Edition 1/2020

PSS STREAMLINER

Constantly Evolving Challenges In The Analytical Laboratory

Digitization, Cloud Computing, Infrastructure as a service (IaaS), Data Integrity, Traceability, Resource-efficient Analysis, Green Chemistry, Sustainability, Plastics Recycling

These are just a few of the buzzwords with which managers and technicians in the analytical laboratory deal with daily. When certain aspects, such as green solvents, become a higher priority, we initially face major changes and challenges. For example, at PSS we recently put GPC / SEC solvents to the test. The current status and our critical assessment of "green" solvents can be found on page 4.

It is undisputed, that single-use plastics and disposable packaging are a major global problem. Plastic recycling and suitability of the recycled materials for production pose new challenges. These topics therefore concern many of our customers. In the article, "Plastics Recycling from an analytical point of view" on page 2, we summarize the most important information and show how indispensable analysis of the materials is during the recycling process.

There are also major changes in the handling of digital data and results. The requirements for data security and protection against data manipulation are ever increasing. The WinGPC Data Safe can help achieve these goals, and the new WinGPC release can make laboratory work easier, as we will explore on page 5. In addition, we give an outlook on new and exciting future developments.

One of our goals at PSS is to always offer fast access to important information. Maybe you have already seen our new website, or you have already generated a quotation in our shop? If not, you can discover what's new on page 6.

We hope you enjoy reading the PSS Streamliner.

In this Issue:

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Plastic recycling

From the perspective of the analytical chemist

The triumphal march of plastics in production has many reasons. They are are inexpensive to manufacture, easily processed materials. They have low density and very specific properties. However, plastics still have a decisive disadvantage. In many cases, recycling is very difficult and impractical.

The following techniques are currently implemented in plastics recycling:

- Material recycling: Macromolecules are recovered (can be used as recyclates)
- Raw material recycling: The macromolecules are broken down into monomers (raw material recovery)
- Energy recovery: Macromolecules are burned (energy generation)

In 2017, plastic recycling comprised of 46% material recycling, 53% energy recycling and <1% raw material recycling. *

However, these 3 techniques can only be used for clean, sorted plastics.

How can sorted plastics now be classified and which plastics can be recycled?

The ASTM International Resin Identification Coding (RIC) is a classification system, which uses symbols on plastic products to indicate the original source material. This system is used in the EU as well as the US.

Table 1 gives an overview of the most important symbols and whether or not the material can be recycled.

Why are some plastics easy to recycle, others not?

Plastics consist of long chains, which can degrade due to stress (mechanical, thermal or chemical). This degradation is undesirable, since it changes the molecular weight distribution and thus also the macroscopic properties.

The chemistry of the plastic plays a crucial role in recycling. In the case of polyolefins, repeated reprocessing often leads to statistical degradation through radical formation. The chains are quickly dismantled from the center into two significantly smaller chains. However, the situation is completely different for polycondensation products, such as PET. These tend to hydrolyse from the chain end, so there is only a small, slow degradation. PET is therefore well suited for recycling, since the molar mass distribution of the starting material changes only slightly with each step and the basic properties are retained.

Can you replace virgin plastic with recycled materials?

For many manufacturers, the question now arises whether a virgin plastic can be replaced by a recyclate or whether recyclate can be added to the virgin material without a negative influence on the product properties and product quality. In order to answer this question, the molecular weight distribution of the polymer and the amount of additives have to be considered. In the case of polyolefins, it is often also worthwhile to examine their crystallinity.

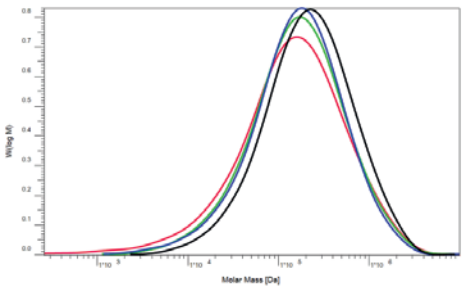

Image 1

Comparison of the molecular weight distribution of a virgin plastic ■ to plastics with varying degrees of recyclate.

- *22% recyclate content*
- *35% recyclate content*
- *61% recyclate content*

The molecular weight distribution is determined by GPC/SEC. Figure 1 shows an overlay of the molar mass distributions of new plastic, and material with differing amounts of recycled materials. A significant change in the molar mass distribution can be observed.

