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Application News

Detailed Hydrocarbon Analysis by Nexis GC-2030 Using ASTM D6730

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User Benefits

- Detailed compositional analysis of gasoline in accordance with ASTM D6730 is feasible using the Nexis GC-2030.
- By employing PONAsolution™, a PONA/DHA analysis software, laborious identification tasks can be reduced, and quantitation calculations and report generation can be performed automatically.

■ Introduction

ASTM D6730 specifies the analysis of hydrocarbons in gasoline and oxygenates such as ethanol, methyl tert-butyl ether (MTBE), and ethyl tert-butyl ether (ETBE) over a boiling point range up to 225 ℃. Identification and quantification of individual compounds in gasoline are critically important for refinery process control and product quality assurance.

In this application news, we report compositional analysis of gasoline conforming to ASTM D6730 using the Nexis GC-2030 gas chromatograph. Gasoline typically comprises over 100 hydrocarbons, making identification tasks highly complex; however, PONAsolution, a PONA/DHA analysis software, simplifies this process.

■ System Configuration and Analysis Conditions

The instrument configuration and analytical conditions are listed in Tables 1 and 2, respectively. ASTM D6730 requires separation of more than 100 components; therefore, a slightly polar pre-column (SH PONA Tuning Column, P/N: 227-36339-01) and a nonpolar 100 m main column (SH-1 PONA, P/N: 221-76196-00), together with CRG, were employed. The inlet pressure was adjusted so that the retention time of methane at 35 ℃ fell within 7.00 ± 0.02 min. Data processing was performed using PONAsolution Ver.6, which contains a retention index library tailored for ASTM D6730.

In contrast, gasoline compositional analysis methods defined in ASTM D8071 and D8369 employ vacuum ultraviolet (VUV) detectors. In those methods, identification is performed using retention indices together with absorption spectral information, enabling deconvolution of coeluting components through spectral matching (see Application News No. 01-00966-EN). Table 3 compares PONA/DHA analyses using FID and VUV detectors.

Table 1 System configuration

GC Model	: Nexis GC-2030 / AOC-30i
Injection Port	: SPL
Liner	: Tapered Split/Splitless Liner with fixed wool - "into wool" (P/N : 221-75191)
Column	: SH PONA Tuning Column* (P/N : 227-36339-01) (5.0 m × 0.25 mm I.D. × 1.0 µm) *cut the column into 3.2 m + SH-1 PONA (P/N : 221-76196-00) (100 m × 0.25 mm I.D. × 0.5 µm)
Detector	: FID-2030
Options	: CRG-2030 (CO_2)
Software	: LabSolutions, PONAsolution

Table 2 Analysis conditions

Injection Temperature	: 250 ℃
Flow Control Mode	: Pressure (He)
Inlet pressure	: 293.0 kPa
Purge Flow	: 3.0 mL/min
Injection Volume	: 0.5 µL
Split ratio	: 150
Column Oven Temp. Program	: 5 ℃ (10 min) → 5.0 ℃/min → 48 ℃ (59 min) → 1.3 ℃/min → 200 ℃ (5.0 min)
Detector Temperature	: 250 ℃
Makeup Gas	: N_2 24 mL/min
Detector Gas	: H_2 32 mL/min, Air 150 mL/min

■ PONAsolution

PONAsolution Ver.6 provides retention index libraries for each relevant standard (ASTM D6730, D6729, D5134, D6733). Identification of n-alkanes automatically corrects the retention times of the remaining several hundred components, thus streamlining the identification process.

When only a specific retention region requires adjustment, the two-point identification function is useful (Fig. 1). In the two-point identification procedure, reference and sample chromatograms are compared while assigning corresponding peaks. First, click on an identified component mark in the reference data (Fig. 1, a), then click the matching sample peak (Fig. 1, b). Repeat this for a second pair of peaks. The retention times of components between these two anchor points are then automatically corrected.

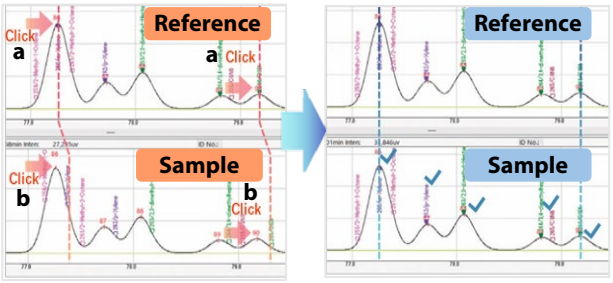


Fig. 1 Two-point identification using PONAsolution

Table 3 Comparison of ASTM D8369, D8071 and D6730

	D6730	D8369	D8071
Report Items	PIONA group Individual compounds	PIONA group Individual compounds	PIONA group select compounds (EtOH、BTX etc.)
Detector	FID	VUV	VUV
Analysis Time (min)	ca. 180	49	35
Qualification	Retention Indices	Retention Indices + VUV spectra	Retention Indices + VUV spectra
Quantification	Corrected Percentage Peak Area Method	Corrected Percentage Peak Area Method	Corrected Percentage Peak Area Method

■ Peak Resolution

Oxy setup blend (RESTEK: 33034) was analyzed to confirm peak shape and resolution. The chromatogram is shown in Fig. 2. Using the ASTM D6730 method with a slightly polar pre-column (SH PONA Tuning Column) connected to a nonpolar main column (SH-1 PONA) allowed separation of pairs that are difficult to resolve on a single column, for example tert-Butanol (3) and 2-Methylbutene-2 (4), or 1-Methylcyclopentene (8) and Benzene (9).

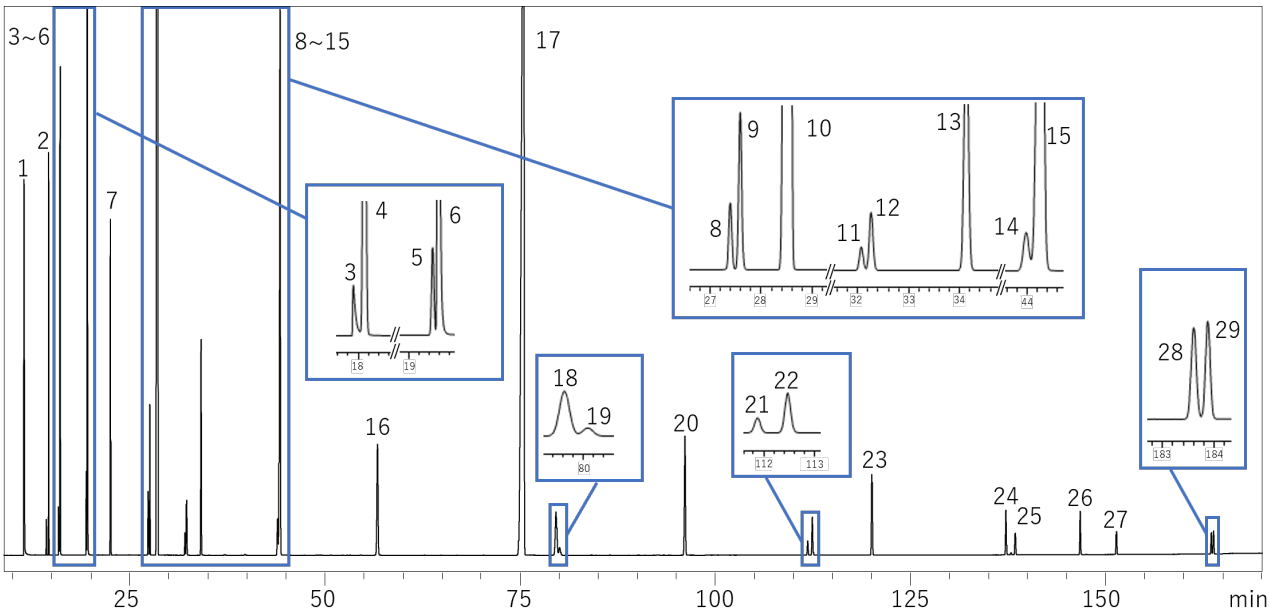
■ Quantification Results

To assess quantitative accuracy, a certified component standard (Tokyo Chemical Industry Co., Ltd., S0429) was analyzed. For all analytes evaluated using ASTM D6730, the difference between measured values and certified values was within 0.5%, indicating excellent agreement.

Table 4 Quantification results for reference material of gasoline components

(vol%)

Compound	a. Conc. of certificate	b. ASTM D6730	|a – b|
Benzene	0.5	0.552	0.052
Toluene	16.2	16.529	0.329
Xylene	10.7	10.755	0.055
MeOH	1.5	1.414	0.086
EtOH	5.3	5.194	0.106
MTBE	5.2	5.268	0.068
ETBE	5.2	5.187	0.013



