

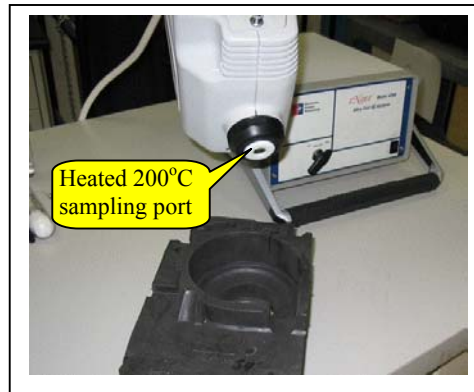
Testing Foam Samples

Procedure Used

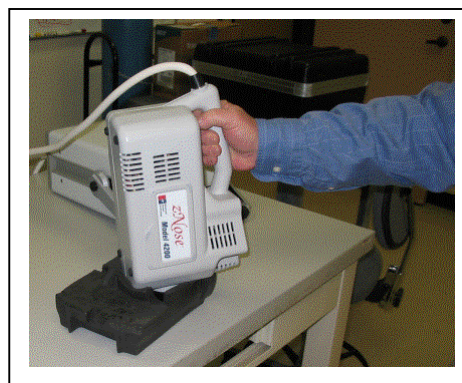
The basic zNose instrument consists of a handheld module attached to a support case (bottom in Figure 1) by means of an 8 foot unbilical cord. To operate the system and to record each chemical analysis a computer with a Windows operating system is required.



Because the inlet of the zNose is heated a wide range of volatile organics can be sampled and analyzed without carryover or cross contamination of samples. In this case the inlet was heated to 200oC.

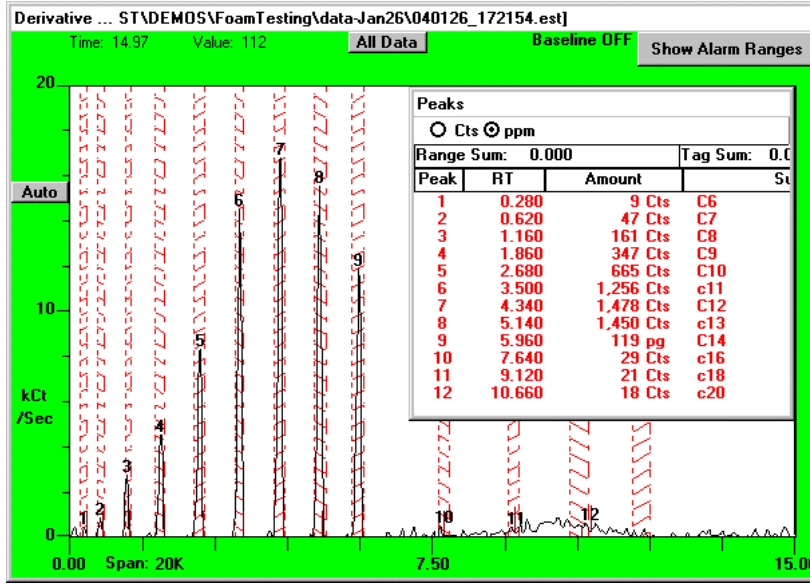


Sampling was done by holding the zNose over the foam sample such that the inlet extended approximately 2 inches into the large circular cavity of the foam piece. A sampling time of 30 seconds was used to collect volatile organics from within a 15 milliliter volume of air.



Chemical Standards

All scientific measurements require machine-independent standards. When the exact compounds are unknown chemical measurements and compound identification can be done relative to linear chain n-alkane vapors. Methanol spiked with n-alkanes C6 through C14 provides a convenient perfume which produces peaks for each of the alkanes. Using a graphical software construct, the position of each alkane is denoted by movable red band.



Positioning of the red bands creates a “peak” file for the n-alkane standards and this file is used to index the retention time of unknown peaks in any test vapor. These indices are referred to as Kovats indices and provide a machine independent identification of any organic. For example a compound with an index of 1250 will have the same index on any instrument which is first calibrated with n-alkane vapors.