In close cooperation with production a maximum tolerance of recycled material can then be established. GPC/SEC, eventually in combination with other separation techniques and FTIR detection, is also a suitable method to assess the additives. The crystallinity in polyolefins can be investigated using TGIC (Temperature Gradient Interaction Chromatography).

Table 1

Symbol	Material		Comment
01 PET	PET or PETE	Polyethylene terephthalate	Largely recycled, suitable for 3D printing
02 PE-HD	PE-HD or HDPE	Polyethylene High Density	Largely recycled
03 PVC	PVC	Polyvinylchloride	In Europe partly recycled
04 PE-LD	PE-LD or LDPE	Polyethylene Low-Density	Rarely recycled
05 PP	PP	Polypropylene	Recycling possible, getting more important
06 PS	PS	Polystyrene	Hardly recycled due to cost
07 O	others	PLA, ABS, PMMA, PA, ...	Rarely recycled, ABS suitable for 3D printing

*Source: Umweltbundesamt/CONVERSIO Market & Strategy GmbH.

D. Held, P. Kilz, How GPC/SEC Can Help to Reduce PET Plastic Waste, The Column 06/2019

P. Montag, plastics recycling from the perspective of the analytical chemist, lecture at the annual symposium at the plastics institute Lüdenscheid on 05.12.2019

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Molar Mass Determination determination of Dextrans

In accordance with USP and EP requirements

Dextrans are water soluble, branched polysaccharides composed of glucose units. Among other uses, dextrans are applied as a blood plasma volume expander. The physiologic activity varies with molar mass.

Pharmaceutical applications of dextrans are only allowed when meeting specific criteria for molar mass and dispersity. The molar mass determination of dextrans has to be performed by Size Exclusion chromatography (SEC, GPC). The requirements are described in European (EP) and US Pharmacopoeias (USP). EP and USP require reporting of the weight average molar mass of the whole sample as well as the upper and lower 10% of the molar mass distribution. In addition, USP require determination of the number average molar mass (Mn) and dispersity, D.

Molar mass calibration in GPC/SEC is usually performed using narrow distributed standards. However, EP and USP regulations require calibration with specific broad distribution reference materials. In addition, a special fit function is required to describe the relation between molar mass and elution volume.

The specific demands of EP and USP on calibration and evaluation of dextrans are not implemented in commercial software packages. As a consequence, users often applied their own routines or determined dextran molar masses using methods differing from the demands of EP and USP. However, in audits, such approaches raise issues with regards to the validity of the results.

To accommodate repeated customer demands, PSS has implemented a software solution for dextran molar mass determination according to EP and/or USP. The solution includes the required calibration routines, a user friendly workflow and report templates for calibration, system suitability test and sample results.

Calibration

To calibrate the GPC/SEC system, the broad distribution standards, glucose and an exclusion limit marker are run, as stipulated by EP and USP. After selecting baselines and integration limits, the chromatograms are overlaid. (Figure 1)

The calibration parameters of the specific fit function are automatically adjusted to obtain the best agreement between the molar masses derived from the chromatograms of the reference materials and their target values. PSS WinGPC reports whether the requirements for EP/USP are fulfilled by the calibration curve. If positive the calibration curve is saved and a report is generated for documentation.

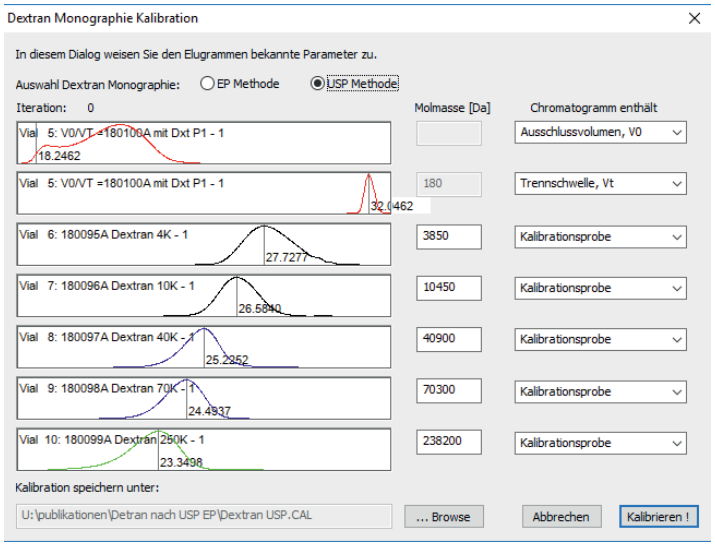

Figure 1

Product Certification Test results
based on product certification requirements as defined in USP monograph

