INTRODUCTION

Peaks eluting from a size exclusion separation are often not completely baseline-separated, due to the inherent polydispersity of the polymer and low efficiency of the separation mechanism. Chemometrical deconvolution provides the possibility of calculating the contribution of each peak separately from the recorded spectrum. Herefore, an in house developed MATLAB script dis-criminates between the different compounds based on their difference in UV-spectrum and retention time, using the entire 3D retention time-UV spectrum. The output of the script provides the calculated chromatograms of each compound as well as their respective UV-spectrum. The latter can be used for peak identification, while quantitative calculations can be performed on the chromatographical peaks. This approach allows for overlap in both retention time as UV-spectrum, speeding up the analyses and extending the separation power of SEC separations. The applicability (both qualitative as quantitative) has been demonstrated on a mixture of three different polymer types.

RESULTS & DISCUSSION

From the overlap of the pure spectra of the three polymers (Figure 2) can be concluded that quantification of PMMA is not possible because of the spectral overlap around 226 nm. Also, the spectra of the pure polymers and the obtained calculated spectra, after deconvolution of a mixture, are depicted. Almost complete overlap confirms the power of the deconvolution method.

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CONCLUSION

• Successful baseline separated deconvolution of a mixture of three different polymers overlapping in both retention times and UV spectra.
• Good accuracy of the calculated concentrations under varying amounts of neighbouring polymers.
• Faster size exclusion chromatography (SEC)-analyses possible because overlap of retention time is allowed.
• Proof of concept of the deconvolution method and proof of applicability in the polymer analysis world.

References: