

Shimadzu Simulated Distillation Gas Chromatograph System



Meets All Simulated Distillation Gas Chromatograph Standards

- Provides Highly Accurate Analysis Results with Excellent Reproducibility-

The Shimadzu simulated distillation system, consisting of a GC-2010 Plus high-performance capillary gas chromatograph and LabSolutions simulated distillation GC analysis software, meets all applicable ASTM, ISO, EN, and JIS standards. Permitting accurate and highly reproducible analysis of high-boiling components in crude oil samples, it is the optimal system for product quality control and process management in oil refinery plants.



Table of Simulated Distillation Gas Chromatograph Standards

The LabSolutions simulated distillation GC analysis software supports measurements that comply with the following simulated distillation gas chromatograph standards.

	Carbon Number	Sample
ASTM D 3710, D 7096	n-C3 ~ n-C15	Gasoline, naptha
JIS K 2254	_	Kerosene, diesel oil
ASTM D 2887 (ISO3924, IP406)	n-C5 ~ n-C44	Jet fuel, diesel oil
ASTM D 6417	n-C8 ~ n-C60	Lubricating oil, base stock oil
ASTM D 7213 (Extended D2887)	n-C7 ~ n-C60	Lubricating oil, base stock oil
ASTM D 6352	n-C10 ~ n-C90	Lubricating oil, base stock oil
ASTM D 7500	n-C7 ~ n-C100	Lubricating oil, base stock oil
EN 15199-1 (IP480, DIN 51435)	n-C7 ~ n-C120	Lubricating oil, base stock oil
ASTM D 5307	n-C44 Max	Crude oil (internal standard method)
ASTM D 7169, EN 15199-2 (IP 507)	n-C7 ~ n-C100	Crude oil (external standard method, n-C120 max. for EN)

LabSolutions Simulated Distillation GC Analysis Software

The simulated distillation GC analysis software features functions for operations from calibration to sample analysis. Reporting functions include all calculations required by the simulated distillation gas chromatograph standards. A distillation characteristics curve and reference oil analysis chromatogram can be overlaid in reports, and flexible report generation allows free arrangement and customization of items. In addition, the software provides comprehensive post-run analysis functions, including calculation of physical properties and creation of summary reports for multiple data.



Retention Time - Boiling Point Curve Display



Simulated Distillation Method Setup Screen



Sample Report

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. As each component elutes from the column in boiling-point order, the retention time – boiling point curve can be created by analyzing a mixture of hydrocarbons with known boiling points. As shown in Fig. 2, dividing the total area of an unknown sample's chromatogram 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 curve and used to obtain the relationship between the elution volume (%) and boiling point, that is, to create the distillation characteristics curve as shown in Fig. 3.

The method above is known as 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.



Support for High-Temperature Simulated Distillation GC Analysis

The Shimadzu simulated distillation gas chromatograph analysis system supports analysis of high-boiling-point samples (up to 120 carbon number). Examples of analyses conforming to ASTM standards are introduced below.

ASTM D7169, D5307, and D7500 High-Temperature GC Analysis Standards

Support for Crude Oil Analysis

ASTM D7169

The ASTM D7169 standard applies to crude oil samples with a final boiling point (FBP) exceeding 720 °C. Reference Oil 5010 was analyzed by the external standard method using a short capillary column with a thin film thickness.

• Using CS₂ quenching factors

ASTM D5307

n-C17) internal standards.

ASTM D7500

• Comparison check against reference oil distillation characteristics standard values

The ASTM D5307 standard applies to crude oil with a FBP exceeding 538 °C. A packed column was used for analysis by the internal standard method of samples, including those spiked with (n-C14 to

The ASTM D7500 standard applies to samples with an initial boiling point (IBP) exceeding 100 °C and a FBP less than 735 °C. In this example, the sample was analyzed by the total area method using a short capillary column with a thin film thickness. Polywax® 655 and Polywax® 1000 are also used to create the retention time – boiling



The chromatogram display screen for unknown samples shows chromatograms for the reference oil and background correction together with other information such as the automatic peak recognition start and end points, and initial and final boiling points.