for sample: Vial 24: Dextran 70

	Test parameter	*Allowed range*	*Test result*	*Status*
Results for detector:	*I2: RID 1, RI Signal*			
Mw	Mw range	63000 ... 77000	75368	passed
Mn	Mn range	34000 ... 48000	34720	passed
Mw/Mn	Mw/Mn range	1.4 ... 1.9	2.2	failed
Mw(high 10%)	Mw result	<= 195000	180000	passed
Mw(low10%)	Mw result	>= 13000	14700	passed
				End of Table

Figure 2

System Suitability and Sample Evaluation

After setting baselines and integration limits, system suitability samples and analyte samples are evaluated using the previously created calibration curve.

PSS WinGPC calculates the parameters required by EP or USP and compares the results to their respective acceptance criteria. Conformity or non-conformity with the requirements is automatically indicated by the status passed/failed flag in the reports. (Figure 2)

Summary

By implementing a routine into WinGPC, PSS has introduced a commercial software solution for the molar mass determination of dextrans. A user-friendly workflow allows for calibration and sample evaluation in agreement with the demands of EP and/or USP.

Specific reports are available for calibration, system suitability and samples to document conformity with these requirements. Application of the WinGPC Compliance Packs allows for data integrity and traceability in regulated environments.

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Green solvents

For organic GPC/SEC

GPC/SEC is a liquid chromatographic method which requires solvents (mobile phase) and produces waste. Water-soluble macromolecules can naturally be analyzed under relatively "green" conditions. For other macromolecules, however, organic solvents that are harmful to the environment and health are often required.

Despite the very challenging special experimental conditions that GPC/SEC requires, strategies have been implemented in the past to reduce solvent consumption.

This includes software-based solutions such as the overlapped injection in PSS WinGPC and, if necessary, utilizing smaller size particles. This enables reduction in the total number or length of the columns used.

In addition to the approaches to solvent reduction, approaches to complete substitution of certain solvents are also being pursued. Of course, it is important to remain critical, to get a comprehensive picture and to assess whether a so-called „green" solvent has any real advantages.

Table 1 summarizes possible environmentally friendly solvent alternatives that are currently being discussed. In order for these alternatives to be completely GPC/SEC-compatible, there are of course other requirements:

- A suitable stationary phase must be available for interaction-free, size-based separation
- Calibration standards for that solvent must be available
- Detection must be possible using compatible detectors

Based on these requirements, the following measures have already been implemented and tested at PSS:

✓ Since DMAc is less harmful than DMF, it is preferred for method development. The standard solvent for the PSS GRAM and PolarSil stationary was changed from DMF to DMAc to avoid using a more harmful solvent.

✓ System test conditions were developed for heptane and ethyl acetate. Both solvents are available as optional solvents for PSS SDV.

✓ For the two THF alternatives, 2-methyl-THF and ethyl acetate, PSS SDV is a suitable stationary phase. For 2-methyl-THF, PS and PMMA can be used for calibration. For ethyl acetate, only PMMA calibration standards should be used.

Certainly there are also many efforts in the laboratory for more sustainable solutions. We are happy to answer any questions and look forward to your feedback on your applications and experience.

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Table 1

Mobile Phase	possible more environmentally friendly alternatives	PSS Comment
Pentane/Hexane	Heptane	Lower health risks, ready to use
DMF/DMAc	Dimethylsulfoxide (DMSO)	DMAc less harmful than DMF, DMSO no H/P warnings, but penetration enhancer, ready to use
THF	2-Methyl THF	Obtained from renewable raw materials such as corn and bagasse
THF	2-Methoxy-2-methylpropane (MTBE)	Less miscible with water and less prone to peroxide formation
THF	Cyclopentylmethyl ether (CPME)	less peroxide formation
THF/Dichlormethane	Ethyllactate	No significant health risks, not teratogenic
THF/Dichlormethane	Ethylacetate	Lower health risks, ready to use

Typical organic GPC / SEC solvents and possible more environmentally friendly alternatives

New WinGPC solutions

Interested in the new WinGPC brochure?

