Expanded Analysis of Fruit Fleuressence

Fast Analysis using 10ps2a1b Method

Ramping the zNose column from 40^o to 160^{o}C at 10^{o}C/sec with a 1 second sample and relatively a low sensitivity sensor temperature of 60^{o}C, provides a quick 20 second analysis of the principal chemical components. The 10ps2a1b method and system operating conditions are shown in Figure 1.

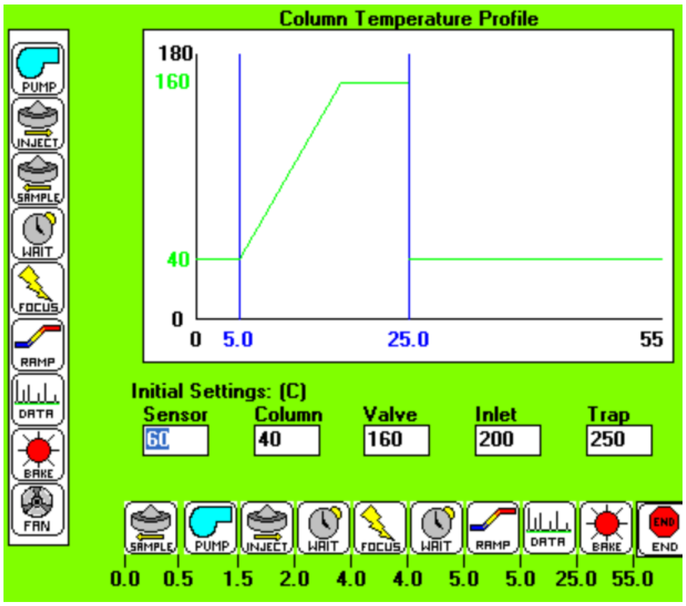

Figure 1- 10ps2a1b method and system parameters.

Using the fast method the fruit fleuressence chromatogram (Figure 2) displayed three major compound peaks with indices of 1111, 1329, and 1461 and concentrations of 34,982, 22,317 and 19,439 counts respectively.

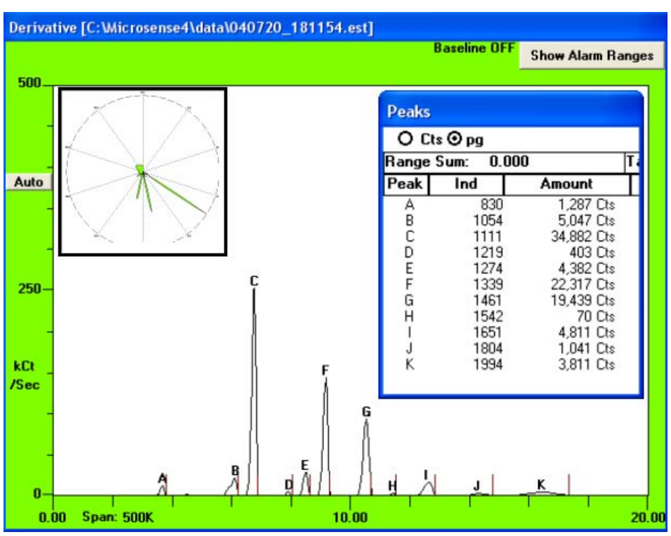

Figure 2- Chromatogram of Fruit fleuressence.

Significant minor compounds with indices of 830, 1054, 1219, 1274, 1542, 1651, 1804, and 1994 were also detected. With the fast method approximately 11 compounds or principal components could be measured in 20 seconds.