Sample Analysis of Calibration Mix Standard

Low Carryover and Excellent Reproducibility

Dedicated Injection Unit Handles High-Boiling-Point Samples

Using an OCI-2010 on-column injection unit with the GC-2010 Plus Capillary Gas Chromatograph achieves low carryover and provides analysis results with high reproducibility.





Reproducibility of ASTM D7500 Reference Oil Analysis (n=5) The FBP of reference oil 5010 is equivalent to the boiling point of 73 carbon number n-paraffin.



Separation of High-Boiling-Point Components in ASTM D7500 Polywax $\ensuremath{\mathbbmm}$ 1000 Analysis

Peak elution up to 120 carbon number n-paraffin (750 °C boiling point) indicates measurement of high-boiling-point samples is possible.

•Display of fractions (mass %) above 538 °C

point curve.

Diverse Analysis Functions

The simulated distillation GC analysis software offers comprehensive functions to support the calculation of the physical properties required for process management in oil refinery plants, multisample data comparison required for product quality control, and statistical calculations.

ASTM D2887 and JIS K2254 Kerosene, Jet Fuel, Diesel Oil Analysis Comprehensive Data Conversion and Customization

The software supports conversions and calculations to acquire information about physical properties from the distillation characteristics. It also supports the following official methods in ASTM, ISO, and DIN standards: estimation of physical distillation (ASTM D86: Normal pressure method; ASTM D1160: low-pressure method; ASTM D2887 Appendix X5: diesel oil and jet fuel conversions), flash point calculations (ASTM D7215), NOACK calculations (DIN 51581-2), MOV calculations (ASTM D6417), Reid vapor pressure calculations, cut point and distillate fraction calculation.

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			1	1		1			
IG-IBP :	+46.566	+0.58289	* GC 10%	+0.34795	* GC IBP	-		1	
No. 2011	+33.300	+0.69002	100 104	+0.30110	* GC 20%	+0.21713	100.103		
36-30%	+14.431	+0.47035	* GC 30%	+0.28369	*GC 20%	+0.22784	* GC 50%		
6-50% :	+4.876	+0.97597	* GC 50%						
6-70% :	+0.911	+0.51975	* GC 80%	+0.33260	* GC 70%	+0.10159	* GC 30%		
6-80% :	+0.279	+0.75936	* GC 80%	+0.28333	* GC 95%	-0.09975	"GC FBP	1	
36-90% :	-1.973	+0.61459	* GC 90%	+0.31909	* GC 95%	-			
G-FBP :	+34.179	+1.14826	* GC 95%	-0.59028	"GC 90%	+0.31542	GC FBP		
FBP:	+34.179	+1.14826	* GC 95%	-0.59028	* GC 90%	+0.31542	GC FBP	1	Initialize

ASTM D86 Conversion Parameter Setting Screen (Normal Pressure Method) Parameters listed in standards such as ASTM or ISO are prepared as default for the conversion and calculation functions. The parameter values can be changed and customized to match the actual physical properties.



Sample Analysis of ASTM D2887-Compliant Diesel Oil



Sample Reports of ASTM D2887-Compliant Diesel Oil Analysis Various reports can be created by overlaying a distillation characteristic curve over the chromatogram or an ASTM D86- or D1160-converted distillation characteristics curve over the distillation characteristic curve.

Data Comparisons and Statistical Calculations Simple Summary Reports of Complex Data

Daily product data management and comparison studies against past data are essential to maintain a high level of product quality. The software permits access to multiple data through simple operations, data comparison between multiple samples, and statistical calculations.



Comparison Window for Distillation Characteristic Curves Permits overlay of distillation characteristic curves for up to 16 samples. Zoom function for target areas is also available.



Summary Report Functions

Multiple distillation characteristics results can be printed in a report. The boiling points for specific elution volumes and fractions, as well as data, maximums, minimums, averages, and relative standard deviations, can be extracted.