Please send an email to
info@pss-polymer.com

The new WinGPC release features exciting innovations to to deal with the latest analytical challenges. These changes are highlighted in the WinGPC change control documents. Below you can find several examples of these new features.

WinGPC Data Safe

The requirements of the FDA and other authorities regarding data security and compliance are constantly growing. The aim is not only to ensure traceability, but also to prevent deliberate manipulation and attempts at deception.
The WinGPC database structure offered a high level of data security right from the start; WInGPC stores data as projects with complete sequences, rather than individual data files but are stored as complete sequences. Each start/ stop automatically creates an entry. The deletion of an entry is not allowed. This ensures the raw data remains available and untouched.

In all previous versions, it was the responsibility of the user or corporate IT to prevent the deletion of complete project databases at the Windows level.

In the current WinGPC with Compliance Pack there is now a solution to this problem. The optional WinGPC Data Safe for data storage is now available. Access to the Data Safe outside of WinGPC is no longer possible.

ChromPilot - More Waters and Shimadzu systems added

The WinGPC ChromPilot supports driver-based control of LC systems from various manufacturers. Additional components have been added for the new WinGPC release:

Waters™ ACQUITY™ APC™:
WinGPC now allows the control of isocratic and gradient systems as well as the digital and analog data acquisition of RI, UV/ PDA, fluorescence and ELS detectors. The new PSS driver supports all ACQUITY APC components as well as ACQUITY UPLC™ and ACQUITY detectors

Shimadzu™ i-Series™:
The i-Series has now been added to the previously supported components and systems. Both analog and digital data acquisition are possible.

Comprehensive 2D for high pressure systems

To support UHPLC systems in the second dimension, PSS now also offers a high pressure 2D transfer valve. Control takes place either via a PSS UDC810 or via the RC.Net driver of WinGPC. The valve can be used at a pressure of up to 1035 bar and supports up to 255 transfer injections per sample.
We would be happy to demonstrate these solutions to you on site or via a live demo on your computer.

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Aqueous ReadyCal Kits

The ReadyCals developed by PSS are very popular, and not just for environmental reasons. You save time avoiding the tedious weighing and filtering in the laboratory. The standards are ready for use immediately after adding solvents. The dextran kit adds another standard to the family of aqueous ReadyCal kits.

The Dextran ReadyCal kit contains a total of 9 standards that ranging from 180 to 298,000 Da for at least 5 calibrations in aqueous solvents or DMSO. The color-coded 1.5 mL vials are suitable for GPC/SEC systems from different manufacturers (e.g. PSS SECcurity (²), Agilent 12x0 etc,).

Other available ReadyCal calibration kits for aqueous applications are

Polyethylene glycol
PSS-pegkitr1, 3x10 vials, Mp 238 - 44 000 Da

Polyethylene glycol / Polyethylene oxide
PSS-peokitr1, 3x10 vials, Mp 238 - 969 000 Da

Pullulan
PSS-pulkitr1, 3x5 vials, Mp 180 - 708 000 Da
PSS-pulkitr1h, 3x5 Vials, Mp 180 - 1 530 000 Da

A new look

www.pss-polymer.com

Maybe you have already seen it? The PSS website has been completely revised and redesigned. Our goal was to present you comprehensive contact and information options in a clear manner.

What is new?

- Improved contact forms ensure faster and more specific response to your inquiry.
- Our chat function is available to get quick answers to simple questions.
- You can now more easily find PSS webinars and WinGPC videos on our webinar channel.

What is the same?

- Our products, application notes, and publication data can be found in the background. This means that all information is still available on a daily basis. If, for example, a new batch is released for a product, you can find the relevant information immediately on the website.
- The search in all databases and for content has also remained unchanged.

We look forward to your visit.

Figure 1

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Welcome to PSS

We are pleased to be able to introduce to you our new colleagues

Mainz

Dr. Moritz Susewind

studied chemistry at the Johannes Gutenberg University in Mainz and received his doctorate on the subject of "Molecularly controlled aggregation of nano-composite crystals". After another year as a postdoc in a group specializing in atomic force microscopy, Dr. Susewind joined PSS. He works as a specialist in the manufacture and development of polymeric spherical materials for column chromatography. He will be happy to advise you on choosing the appropriate columns for your application.

