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Application Note

Efficient Processing of Data for Polymer Analysis Using Empower 3 Software with GPC Option

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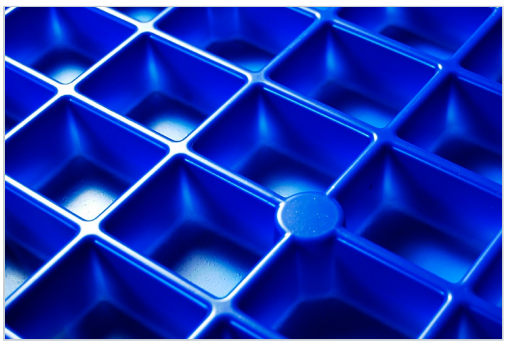


This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief demonstrate the efficiency and simplicity of using Empower Software to process GPC/APC data, calculate the molecular weight parameters, and effectively characterize polymer samples.

Benefits

A powerful and efficient tool to calculate molecular weight distributions and automatically generate characterization data for polymer samples.

Introduction

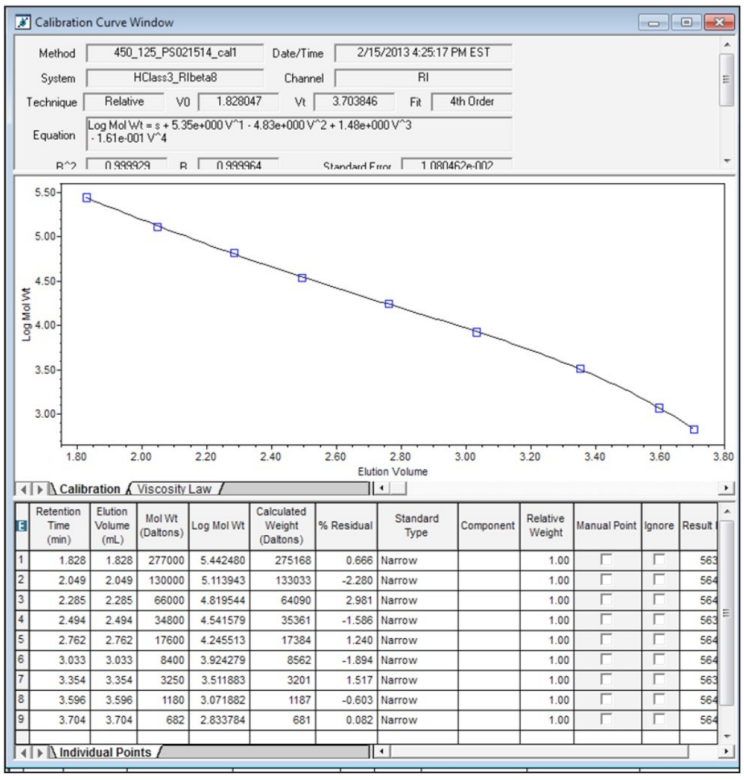
Empower Software is Waters' compliance-ready chromatography data software (CDS) package for advanced data acquisition, management, processing, reporting, and distribution. It is widely used in many analytical laboratories for applications ranging from pharmaceutical, chemical, food, and environmental analysis. In addition, it offers powerful processing options for gel permeation chromatography for polymer analysis. With recent technological advances in instrumentation, Waters ACQUITY Advanced Polymer Chromatography (APC) System combined with the sub-3 µm particle column technology delivers unprecedented high resolution, chromatographic characterization of polymers, and particularly low molecular weight species, faster than ever before.

To illustrate the capabilities of Empower, a polysulfone sample was analyzed using Waters ACQUITY APC System with two columns connected in series. The molecular weight calibration was performed using a set of polystyrene standards with narrowly distributed molecular weights. The calibration data were processed and the curve was generated using Empower 3 Software with GPC option. Finally, the molecular weight parameters of this polysulfone sample were automatically measured against the polystyrene calibration curve to characterize the polymer.

Results and Discussion

There are two ways to calibrate GPC/APC systems: relative and universal. Relative calibration can be achieved by comparing the unknown to a well-characterized polymer with broad molecular weight distribution, or to a set of narrowly distributed polymers. This is typically based on data acquired from various detectors including but not limited to UV, ELSD, RI and CAD. Universal calibration requires the use of molecular weight sensitive detectors, such as a viscometer, low-angle light scattering detector (LALLS), or multi-angle light scattering detector (MALLS). Empower 3 Software with GPC option can accommodate all modes of calibration.

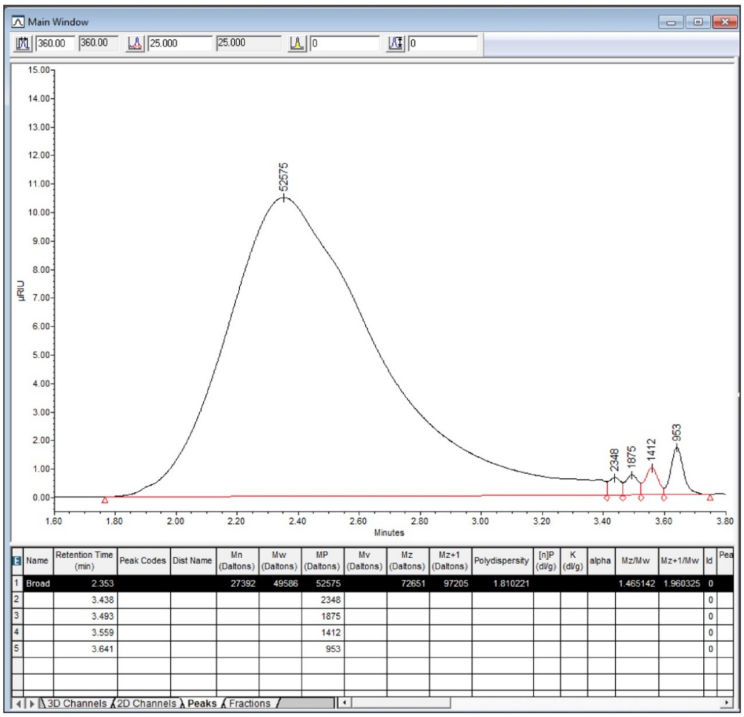
In this example, the calibration of the ACQUITY APC System is illustrated by analyzing a set of polystyrene standards with narrow dispersity. The molecular weights at peak maximum (Mp) of each polystyrene standard are utilized to establish the molecular weights relative to the retention time or retention volume. The creation of the processing method is easily performed using a processing method wizard, or customized integration events can be set manually. Once the data is automatically integrated and quantified, a calibration curve is generated. The polystyrene calibration curve plotting log Mp versus the retention volume is shown in Figure 1.



	Retention Time (min)	Elution Volume (mL)	Mol Wt (Daltons)	Log Mol Wt	Calculated Weight (Daltons)	% Residual	Standard Type	Component	Relative Weight	Manual Point	Ignore	Result
1	1.828	1.828	277000	5.442480	275168	0.666	Narrow		1.00			563
2	2.049	2.049	130000	5.113943	133033	-2.280	Narrow		1.00			564
3	2.285	2.285	66000	4.819544	64090	2.981	Narrow		1.00			564
4	2.494	2.494	34800	4.541579	35361	-1.586	Narrow		1.00			563
5	2.762	2.762	17600	4.245513	17384	1.240	Narrow		1.00			564
6	3.033	3.033	8400	3.924279	8562	-1.894	Narrow		1.00			564
7	3.354	3.354	3250	3.511883	3201	1.517	Narrow		1.00			563
8	3.596	3.596	1180	3.071882	1187	-0.603	Narrow		1.00			564
9	3.704	3.704	682	2.833784	681	0.082	Narrow		1.00			564

Figure 1. Calibration curve for polystyrene standards generated using Empower 3 Software with GPC option.

Once the calibration curve is generated, the sample is processed and molecular weight distributions are calculated and displayed in a conventional Empower data table, as shown in Figure 2. Further data processing using the GPC option in Empower 3 allows users to visualize polymer data in many ways, including molecular weight distribution plots where both dwt/d(logM) and % cumulative versus the slice log MW are displayed in the same graph, shown in Figure 3. Data may be exported, or a report containing any or all of the results (including molecular weights, chromatograms, distribution plots, and calibration curves), can be generated using an existing template or a customizable report template.



	Name	Retention Time (min)	Peak Codes	Dist Name	Mn (Daltons)	Mw (Daltons)	MP (Daltons)	Mv (Daltons)	Mz (Daltons)	Mz+1 (Daltons)	Polydispersity	[n]P (dl/g)	K (dl/g)	alpha	Mz/Mw	Mz+1/Mw	Id
1	Broad	2.353			27392	49586	52575		72651	97205	1.810221				1.465142	1.960325	0
2		3.438					2348										0
3		3.493					1875										0
4		3.559					1412										0
5		3.641					953										0

Figure 2. Chromatogram of polysulfone. The molecular weight parameters such as Mw, Mn, Mz, and polydispersity were calculated from a calibration curve generated using a set of narrow polystyrene standards.

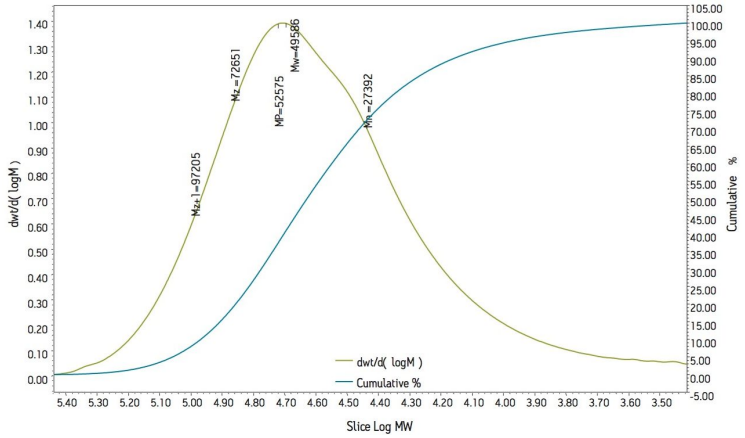


Figure 3. Molecular weight distribution plot of a polysulfone sample that was analyzed using APC XT 450Å and 125Å columns connected in series.

Conclusion

A set of narrow polystyrene standards and a polysulfone sample were rapidly analyzed using the ACQUITY APC System and processed using Empower 3 Software with GPC option. A relative calibration curve was established based on the polystyrene standard injections, and the polymer was characterized by molecular weight distributions that were automatically calculated by the software. Empower 3 Software with GPC option has proven to be straightforward yet versatile for its capabilities to calculate molecular weight distributions and automatically generate characterization data for polymer samples. Combining the vast capabilities of Empower 3 Software with the GPC option with the analysis speed and resolution of the ACQUITY APC System results in a powerful and efficient tool for the effective characterization of new and existing polymers.

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ACQUITY UPLC Refractive Index Detector

Empower 3 Chromatography Data Software

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