Date: October 29, 2021

Using isosorbide to make sustainable polycarbonates with excellent mechanical and optical properties.

Polycarbonates are highly prized as engineering plastics, combining transparency and other optical benefits with excellent mechanical and thermal properties. These characteristics support broad application in the manufacture of, for example, food and beverage containers, optical displays, protective shields and lenses. However, conventional polycarbonate production is based on bisphenol A (BPA), a petrochemical feedstock known to be an endocrine disrupter, with potential to cause reproductive, developmental, and other health issues[1]. BPA-free polycarbonates are therefore highly desirable.

Isosorbide is a bio-based diol that can be used in place of BPA to eliminate health concerns and synthesize more sustainable polycarbonates. At the same time, isosorbide-based polycarbonates demonstrate significantly improved properties relative to conventional analogues. In this article we introduce POLYSORB® from Roquette, a commercial 100% bio-based isosorbide of exemplary quality, and explore its exciting potential for polycarbonate production.

Switching to isosorbide for polycarbonate production

Isosorbide is a plant derived monomer, increasingly recognised as a core biochemical building block. Roquette (Lestrem, France) is the global leader in isosorbide production and supply, and operates the world's first industrial scale plant, manufacturing POLYSORB®, a high purity, highly stable isosorbide in a range of grades. POLYSORB® PSA, which is supplied in the form of white pellets that dissolve to form a solution with a pH in the range 8.0 – 9.5, is especially suitable for polycarbonate production.

Roquette produces POLYSORB® by hydrolysing plant-based starches from annually renewable feedstocks to glucose, which is then converted to sorbitol (see below). The hydrogenation of sorbitol is the final step. By rigorously refining and optimizing this process, the carbon footprint of the product has been reduced to just 0.09 kg CO_2/kg of product.* Sustainable, non-toxic/non-carcinogenic and REACH compliant, POLYSORB® is a highly desirable biomonomer/feedstock from the perspective of environmental impact.

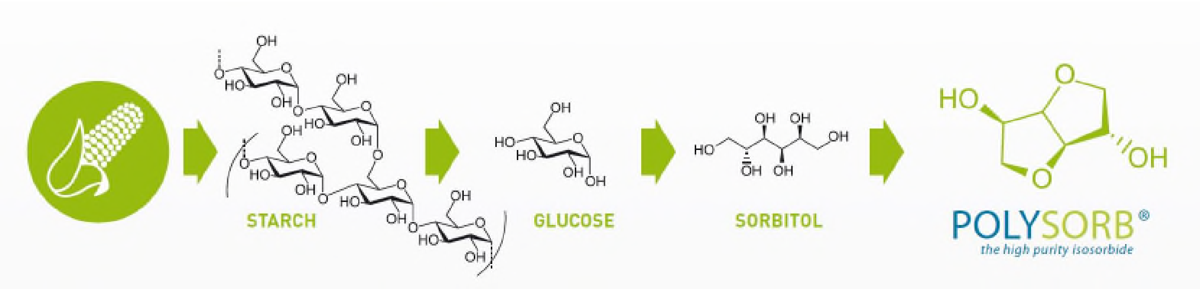


Figure 1: Roquette produces POLYSORB®, a high purity isosorbide at an industrial scale from annually renewable plant-based feedstocks.

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

Switching to isosorbide directly addresses the health concern that has led to the banning of BPA for the manufacture of products such as baby bottles, which is its endocrine-disrupting properties, i.e. its impact on hormone-regulated processes[2,3]. Substituting other bisphenols is an alternative strategy but some argue that this risks exposure to less extensively tested chemicals likely to have similar properties and that minimising the use of bisphenols, as a chemical class, is preferable[3].

