SIMDIST Analysers

- Solutions comply with ASTM, CEN, DIN, IP and ISO SIMDIST methods
- SIMDIST software fully integrated in Chromeleon datasystem
- Optimised injector technology
- Data merge of High Temp SIMDIST and DHA Front End

AN 205WA0620L

GAS offers custom configured GC analysers for many application fields since 40 years. GAS analysers are designed to meet many standardised methods from GPA, ASTM, UOP, ISO, EN and others. The efficient configurations are based on proven GC technology, resulting in robust instruments with an optimal return on investment.

The determination of boiling point distribution of petroleum products and crudes by GC is a fast and reliable tool, which is widely used to replace conventional labour intensive distillation methods like D86 and D1160. This proven technology is supported by several standardised methods.

GAS offers fully automated solutions for SIMDIST which enables you to generate TBP data according to international reference methods. The instruments are fully factory calibrated, fine-tuned to the specified method and tested to certified reference materials. Proven GC technology with optimised inlets offer reliable SIMDIST results. GAS SIMDIST Calculator software is completely integrated in Chromeleon data system, providing a clear and user friendly workflow as a result. Figure 1 shows the sample sequence list with samples, calibrations runs, blanks and check standards, while figure 2 displays a typical SIMDIST chromatogram with baseline subtraction.

Figure 1. Chromeleon datasystem with SIMDIST Calculator software showing clear and accessible acquisition list
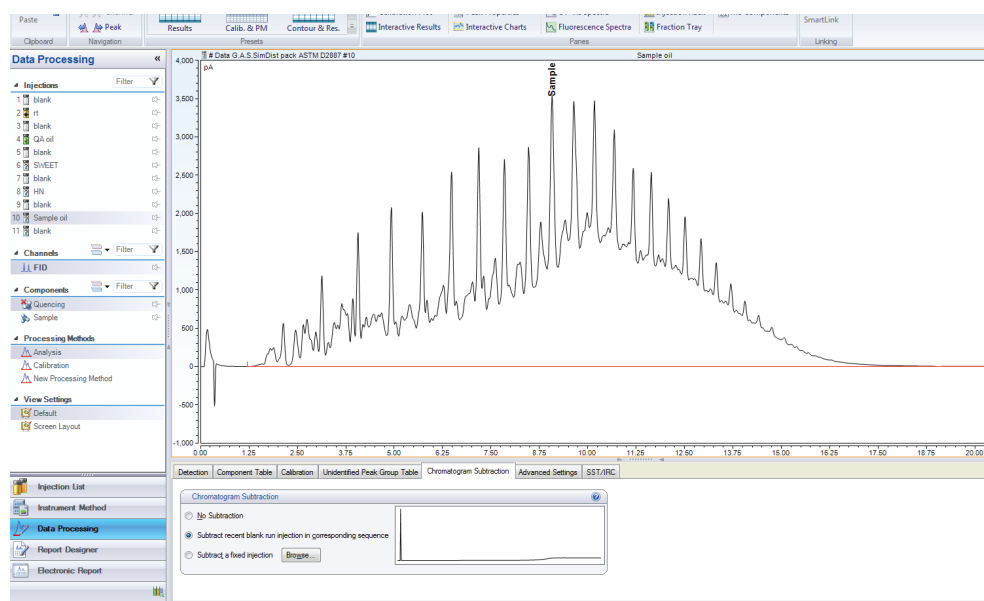

Figure 2. SIMDIST D2887 chromatogram with baseline subtraction

Figure 3. GC Trace 1310 with RSH autosampler

SIMDIST Calculator software provides:

▲ ASTM D86 and D1160: correlation for atmospheric and vacuum distillation

▲ Custom correlation models can be added by the user

▲ DIN 51.581 (NOACK): evaporative loss in mass% of lubricants at 250ºC

▲ ASTM D6417 (MOV): evaporation loss in mass% of lubricants at 371ºC

▲ Flashpoint correlations according to ASTM D56, D93 and D3828

▲ Cut point tables

▲ SIMDIST/DHA MERGE of ASTM D7169/ IP545 data according to ASTM D7900

▲ Carbon number report: list of carbon numbers with their appropriate boiling points. See figure 7.

Besides the boiling point distribution report (figure 4), a quality control report is available as well (figure 5). This report shows the conformity with reference samples, and is therefore very important for the overall reliability of the method.

