol to concentrations of 4 ppm, 10 ppm, 40 ppm, 100 ppm, and 400 ppm respectively, were prepared in addition to the standard toluene samples so as to create the calibration curves. The mixed standard samples prepared were then added 1 µL at a time to a TENAX-TA collection tube, and analyzed. Mixed standard samples of 100 ppm hexane and hexadecane were similarly prepared and analyzed. In terms of the actual sample, air from laboratory A was collected for 30 minutes at a rate of 100 mL per minute, and measured. The collection method is shown in Fig. 2, and the analysis conditions are shown in Table 1.

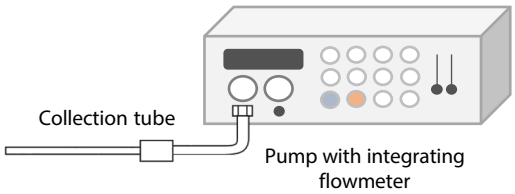

Fig. 2 Air Collection Method

Table 1 Analysis Conditions

Model:	GCMS-QP2020 NX
Autosampler:	TD-30R
[TD-30R]	
Tube Desorb Temp.:	280 °C (10 min)
Tube Desorb Flow:	60 mL/min
Trap Cooling Temp.:	-20 °C
Trap Desorb Temp.:	280 °C (10 min)
Joint Temp.:	250 °C
Valve Temp.:	250 °C
Transfer Line Temp.:	250 °C
[GC]	
Injection Mode:	Split
Split Ratio:	10
Carrier Gas:	He
Carrier Gas Control:	Linear velocity (30 cm/min)
Column:	SH-I-1MS (P/N 227-36005-02) (60 m × 0.25 mm I.D., 0.25 µm)
Column Temp.:	40 °C (5 min) - 5 °C/min – 250 °C (5 min)
[MS]	
Ion Source Temp.:	200 °C
Interface Temp.:	280 °C
Acquisition Mode:	Scan
Event Time:	0.3 sec
m/z Range	*m/z*=35-350

■ Calibration Curves for Toluene and Target Compounds

When calibration curves were created for the range from 4 ppm to 400 ppm by measuring the mixed standard samples of benzene, toluene, ethylbenzene, m,p-xylene, o-xylene, 1,4-dichlorobenzene, and tetradecane, favorable results were obtained, with R > 0.999 for all compounds. The TVOC was calculated using the TIC for toluene.

The standard samples apart from toluene should be changed as needed in accordance with the compounds to be quantitated precisely. When only calculating quantitative values using toluene conversion, it is sufficient just to measure the toluene standard sample.