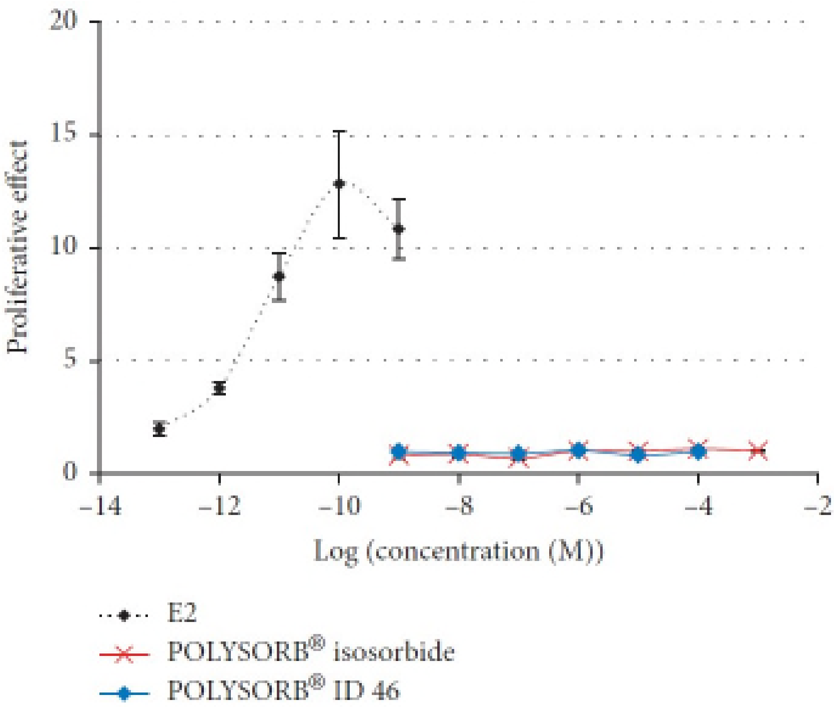


Figure 2: E-screen assay data provide evidence of the safety of POLYSORB® with respect to endocrine activity. [Note POLYSORB® ID 46 is an isosorbide diester used as a plasticizer which was also included in the tests][4]

Figure 2 shows data from an E-screen assay assessing the estrogenic activity of POLYSORB®[4]. The results are part of a wider study investigating the estrogenic, androgenic and steroidogenesis disrupting properties of POLYSORB® via a battery of *in vitro* tests and provide evidence of its saftey with respect to endocrine activity.

Polycarbonates are conventionally synthesized via the condensation polymerization of BPA with either carbonyl chloride or diphenyl carbonate. Like BPA, isosorbide is a diol and direct substitution produces polycarbonates as illustrated in the schematic below:

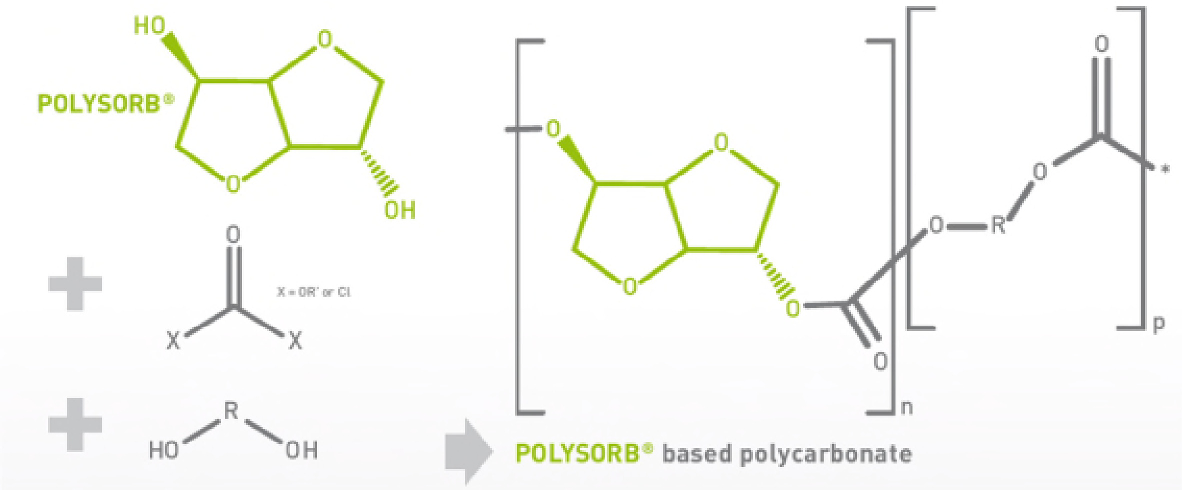


Figure 3: Isosorbide is an attractive substitute for BPA, producing polycarbonates that combine desirable properties with an enhanced safety and environmental profile.

