Case study
January 28, 2021

Improving the Performance and Sustainability of PET

Incorporating isosorbide to develop eco-friendly polyesters with exciting potential for hot fill and cosmetic packaging

As a copolyester, polyethylene terephthalate (PET) lends itself to the incorporation of alternative comonomers to access modified performance profiles. Isosorbide is a plant starch-derived bicyclic diol with considerable potential for this application. Isosorbide manufactured on an industrial scale (POLYSORB®, Roquette - Lestrem, France) has a carbon footprint of just 0.09 kg CO_2/kg* of product and the ability to enhance the performance of PET in areas of recognized weakness. In this article we discuss how SK chemicals (Seongnam-si, South Korea) a global leader in the field of eco-friendly materials, has capitalized on the potential of isosorbide to commercialize new polymers (ECOZEN®) that deliver high performance in areas where PET has limitations.

Introducing isosorbide

"Isosorbide is a really versatile, safe, environmentally benign performance chemical with great potential as a co-monomer," said Bruno Plancke (Head of Global BU Industry, Roquette). "Now that a reliable, high purity industrial-scale supply of POLYSORB® *isosorbide is in place, polymer manufacturers are free to exploit its full potential. Incorporation into PET is already demonstrating proven value."*

Isosorbide is produced from annually renewable plant feedstocks by a process of sequential hydrolysis and hydrogenation. Hydrolysis converts plant starches to glucose which are subsequently converted to sorbitol; the hydrogenation of sorbitol to isosorbide is the final step (see figure 1).

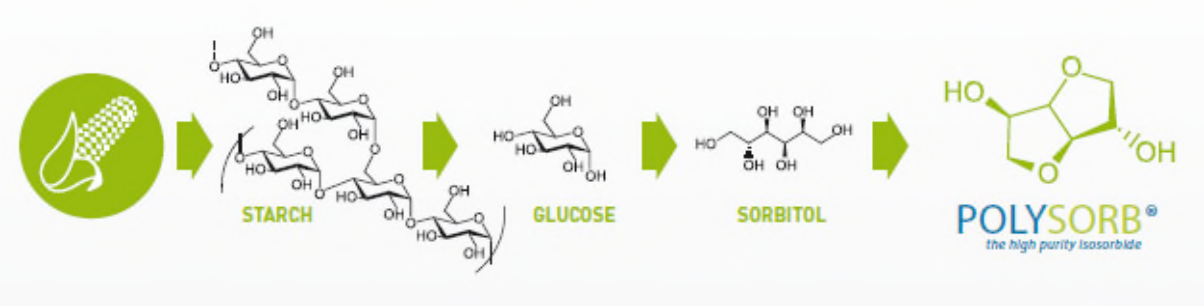


Figure 1: Isosorbide is produced from renewable plant feedstocks by a processs involving hydrolysis and hydrogenation.

Isosorbide production technology has been optimized over the last two decades, to minimize carbon footprint and deliver consistently high purity, in excess of 99.5%. The resulting product is completely safe, REACH compliant, non-toxic, non-endocrine disrupting, suitable for food contact, and compatible with cosmetic and pharmaceutical requirements.

These credentials make isosorbide a valuable feedstock for multiple applications [1], but its potential as a substitute diol in the production of PET, a copolyester of ethylene glycol and terephthalic acid, is especially promising. Ethylene glycol is still predominantly a petrochemical feedstock so (partial) substitution is potentially appealing from the perspective of environmental impact. More importantly, incorporating isosorbide beneficially modifies the properties of PET, improving its glass transition temperature *(T_g)*, for example, and the optical properties of finished packaging.

Improving thermal properties for hot fill applications

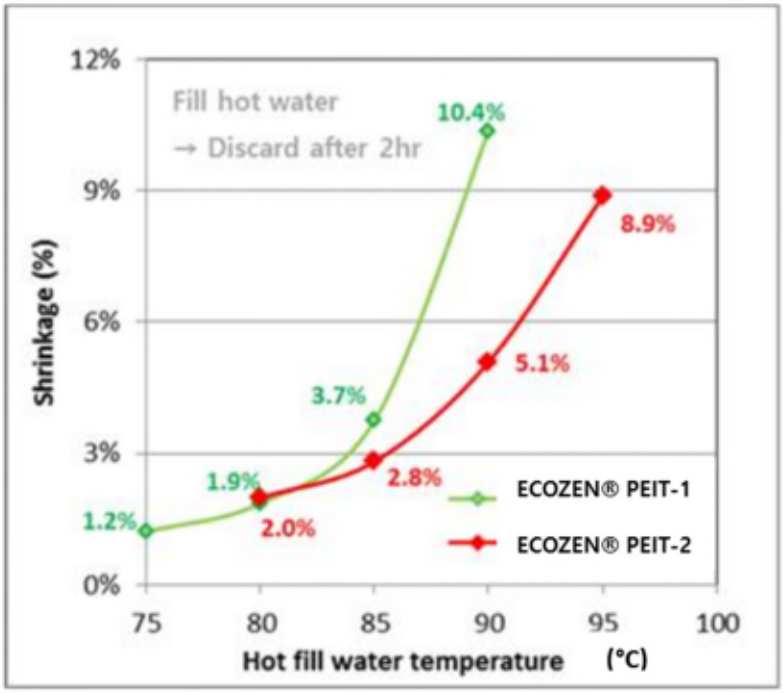
"We've found that incorporating isosorbide can help PET to perform perfectly in areas where it currently fails," said Eung-Soo Kim (Head of Copolyester business, SK chemicals). "Hot fill for food and beverage is a primary example. Isosorbide is highly effective at increasing T_g and allows us to produce a stretchable, transparent, heat-resistant plastic that can be directly substituted into existing blow molding processes."