Aroma chemistry can be used to create polar olfactory diagrams (VaporPrint®) in which the radial dimension is proportional to aroma impact (chemical concentration) and the angular dimension maps the retention time (index) starting and ending at the 12 o'clock position. Aroma impact (radial distance) can be displayed as a linear or

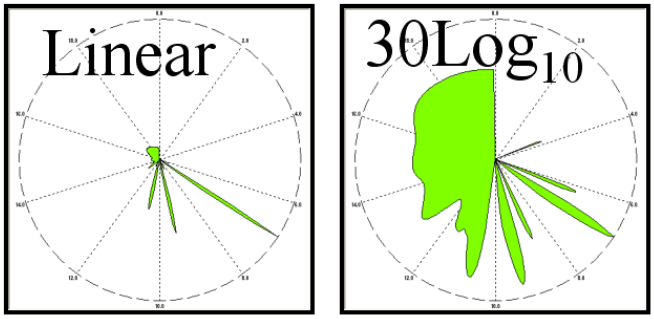

Figure 3- High-resolution VaporPrint® images provide a visual pattern representing aroma impact and chemistry.

logarithmic image as shown in Figure 3. Olfactory images provide a user-friendly visual display of aroma chemistry for perfumery experts. Humans are extraordinarily adept at judging and comparing visual figures and such comparisons combined with olfactory impressions give the perfumer a much-improved ability to judge the finished product.

Software provides tools for creating virtual sensor arrays specific to aroma types. Each sensor measures the concentration of a specific chemical within that aroma and is useful for quickly assessing quality of that chemical mixture. The principal chemical components of fruit fleuressence are graphically defined by placing bands or regions over the main chromatogram peaks as shown in Figure 4. Each peak is described by a user-defined name containing the peak's retention index. Once defined, the sensor array can record, track, and display the concentration of each principal component of the aroma.

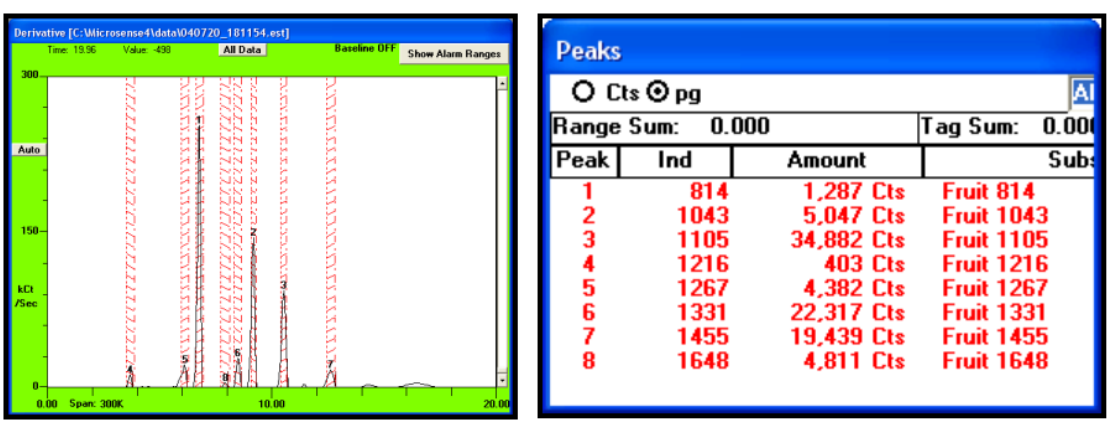

Figure 4- Vvirtual chemical sensors the concentration of an aroma's principal components.

The principal chemical components of each aroma type form a virtual sensor array specific to that type or fleuressence base. Once defined it is possible to monitor the sensor array readins, define thresholds, scale factors, and set alarm values without ever actually viewing the chromatogram. As an example, a virtual sensor array for the 8 principal components of the fruit fleuressence aroma is shown in Figure 5.

