

New SimDist Software and Applications

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Introduction

Simulated distillation by Gas Chromatography has been widely used in the petro-refinery industry to predict boiling point distribution properties of a feedstock. Sample boiling point information is of utmost importance in quality and process control, regulatory compliance, and the prediction of various product yields.

In most cases, special SimDist software is needed to perform peak integration, distillation curve calculation and

simulation. In this study, a new SimDist software fully integrated into GC control software will be evaluated. GC operation conditions and SimDist parameters in the same GC method file. The raw chromatogram and simulated distillation results are stored in the same data file. ASTM D2887 method is used to demonstrate the new software functions.

What is Simulated Distillation GC Analysis?

Simulated distillation GC analysis applies a gas chromatograph with a nonpolar column to the boiling-point distribution analysis of petroleum fractions, such as kerosene, diesel oil, and heavy oil. A **boiling point calibration curve** (as shown in Fig. 1) can be created by analyzing a mixture of hydrocarbons with known boiling points.

As shown in Fig. 2, dividing the total area of the chromatogram for an unknown sample into equal time intervals and calculating the area of each time interval allows the proportion of elution volume (%) in each time interval to be calculated as the time interval area value divided by the total area. The elution volume (%) in each

boiling point range can be determined from the retention time – **boiling point calibration curve** and used to obtain the relationship between the elution volume (%) and boiling point, that is, to create the **distillation curve** as shown in Fig. 3.

The method above is called the "total area method," as it applies when all components in the entire sample elute from the column. The internal standard method, which involves adding an internal standard substance, and the external standard method, which compares the analysis results with an external standard sample, are used for the analysis of crude oil and other samples that contain components that do not elute.

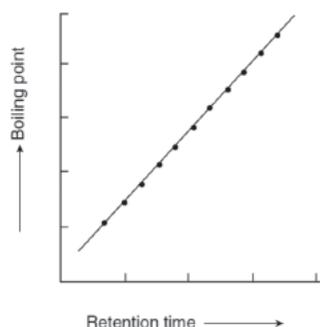


Fig. 1 Retention Time – Boiling Point Calibration Curve

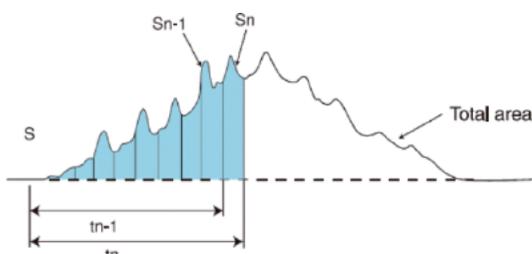


Fig. 2 Calculating the Elution Amount

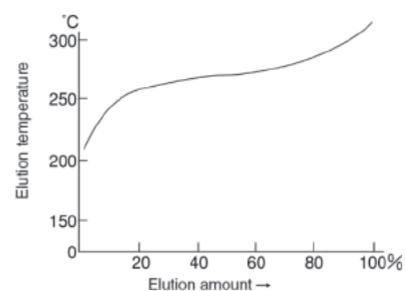


Fig. 3 Distillation Curve

Support of all SimDist Official Methods

Simulated Distillation GC Official Methods

LabSolutions simulated distillation GC analysis software supports the following simulated distillation GC standards.

Official Method	Carbon Number	Sample
JIS K 2254	-	Kerosene, diesel oil
ASTM D 2887 (ISO3924, IP406)	n-C ₅ to n-C ₄₄	Jet oil, diesel oil
ASTM D 3710, D 7096	n-C ₃ to n-C ₁₅	Gasoline, naphtha
ASTM D 6417	n-C ₈ to n-C ₆₀	Lubricating oil, base stock oil
ASTM D 7213 (Extended D2887)	n-C ₇ to n-C ₆₀	Lubricating oil, base stock oil
ASTM D 6352	n-C ₁₀ to n-C ₉₀	Lubricating oil, base stock oil
EN 15199-1 (IP480, DIN 51435)	n-C ₇ to n-C ₁₂₀	Lubricating oil, base stock oil
ASTM D 5307	n-C ₄₄ max.	Crude oil (internal standard method)
ASTM D 7500	n-C ₇ to n-C ₁₁₀	Crude oil
ASTM D 7169, EN 15199-2 (IP 507)	n-C ₇ to n-C ₁₁₀	Crude oil (external standard method, n-C ₁₂₀ max. for EN)
EN 15199-3 (IP545)	n-C ₁₂₀ max.	Crude oil (external standard method + backflushing)

There are various methods for each analysis sample, and a different analytical method and functions are required.