Peak File: ... \DEMOS\FoamTesting\data-Jan26\alkanes_10ps2a1b.pkd

File Close Calibration Form

No.	Indice	Percent Spread	Substance	Alarm Level (in Cts)	Alarm Level (User units)	Calc. Method	Scale Factor	Tag
1	600	25.950	C6	0 Cts	0	Area	0.00	
2	700	10.990	C7	0 Cts	0	Area	0.00	
3	800	5.180	C8	0 Cts	0	Area	0.00	
4	900	5.410	C9	0 Cts	0	Area	0.00	
5	1000	4.370	C10	0 Cts	0	Area	0.00	
6	1100	2.420	c11	0 Cts	0	Area	0.00	
7	1200	2.470	C12	0 Cts	0	Area	0.00	
8	1300	2.610	c13	0 Cts	0	Area	0.00	
9	1400	2.060	C14	0 Cts	0	Area	10.12	
10	1600	1.540	c16	0 Cts	0	Area	0.00	

Units to Display: Concentration (ppm) Mass (pg) User

Retention Time Units: Seconds Indices

File Name: alkanes_10ps2a1b.pkd

File Notes: alkane peak file 10ps2a1b db624

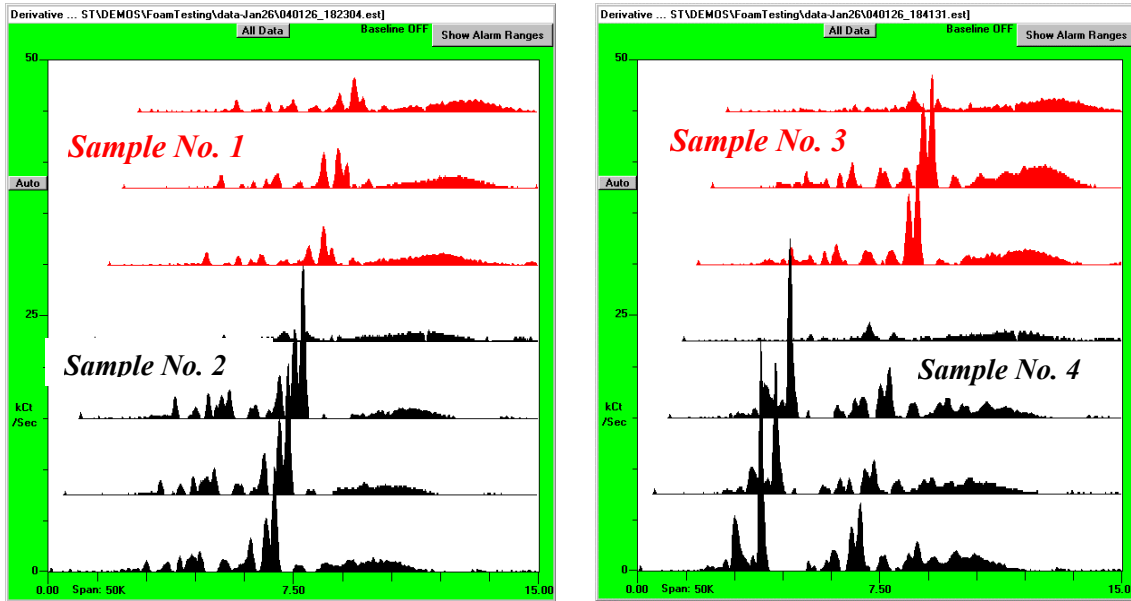
Conversion Selection: Use Scale Factors Use Calibration Factors

Range Settings: From 0.0 To 0.0

Re-Index

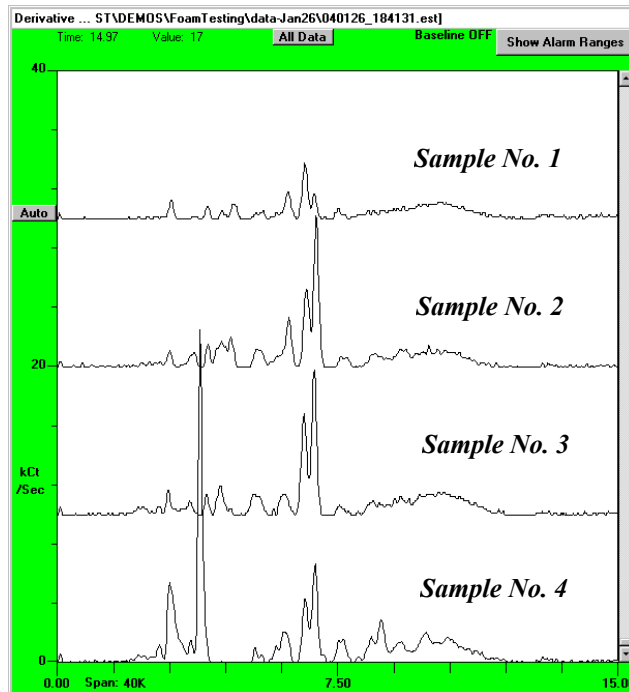
Sample Testing Results

Each foam sample was measured in triplicate with good overall precision and repeatability.



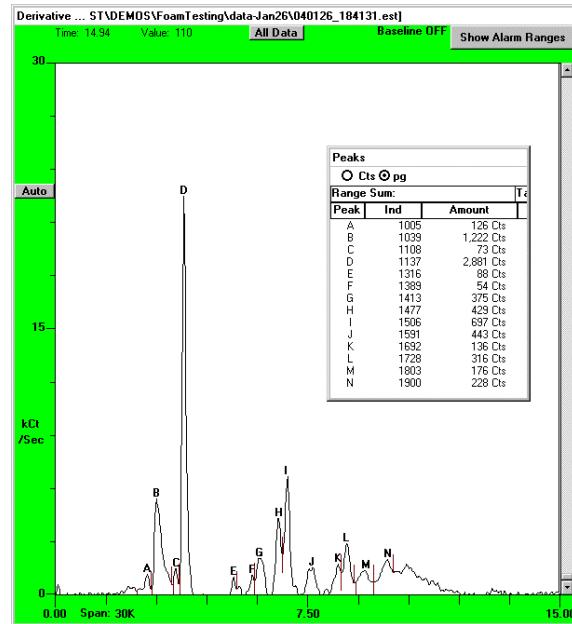
One measurement of each foam sample is plotted vertically offset so as to illustrate the differences between the chemistry of each odor sample. Sample No.1 (no odor) gave the lowest overall odor concentration while sample 2 (bake) and sample 3 (unbaked) gave nearly identical odors. Sample 4 made from a different material introduced several lower molecular weight compounds with relatively high concentrations.

The exact name of each compound and its individual odor threshold for human perception is at present unknown. Nevertheless, the individual compounds are clearly separated and the relative intensity of the entire odor signature is readily apparent.

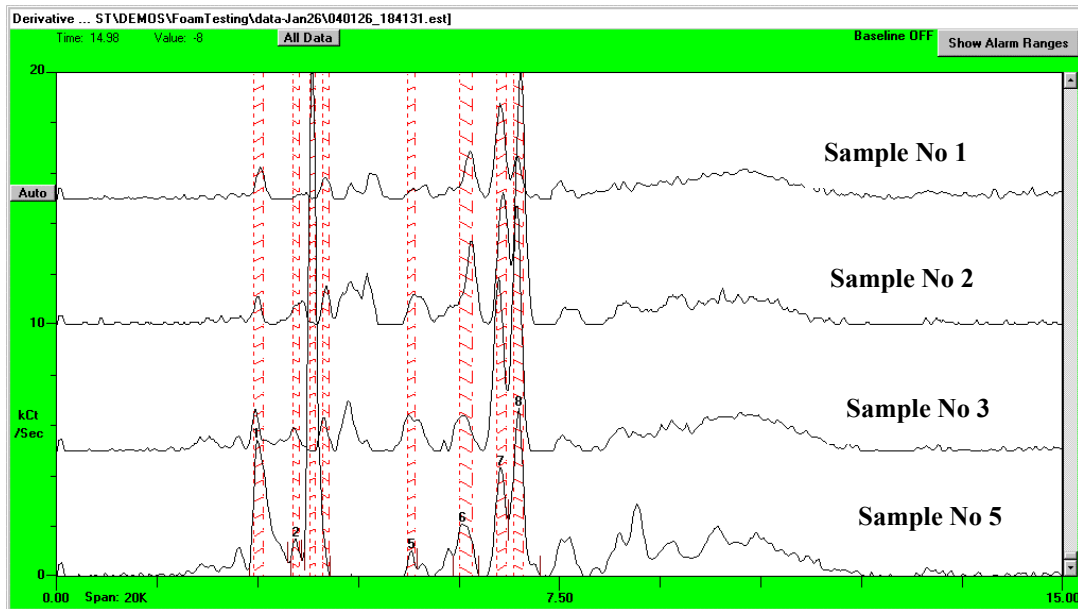


Quantification and Compound Identification (Kovats Indices)

In any analysis of a given odor sample the individual compounds are separated and can be identified by their unique Kovats index as shown in the figure on the right for sample No. 4. In addition the odor intensity of each compound can be measured and tabulated as detector counts.