Dr. Moritz Susewind
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Mainz

Dr. Anna-Katharina Krumpfer

studied chemistry at the Johannes Gutenberg University in Mainz and did her doctorate there on the topic „Synthesis and surface properties of hydrophilic and amphiphilic poly (dimethyl siloxane) copolymers". In 2016 she joined IBM Research in Yorktown Heights, NY working in the field of photolithography for the manufacture of semiconductors and microelectronics. Dr. Krumpfer started at PSS in October 2019 in the equipment and software department. She is responsible for device installation and maintenance and will be happy to help you with technical problems.

Dr. Anna-Katharina Krumpfer
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Quotation in the PSS Shop

The PSS shop: your main source for quick information

New in the PSS web shop for columns, standards and consumables is the option to create your own quotation. This requires the free, one-time creation of a PSS web shop account. You can then create your own quotes with just a few clicks of the mouse.

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How it works:

- Open www.pss-shop.com
- If this is your first visit: select your country. If you don't already have one, create an account using „My Account".
- Place products in the „offer/ order basket" When you are finished: log in and select „create offer"
- You can then download your offer directly and share.

University discounts on columns are shown directly. We are happy to modify and extend your quotes with regard to our refill option. Please feel free to contact us.

Of course, you can still have quotes completed by PSS, especially if you are in need of advice.

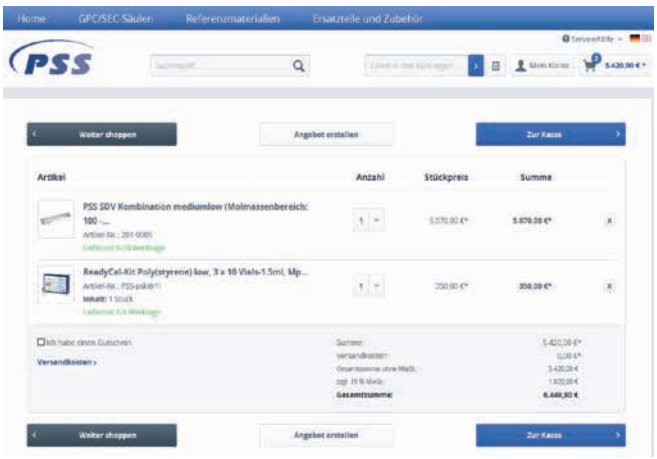

Figure 1

We are looking forward to a good cooperation!

Mainz

Tamara Pfeifer

completed her training as an office communication clerk at Schott Glas in Mainz. Mrs. Pfeifer has been responsible for order processing in Germany and the USA at PSS since April 2018 and will be happy to help you with questions about orders and deliveries.

Tamara Pfeifer

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Amherst, United States

Stephen J. Rosa

is a graduate of the University of Massachusetts (UMass) in Amherst. In 2015 he was appointed as a research assistant at the UMass Department of Polymer Science and Engineering and was involved in the synthesis and characterization of macromolecules for use in organic electronics and in flame retardant applications. He started at PSS USA in October 2019 and supports our American hardware and software customers.

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PSS Events 2020

Face-to-face training

GPC-Theory & Practice
September 28 – 29, 2020

Hands-on Training Visco/LS
June 25 – 26, 2020

User Meetings

GPC/SEC Separations
June 16, 2020
Eindhoven, The Netherlands

WinGPC Usermeeting
June 17, 2020
Eindhoven, The Netherlands

GPC/SEC Troubleshooting and SECcurity(²) Training
June 16, 2020
Eindhoven, The Netherlands

IPC course

Interaction chromatography of Polymers
June 24, 2020

Software training

WinGPC Visco/LS
September 14, 2020

WinGPC Basic training
September 15, 2020

WinGPC ChromPilot
September 16, 2020

WinGPC ReportDesigner
September 17, 2020

WinGPC Compliance Pack
September 18, 2020

Conferences/Trades Shows

October 19 – 22, 2020
Hall A1, Booth 420
Analytica, Munich

Single day booking available.
All software trainings in Mainz, Germany

On demand:
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