Work with LabSolutions

LabSolutions ver.5.54SP2~(File) /
ver.6.11 SP1~(DB/CS)



Win7 64 bit OS compatible

LabSolutions SIMDIS Software
(CD + USB dongle)



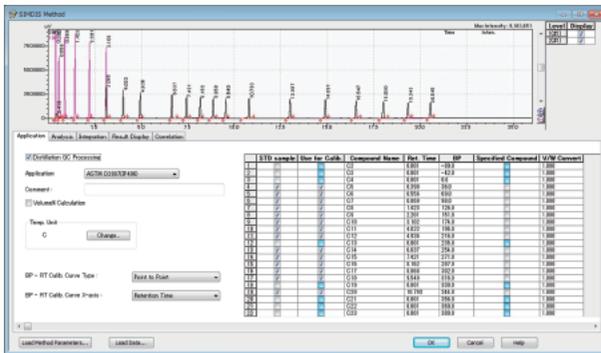
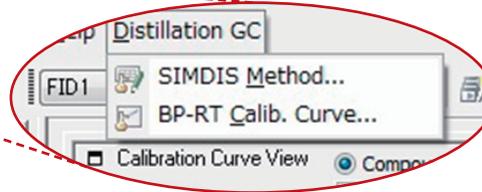
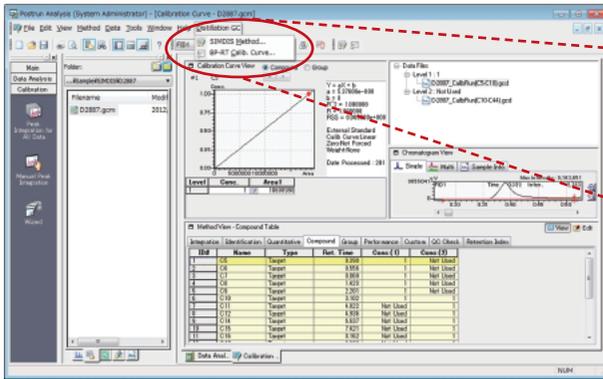
New SimDist Software and Applications

Ease of Operation I

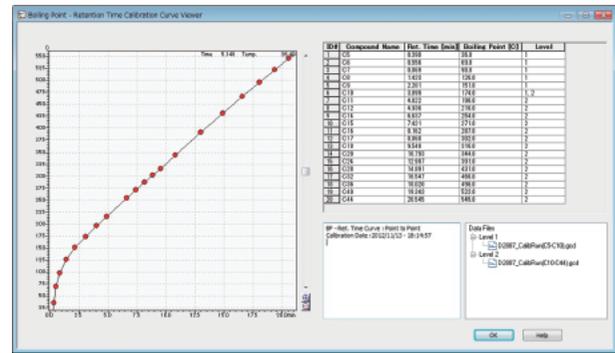
Menus for simulated distillation are added in LabSolutions

- The window to set methods, check distillation data and compare the result is available from menus in the LabSolutions window.

ex. LabSolutions [Calibration Curve] Window



[SIMDIS Method] Window



[BP-RT Calib Curve] Window

Ease of Operation II

Parameters and Result are saved in a LabSolutions File

- Method parameters for simulated distillation GC analysis are saved in LabSolutions method file (.gcm)
- The parameters and distillation results are saved in LabSolutions Data File (.gcd)

Method Parameters for Simulated Distillation GC Analysis

- Settings for RT-BP calibration curve / Analysis method / Integration / Result display / correlation

Simulated Distillation GC Analysis result

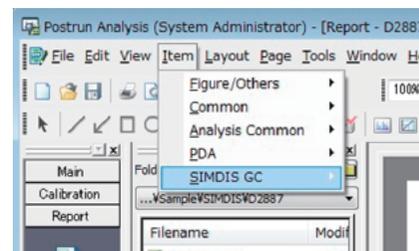
- Distillation Curve / Table (Temperature to Recovery, Recovery to Temperature)
- Sample Data Information (Eluting zone, Internal standard / External standard information, etc.)

Customizable Report format

- 6 new report items for simulated distillation GC analysis are prepared.
- User can customize the report layouts and output reports on LabSolutions report function.