1: Ethanol
2: C5 (n-pentane)
3: tert-Butanol
4: 2-Methylbutene-2
5: 2,3-Dimethylbutane
6: Methyl tert-butyl ether (MTBE)
7: C6 (n-hexane)
8: 1-Methylcyclopentene
9: Benzene
10: Cyclohexane
11: 3-Ethylpentane
12: trans-1,2-Dimethylcyclopentane
13: C7 (n-heptane)
14: 2,3,3-Trimethylpentane
15: Toluene
16: C8 (n-octane)
17: Ethylbenzene
18: p-Xylene
19: 2,3-Dimethylheptane
20: C9 (n-nonane)
21: 5-Methylnonane
22: 1-Methyl-2-ethylbenzene
23: C10 (n-decane)
24: C11 (undecane)
25: 1,2,3,5-Tetramethylbenzene
26: Naphthalene
27: C12 (dodecane)
28: 1-Methylnaphthalene
29: C13 (tridecane)

Fig. 2 Chromatogram of oxy setup blend

■ Data Processing of gasoline sample

After system suitability tests were completed, real gasoline samples were analyzed. Quantitation results are presented as two-dimensional tables by PIONA group and carbon number, and as individual component concentration reports (Fig. 3).

In the chromatogram view of PONAsolution, the identified reference data can be displayed above while performing identification of sample peaks in the lower pane (Fig. 4). By using AART for DHA, alkanes can be identified automatically, and the remaining components are subsequently identified automatically, substantially reducing analysis time*1.

*1 Once the library is adjusted, re-adjustment is generally unnecessary until retention time shifts occur due to column degradation.

■ Conclusion

Compositional analysis of gasoline in accordance with ASTM D6730 was performed. The combination of SH PONA Tuning Column and SH-1 PONA main column enabled separation of compounds with closely spaced retention times. Moreover, use of PONAsolution software greatly simplifies complex identification tasks.

<Related Applications>

1. Detailed Hydrocarbon Analysis by GC-VUV Using ASTM D8369, Application News No. 01-00966-EN

Summary by Group

Group	Area%	Wt%	Vol%	Mol%
Paraffins	15.547	15.802	17.480	15.322
Iso-Paraffins	31.555	32.030	34.956	29.396
Olefins	8.781	8.719	9.145	8.105
Naphthenes	3.571	3.548	3.425	3.263
Aromatics	25.555	24.062	20.245	18.955
Oxygenates	14.232	15.069	14.184	24.958
Unknowns	0.759	0.769	0.565	0.000
Total	100.000	100.000	100.000	100.000

Summary by Carbon

C#	Area%	Mass%	Vol%	Mol%
C1	2.802	3.184	2.955	8.649
C2	4.129	4.398	4.094	8.307
C3	1.451	1.511	1.384	2.188
C4	3.409	3.503	3.810	4.664
C5	13.076	13.317	15.397	15.904
C6	16.121	16.220	17.089	16.063
C7	21.727	21.529	21.857	19.133
C8	16.258	15.881	15.012	12.528
C9	9.279	8.956	8.113	6.355
C10	5.614	5.448	4.909	3.461
C11	1.803	1.751	1.543	1.010
C12	2.175	2.131	1.923	1.117
C13	0.587	0.588	0.573	0.278
C14	0.322	0.323	0.310	0.142
C15	0.488	0.489	0.466	0.200
C16	0.000	0.000	0.000	0.000
Unknowns	0.759	0.769	0.565	0.000
Total	100.000	100.000	100.000	100.000

