

“Polymer Status” of Synthetic Oil Under REACH Context

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Under the registration, evaluation and authorization of chemicals (REACH) Regulations (EG) no. 1907/2006 the producer, manufacturer or importer of chemical substances/formulations have to register their products (more than 1 ton/year) at the chemical agency.

For the registration a technical dossier is required. Producer or importer of chemical substances in a quantity of more than 10 ton/year is committed to give more information about the effect of the human health and environment.

Polymers are substances in the context of REACH; however, polymers are defined in REACH under article 3, No.5, as “special” substances, based on their composition and structure.

Polymers are macromolecules that are synthesized by the reaction of an initiator (reactant) and monomers. During the polymerization process polymer chains grow with different chain length. Even if the average chain length is large there will be a fraction of either free monomer or of smaller chain lengths (oligomers). It is usually those fractions, which lead to any polymer toxicity.

Polymer Definition Under REACH

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

This definition is equal to the so called (3M+1)-rule.

- 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.

Example	Content	Comment	Polymer
R-M	10%	only 25% below (3M+1)	
R-M-M	15%		

R-M-M-M	30%	no individual chain >50%	yes
R-M-M-M-M	25%	(3M+1)-rule	yes
R-M-M-M-M-M	15%	Polymer	yes
R-M-M-M-M-M-M	5%		

R: Reactant M: Monomer

Determination of “Polymer Status”

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).

Because GPC is a relative method, a calibration is required. Mostly narrowly, linear polystyrene molar mass standards are used for calibration.

The calibration curve can be used in the determination of the molecular weight of the unknown sample if the conditions for the separation of the sample and the standards are identical.

In the instance of oligomeric compounds a high separation capacity for small molecules is essential to get oligomer-peaks separation.

From the GPC elugram it is possible to calculate the molecular weight and the molecular weight distribution of the unknown sample using the slice-by-slice method. Furthermore, the relative mass content of oligomeric species can be calculated easily to proof the polymer status under REACH context.

Figure 1: GPC elugram of synthetic oil.

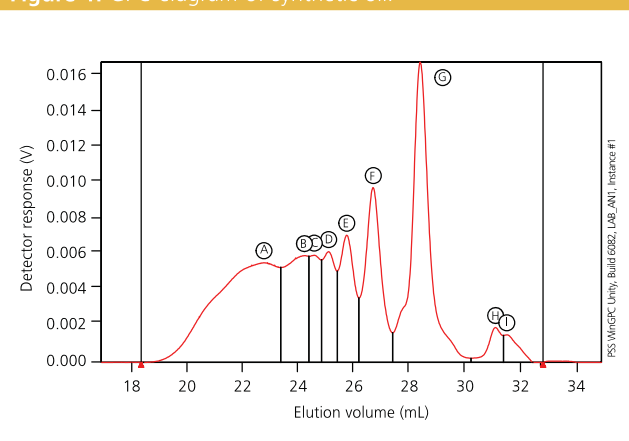
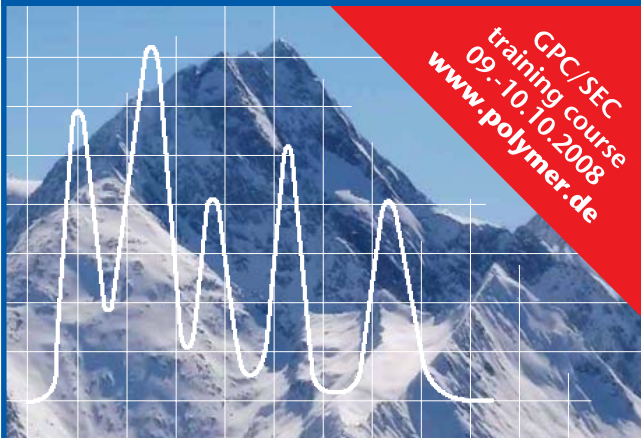


Table 1: Mass fraction of oligomers in synthetic oil.

Peak	Area (%)	Molar mass at peak-maximum, Mp (Da)	Comment	Polymer
A	28.53	17 100	(3M+1)-rule	yes
B	11.03	8340	(3M+1)-rule	yes
C	5.29	7100	(3M+1)-rule	yes
D	6.35	5630	(3M+1)-rule	yes
E	8.31	4250	(3M+1)-rule	yes
F	12.64	2850	(3M+1)-rule	yes
G	23.93	1430	(3M+1)-rule	yes

H	2.17	450		
I	1.77	378	Only 3.94% below (3M+1)	

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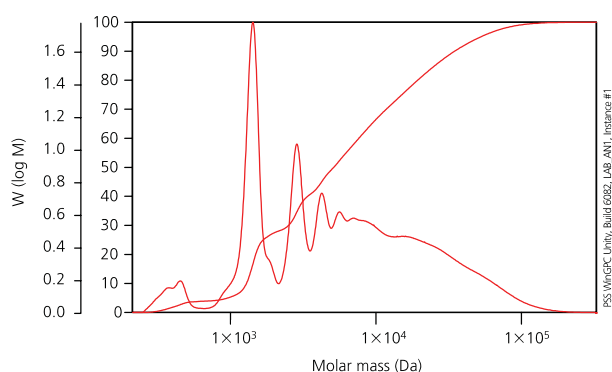
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Figure 2: Plot of the differential and integral distribution of a synthetic oil.



GPC-Conditions

SEC/GPC analysis was performed on a SECcurity GPC1200 System
Mobile phase: THF

Pre-columns: PSS-SDV, particle size 5µm, porosity 100 Å, i.d. 8 mm × 50 mm

Columns: PSS-SDV, particle size 5µm, porosity 100 Å, 1000 Å, 100000 Å, each i.d. 8 mm × 300 mm

Flow: 1 mL/min

Sample conc.: 3 g/L

Inject-volume: 20 µL

Detector: refractive index detector (RID)

Calibration: PSS polystyrene ReadyCal standards

Conclusion

The analysed synthetic oil is a polymer under REACH definition

Literature:

1. ECHA (European Chemicals Agency), Guidance for monomers and polymers, 2007.



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