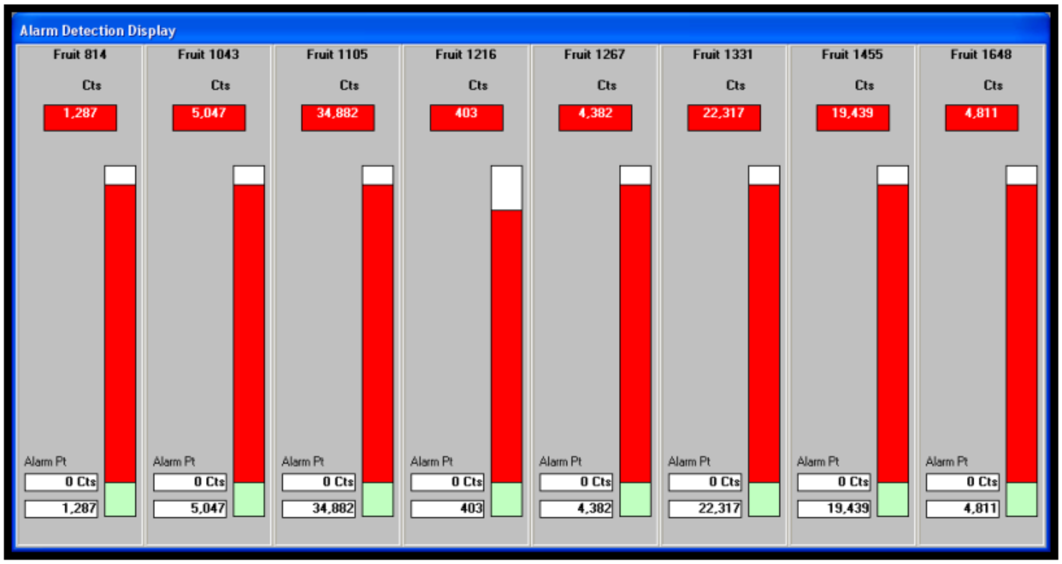

Figure 5- Virtual sensor array using the 8 principal components of the fleuressence aroma.

Detailed Analysis Using 3ps2a1b Method

Ramping the column at 3°C/sec and a high sensitivity sensor temperature of 20°C, slows the analysis time to 50 seconds but provides a much more detailed analysis of the chemical components of the mixture aroma. The 3ps2a1b method and system operating conditions are shown in Figure 6.

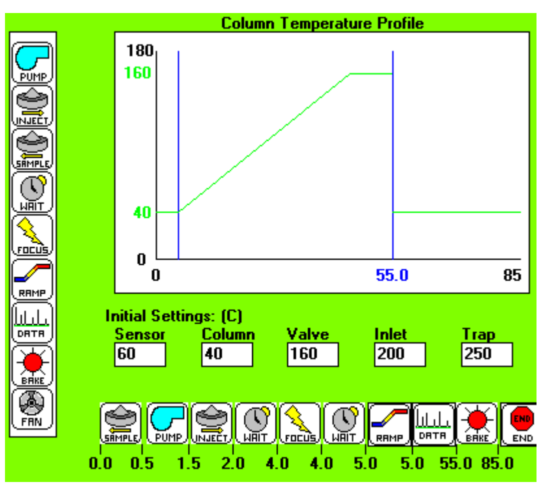

Figure 6- 3ps2a1b method and system parameters.

The n-alkane response used for indexing with the 3ps2a1b method is shown in Figure 7.

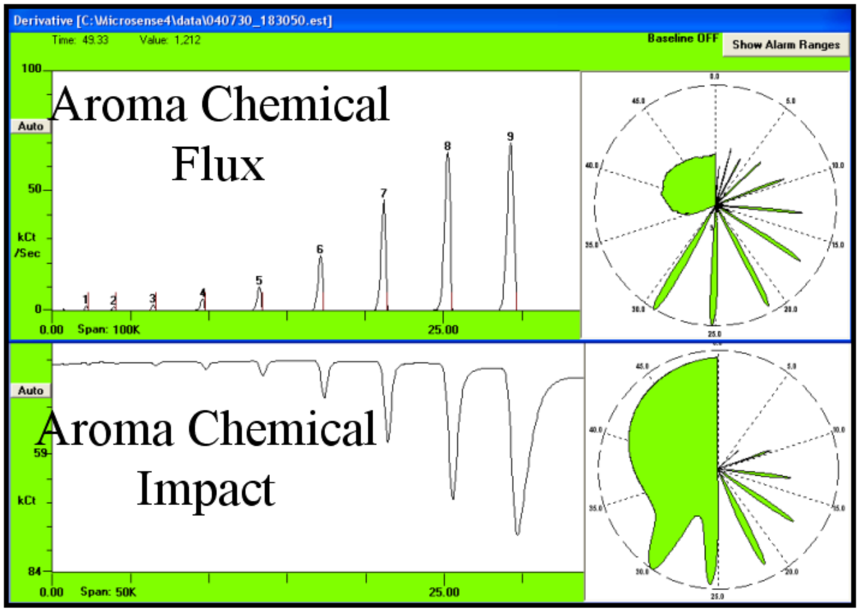

Figure 7- Alkane perfume response using 3ps2a1b method.

