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Agilent WinGPC Multi-Area Evaluation

Introduction

Agilent WinGPC can be used to extract extensive information from a single polymer peak. These data include the mass distribution and the derived molecular weight averages obtained with different types of calibration such as conventional, universal, and light scattering, depending on the type of detection. The sample mass distribution can also be cut into strips to output area fractions and thus (semiquantitatively) molecular weight fractions as area percent.[1]

However, the mass distribution and the calculation of the molar mass averages always relate to the entire section of the elugram defined by the integration limits. Where there are multiple peaks or shoulders, several areas of interest must be evaluated one after the other, each delimited by the corresponding integration limits. The molar mass averages calculated based on the total area cannot provide a differentiated and meaningful picture. The multi-area evaluation tool in WinGPC can be used to divide the elugram into areas that are evaluated separately, with individual molar mass averages.[2] This technical overview describes how the elugram can be divided into up to eight areas, combining eight individual evaluations into one.

Experimental

The multi-area functionality is located in the Raw Data window menu under Options > Analysis > Multi area. First, set the baseline as usual and then select **Multi-area create**. WinGPC opens the multi-area evaluation properties window and assumes the peak limits automatically found in the elugram (Figure 1). If the measurement contains more than one (concentration) detector signal, check which signal is selected as the "active detector" in the status area in the top left. The automatic peak search or integration carried out in the elugram window is based on the minima found for the active detector. A total of eight areas can be defined using the limits entered for the start and end. These limits can be given in mL, min, or in g/mol if the X-axis is calibrated. WinGPC also allows areas to overlap. Eight evaluations can be defined, which also determines which results WinGPC should output in each case (similarly to the MWD window).

Figure 1. Multi-area evaluation properties window

Naming the areas is recommended: the user-defined designations appear both in the elugram, when the areas are drawn in, and on the printout of the results.

The evaluation usually only covers the relevant area, and so WinGPC also initializes the multi-area evaluation by default. However, several areas can also be combined in one evaluation. This step may not be useful for molar mass averages, but it is interesting for area fractions. The reference area (= 100%), to which the calculations of the area percentages are related, must be specified globally. Normally, Fl. MWD is the area of the total mass distribution defined via the integration limits in the elugram window and calculated in the MWD.

The area limits can also be drawn in the elugram, which significantly increases clarity (click the **Draw** option). With the "Auto search" option, WinGPC is enabled to search for peaks in the elugram of a new sample, applying the previously defined range limits with the flexibility specified under **Search within...**. By clicking **Save** or **Load**, recently created definitions can be made available for later (automatic) evaluations or opened for editing. **Delete** clears the entire input mask. By clicking **OK**, the elugram window is closed, and WinGPC opens an overview of the results (Figure 2).

In the top left of the results window, the detector signal for the evaluation can be selected. Just as a separate column with results is generated for each concentration detector displayed in the MWD window, the multirange evaluation produces a whole page with values for each detector. Save this overview as an ASCII report to make the results available for other programs. The results of the multi-area evaluation can be summarized and presented with the WinGPC ReportDesigner. All the necessary variables are available. The required data can also be exported directly to Excel format using a simple report.

Via the path Options > Analysis > Multi-area results, the user can return to the results window at any time. The menu item "Multi-area edit" opens the current multi-area settings for editing without updating the area definitions. If the Draw option is activated, it can be seen from the range limits drawn in the elugram window that the multi-area evaluation is active. The evaluation can be switched on and off in a controlled manner via the menu **Multi-area activate**.
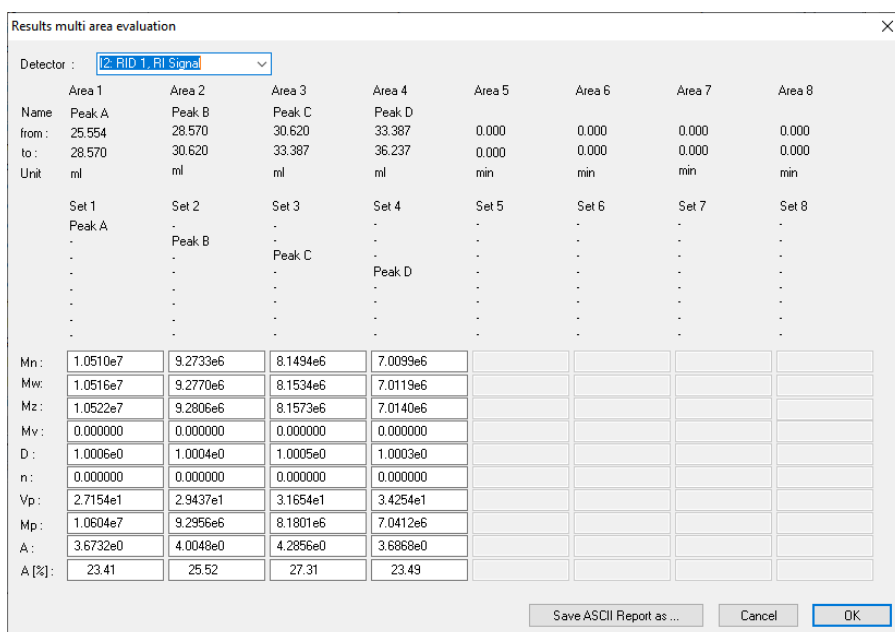
Figure 2. Multi-area evaluation results window

The multi-area evaluation is also integrated into Quick analysis: click **Options**, **Analysis**, then **Quick Analysis** in the raw data window.[3] Here, saved area definitions can be opened and applied to the sample. This means that a suitable multi-area definition can be created for a sample or a sample type beforehand, with all areas found by WinGPC. Limits can be adjusted if necessary or undesired areas removed, necessary evaluations and results can be selected, and this multi-area definition can be saved with all parameters. As part of a repeated evaluation of the same samples, this multirange evaluation can be carried out automatically.

The Auto search option in combination with Search within… is particularly effective in the context of quick analysis with previously created multi-area definitions. Slight variations in the peak position are automatically and flexibly adjusted. It is also possible to work in WinGPC HPLC mode to have peaks or peak limits determined automatically with the peak integrator, then to edit them in a targeted manner (e.g., delete, add, adjust limits…). The user can transfer the peak limits directly to the multi-area mode and continue working with them (click **Options**, **Send peak list to**, then **Multi-area evaluation** in the elugram window).[4]

Conclusion

The multi-area evaluation tool in Agilent WinGPC facilitates the assessment of elugrams with several peaks or shoulders. By making it possible to divide an elugram into eight areas for individual evaluation, this feature enables meaningful analysis of complex data.

References

1. Tips & Tricks #69, Newsletter 01/2011.

2. Appl. # 17, Newsletter 04/2001.

3. Revised Quick Analysis: Re-Processing with Agilent WinGPC. *Agilent Technologies technical overview*, publication number 5994-5945EN, **2023**.

4. Transferring HPLC Peaks into Agilent WinGPC Multi-Area Analysis. *Agilent Technologies technical overview*, publication number 5994-5941EN, **2023**.

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