Simulated Distillation GC Report Items

- Method / Calibration Curve / Result Table / SIMDIS Chromatogram / Distillation Graph / Summary



New SimDist Software and Applications

Ease of Operation III

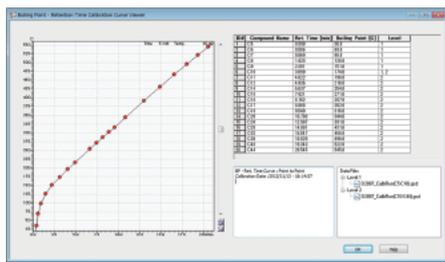
All Samples can be acquired thru a LabSolutions Batch.

- Blank analysis
- Retention Time – Boiling point Calibration analysis (n-paraffin mixture)
- Distillation characteristics calculation of unknown samples analysis
- Report generation.

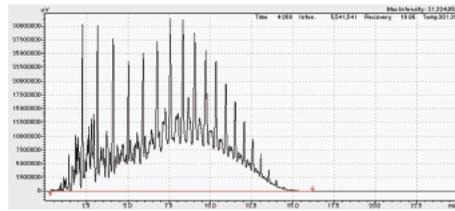
LabSolutions Batch Table

Postrun	Sample Name	Sample ID	Sample Type	Level#	Method File	Data File	Background	Background Data File	Report Output	Report Format File
1	CalibRun_1		1:Standard(D)	1	D2887.gcm	D2887_CalibRun(C5-C10).gcd	<input checked="" type="checkbox"/>	D2887_Blank.gcd		
2	CalibRun_2		1:Standard	2	D2887.gcm	D2887_CalibRun(C10-C44).gcd	<input checked="" type="checkbox"/>	D2887_Blank.gcd		
3	light oil-Std		0:Unknown	3	D2887.gcm	D2887_lightOil(Std).gcd	<input checked="" type="checkbox"/>	D2887_Blank.gcd	<input checked="" type="checkbox"/>	D2887.lsr
4	light oil-Unk		0:Unknown	4	D2887.gcm	D2887_Unk_lightOil.gcd	<input checked="" type="checkbox"/>	D2887_Blank.gcd	<input checked="" type="checkbox"/>	D2887.lsr

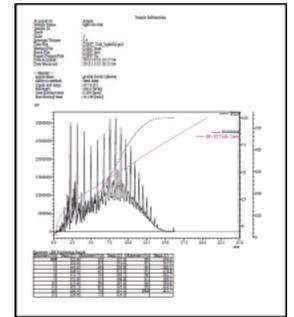
Set Report format for distillation result.



Create RT – BP calibration curve



Analyze unknown sample

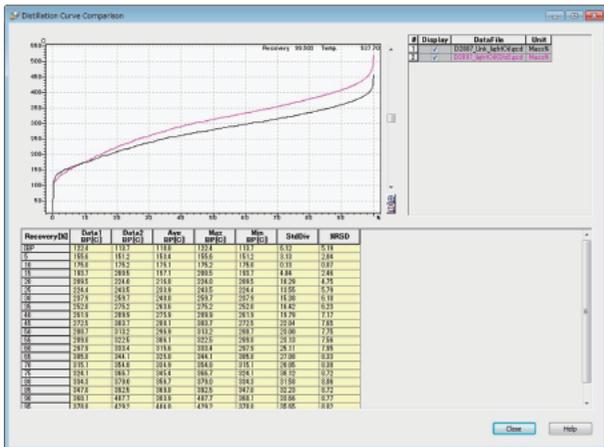


Create report

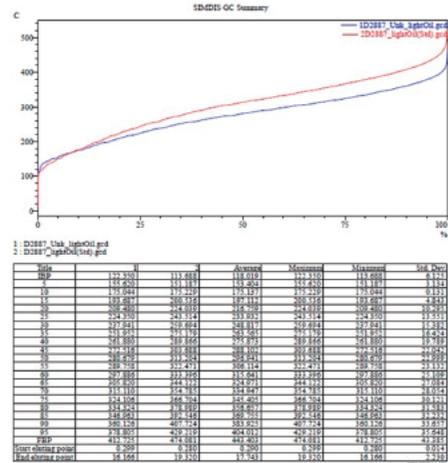
Data Comparison - Multiple Data Overlay

Comprehensive Functions for Statistic Calculations and Comparison of Multiple Distillation Results

- Up to 16 distillation results can be displayed in the [Distillation Curve Comparison] window.
- Multiple distillation results can be printed with a summary report.
 - √ Maximums, minimums, averages, and relative standard deviations of distillation result can be calculated and output in a report.



[Distillation Curve Comparison] window



Summary Report

For quality control and process control, daily product data management or comparison with past collected data may be required.

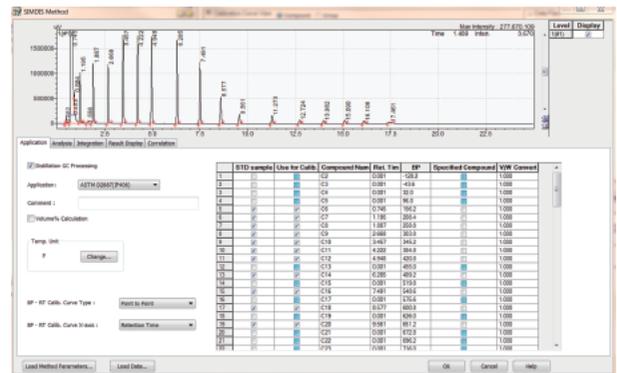
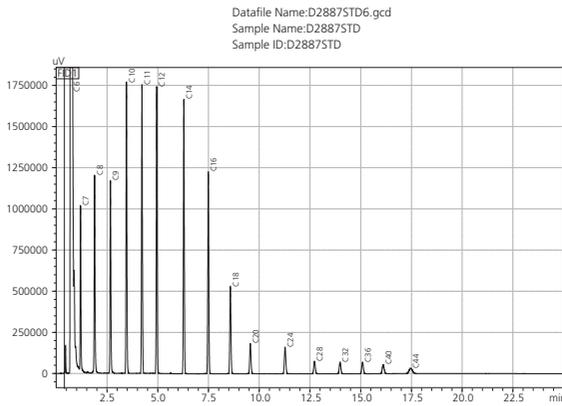
New SimDist Software and Applications

Method ASTM D2887

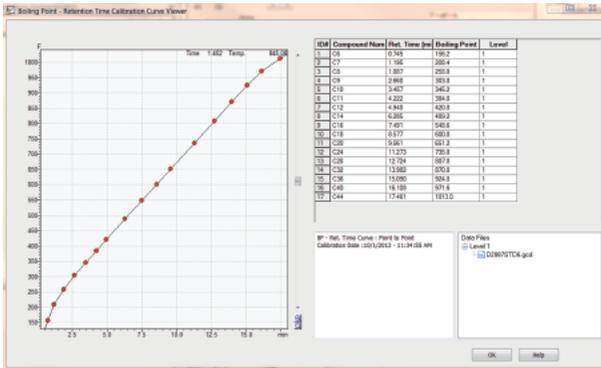
ASTM D 2887, simulated distillation (SIMDIS), is one of the most basic tests in the petroleum lab. It has eliminated the need for the time-consuming and complicated D-86 true distillation method.

This method is applicable to petroleum products and fractions up to 538°C (1000°F), and SimDist GC results can be reported independently as well as a correlation to method ASTM D86.

