Quantitative Analysis of Food Packaging by Thermal Desorption–GC–MS Method

Author:

Xiaohui Zhang

Application Note
Food

Abstract
This application note demonstrates quantitative analysis of food packaging samples by thermally desorbing the sample into a GC-MS.

Introduction
Food packaging is used to protect food against microbiological, chemical and physical contamination. However, the interactions between the food packaging and the content may actually lead to alterations in the food quality. Two types of such interactions have been extensively studied as (1) migration of substances from packaging to food[1,2], where organic compounds, such as adhesive, ink solvent, plasticisers, photoinitiators, perfluorochemicals, leached from the container into the content, and (2) scalping by the packaging[3], where the flavor and antioxidant in the food are absorbed by the container.

In this application note, various types of food packaging samples were tested against a list of volatile organic compounds (VOCs) that are either known as compounds that may migrate into food or flavor additives that were adsorbed by the packaging. The analysis was performed on a CDS 7550S thermal desorber that was connected to a GC-MS.

Experiment Setup
Six food packaging samples were cut from two different brands of chocolate, one sandwich cookie, one instant noodle, one potato chips, and one energy bar. All samples had the same dimension as 1" x 1". Each sample was individually weighed and folded into a ¼" OD x 3.5" L empty quartz tube (Camsco, Houston, TX). Then each tube was loaded into the 7550S thermal desorber, purged at 35 °C with purging gas to remove air, and sequentially heated at 60 °C for 10 minutes to release VOCs, which were collected onto a 1/8" x 115 mm inert coated refocusing trap packed with Carbograph 1 60/80 and Carbograph 5 60/80. The trap was heated at 300 °C for 3 minutes to transfer all the analytes to a Shimadzu GC-MS QP-2010 for analysis.

7550S Thermal Desorber:	
Valve oven:	220 °C
GC transfer line:	250 °C
Tube purge flow:	30 mL/min
Pre-heat time:	15 s
Tube desorber:	
Rest temp.:	35 °C
Dry purge temp.:	35 °C
Dry purge time:	1 min
Desorb temp.:	60 °C
Desorb time:	10 min
Trap:	
Rest temp.:	30 °C
Desorb temp.:	300 °C
Desorb time:	3 min

GC-MS:	
GC conditions	
Column:	GsBP-5ms,
30 m x 0.25 μ m x0.25 mm	
Oven temp.:	40.0 °C
Injection temp.:	230.00°C
Injection mode:	Split
Column Flow:	1.01 ml/min
Split Ratio:	10.0
Temp. program:	40.0 °C hold 1 min
40.0 °C ramp to 120.0 °C	
16.0 °C ramp to 320.0 °C hold 35 min	
Mass conditions	
Ion Source:	200.00 °C
Interface Temp.:	250.00 °C
Start m/z:	29.00
End m/z:	450.00

Results and Discussions

Figure 1 (a-f) showed the total ion chromatogram of VOCs from six food packaging samples, which had dramatically different composition.

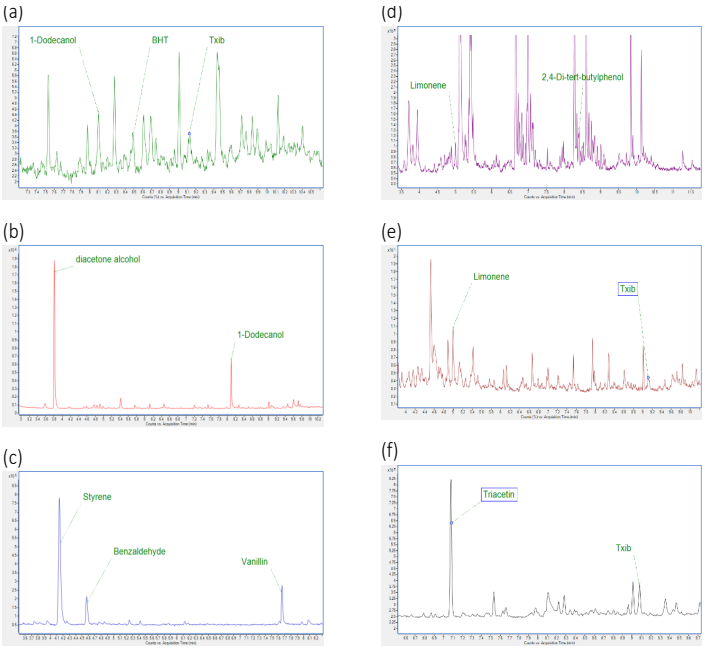

Figure 1 (a-f): Chromatograms of VOCs from six food packaging samples

These varieties of VOCs were grouped as migration of substances from packaging to food shown in Table 1, and scalping by the packaging summarized in Table 2. Table 1 was further categorized into three subgroups as adhesive, ink solvent and plasticizer. Table 2 was also sorted into subgroups as antioxidant, flavor, flavor solvent and surfactant.