Using the slower 3ps2a1b method the fruit fleuressence aroma chemistry is shown in Figure 8.

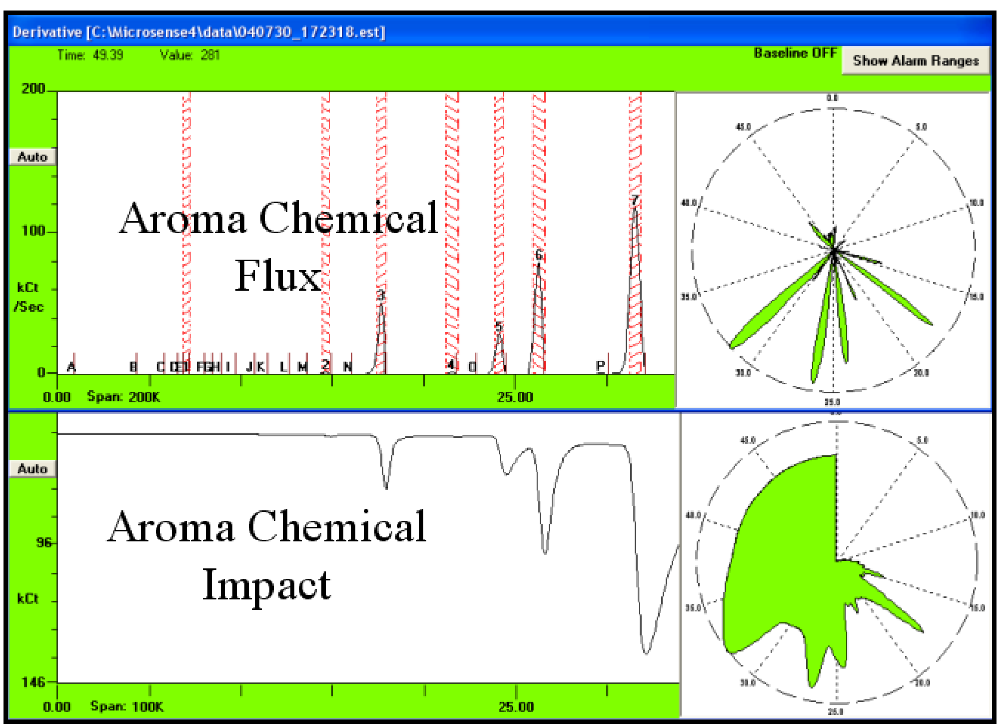

Figure 8- Fruit fleuressence response using 3ps2a1b method.

Using the more detailed method a virtual chemical sensor array for the fleuressence base shows approximately 22 distinct chemicals or sensors in figure 9.