SK chemicals has developed a range of poly(ethylene-co-isosorbide) terephthalate (PEIT) polymers tailored to the requirements of hot-fill applications. Semi-crystalline and offering high thermal stability, these polymers have a glass transition temperature of 90 or 95°C, depending on grade, which compares favorably with that of PET (70°C) and PETG (70 – 80°C, where PETG is a class of PET incorporating alternative glycols such as cyclohexanedimethanol (CHDM)) .

Property	**Overall stretch ratio**	**X10**	**X6**
	Tg	90	95
Application suitability	Aerosol container (IBM/ISBM)	***high***	-
	Hot fill (IBM/ISBM)	***high***	***high***
	Heat resistant bi-oriented film	***high***	***moderate***
	Injection	***moderate***	***high***

Table 1: A summary of the properties and application of PEIT grades developed for hot fill applications

The intrinsic viscosity (IV) of the new polymers compares with a range of 0.6 to 0.85 for PET, depending on application; PET for bottles typically has an IV of around 0.73 to 0.80 [2]. IV is indicative of the flow properties of the molten polymer so these values suggest that the new polymers will work efficiently in existing manufacturing processes; stretch ratios are also comparable with PET. All the new grades are suitable for use with food in accordance with EU 10/2011 [3].



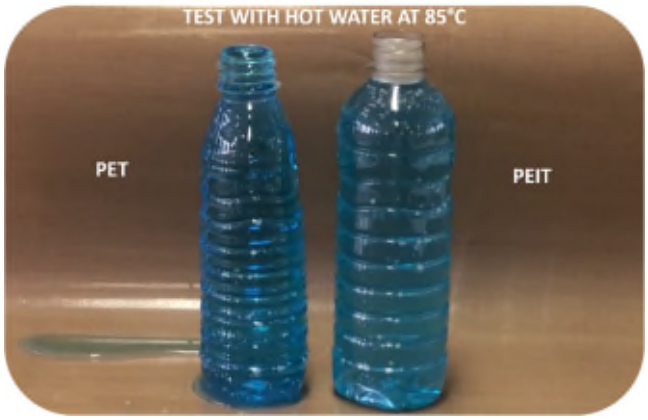


Figure 2: PEIT grades exhibit much less shrinkage than PET when subjected to temperatures comparable to those associated with hot fill.

Figure 2 shows shrinkage data relevant to the use of PEIT to produce packaging for hot fill applications. This test involves filling a bottle with hot water (75 – 90°C), allowing it to stand for 2 hours, and then measuring any change in volume, as the water is discarded. The results for both

grades demonstrate substantially enhanced performance relative to PET which exhibits shrinkage of 7% at 85°C rising to 28% at 90°C. This is an important gain for hot fill applications. Furthermore, bottles made with the new polymers have a burst pressure of 27 bar – most applications require 20 bar maximum – and exhibit good color and transparency.

These and other tests confirm the suitability of these new polymers as a packaging material for hot fill applications and they are already in commercial use. For example, Morning Recovery (More Labs, Los Angeles, USA), a blend of electrolytes and other ingredients for rehydration and replenishment, now uses a PEIT-based polymer in place of glass for export applications. Produced in an established injection molding line the resulting packaging is lightweight and hot filled at 85°C to confer good shelf-life.

Improving transparency, colour and chemical resistance for cosmetic packaging

"We also see great potential for incorporating isosorbide to improve the properties of PET for cosmetic packaging ," said Eung-soo Kim (Head of Copolyester business, SK Chemicals). "We've developed several grades for this application that combine excellent optical properties, good chemical resistance and the high flowability required for easy injection molding."