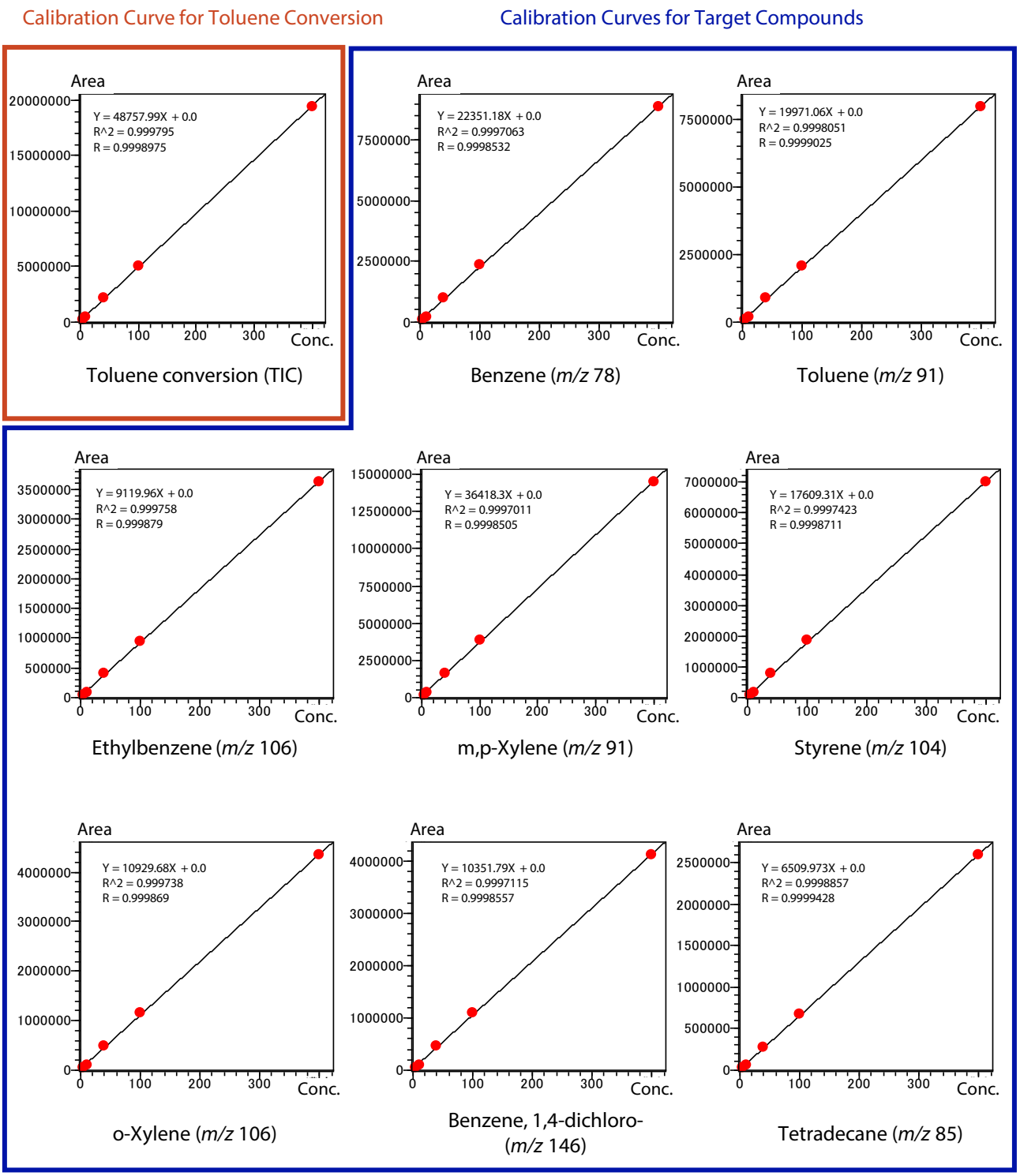

Fig. 3 Calibration Curves for Toluene and Target Compounds (4 ppm, 10 ppm, 40 ppm, 100 ppm, and 400 ppm)

■ Calculation of TVOC (Toluene Conversion and Precise Quantitation)

Fig. 4 shows the TIC chromatogram for the actual sample. Of the peaks detected here, those in the interval from hexane to hexadecane were defined as VOCs, and were used for the TVOC calculation. After peak integration and qualitative analysis, the results obtained were read into TVOC Calculation Tool. Following this, the total value for the concentrations of all the peaks was calculated automatically and used to indicate the TVOC value in Fig. 5 (2). In addition, the concentrations found using the respective toluene conversions for each peak were calculated individually as shown in Fig. 5 (3) and (4) and could be printed in a report as is, heightening the procedural efficiency. In (4) for example, only some of the compounds detected are displayed.

In addition, as shown in Fig. 5 (1), either [Show Result of equiv.] (Toluene conversion quantitation) or [Show Result of precise quant.] (Precise quantitation) could be selected. As shown in Fig. 6 (3), if [Show Result of precise quant.] is selected here, recalculation is performed so as to calculate precise quantitative values for the target compounds (benzene, toluene, ethylbenzene, m,p,o-xylene, styrene, 1,4-dichlorobenzene, and tetradecane) which were measured to produce the calibration curves. Switching between quantitation using toluene conversion and precise quantitation can be performed with one click, to suit the analysis objective.

