Pegasus®

Semi-Quantification

The analysis of complex materials such as petroleum and petroleum derivatives result in a relatively large number of volatile components. In complex mixtures such as these, it becomes very hard to quantitate data due to the large number of components present along with the large number of coeluting peaks. For these reasons, analytical conditions have been focused on the complete chromatographic resolution of as many individual analytes as possible. A number of methods have been developed for the analysis of complex samples using GC-MS. While all mass spectrometers offer multi-channel detection capabilities that may be used to identify coeluting analytes, slow spectral acquisition rates, and under-developed software algorithms have minimized the impact of MS detectors on faster GC separation times.

Since the number of isomers increase dramatically as the number of carbon atoms increases, it may not be possible to quantify each analyte present in a complex mixture. What is done instead is to group compounds that have similar structures and quantitate them against the calibration curve of another compound. This type of analysis is known as semi-quantification. It is assumed in this type of quantification that the response of each analyte is similar to the response of the component used to build the calibration table. This assumption is only valid if used with compounds that have similar structures (isomers). However, in the case where there is a known substantial difference in the response factors, a multiplier can be used to correct.

An example where semi-quantification is used is in the analysis of Gasoline by ASTM Method D5769 (LECO Application Note #203-821-094; Rapid Determination of Benzene, Toluene, and Total Aromatics in Finished Gasoline). The LECO Pegasus contains built-in software specifically designed for the purpose of semi-quantification. As specified in this method, the C10 aromatics are quantified by using a selected mass of 134. In Figure 1, the aromatics containing 10 carbon atoms are quantified using the calibration curve for 1,2-diethylbenzene. The results obtained using this method are only approximate. In order to get more accurate results, the response factor for each C10 isomer with respect to 1,2-diethylbenzene must be known. This same process is then repeated for the C11 and C12 benzenes using other quantification masses. A typical chromatogram is shown in Figure 2. The masses selected are those used for the semi-quantification as specified by the method. Table 1 shows what the typical results are for total aromatics using semi-quantification.

A semi-quantification method is accessed from the “Data Processing Methods” section of Pegasus' software. Once semi-quantification is selected a new field becomes active where the quantification mass is selected along with the calibration curve to be used. A calibration curve must exist before it can be assigned in the semi-quantification section of the data processing method.

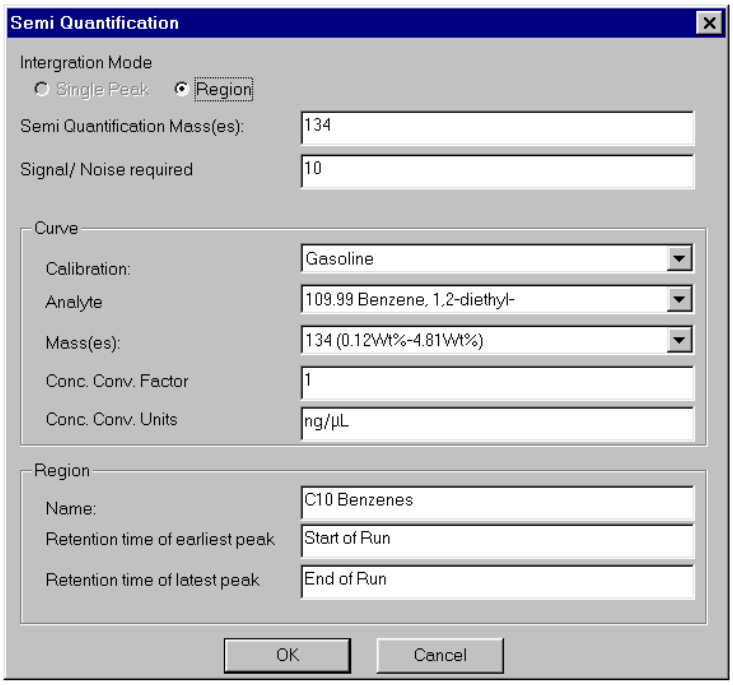

Figure 1: Semi-quantification of C10 Aromatics using m/z 134.

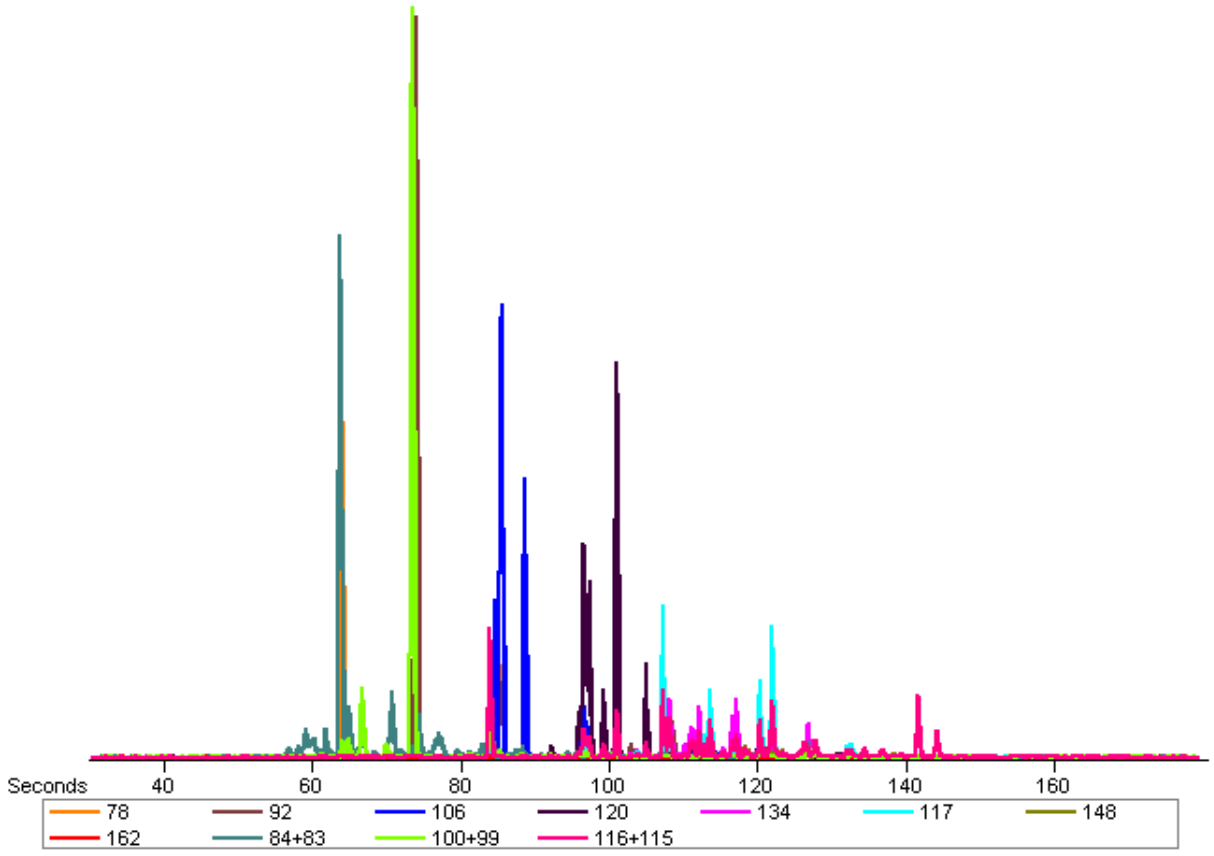

Figure 2: Typical Chromatogram of Aromatics in Gasoline Using Selected Masses

Table 1

Name	R.T.	Type	Quant Masses	Area	Concentration
Perdeuterobenzene	63.905	Quantified	84+83	8566800	2.00 Wt%
Benzene	64.125	Quantified	78	3446700	0.82 Wt%
Toluene-d8	73.645	Quantified	100+99	14814000	7.00 Wt%
Toluene	74.125	Quantified	92	10029000	5.27 Wt%
Ethylbenzene-d10	84.225	Quantified	116+115	1763700	2.00 Wt%
Ethylbenzene	84.945	Quantified	106	1224000	1.01 Wt%
p/m-Xylene	85.825	Quantified	106	7069400	7.72 Wt%
Benzene, 1,2-dimethyl-	89.065	Quantified	106	2543500	2.00 Wt%
Benzene, (1-methylethyl)-	92.765	Quantified	120	79161	Out of calibration range: 0.01 Wt%
Benzene, propyl-	96.545	Quantified	120	369490	0.32 Wt%
Substituted Alylindanes		Summed	117	5028700	0.40 Wt%
Benzene, 1-ethyl-3-methyl-	97.185	Quantified	120	1842600	1.74 Wt%
Benzene, 1-ethyl-4-methyl-	97.585	Quantified	120	638030	0.59 Wt%
Benzene, 1,3,5-trimethyl-	98.025	Quantified	120	1114500	0.69 Wt%
Benzene, 1-ethyl-2-methyl-	99.985	Quantified	120	541920	0.43 Wt%
Benzene, 1,2,4-trimethyl-	101.81	Quantified	120	4513500	3.85 Wt%
C10 Benzenes		Summed	134	612530	0.74 Wt%
Benzene, 1,2,3-trimethyl-	105.97	Quantified	120	734850	0.51 Wt%
Indane	108.31	Quantified	117	1216900	0.24 Wt%
Benzene, 1,4-diethyl-	109.23	Quantified	134	639190	0.82 Wt%
Benzene, butyl-	109.67	Quantified	134	279210	0.34 Wt%
Benzene, 1,2-diethyl-	110.57	Quantified	134	21126	Out of calibration range: 0.01 Wt%
C11 Benzenes		Summed	148	902820	0.86 Wt%
Benzene, 1,2,4,5-tetramethyl-	117.97	Quantified	134	342660	0.28 Wt%
Benzene, 1,2,3,5-tetramethyl-	118.51	Quantified	134	505590	0.38 Wt%
Naphthalene-d8	128.31	Quantified	136+135	4746800	1.00 Wt%
Naphthalene	128.75	Quantified	128	2113800	0.34 Wt%
C12 Benzenes		Summed	162	51996	0.01 Wt%
Naphthalene, 2-methyl-	143.37	Quantified	142	739050	0.29 Wt%
Naphthalene, 1-methyl-	145.95	Quantified	142	305990	0.12 Wt%
Total				76798000	41.85 Wt%

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