The low isosorbide PEIT grades that SK chemicals has developed enable the manufacture of light, clear, glossy packaging for demanding cosmetic applications. Figure 3 shows how color and transparency compares with competing materials, for a 6mm thick sample. Col L is a metric used to define clarity or transparency on a scale from 0 (black) to 100 (perfectly transparent) while Col-a and Col-b relate to colour, green-red and blue-yellow respectively. The results show the superior transparency of the new polymer which is also very close to being completely colourless. A Col-b score of 0.2 (Competitor B) is indicative of yellowing with the higher 0.6 score (Competitor A) producing a clearly visible tinge.

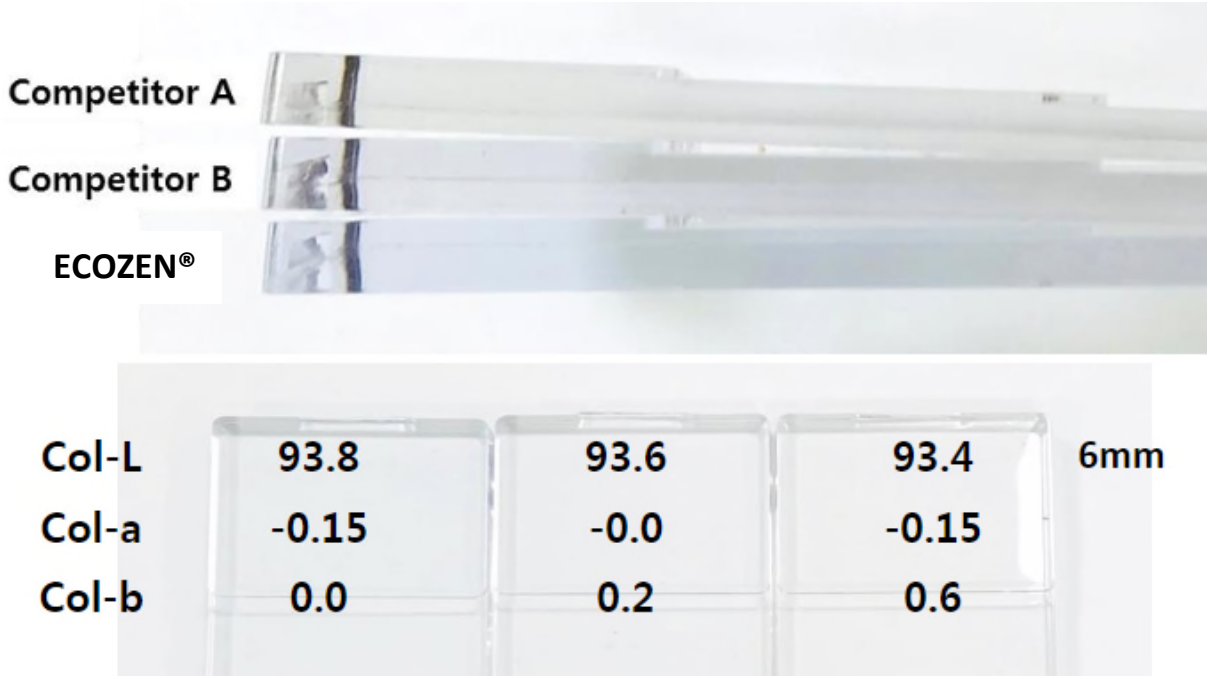


Figure 3: PEIT grades containing low levels of isosorbide produce clear, transparent, almost colourless samples making them highly suitable for high quality cosmetic packaging.

The chemical resistance of the new polymers has also been assessed, for multiple products. For example, sunblock was applied to polymer samples subject to 1% curvature, held at 50°C for 24 hours, to assess environmental stress cracking. The PEIT showed no evidence of deterioration while alternative PET samples, incorporating comonomers such as CHDM, either cracked or broke. Figure 4 shows the results of testing resistance to perfume (exposure for 72 hours @50°C). Here too, the PEIT (right hand sample) exhibits excellent performance, retaining clarity, while alternative grades developed a haze.

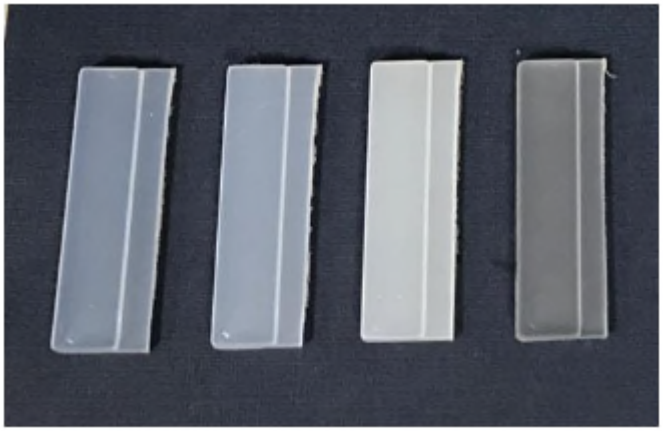


Figure 4: PEIT (right hand sample) exhibits superior resistance to perfume with no evidence of haze, unlike competing polymer samples.

These new polymers have semi-crystalline properties but perform well across a wide processing window, exhibiting slow crystallization rates during processing. This means flexibility with respect to mold temperature and makes it possible to produce parts up to 8mm with relative ease and no hazing. Taken together this suite of attributes makes the new PEIT grades a versatile and highly competitive solution for high quality cosmetic packaging.

Polymers for the future: the importance of re-use and recycling.

Polymer use is coming under increasing scrutiny as countries work towards the realisation of the Sustainability Development Goals advanced by the UN in 2015. In the EU, for example, the target is to make all polymer packaging recyclable by 2030[4]. Furthermore, there are initiatives in place to encourage the use of recycled polymers, with Post Consumer Recycle (PCR) material an increasingly important consideration for polymer manufacturers.

The new polymers developed by SK chemicals sit easily within the developing Circular Economy. Completely compatible and miscible with PET, they carry resin identification code 1 (RIC 1), the code reserved for PET. This means that after use the polymers can be disposed of and reused/recycled via existing PET-handling channels. Furthermore, tests show that the inclusion of PEIT in a blend with PET enhances properties, an encouraging result for the use of PCR materials.

In conclusion

With a secure, high purity, industrial-scale supply of isosorbide now in place at Roquette, polymer manufacturers are free to exploit the potential of this plant-based performance chemical as a comonomer. SK chemicals has already done just that. New PEIT grades optimized for specific applications such as hot fill and cosmetic packaging illustrate how incoporating isosorbide can address the widely recognized limitations of PET, producing valuable polymers that fit easily into established recycling and re-use channels.

**Internal comparative study based on life cycle analysis methodology, peer-reviewed by an external auditor.*

References:

[1] D. Saxon et al. “Next Generation Polymers: Isosorbide as a Renewable Alternative.” Progress in Polymer Science 101 (2020) 101196

[2] F. Awaja et al. “Recycling of PET”. European Polymer Journal 41 (7): 1453-1477

[3] Commission Regulation (EU) No 10/2011 of 14 January 2011 on plastic materials and articles intended to come into contact with food.

[4] A European Strategy for Polymers in a Circular Economy. Available to view at:

https://ec.europa.eu/environment/circular-economy/pdf/plastics-strategy-brochure.pdf

For more information:

About Roquette's Performance Materials :

Roquette's Performance Materials provides various ingredients from 100% biomass feedstock to serve brand owners and consumers. In the global development of plant-based chemistry, Roquette offers the industrial markets new, innovative and sustainable monomers to create solutions for safer and more sustainable polymers used in packaging, automotive, CASE, sports and leisure.

⇨ *For more information, visit our website or contact : jiae.kim@roquette.com*

About Roquette: "Offering the best of nature"

Roquette is a global leader in plant-based ingredients, a pioneer of plant proteins and a leading provider of pharmaceutical excipients. In collaboration with its customers and partners, the group addresses current and future societal challenges by unlocking the potential of nature to offer the best ingredients for food, nutrition and health markets.

These ingredients respond to unique and essential needs, enable healthier lifestyles and are critical components of life-saving medicines.

Thanks to a constant drive for innovation and a long-term vision, the group is committed to improving the well-being of millions of people all over the world while taking care of resources and territories.

Roquette currently operates in over 100 countries, has a turnover of around 3.7 billion euros and employs 8,670 people worldwide.

About SK chemicals' Copolyester

SK chemicals' copolyester products can replace diverse plastic materials including PC, PVC, PMMA and PS. The safety of our BPAfree products also enables the products to cover various applications encompassing containers for food we eat and cases for cosmetics we touch.

About SK chemicals : "We care for the future, healthcare, earthcare."

SK chemicals' mission statement says, "We enhance human health and protect the Earth's environment" and we have reorganized our business structure to focus on the two large sectors of green chemicals and life sciences.

Providing distinguished chemical and life sciences products and solutions based on the world's highest technology standards, SK chemicals is recognized as a leading global company of environmentally-friendly materials and total healthcare solutions.

Our green chemical business is steadily progressing as a leading global company in the environment friendly materials business by using the world's best technology, knowledge, and production facilities. To achieve this goal, SK chemicals has selected four new core areas of business: bio-materials, composites, high-performance materials, and energy saving materials while continuing a commitment to R&D activities.

Our life sciences business, dominated by pharmaceuticals and bio, is anchored by the comprehensive healthcare solutions that cover patient care from diagnosis to treatment and prevention. The creation of new medicines is bolstering our global position.