SUSTAINABLE POLYMERS FOR HEALTHCARE HELP ADVANCE THE CIRCULAR ECONOMY

In this article, Alexander Fix, Business Development Leader, and Hans de Brouwer, PhD, Chief Scientist, both of SABIC, provide an update on activities undertaken by the company's Specialties business to address the need for sustainable materials in the pharma world.

Sustainable materials are receiving increased attention by customers across industries. While efforts are primarily focused on food packaging, the healthcare industry is also looking for more environmentally responsible solutions. This article looks at the activities SABIC's Specialties business is undertaking in order to address the use of sustainable materials in the pharmaceutical industry.

THE PLASTIC DILEMMA

As they have for many decades, plastics support innovation in the healthcare industry and can help improve medical treatment and outcomes for patients. At the same time, plastics have received criticism due to plastic waste being discarded in the environment. A 2018 article from McKinsey and Company reported that around 260 million tonnes of plastic waste are being created every year.[1] This quantity of plastic waste is equal to the mass of around 26,000 Eiffel Towers.[2]

Only 16% of plastic waste is collected for recycling.[1] Eight million metric tons of plastic escape into the oceans every year, as reported in National Geographic.[3] A study from McKinsey and the Ocean Conservancy shows that land-based plastic waste ending up in the oceans will reach up to 20 million metric tons by 2030 if necessary corrective actions are not taken.[4] Beverage bottles, caps and lids are among the top single-use items found on ocean shores.[5]

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Next to these waste problems, production, processing and incineration of plastics generate carbon dioxide (CO_2) contributing to increased climate change.

CHEMICAL UPCYCLING OF PLASTIC WASTE

How can polymer technology continue to drive innovation in the medical industry while helping to create meaningful uses for plastic waste and reduce CO_2 emissions?

One answer is chemically upcycled polybutylene terephthalate (PBT) resin that

Alexander Fix
Business Development Manager
T: +49 174 3079133
E: alexander.fix@sabic.com

Dr ir Hans de Brouwer
Chief Scientist Healthcare
T: +31 164 292149
E: hans.debrouwer@sabic.com

SABIC
Plasticslaan 1
4612 PX
Bergen op Zoom
The Netherlands

www.sabic.com

is synthesised from single-use polyethylene terephthalate (PET) bottles. This solution is created by reusing post-consumer plastic waste to produce a drop-in replacement for virgin PBT, which avoids the need to consume fossil-based feedstocks to produce more virgin resin. This approach can help support the reduction of CO_2 emissions, plastic waste, energy demand and water consumption, according to a Lifecycle Assessment study completed by SABIC in 2020.[6] The study featured a comparison with virgin PBT produced with the terephthalic acid process.

MAKING PBT MORE SUSTAINABLE

PBT is an engineering plastic that is often used in the healthcare industry. It processes more predictably than PET and, being a semi-crystalline resin, offers excellent chemical resistance. PBT is made from 1,4-butanediol and either terephthalic acid or dimethyl terephthalate building blocks. These monomers are derived from crude oil – a fossil-based, non-renewable resource – through several intermediate steps. At each step, purification takes place, resulting in a well-defined polymer product.

Efforts to replace both the diol monomer and the diacid monomer with alternatives that are more sustainable, such as bio-sourced components, typically lead to polymers with different processing behaviour and material performance. Even small structural changes to either monomer can have large effects on processing, crystallisation behaviour and material performance. The resulting polymer may be interesting on its own, but it is never a drop-in solution for an existing application.

> "SABIC is using its chemical upcycling technology to produce PBT from post-consumer PET. Rather than mixing molten recycled PET into a new plastic, SABIC uses PET as a feedstock in a chemical process that deconstructs the material down to its basic building blocks."

Figure 1: Approximately 67 0.5 L PET bottles go into each kilogram of virgin-quality LNP™ ELCRIN™ iQ engineering resin.

Performance changes can also occur when mechanically recycled plastics are mixed with new material. First, the composition of most mechanically recycled plastics from post-consumer sources shows greater variation compared with non-recycled plastics. Mechanically recycled plastic may also be a mixture of different types of plastic and contain traces of its first life: colourants, stabilisers, flame retardants and the like. Some of these components are unacceptable in healthcare-grade plastics. They can restrict colour options and affect food contact compliance and biocompatibility.

UPCYCLING PET TO HIGHER-VALUE PBT

To help address this challenge, SABIC is using its chemical upcycling technology to produce PBT from post-consumer PET. Rather than mixing molten recycled PET into a new plastic, SABIC uses PET as a feedstock in a chemical process that deconstructs the material down to its basic building blocks. These building blocks are then purified with similar rigor as chemicals coming from a fossil source, before being fed into the polymerisation process to prepare PBT resin. SABIC's process uses dissolved monomers and oligomers from PET and adds fossil-based 1,4-butanediol to produce LNP™ ELCRIN™ iQ resin (PBT).

This upcycling process converts commodity plastic waste into virgin-quality engineering resin (approximately 67 0.5 L PET bottles – see Figure 1 – go into each kilogram) at reduced CO_2 emission levels compared with the production of virgin resin. Not only does 60% of the material originate from the waste stream, but this resin's performance is equivalent to that of traditional PBT resin. In addition, PBT may be used for more-durable applications than PET, such as medical device housings. In this way, upcycling can extend the lifespan of PET beyond its original application in disposable water bottles.

As shown in Figure 2, the upcycled PBT reduces global warming impact by 29%, has 43% less cumulative energy demand and consumes 15% less water compared with virgin PBT. All these values contribute to an improved environmental footprint.[6]

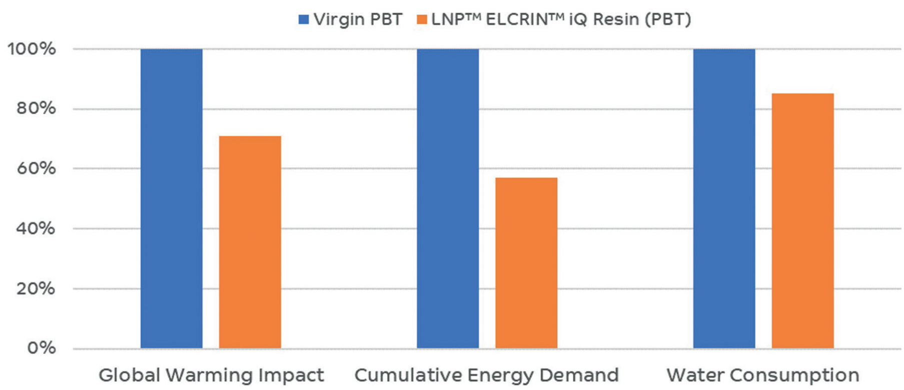

Figure 2: Comparison of resin cradle-to-gate footprint data.[6]

MATERIAL PROPERTIES FOR HEALTHCARE APPLICATIONS

The medical industry typically requires healthcare-grade materials to meet specific criteria, such as biocompatibility pre-assessment; management of change; plant and formulation lock; long-term supply guarantee; and production according to good manufacturing practices (GMPs). Further, each end application has its own set of material requirements.

Technical datasheets provide many of the important properties of a material: mechanical performance, electrical properties, rheological parameters and heat resistance, for instance. The properties of the upcycled PBT material are similar to those of a standard, unfilled PBT of comparable viscosity. Table 1 compares key properties of a representative grade for the upcycled PBT, LNP ELCRIN W1000JiQ resin, with those of a reference PBT material, SABIC's VALOX™ HX260HPR resin. This comparison reveals the strong similarities between the two materials. Even a parameter such as mould shrinkage, which is sensitive to small material differences, was identical (1.2%) in a side-by-side comparison on a tensile part specimen.

Environmental stress cracking resistance (ESCR) was tested using PDI's (NJ, US) Sani-Cloth® AF3 Germicidal Disposable Wipes, which include one of the strongest chemicals used on medical devices, as well as Banana Boat® Sunscreen lotion (Edgewell Personal Care, CT, US), which represents an aggressive skin contact situation. The tests featured tensile bars in continuous contact with these chemicals under 1% strain at room temperature for seven days. Table 2 shows that both materials performed very well against these harsh chemicals. A positive rating (+) in this table indicates over 90% retention of yield strength and 80–140% retention of elongation after exposure, indicating no significant change.

		LNP™ ELCRIN™ W1000JiQ resin	VALOX™ HX260HPR resin	Test Method
Tensile modulus	MPa	2450	2400	ISO 527
Stress at Yield	MPa	54	54	ISO 527
Stress at Break	MPa	25	28	ISO 527
Strain at Yield	%	3.3	3.5	ISO 527
Strain at Break	%	93	84	ISO 527
Impact Strength (23C)	kJ/m²	5	5	ISO 180/1A
Impact Strength (-30C)	kJ/m²	5	5	ISO 180/1A
Vicat softening temp.	°C	165	170	ISO 306, 50N
Heat deflection temp.	°C	122	123	ISO 75 0.45MPa
Heat deflection temp.	°C	52	54	ISO 75 1.8MPa
Mould shrinkage parallel	%	1.2	1.2	SABIC method

Table 1: Mechanical performance comparison.

Retention of:	LNP™ ELCRIN™ W1000JiQ resin		VALOX™ HX260HPR resin	
	Yield Strength	Elongation at break	Yield Strength	Elongation at break
PDI Sani-Cloth® AF3	+	+	+	+
Banana Boat® Sunscreen	+	+	+	+

Table 2: ESCR testing results.

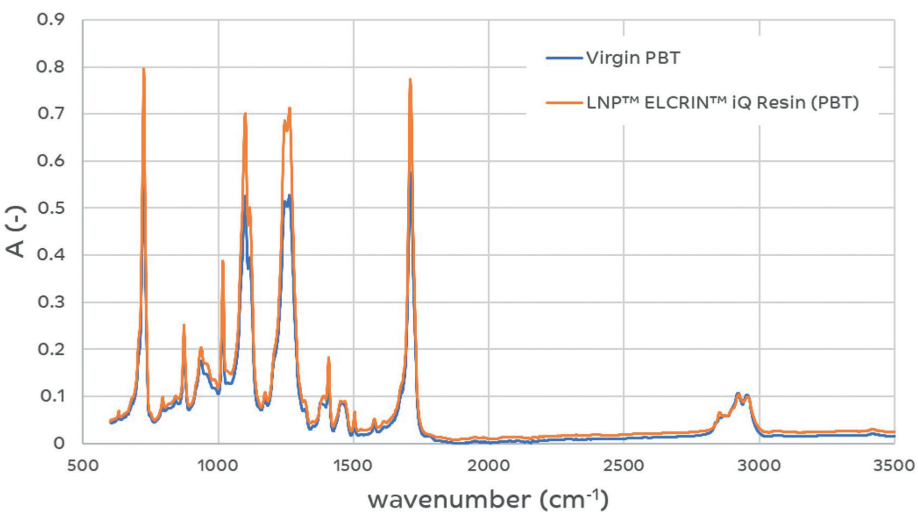

Figure 3: Infrared spectra of the two types of PBT indicate no structural differences. Peaks are the same in both samples.

ANALYSING TWO PBT MATERIALS

However, there is much more to a material than what is shown on a datasheet. Analytical techniques allow us to collect additional information, down to a material's molecular level. Infrared spectroscopy detects molecular vibrations and is often used for fingerprinting purposes: it can determine if materials are the same without interpreting and labelling every individual peak in the spectrum.

The infrared spectra overlay graph (Figure 3) shows matching fingerprints for the standard PBT and the upcycled PBT materials, indicating no significant difference between the two.

Other analytical techniques allow us to study extractables. These components can potentially migrate out of a material under extreme conditions. Extractables depend, not only on the type of polymer, but also on the quality of the raw materials used to build the molecules and the specifics of the chemical process. We studied both volatile and nonvolatile organic components and ran an elemental analysis with a focus on metals.

The elemental analysis was conducted using inductively coupled plasma mass spectrometry (ICP-MS) on an acidic liquid extract that had been in contact with the polymer material for three hours. This mimics a worst-case scenario as metal ions are typically extracted more actively under such conditions than in a pH-neutral aqueous environment. Of the 39 elements analysed, 34 were not detected above their individual quantification limits or the 0.010 ppm reporting limit.* Quantified elements, which are listed in Table 3, are low levels of common elements of no particular concern. In this particular data set, the levels of these elements in the upcycled PBT are lower than those in the virgin PBT.**

Volatile organic components (VOCs) were measured by analysing the gas emitted from a sample kept at 150°C for 45 minutes using gas chromatography with time-of-flight mass spectroscopy (GCMS). Under these extreme conditions, tetrahydrofuran (THF) was detected in both samples (Table 3). THF is a known by-product of PBT synthesis. In a polymerisation with terephthalic acid (virgin PBT), it is present at higher levels than in the chemically upcycled PBT, which is formed from transesterification, consistent with the literature.[7]

Further, ethanol was used to extract organic components from the samples at 70°C for 24 hours. The extracts were analysed for semi-volatiles with liquid chromatography coupled to a quadrupole mass spectrometer (LCMS), and for volatiles using GCMS. Quantification was executed using an internal standard. Both techniques revealed the presence of short cyclic polymer chains of PBT (Figure 4, Table 3).

These molecules are an integral part of the PBT molecular weight distribution. During the polymerisation process, all molecules pass through the stage of short chain oligomers. Molecules that happen to react with themselves form cyclic structures that stop growing due to the absence of a reactive chain end (either a carboxylic group or a hydroxyl group). As such, their presence is to be expected. The process to form LNP ELCRIN iQ resin results in fewer of these structures than the virgin PBT process in the current comparison. Neither sample showed any unidentified components. In a similar extract using hexane, lower levels of the same components were found.

DROP-IN SOLUTION FOR TRADITIONAL PBT

All snowflakes appear the same but none are identical. The same is true of plastics. It all depends on how deeply they are evaluated. This study was not restricted to a high-level comparison of macroscopic properties for upcycled and traditional PBT. It looked closely at the subtle differences between SABIC's sustainability driven PBT material and the oil-derived commodity product. Importantly, there were no significant differences between the two products: the same components were observed, and a quantitative comparison confirmed the cleanliness of the upcycled PBT product.

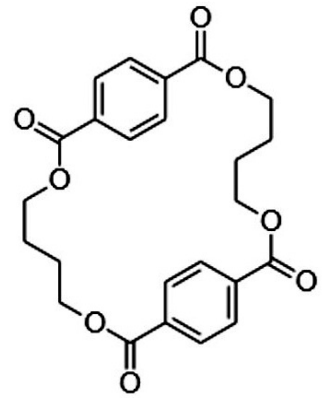

Figure 4: Structural formula of cyclic PBT dimer.

This analysis indicates that LNP ELCRIN W1000JiQ resin can be considered a more-sustainable, drop-in replacement for traditional PBT in many healthcare applications. This material also features formulation lock, US FDA food contact compliance and a stringent management of change process – and is produced according to GMPs.

Element	LNP™ ELCRIN™ W1000JiQ resin (ppm)	VALOX™ HX260HPR resin (ppm)	Method
Sodium (Na)	0.19	0.50	Elemental analysis, ICP-MS
Magnesium (Mg)	0.07	0.14	Elemental analysis, ICP-MS
Sulphur (S)	< 0.02	0.05	Elemental analysis, ICP-MS
Potassium (K)	0.07	0.25	Elemental analysis, ICP-MS
Calcium (Ca)	0.40	0.60	Elemental analysis, ICP-MS
THF	4.9	36.8	headspace, GCMS
cyclic PBT dimer	<0.1	12.0	ethanol extract, GCMS
cyclic PBT dimer	3.2	12.0	ethanol extract, LCMS
cyclic PBT trimer	0.7	2.2	ethanol extract, LCMS
cyclic PBT tetramer	<0.1	0.1	ethanol extract, LCMS

Table 3: Results from elemental analysis.

** Not detected above quantification or reporting limit: Li, Be, B, Al, P, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ge, As, Se, Sr, Zr, Nb, Mo, Ag , Cd, Sn, Sb, Cs, Ba, La, Ce, Hf, W, Hg, Tl, Pb*

*** Please note that even though the data in this document have been generated with the utmost care and most analyses have been executed in duplicate, the sample set is restricted to a single representative sample of LNP ELCRIN W1000JiQ PBT resin and VALOX HX260HPR PBT resin. It does not include statistical analyses of multiple lots, nor does it provide a complete picture of all available virgin PBT materials. Hence, a customer should always independently assess suitability of the material for the intended application.*

ABOUT THE COMPANY

SABIC is a global diversified chemicals company, headquartered in Riyadh, Saudi Arabia. SABIC manufactures on a global scale in the Americas, Europe, the Middle East and Asia Pacific, making distinctly different kinds of products: chemicals, commodity and high-performance plastics, agri-nutrients and metals.

SABIC supports its customers by identifying and developing opportunities in key end-use applications such as construction, medical devices, packaging, agri-nutrients, electrical and electronics, transportation and clean energy. Production in 2019 was 72.6 million tonnes.

SABIC has more than 33,000 employees worldwide and operates in around 50 countries. Fostering innovation and a spirit of ingenuity, SABIC has 12,540 global patent filings, and has significant research resources with innovation hubs in five key geographies – US, Europe, the Middle East, South Asia and North Asia.

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ABOUT THE AUTHORS

Alexander Fix is a business development leader for healthcare for SABIC's Specialties business. He has been with SABIC for five years and has held different roles in account management and marketing in the healthcare industry. As a business development leader, Mr Fix focuses on the advancement of material solutions for drug delivery devices and works closely with customers to provide technical application development support. He holds a diploma in business administration from AKAD Private University of Applied Sciences in Stuttgart, Germany.

Dr ir Hans de Brouwer is Chief Scientist Healthcare for SABIC's Specialties business, developing products to meet the future needs of the healthcare industry. He has 20 years of experience in a range of technical roles including the development of plastics for the healthcare, telecom, lighting and automotive markets and execution of continuous improvement projects in production and technology. Dr de Brouwer holds an engineering degree in chemical technology and a doctorate in polymer chemistry from Eindhoven University of Technology (the Netherlands) and is a certified Six Sigma Black Belt.

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INNOVATION FOR PATIENT SAFETY

SABIC's healthcare business is driven by our passion to support our customers and improve patient experiences and outcomes.

Leveraging our global capabilities and creating new collaborations, we develop advanced materials and technologies that help drive innovation for the next generation of medical devices.