High resolution GC/Q-TOF x Multivariate analysis Elucidating hidden odor components

Although GC/MS measurements are usually used to elucidate the cause of odor, even trace amounts of compounds can be odor-causing substances, and there are cases where they cannot be identified because they are hidden by other components. In this paper, we investigated the causes of filter odor in air purifiers using multivariate analysis and odor libraries.

Equipment

GC/Q-TOFMS with Thermal desorption system
■Features
・High-mass resolution（25000 at m/z 271）
・Equipped with re-collect system
・CI measurement is possible
・Equipped with deconvolution function *1)
・Multivariate analysis is possible
・GC×GC   MS/MS analysis is available.

Sample and pre-treatment

■Sample
Deodorizing filters (activated carbon) for air purifiers
✔New
✔Used (1 week use)

■pre-treatment
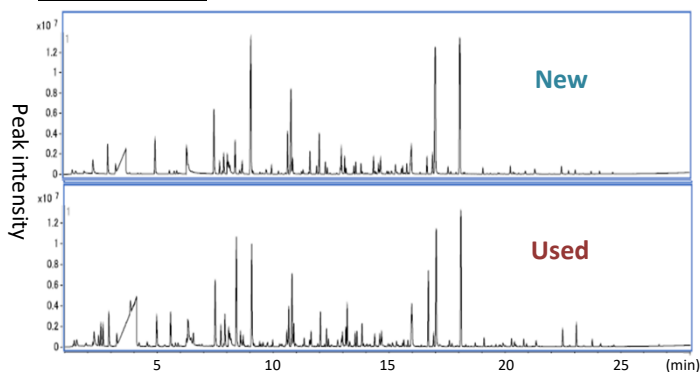Heating conditions: 300℃, 60 minutes collection

Strong Point!
Out gas analysis is possible!

1: Overlapping mass spectra are separated to identify individual components. A mathematical method for extracting "appropriate" mass spectra.

Result

■GC/MS data

Peak intensity

New

Used

multivariable Analysis

Visualization of differences

■Results of multivariate analysis

Characteristic peaks of "New"

Characteristic peaks of "Used"
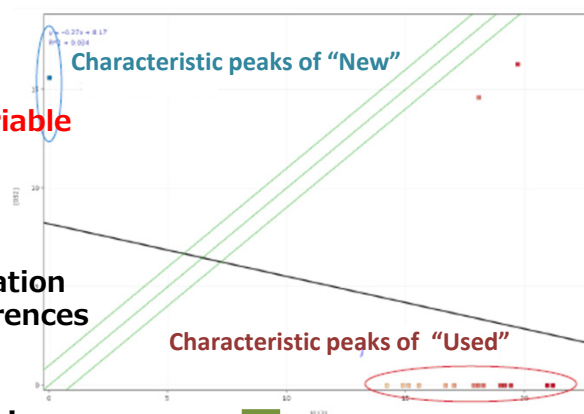
Deconvolution analysis Extract even the buried peaks!

Identification by odor library

■ Identification of characteristic peaks of "Used" and results

Retention time	Compound name	threshold	Features
9.4	butyl acetate	Several tens of ppb	Solvent-like Fruity
10.6	N,N-dimethylacetamide	10ppm	Fishy solvent, amine smell
12.8	phenol	1ppb	Disinfection, solvent
13.8	Dimethyl succinate	Several hundred ppb	fruity smell
13.8	2-Ethyl-1-hexanol	10 ppb	Solvent, plastic-like
13.8	1,4-Dichlorobenzene	Several hundred ppb	Solvent, disinfectant odor
14.1	1-methyl-2-pyrrolidone	several ppm	smell of fish
14.7	Acetophenone	Several hundred ppb	Almonds, insecticide
15.6	Dimethyl glutarate	Several hundred ppb	sweet solvent-like
16.4	Methyl Benzoate	A few 10 ppb	Berries, flowers, vanilla
16.9	Naphthalin	Several hundred ppb	insecticide

Comprehensive analysis considering the quantitative results.

The source of the odor is estimated to be phenol.

By combining high-resolution GC/MS measurements with deconvolution analysis and multivariate analysis, it is possible to identify hidden odor components.
(Other examples of application)
✔Examine the difference in gas components generated between lots.
✔Elucidation of the cause of defects in recycled polymers

Toray Research Center, Inc.