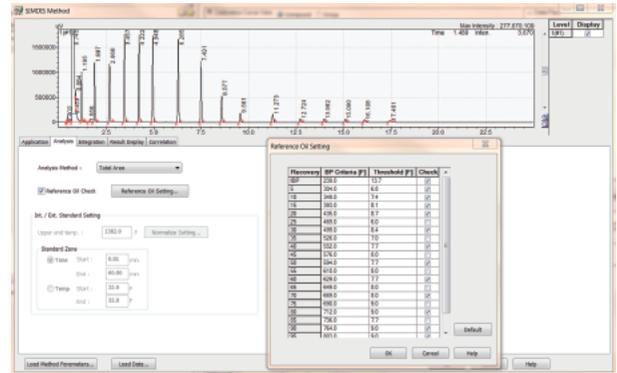
ASTM D2887 Calibration



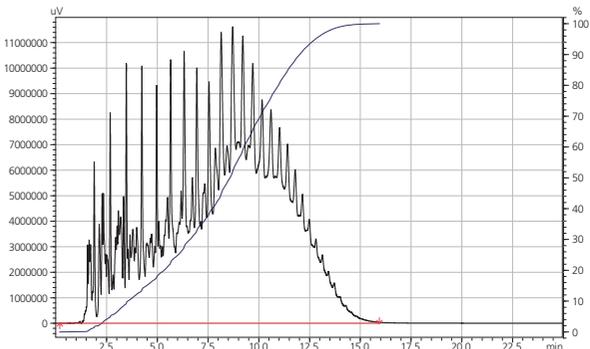
ASTM D2887 Calibration Curve



ASTM D2887 Reference Oil Criteria Setup



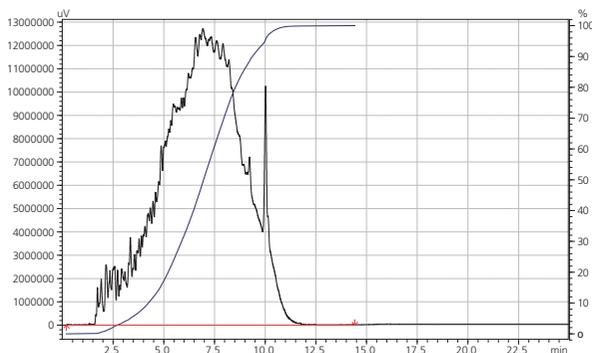
ASTM D2887 Reference Oil QC Results



Recovery (%)	Temp (F)	BP Criteria	Threshold	Check	Recovery (%)	Temp (F)	BP Criteria	Threshold	Check
5	304.6	239	13	Pass	30	505.4	499	8	Pass
10	349.6	304	6	Pass	35	533.6	552	7	Pass
15	397.0	349	7	Pass	40	559.2	580.6		
20	440.6	435	8	Pass	45	580.6			
25	475.8	455	8	Pass	50	600.8	594	7	Pass
60	636.0	629	7	Pass	90	772.6	764	9	Pass
65	656.6				95	811.0	803	9	Pass
70	676.8	669	8	Pass	FBP	890.8	887	21	Pass
75	698.4								
80	720.4	712	9	Pass					
85	743.8								

New SimDist Software and Applications

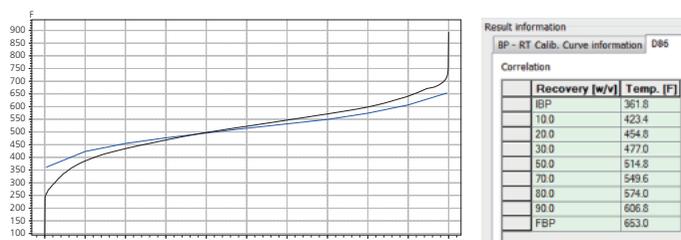
ASTM D2887 Diesel Fuel Results



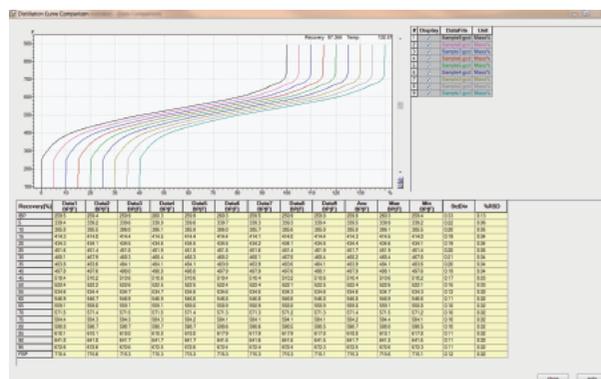
Recovery - BP Distillation Result

Recovery (%)	Temp.(F)	Recovery (%)	Temp.(F)	Recovery (%)	Temp.(F)
IBP	259.8	30	468.4	80	598.6
1	273.8	35	484.2	85	617.8
2	292.4	40	498.0	90	641.4
3	308.8	45	510.6	95	672.2
4	325.4	50	522.6	96	675.4
5	339.4	55	534.6	97	680.6
10	385.8	60	546.8	98	689.6
15	414.4	65	559.0	99	703.0
20	434.6	70	571.4	FBP	715.2
25	451.8	75	584.2		

ASTM D2887 Diesel Fuel D-86 Correlation



ASTM D2887 Diesel Sample Data Comparison



Conclusions

- New Shimadzu SimDist software supports all simulated distillation official methods.
- All operations are controlled with one software - LabSolutions.
- Software can generate summary reports and compare multiple simulated distillation results.
- ASTM D2887 method has been demonstrated that the new software is quick, easy and rugged.