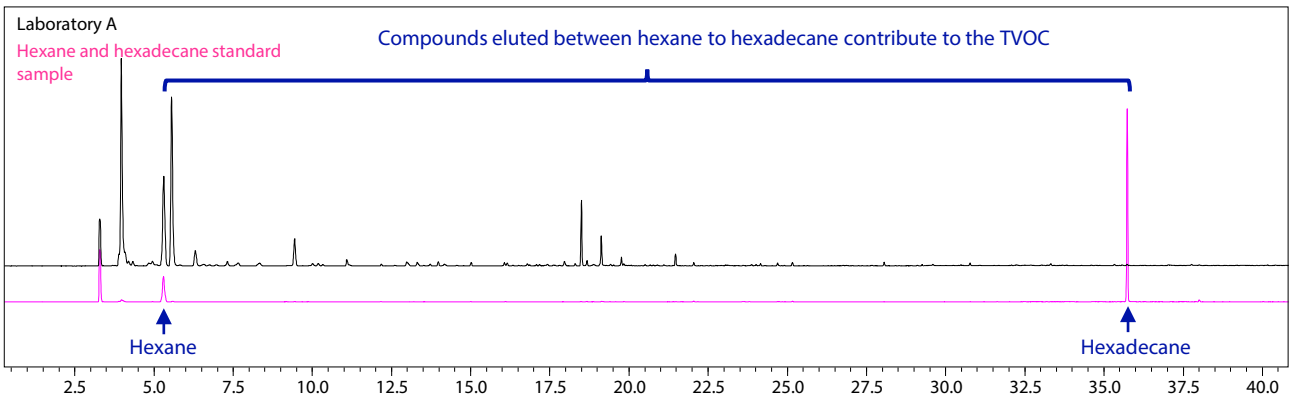

Fig. 4 TIC Chromatograms for Air Collected in Laboratory A and Hexane/Hexadecane

Imported into the toluene conversion program after peak integration and qualitative analysis

(1)

Display mode: Show Result of equiv. | Labguage: English | RF for equiv.: Auto

Load data and calculate

Recalculate

Report Title

Data File Name: Data File.qdg

RF for equiv.: Y= 48758 X

equiv. Comp. Name: Toluene conversion

Start R.T.: 5.300 min

End R.T.: 35.738 min

nt Peak by RT allowance: ± 0.050 min

ent Peak by CAS Number: Not use

(2)

Total conc.(equiv.) 578.827 ng

Quant Results of target Compounds (equiv.): Sum of conc 66.883 ng

ID#	Compund Name	R.T. [min]	CAS#	Similarity	Area	Conc.[ng]
1	Benzene	6.309		80	1034173	21.210
2	Toluene	9.444		99	1488708	30.533
3	Toluene conversion			98		
4	Ethylbenzene	13.025		98	109029	2.236
5	m,p-Xylene	13.315		98	190992	3.917
6	Styrene	13.980		96	168043	3.446
7	o-Xylene	14.169		93	108271	2.221
8	Benzene, 1,4-dichloro-	18.303		97	76143	1.562
9	Tetradecane	30.772		95	85709	1.758

(3)

Quant Results of TIC peaks (equiv.): Sum of conc 511.944 ng

No	Compund Name	R.T. [min]	CAS#	Similarity	Area	Conc.[ng]
10	n-Hexane	5.312	110-54-3	91	6415428	131.577
11	Tetrahydrofuran	5.559	109-99-9	98	10097733	207.099
12	Cyclopentane, methyl-	5.830	96-37-7	89	58213	1.194
14	Cyclohexane	6.575	110-82-7	91	156421	3.208
15	Hexane, 2-methyl-	6.764	591-76-4	91	77825	1.596
16	Hexane, 3-methyl-	6.969	589-34-4	91	74181	1.521
17	Pentane, 2,2,4-trimethyl-	7.320	540-84-1	97	226003	4.635
18	Cyclopropanecarboxylic acid, methyl e	7.575	2868-37-3	74	42673	0.875
19	Heptane	7.664	142-82-5	95	215743	4.425

(4)

Fig. 5 Quantitation Using Toluene Conversion for All Compounds Detected

Precise quantitation of only the target compounds from which the calibration curves were produced by measuring standard samples

