Analysis of Volatile Organic Compounds in a Proprietary Commercial Coating

Application Note

Rapid Chemical Screen

Author

Charles Spanjers, Ph.D.
Berd LLC
Minneapolis, MN
charlie.spanjers@berdspokes.com

Abstract

Activated Research Company's Rapid Chemical Screen program, which uses the combined Polyarc® and Mass Spectrometry system, was used to analyze a commercial coating for a small company. The results of the testing helped to make informed decisions about safety, which couldn't be done using the manufacturer-supplied safety data sheet (SDS) alone.

Introduction

Pigments and coatings are used across many industries for a wide variety of applications. The compositional information of such coatings is often proprietary, and the only information available to the user is what is shown in the SDS. However, SDSs never contain a complete list of the compositional information; they simply list the most prevalent compounds as well as any potential carcinogens or otherwise dangerous compounds.

Determining the identity and concentration of volatile organic compounds in a proprietary commercial coating is not feasible for a small company to do directly. Instead, the company must send the sample to an outside lab. However, this is typically an extremely costly service for detailed results and outside of the reach of what small companies can afford. On the other hand, Activated Research Company's new Rapid Chemical Screen program is a low-cost, fast service that is accessible to small companies.

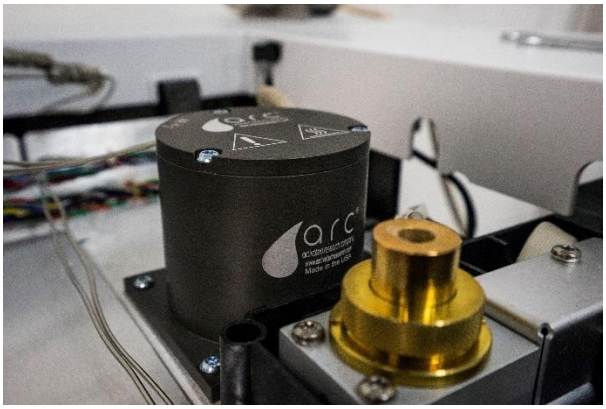

Figure 1. Polyarc System on an Agilent 7890 GC.

In this application note, it is shown how the Polyarc System (Figure 1) can be used to determine the volatile organic compounds in a proprietary commercial coating. The Polyarc is a catalytic microreactor that is an intermediate step after the column and before detection in the FID, in which all organic compounds are converted to methane through a two-step catalytic reaction:

$$\underset{\text{Compounds}}{\text{Carbon-Containing}} + \text{Air} + H_2 \rightarrow \underset{(CH_4)}{\text{Methane}} + \underset{\text{Byproducts}}{\text{Non-Carbonaceous}}$$

The response-per-carbon in the FID is equivalent for all molecules because the FID only ionizes methane. Thus, the relative response of the FID to a single internal standard (or an external standard) can be used to quantify all other components in the mixture, without the need for calibration factors.

Experimental

A single alcohol ink coating sample was injected into the GC/MS/Polyarc split system without the addition of an internal standard. The conditions for the system are shown below.

GC conditions

Front inlet	MMI, Split
Inlet temperature	250 °C
Inlet linter	Agilent 5190-2295
Carrier gas	He; 40 cm/s constant flow
Septum purge flow	3 sccm
Oven	40 °C (hold 5 min) to 270 °C at 5 °C/min (hold 10 min)
Column	DB-5MS UI (30 m x 0.25 mm x 0.25 µm film)
Syringe	10 µL
Injection volume	0.5 µL

FID conditions

Temperature	315 °C
H_2	1.5 sccm
Air	350 sccm
Makeup	5 sccm

Polyarc® System conditions

Setpoint	293 °C
H_2	35 sccm
Air	2.5 sccm

Analysis Procedure

The area-per-mol of carbon is equivalent for all carbon-containing analytes because every molecule is completely converted to methane. This property allows for the determination of the concentration of any analyte using no internal or external standard. Tetrachloroethylene was chosen arbitrarily as the reference standard for calculating the RMRF terms, though any compound can be used. For unknowns, an average of the known RMRF values were applied to the calculations. The concentrations of all analytes were then calculated using the following equations:

$$C_A = \frac{(Area_A \cdot RMRF_A)}{\sum_{i=1}^{n}(Area_i \cdot RMRF_i)} * 100 \quad (1)^*$$

$$RMRF_A = \left(\frac{Mw_A}{Mw_S}\right)\left(\frac{\#C_S}{\#C_A}\right) \quad (2)^*$$

where:

C_A = Wt. % of analyte
$Area_A$ = Integrated peak area of the analyte
Mw_A = Molecular weight of the analyte
Mw_S = Molecular weight of the standard
$\#C_S$ = Number of carbon atoms for standard
$\#C_A$ = Number of carbon atoms for analyte

*See "Quantification with the Polyarc.pdf" at https://www.activatedresearch.com/documents/ for more information.

Results and Discussion

An alcohol-based ink similar to the ink that is used in permanent markers was analyzed. It contains predominantly ethanol with a small amount of other solvents, pigments, and binders/polymers. The compositional information on the SDS for the sample tested is shown in Figure 2.