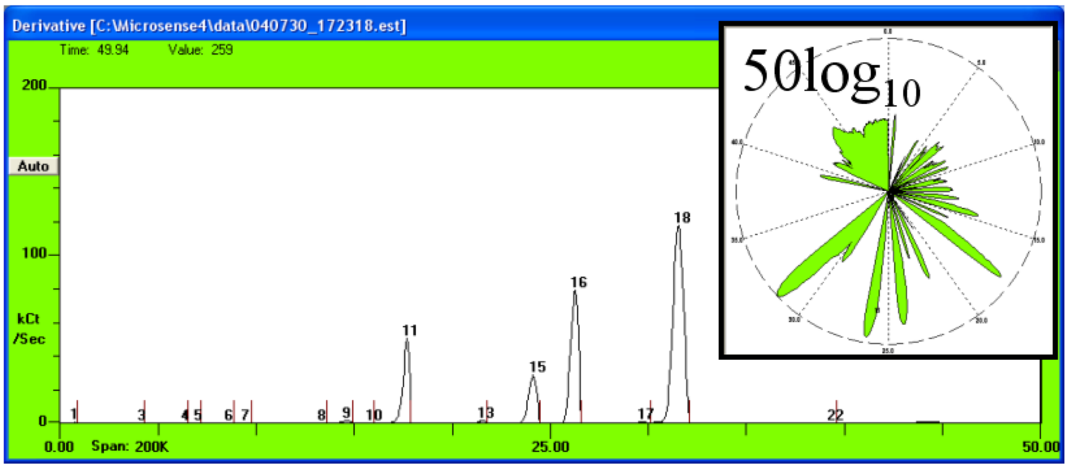

Figure 9- Detailed analysis showing 20 principal chemical components in aroma.

Using graphical bands to define sensors a 22 element virtual sensor array quantifies the concentration and index of each chemical in the aroma as shown in Figure 10.

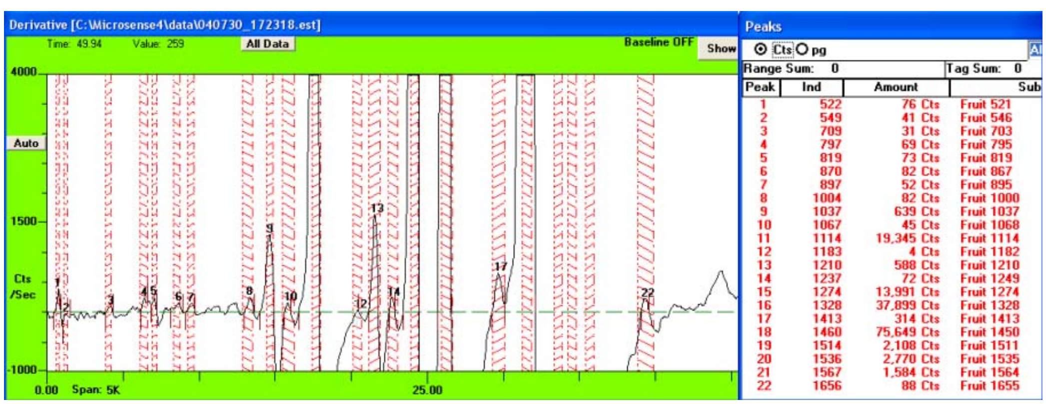

Figure 10- Creation of 22 virtual sensor array for fruit fleuressence aroma.

Relative Concentration Comparison

The zNose vapor analyzer uses acoustic waves to measure the condensation of volatile organic vapors on to a temperature-controlled crystal as they elute from a capillary column. Because sensitivity is an exponential function of retention time for organic vapors that do not completely condense on the crystal surface, the measured concentration values must first be corrected and then normalized in order to compare relative chemical concentrations. Such an analysis and comparison for fruit fleuressence aroma is shown in Table I using peak No. 11 for normalization.

Table I - Quantification of Results

Peak No.	Index	Measured	Corrected	Normalized
1	522	76	1189131	264.47%
2	549	41	476666	106.01%
3	709	31	62006	13.79%
4	797	69	52423	11.66%
5	819	73	43541	9.68%
6	870	82	27909	6.21%
7	897	52	13151	2.92%
8	1004	82	6391	1.42%
9	1037	639	34645	7.71%
10	1067	45	1754	0.39%
11	1114	19345	449634	100.00%
12	1183	50	544	0.12%
13	1210	588	4754	1.06%
14	1237	101	607	0.13%
15	1274	13991	55948	12.44%
16	1328	37899	83674	18.61%
17	1413	314	314	0.07%
18	1460	75649	75649	16.82%
19	1514	24040	2108	0.47%
20	1536	12032	2770	0.62%
21	1567	7120	1584	0.35%
22	1656	200	200	0.04%