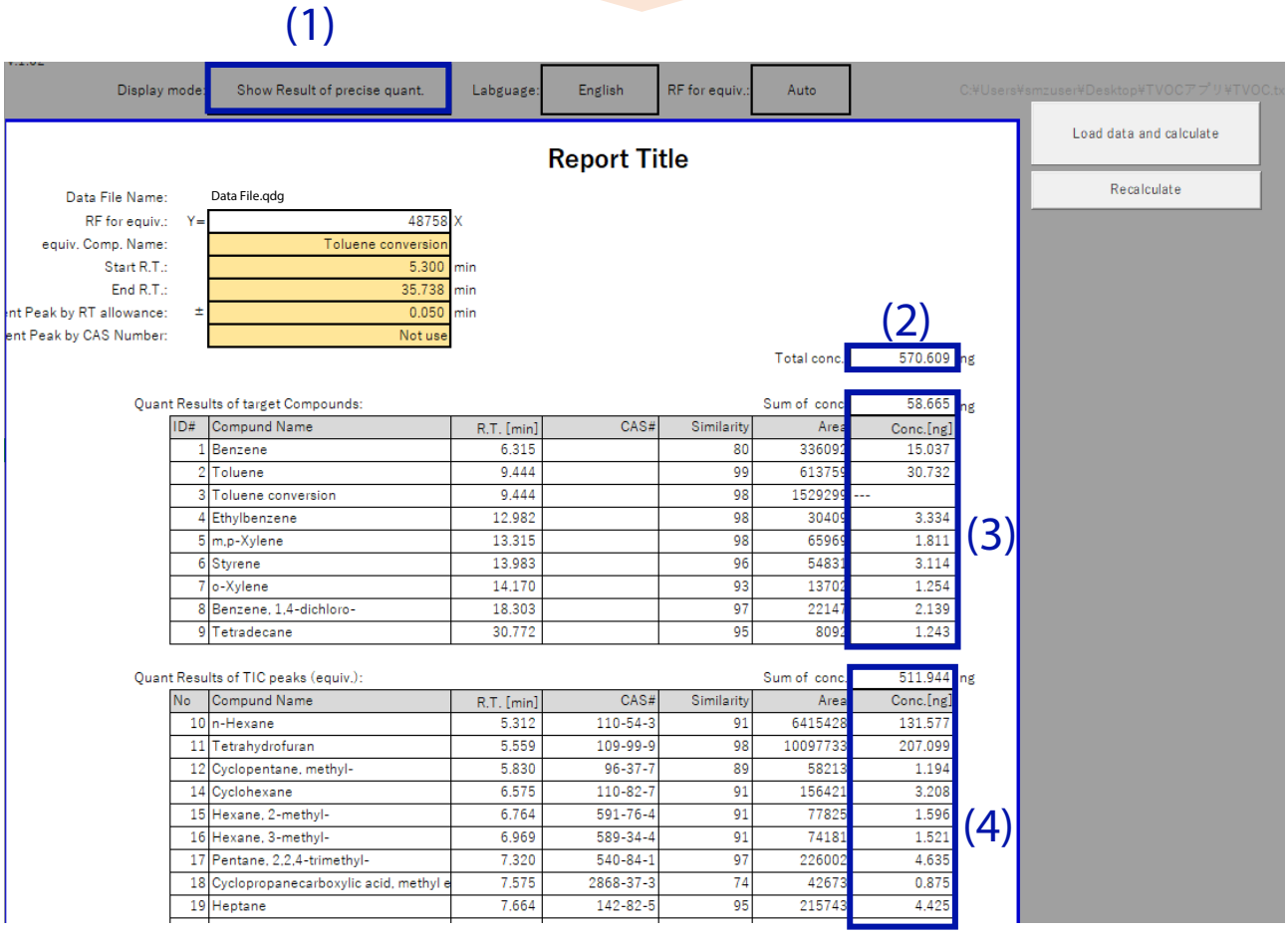

Fig. 6 Precise Quantitation of Target Compounds Only, and Quantitation of the Other Detected Compounds Using Toluene Conversion

■ Conclusion

This article introduced a simple method for calculating the TVOC in a laboratory air sample measured with the TD-30R + GCMS QP2020 NX, using TVOC Calculation Tool. Precise quantitative values for the target compounds for which calibration curves were created by measuring standard samples can be calculated with just one click, heightening extendibility.

TVOC Calculation Tool heightens productivity by automating the calculation of TVOC and the production of reports.

Fig. 7 TD-30R + GCMS-QP2020 NX

• TVOC Calculation Tool is optionally available software compatible with new models of GCMS. For further details, contact your Shimadzu sales representative.

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