High Data Reliability

The keys to obtaining reliable and reproducible data are daily system accuracy management and a robust system configuration. Optimized software and hardware are combined to deliver the highest data accuracy.

Support for Reference Oil Analysis Comprehensive System Check Functions

The system performance must be comprehensively checked in advance to ensure high-accuracy data when analyzing high-boiling-point samples. It is possible to check whether the system performance specifications prescribed in official methods, such as peak resolution, peak symmetry, and relative sensitivity calculations, are satisfied for standard sample analysis and to check for differences from standard values in reference oil analysis.



Sample Reference Oil Standard Value Setting Screen and Analysis Results Report



Data File Structure

Data files have an "All-in-One" structure that contains not only chromatograms and data processing results, but also information related to analysis methods and batch files used for serial analysis. The files also contain parameters related to the simulated distillation gas chromatograph system that permit accurate tracing of the analysis parameters from the data.

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Templates Provided for Each Analysis Method

Using the analysis parameters contained in the method and report file templates supplied with the system allows analysis to be started immediately. These files are not fixed but can be freely created from new or expanded parameters.

Network Compatibility Compatible with LabSolutions Network Functions

Data acquired using the Shimadzu simulated distillation gas chromatograph system can be registered to the LabSolutions database, together with data acquired using other instruments. The highly secure database system permits optimal analysis operations. Configuring a network system with LabSolutions CS permits analysis directions and instrument monitoring and control from a remote PC.

Notes

- 1.The acquisition controller PC controls the analytical instruments. Analysis directions and re-analysis of data can be performed using a client PC.
- 2.1t is not necessary to install LabSolutions software on the client PC for terminal service. 3.iPad is a registered trademark of Apple Inc.
- 4. When using an iPad, the installation of Citrix's XenApp is required.



LabSolutions Simulated Distillation GC Analysis Software Specifications

Basic Specifications	Create retention time - boiling point curves (tables, retention time - boiling point curves, °C or °F temperature units) Create distillation curves (tables, distillation characteristics curves, °C or °F temperature units) Unknown sample - blank difference chromatogram Analysis methods: total area method, internal standard method (single, double), external standard method
Supported Simulated Distillation Gas Chromatograph Standards	ASTM D2887 (ISO3924,IP406), ASTM D3710, ASTM D5307, ASTM D5399, ASTM D6352, ASTM D6417, ASTM D7096, ASTM D7169, ASTM D7213 (Extended D2887), ASTM D7500, EN 15199-1 (IP480, DIN 51435), EN 15199-2 (IP 507), JIS K 2254
Requirements of Simulated Distillation Gas Chromatograph Standards	Automatic evaluation of distillate peak start and end points Distillation calculation (mass%, volume%) Quenching factor calculation MOV calculation (elution volume % to 371 °C, ASTM D6417) Specific component volume % calculation (ASTM D3710, D7096) Cut point and distillate fraction calculation
System Check Support	Peak resolution calculations, peak symmetry calculations, relative sensitivity calculations, reference oil distillation, characteristics checks
Conversions and Calculations from Distillation Characteristics (Factors can be customized.)	ASTM D86 and D1160 conversion Diesel oil and jet fuel conversions (ISO3924, ASTM D2887, IP 406) NOACK conversion (DIN 51.582-2) Flash point calculations (ASTM D7215) Reid Vapor Pressure calculations (ASTM STP577)
Chromatogram Output	Display of IBP, FBP, distillate peak start and end points, standard substance intervals, maximum distillation temperatures, quenching intervals Background chromatograms, distillation characteristics curves, ASTM D86 and D1160 conversion, diesel oil and jet fuel conversions, overlay of reference oil standard curves
Distillation Characteristics Curve Output	Display of cut points and fractions ASTM D86 and D1160 conversion, diesel oil and jet fuel conversions, overlay of reference oil standard curves
Comparison of Multiple Data	Distillation characteristics comparison, summary reports of conversion and calculation results





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