Available hardware solutions:

▲ Thermo Trace 1300/1310 GC with InstantConnect injector and detector modules

▲ Split/Splitless Injector (medium volatile sample range)

▲ Optimised PTV injector module for true quantitative analytical results for all sample types

▲ PTV-Backflush for ASTM D7900 (application note available)

▲ Optional On-Column injector

▲ Triplus RSH or AI/AS 1310 autosamplers

SIMDIST application package including:

▲ Set of standards, Polywax (500, 655 or 1000) or hydrocarbon mix according to the required method to set the boiling point distribution versus retention time

▲ External reference sample, for quantification and performance verification

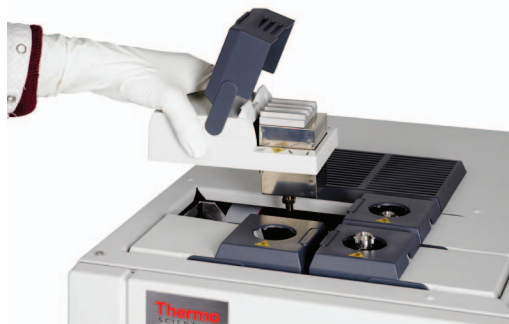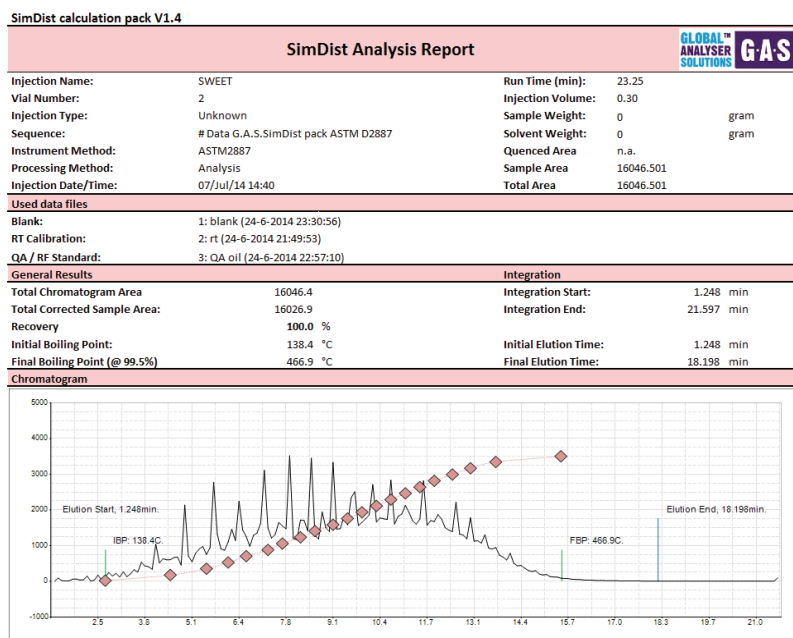▲ Analytical column, MXT-1 2887, or MXT-1HT for high temperature SIMDIST up to FBP 750 ºC

Figure 6. Easy injector/detector exchange with InstantConnect modules

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SimDist calculation pack V1.4

SimDist Analysis Report — GLOBAL ANALYSER SOLUTIONS G·A·S

Injection Name:	SWEET	Run Time (min):	23.25	
Vial Number:	2	Injection Volume:	0.30	
Injection Type:	Unknown	Sample Weight:	0	gram
Sequence:	# Data G.A.S.SimDist pack ASTM D2887	Solvent Weight:	0	gram
Instrument Method:	ASTM2887	Quenced Area	n.a.	
Processing Method:	Analysis	Sample Area	16046.501	
Injection Date/Time:	07/Jul/14 14:40	Total Area	16046.501	

Used data files

Blank:	1: blank (24-6-2014 23:30:56)
RT Calibration:	2: rt (24-6-2014 21:49:53)
QA / RF Standard:	3: QA oil (24-6-2014 22:57:10)

General Results / **Integration**

Total Chromatogram Area	16046.4	Integration Start:	1.248	min
Total Corrected Sample Area:	16026.9	Integration End:	21.597	min
Recovery	100.0 %			
Initial Boiling Point:	138.4 °C	Initial Elution Time:	1.248	min
Final Boiling Point (@ 99.5%):	466.9 °C	Final Elution Time:	18.198	min

Chromatogram

Elution Start, 1.248min. IBP: 138.4C. FBP: 466.9C. Elution End, 18.198min.

Boiling Point Distribution Table / Correlation Results / Cut Points

%OFF	BP (°C)		Model:	D86		BP (°C)	%OFF
0.5	138.4		**%OFF**	**BP (°C)**		150.0	1.0
5.0	185.1		IBP	192.9		200.0	8.1
10.0	208.7		5.0	219.8		250.0	23.4
15.0	226.6		10.0	231.6		300.0	44.2
20.0	238.9		20.0	252.0			
25.0	253.4		30.0	272.2			
30.0	265.5		40.0				
35.0	277.5		50.0	307.1			
40.0	288.3		60.0				
45.0	301.2		70.0	341.3			
50.0	311.8		80.0	357.0			
55.0	321.8		90.0	377.2			
60.0	332.3		95.0	393.4			
65.0	343.9		FBP	404.9			
70.0	354.6		**%vol @ 350°C**	75.5			
75.0	365.2						
80.0	376.1						
85.0	388.3		**Flash point (°C):**				**mass %**
90.0	401.6		D56 (Jet Fuel)	79.3	DIN 51581 (Noack)	Not valid	
95.0	420.0		D93 (Diesel)	78.9			**mass %**
99.5	466.9		D3828 (Jet Fuel)	82.8	ASTM D6417(MOV)	77.5	

