

Reach Polymer Status Analysis of Polyols

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Introduction

Polyols are alcohols with multiple hydroxyl groups. They are used for very different applications, such as, for example, in Feed and Food as sugar substitutes or in polymer chemistry as reactants to produce high quality products.

REACH (Registration, Evaluation and Authorization of Chemicals) is a European Union (EU) regulation for the production and use of chemical substances. Companies using polyols need a technical dossier to register under regulation EG No. 1907/2006.

Polymers are "special substances" in terms of REACH. However, companies have to prove that their products/educts ARE polymers. The preferred method to identify whether a

substance falls under the definition of a polymer is gel permeation chromatography (GPC).

Guidelines on the determination of the molecular weight distribution using GPC are available in the OECD TG118 (1996).

Analytical Conditions

The samples were dissolved in THF.

Eluent:	THF
Columns:	PSS SDV 5 μm 50 Å, 100 Å and 1000 Å (8 \times 300 mm) + precolumn
Calibration standards:	PSS Polystyrene
Data acquisition:	PSS WinGPC Unity 7.3
Detectors:	PSS SECcurity GPC1200 RI
Flow rate:	1.0 mL/min

Concentration: 5 g/L
Injection volume: 20 μL

Results

A polymer molecule in the sense of REACH is a molecule that contains a sequence of at least 3 monomer units (M), covalently bound to at least one other monomer unit or reactant (initiator).

This definition is equal with the so called (3M+1)-rule. Additional requirements are:

- Over 50 percent of the weight for that substance consists of polymer molecules.
- The amount of polymer molecules presenting the same molecular weight must be less than 50 weight percent of the substance.

To determine if the above stated requirements

are true, a GPC/SEC experiment using high resolution columns is performed. Figure 1 shows the elugram of a Polyol showing separation into individual R-(M)_x peaks. The results for the detailed analysis are summarized in Table 1.

Conclusion

The Polyol is a polymer in the context of REACH because:

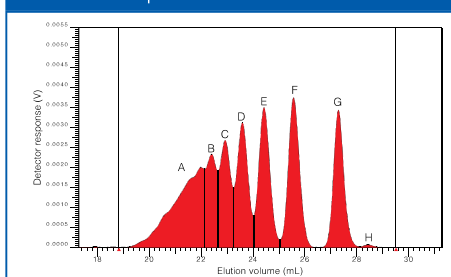
- Less than 50 weight percent of the sample is below (3M+1), the sample consists mainly of polymer molecules with $n > 3$. The (3M+1)-rule is met.
- None of the different constituents present has a concentration above 50 weight percent.

Table 1: Content and molar mass average report for a Polyol and comments to the REACH requirements.

Example polyol	Content (%)	Molar mass M_p (Da)*	Comment	Polymer
R-M Peak H	0.20	200	Less than 50% below (3M+1)	Yes
R-M-M Peak G	13.4	490		
R-M-M-M Peak F	15.7	790	(3M+1)-rule	Yes
Peak E	14.8	1090	No individual chain > 50%	Yes
Peak D	13.3	1400		
Peak C	11.0	1810		
Peak B	9.30	2190		
Peak A	22.3	2550		

* Polystyrene equivalents

Figure 1: Elugram of a Polyol sample. The column combination separates into different constituents.



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