ID No.	Component	R.T.	R.I.	Group	C#	Area	Wt%	Vol%	Mol%
6	Isobutane	8.299	354.168	I	4	24892.157	0.177	0.233	0.265
7	Methanol	8.594	368.593	X	1	406299.910	3.184	2.955	8.649
9	iso-Butylene	8.976	386.523	O	4	2482.278	0.017	0.021	0.026
11	Butane	9.274	400.000	P	4	192520.754	1.367	1.734	2.046
13	trans-2-Butene	9.658	408.900	O	4	7647.724	0.052	0.064	0.081
14	2,2-Dimethylpropane	9.776	411.568	I	5	2495.263	0.018	0.022	0.021
15	cis-2-Butene	10.249	421.930	O	4	9797.340	0.067	0.079	0.104
16	Ethanol	11.465	446.522	X	2	598700.323	4.398	4.094	8.307
18	3-Methyl-1-butene	11.837	453.519	O	5	4565.683	0.032	0.037	0.040
19	Isopentane	12.875	471.955	I	5	874250.487	6.163	7.306	7.434
24	1-Pentene	13.871	488.297	O	5	13582.111	0.093	0.107	0.115
25	Isopropanol	14.061	491.285	X	3	94432.623	0.678	0.623	0.982
26	2-Methyl-1-butene	14.356	495.834	O	5	36568.783	0.251	0.283	0.311
27	Pentane	14.631	500.000	P	5	642188.562	4.527	5.310	5.461
29	trans-2-Pentene	15.232	509.343	O	5	39714.292	0.272	0.308	0.338
31	cis-2-Pentene	15.793	517.731	O	5	22063.049	0.151	0.169	0.188
32	2-Methyl-2-Propanol (tert-Butanol)	15.930	519.723	X	4	138623.456	0.984	0.916	1.155
33	2-Methyl-2-butene	16.128	522.599	O	5	78572.850	0.538	0.597	0.668
37	2,2-Dimethylbutane	17.184	537.296	I	6	38316.037	0.269	0.304	0.272
39	Cyclopentene	18.459	553.907	O	5	7440.675	0.050	0.047	0.063
40	n-Propanol	18.697	556.878	X	3	116010.020	0.833	0.761	1.206
42	3-Methyl-1-pentene	18.914	559.551	O	6	2769.916	0.019	0.021	0.020
43	Cyclopentane	19.263	563.790	N	5	33353.744	0.229	0.225	0.284
44	2,3-Dimethylbutane	19.446	565.977	I	6	160298.736	1.125	1.249	1.136
45	Methyl tert-butyl ether	19.588	567.667	X	5	140932.910	0.994	0.985	0.981
47	2,3-Dimethyl-1-butene	19.745	569.522	O	6	2925.882	0.020	0.022	0.021
48	2-Methylpentane	19.846	570.703	I	6	451411.524	3.168	3.562	3.199
49	trans-4-Methyl-2-pentene	20.013	572.650	O	6	7672.537	0.053	0.057	0.054
53	3-Methylpentane	20.983	583.625	I	6	279713.239	1.963	2.170	1.982
54	2-Methyl-1-pentene	21.477	589.021	O	6	12837.827	0.088	0.094	0.091
55	1-Hexene	21.578	590.107	O	6	5031.440	0.034	0.037	0.036
56	2-Butanol	21.898	593.524	X	4	118216.776	0.839	0.763	0.985
58	Hexane	22.518	600.000	P	6	474371.965	3.329	3.708	3.362

Fig. 3 Two-dimensional PIONA/carbon number table and component concentration report

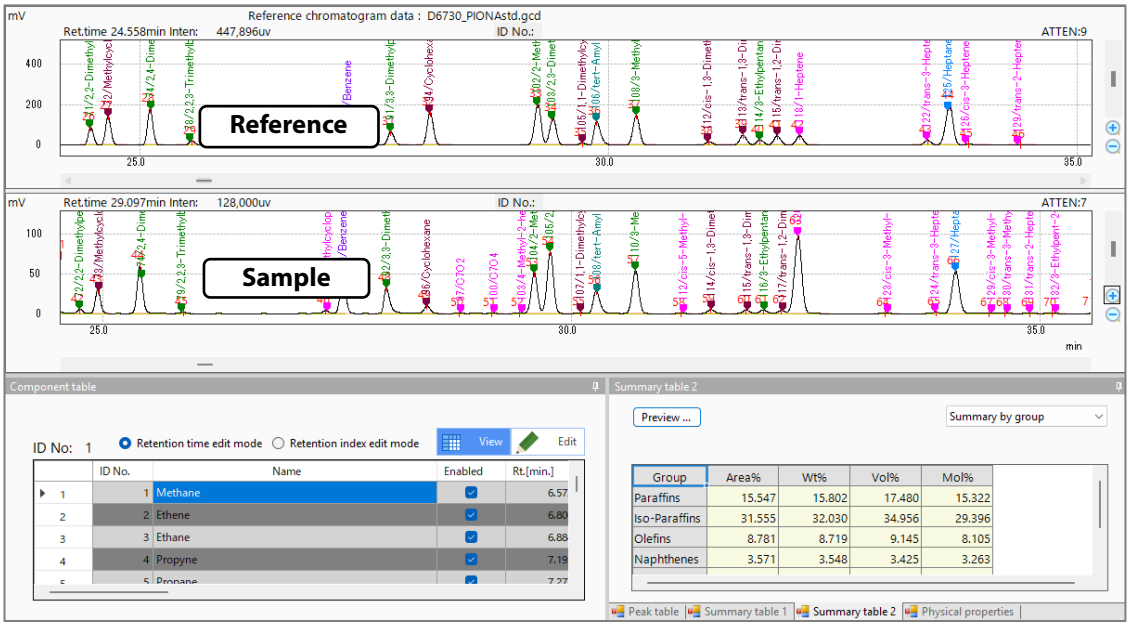


Fig. 4 PONAsolution chromatogram view

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