Figure 4. Sample report

SimDist calculation pack V1.4

QA System Check Report — GLOBAL ANALYSER SOLUTIONS G·A·S

Injection Name:	QA oil
Vial Number:	3
Injection Type:	Check Standard
Sequence:	# Data G.A.S.SimDist pack ASTM D2887
Instrument Method:	ASTM2887
Processing Method:	Analysis
Injection Date/Time:	41814.95637
Injection Name:	QA oil

Used data files

Blank:	1: blank (24-6-2014 22:23:18)
RT Calibration:	2: rt (24-6-2014 21:49:53)
QA / RF Standard:	3: QA oil (24-6-2014 22:57:10)

General Results

Reference Check PASSED

Boiling Point Table:

Reference material: Ref D2887

%OFF	Expected BP	Allowable Diff	Boiling Point	Difference	Pass/Fail
0.5	115	7.6	114.8	0.2	Pass
5	151	3.8	151.1	0.1	Pass
10	176	4.1	178.1	2.1	Pass
15	201	4.5	204.2	3.2	Pass
20	224	4.9	227.7	3.7	Pass
25	243	4.9	246.7	3.7	Pass
30	259	4.7	262.7	3.7	Pass
35	275	4.7	278.1	3.1	Pass
40	289	4.3	291.8	2.8	Pass
45	302	4.3	302.3	0.3	Pass
50	312	4.3	313.2	1.2	Pass
55	321	4.3	322.1	1.1	Pass
60	332	4.3	331.3	0.7	Pass
65	343	4.3	342.8	0.2	Pass
70	354	4.3	353.6	0.4	Pass
75	365	4.3	365.7	0.7	Pass
80	378	4.3	378.5	0.5	Pass
85	391	4.3	391.8	0.8	Pass
90	407	4.3	409.1	2.1	Pass
95	428	5	432.1	4.1	Pass
99.5	475	11.8	484.9	9.9	Pass

Figure 5. Quality control report

Specifications

Configuration: 1 or 2 channel instrument based on Thermo GC Trace 1300, with InstantConnect SSL, PTV or Cold-On-Column injector module and InstantConnect FID detector module, Triplus RSH or AS/AI-1310 liquid autosamplers

Optional: Cryogenic oven cooling (liquid N_2 or liquid CO_2)

Application: Custom configured analyser for light hydrocarbon products up to crude oil, lube oil and residual samples SIMDIST analyser tuned for applications according to the standardised methods

Sample requirements: Neat or dissolved in CS_2 (safety issue: CS_2 is extremely flammable and toxic)

Analysis time: Depending on method

Software   **GAS** SIMDIST Calculator for Chromeleon. See page 3 for specification SIMDIST/DHA MERGE of ASTM D7169/ IP545 data according to ASTM D7900 (application note available)
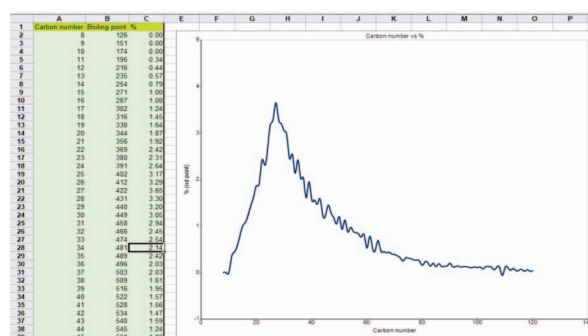

Figure 7. Optional carbon number report

Boiling point	-200	-100	0	100	200	300	400	500	600	700	800
ASTM D3710			gasoline								
ASTM D7096			gasoline + ethanol								
ASTM D5399			solvents								
ASTM D2887				petroleum fractions							
ASTM D5442					petroleum wax						
ASTM D7213				medium petroleum destillates							
ASTM D6417				medium petroleum destillates							
ASTM D6352				medium and heavy petroleum destillates							
ASTM D5307			crude petroleum								
ASTM D7500				medium and heavy petroleum destillates							
ASTM D7169			crude oil and residues								
DIN 51581-2				medium petroleum destillates							
DIN 51435				medium and heavy petroleum destillates							
IP 406				petroleum products							
IP 480				middle destillates and lubricating base oils							
IP 507				vacuum destillates and residues							
IP 545			crude oil								
EN 15199-1				middle destillates and lub base oils							
EN 15199-2				vacuum destillates and residues							
EN 15199-3			crude oil								
ISO 3924				petroleum fractions							

Figure 8. Available standardised methods with boiling point and application range

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