By placing graphical bands over selected compounds a “peak” file specifically for foam samples can be created which enables these compounds and their relative concentration counts to be logged to other programs like Excel.



The peak file specific to forms simply uses identification names derived from the compounds unique Kovats index e.g. compound – ID-1163. In this case the eight compounds can also be added to a library of Kovats indices which can be used by other gas chromatographs for identification purposes.

Peak File: C:\ved\EST\DEMOS\FoamTesting\data-Jan26\Foam.pkd

File Close Calibration Form

No.	Index	Percent Spread	Substance	Alarm Level (in Cts)	Alarm Level (User units)	Calc. Method	Scale Factor	Tag
1	1041	2.500	ID-1041	0 Cts	0	Area	0.00	X
2	1108	1.460	ID-1108	0 Cts	0	Area	0.00	X
3	1139	1.100	ID-1139	0 Cts	0	Area	0.00	X
4	1163	1.100	ID-1163	0 Cts	0	Area	0.00	X
5	1316	1.100	ID-1316	0 Cts	0	Area	0.00	X
6	1419	1.580	ID-1413	0 Cts	0	Area	0.00	X
7	1477	1.110	ID-1477	0 Cts	0	Area	0.00	X
8	1506	1.000	ID-1506	0 Cts	0	Area	0.00	X

Units to Display: Concentration (ppm) Mass (pg) User

Retention Time Units: Seconds Indices

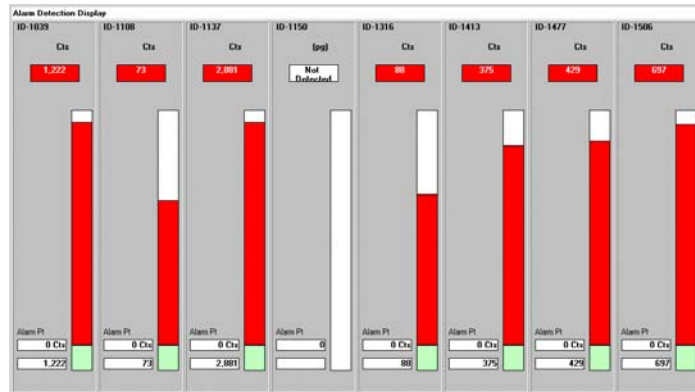
File Notes: alkane peak file 10ps2a1b db624

Conversion Selection: Use Scale Factors Use Calibration Factors

Range Settings: From: 0.0 To: 0.0

Re-Index

Denoting the eight compounds of the peak file as tagged peaks allows the software to display an array of virtual chemical sensors for each of the compounds. This is often a simpler display for unskilled production workers wishing to quantify odors from foam samples.