SECTION 3 *Composition/Information on Ingredients*

Contents	Synonyms	Percent by Weight	CAS No.	OSHA PEL	ACGIH TLV	LISTED CARCINOGEN (IARC/OSHA/NTP)
Ethanol	Ethyl Alcohol	55% - 80%	64-17-5	1000 ppm	1000 ppm	No
2-Propoxyethanol	EP Solvent	10% - 15%	2807-30-9			No
n-Propanol (Black only)		1% - 5%	71-23-8	200 ppm	100 ppm	No
Modified Polymers/Binders		5% - 10%	Proprietary			No
Colored Pigments		1% - 2%	Proprietary			No

Figure 2. Compositional information given on SDS.

In addition to ethanol, the SDS lists 2-propoxyethanol, n-propanol, polymers/binders, and colored pigments.

The sample was analyzed using ARC's Rapid Chemical Screen program, and the results are shown in Table 1 and Figure 3. In addition to the solvents listed on the SDS, the sample contained 4% isopropyl alcohol, 4% n-propyl acetate, 1% aniline, and 5 other identified solvents in concentrations less than 1%. Of particular interest, aniline was identified by ARC, but was not displayed on the SDS. The EPA has determined that aniline is a "probable human carcinogen." It is surprising that the SDS did not report aniline, as knowledge of this compound will help determine the appropriate safety considerations to use when working with this coating.

Table 1. Concentrations and retention times

Ret. Time (min)	Compound	Area	MW	C#	Wt. %
1.537	Ethanol	890359775	46	2	74.16%
1.607	Isopropyl Alcohol	58937713	60	3	4.27%
1.801	1-Propanol	70948289	60	3	5.14%
3.224	N-Propyl Acetate	62246490	78	5	3.52%
5.867	Ethanol, 2-propoxy-	208444822	70	5	10.57%
13.155	Aniline	16328993	93	6	0.92%
21.693	Cyclooctane	8381443	112	10	0.34%
23.681	Acetamide, N,N dibutyl-	15036922	135	10	0.74%
24.173	Acetamide, N-phenyl-	968255	135	10	0.07%
33.359	Nonadecane MW	2014717	268	19	0.10%
45.835	Dehydroabietic acid	3265027	300	20	0.18%

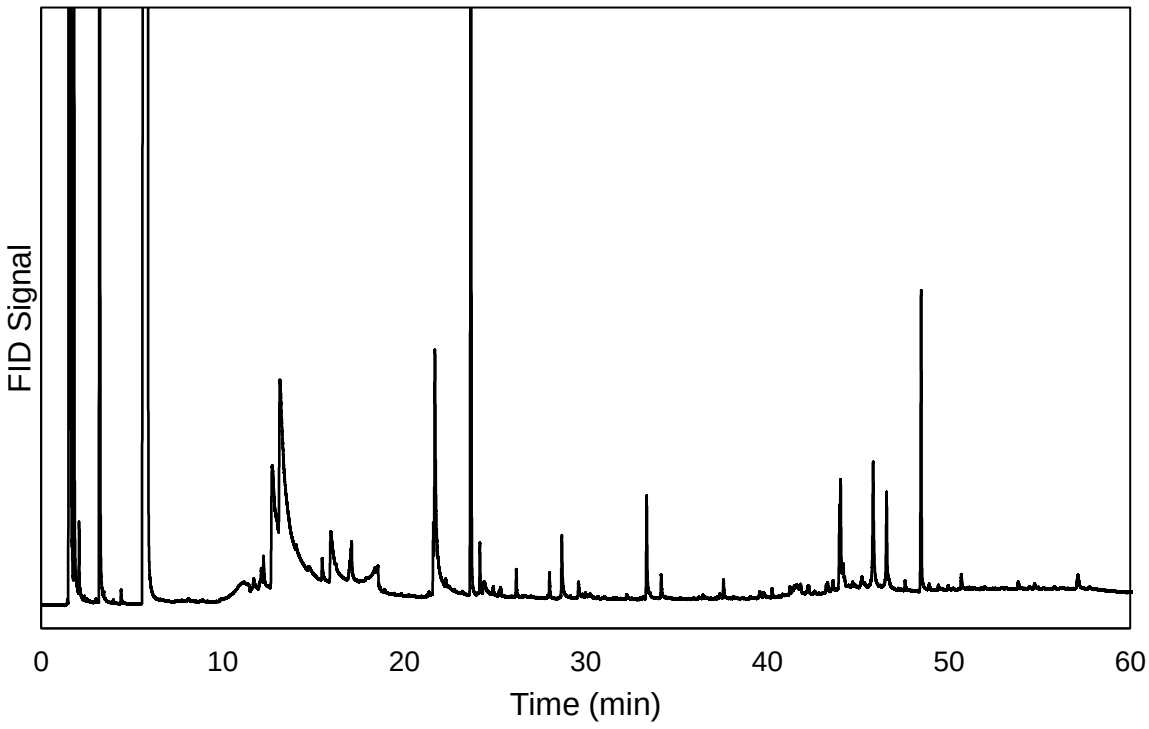

Figure 3. FID chromatogram

Conclusions

Activated Research Company's Rapid Chemical Screen program was used to determine the identity and composition of volatile organic compounds in a proprietary commercial coating. The testing uncovered a probable human carcinogen, among other compounds not reported on the SDS. ARC's testing makes knowledge of chemical composition accessible to small companies and can be used for the analysis of many types of samples and mixtures.

Contact Us

For more information or to purchase a Polyarc® system, please contact us at 612-787-2721 or contact@activatedresearch.com.

Please visit our website for details and additional technical literature.

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