Among the detected compounds in Table 1, styrene, phthalates, Txib, diacetone alcohol and 1-(2-methoxypropoxy)-2-Propanol all have direct impact on human health and quantification is required as part of the food safety regulation.

Figure 2 showed a 6-point calibration curve by spiking 1 ng, 2 ng, 5 ng, 10 ng, 25 ng and 50 ng styrene standards into a thermal desorption tube packed with Tenax and desorbed under the same condition by 7550S into GC-MS. Based on the calibration curve, the styrene in the sandwich cookie bag was quantified as 3.3 ppm.

Conclusions:

Six food packaging samples were analyzed quantitatively by thermal desorption method on the VOC contents. The CDS 7550S thermal desorber was demonstrated as a useful tool in investigating the migration and scalping processes for food industry.

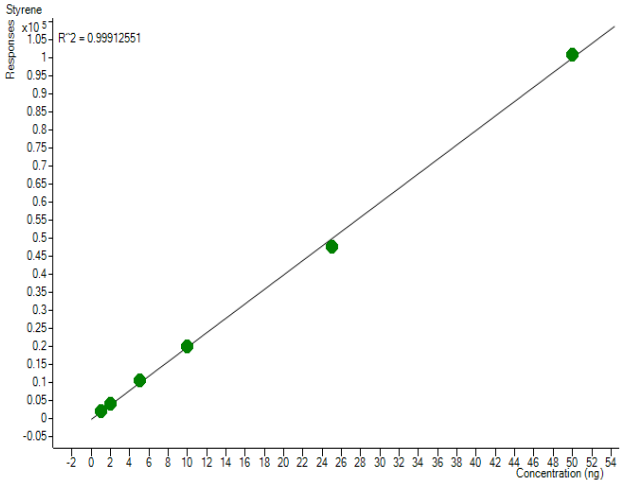

Figure 2: Styrene 6-point calibration curve with R^2=0.999

References

(1) de Quirós, Ana Rodríguez Bernaldo, et al. Food Contamination by Packaging: Migration of Chemicals from Food Contact Materials. Walter de Gruyter GmbH & Co KG, 2019.

(2) Lau, Oi-Wah, and Siu-Kay Wong. "Contamination in food from packaging material." Journal of Chromatography A 882.1-2 (2000): 255-270.

(3) Sajilata, M. G., et al. "Scalping of flavors in packaged foods." Comprehensive reviews in food science and food safety 6.1 (2007): 17-35.

Table 1: Detected VOCs in packaging that may contaminate food (Migration)

Compound	Type	m/z	Chocolate A packaging (87 mg)	Chocolate B packaging (78 mg)	Sandwich packaging (87 mg)	Noodle packaging (80 mg)	Potato chip packaging (97 mg)	Energy bar packaging (97 mg)
Txib	Packaging adhesive	71,43,159	Detected	Detected	N/D	Detected	Detected	Detected
diacetone alcohol	Packaging ink solvent	43,59,101	Detected	Detected	N/D	N/D	N/D	N/D
1-(2-methoxypropoxy)-2-Propanol	Packaging ink solvent	59,73,104	N/D	Detected	Detected	N/D	N/D	N/D
Styrene	Packaging plasticizer	104,103,78	N/D	N/D	Detected	Detected	Detected	N/D
Diethyl Phthalate	Packaging plasticizer	149,177,150	Detected	Detected	Detected	Detected	Detected	Detected
Diisobutyl Phthalate	Packaging plasticizer	149,57,29	N/D	N/D	Detected	Detected	Detected	Detected
Dibutyl Phthalate	Packaging plasticizer	149,150,76	Detected	Detected	Detected	Detected	Detected	Detected

Table 2: Detected VOCs adsorbed by packaging from food (Scalping)

Compound	Type	m/z	Chocolate A packaging (87 mg)	Chocolate B packaging (78 mg)	Sandwich packaging (87 mg)	Noodle packaging (80 mg)	Potato chip packaging (97 mg)	Energy bar packaging (97 mg)
2,4-Di-tert-butylphenol	Food antioxidant	191,57,206	Detected	Detected	Detected	Detected	Detected	Detected
BHT	Food antioxidant	205,57,220	Detected	Detected	Detected	Detected	Detected	Detected
Benzaldehyde	Food flavor	106,105,77	Detected	Detected	Detected	Detected	Detected	Detected
Limonene	Food flavor	68,93,67	Detected	Detected	N/D	Detected	Detected	Detected
Vanillin	Food flavor	151,152,81	N/D	Detected	Detected	Detected	Detected	Detected
Ethyl Vanillin	Food flavor	137,166,138	N/D	N/D	Detected	N/D	N/D	Detected
Triacetin	Food flavor solvent	43,103,145	N/D	N/D	N/D	N/D	N/D	Detected
1-Dodecanol	Food surfactant	55,43,69	Detected	Detected	N/D	N/D	N/D	Detected