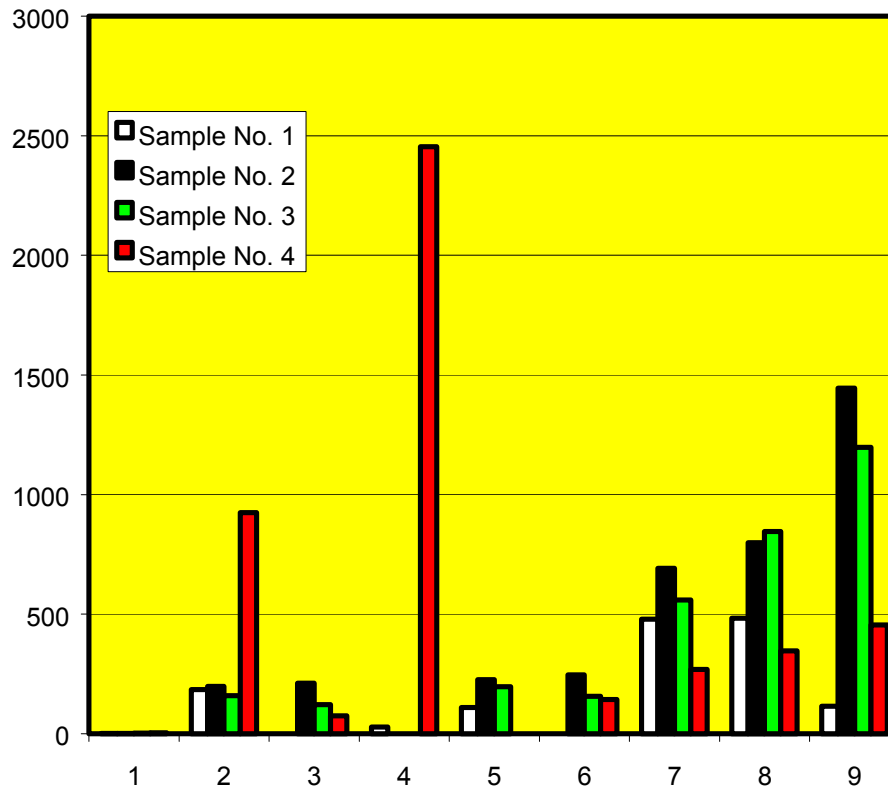


Peak Logging and Tabulation of Results with Excel

The supplied software for the zNose enables creation of spreadsheets listing the concentration of each peak called out in the peak file. This function is called peak logging and an example is the spreadsheet below listing the concentration of the compounds shown in the Foam peak file.

Substance:	ID-1041	ID-1108	ID-1139	ID-1163	ID-1316	ID-1413	ID-1477	ID-1508	Notes:
File Name:	Amt	Amt	Amt	Amt	Amt	Amt	Amt	Amt	
D40126_180341.est	138		72	127		289	423	65	Sample No. 1
D40126_180547.est	239		11	73		706	506	165	Sample No. 1
D40126_180742.est	178		2	131		441	519	114	Sample No. 1
Average	185		28	110		479	483	115	
D40126_181919.est	247	230		293	307	677	1005	1824	Sample No. 2
D40126_182115.est	196	183		213	105	653	824	1421	Sample No. 2
D40126_182304.est	150	220		174	326	746	569	1091	Sample No. 2
Average	198	211		227	246	692	799	1445	
D40126_182956.est	121	74		213	148	594	959	1094	Sample No. 3
D40126_183316.est	158	82		150	77	392	777	1052	Sample No. 3
Average	159	122		197	157	559	845	1197	
D40126_183644.est	750	89	2531		126	281	328	448	Sample No. 4
D40126_183832.est	800	62	1952		217	149	283	220	Sample No. 4
D40126_184131.est	1222	73	2881		88	375	429	697	Sample No. 4
Average	924	75	2455		144	268	347	455	

In this way it is possible to average replicate runs and to compare samples on a compound-by-compound basis and plot the results using the many functions of Excel.



Summary

Polyurethane foam is produced using a wide assortment of volatile organic compounds. Frequently foam outgases organic vapors leading to unwanted odors associated with foam products. The odors are complex, frequently containing 10 to 20 principal chemical components. These compounds can be separated and their concentration measured using a gas chromatograph. The zNose, an ultra-fast GC with a non-specific solid-state detector, is able to do this in less than 1 minute run-to-run. In fact the zNose can perform more than 300 such analyses in an 8-hour shift. The zNose is portable and able to be used as a quality control tool based upon odor chemistry. This is in contrast to conventional GCs, which typically are not portable and do less than 10 runs in the same period of time.

Identification of the compounds by their chemical name is not possible with a straight GC without a mass spectrum detector (GC/MS). With a mass spectrum detector the compounds are split apart into their atomic sub-components and the mass spectra of the fragmentation pattern used as a fingerprint to identify the individual compounds. Because GC/MS instruments are large and expensive they are only found in well-equipped laboratories. Hence to identify compounds by their correct chemical name it is best to send samples to a laboratory equipped with GC/MS for this purpose. Once the compound has been identified, chemical standards can be purchased and used to calibrate the zNose in the field.

Identification of the compounds name only changes the name assigned to the peak. For odors which are detected by people, it is necessary to know the odor threshold or sensitivity to each compound within an odor or fragrance. Often humans are more sensitive to some compounds and not to others. Once the compounds have been identified, the odor threshold can be measured using pure standards of that compound.

Often a fragrance contains a group of compounds with a definite relationship to each other in concentration. Knowledge of the correct chemical name of each compound is not as important as knowing the overall concentration of the total group since any one compound will have the same level relative to the group level. In this case the zNose can be used as a tool to measure the concentration of the total aroma or fragrance as a sum of all peaks detected. In addition, since the peaks are separated and can be assigned unique names (albeit not correct chemical names) they can be identified for the purpose of tracking down their source within a process. In the case of the foam samples tested the peaks were given names based upon their Kovats index number. In this case the only standard needed is a perfume containing n-alkanes for reference. Since the Kovats index is machine independent it allows the zNose to uniquely assign a time slot relative to the n-alkane response.