Numerous studies[5-7] have identified isosorbide as an ideal alternative to BPA not just because it reduces environmental impact and addresses health and safety issues but because it produces polycarbonates with an enhanced property profile. This latter point is crucial since enhancing the properties of polycarbonates improves suitability for existing applications while at the same time extending use into new areas. Unfortunately, direct, like-for-like substitution, using isosorbide as the only diol, results in polycarbonates that are relatively brittle and fragile because of their low molecular weight[5]. But this issue has been successfully addressed through the use of comonomers, notably cyclohexanedimethanol (CHDM), a monomer used routinely in PET production. Results suggest that this system can be tailored to produce isosorbide-based polycarbonates with improved mechanical properties relative to homo-polycarbonates based on isosorbide alone and on BPA.

Exploring the enhanced properties of isosorbide-based polycarbonates

Relative to conventional BPA polycarbonates, isosorbide-based polycarbonates offer improved:

- Scratch resistance
- UV resistance
- Heat resistance
- Impact resistance and strength
- Birefringence and other optical properties

With respect to optical properties, UV resistance and surface hardness, such polycarbonates are comparable to polymethylmethacrylate (PMMA), an engineering plastic similarly used as an alternative to glass. And while the heat resistance and flame retardance of isosorbide-based polycarbonate may not quite match that of BPA-based products, it significantly exceeds that of PMMA. Isosorbide-based polycarbonates can therefore be considered as meshing desirable characteristics of two core, conventional engineering polymers.

The following comparative datasets illustrate in greater detail the performance improvements that are accessible.

Hardness/scratch resistance

Figure 4 shows images comparing the scratch resistance of isosorbide-based polycarbonate with that of a conventional BPA-based sample, from comparative linear Taber scratch testing (5N loading, 10 cycles). This automated technique can be used to determine pencil hardness on a scale ranging from 9B (very soft) to 9H (very hard). In this test, the POLYSORB®-based polycarbonate proved to be substantially harder (B) than the BPA-based alternative (4B).

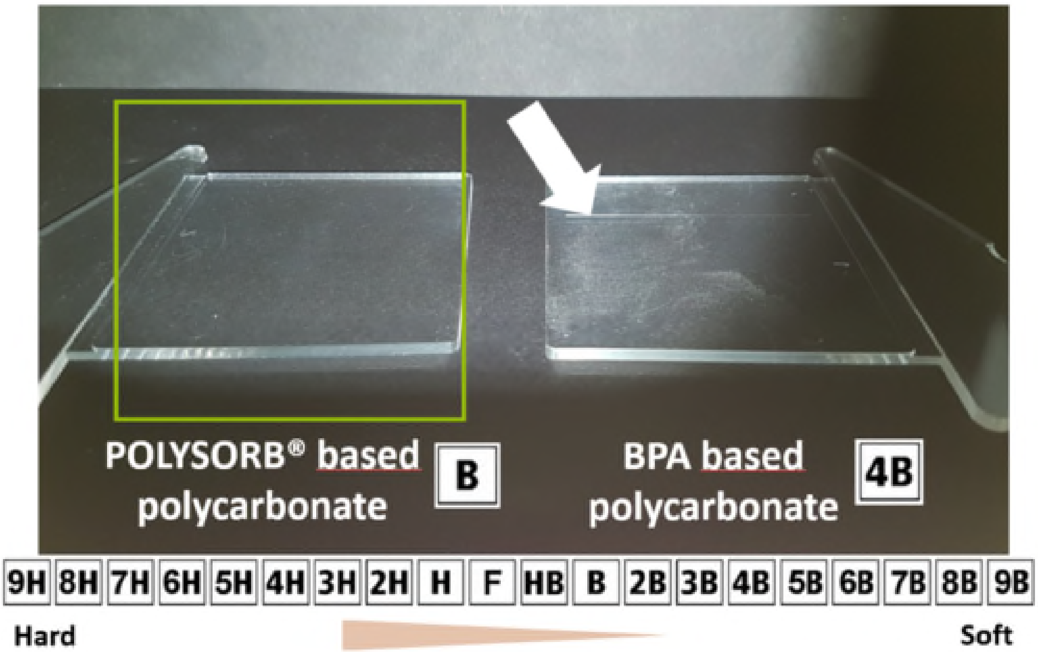


Figure 4: Isosorbide-based polycarbonates exhibit enhanced scratch resistance relative to BPA-based polycarbonate as evidenced by pencil hardness testing.

Table 1 shows data from a second study, this time of isosorbide/CHDM copolycarbonates[5]. These results show how increasing the amount of isosorbide in the copolycarbonate progressively increases scratch resistance. Levels of 70% and 85% isosorbide (molar % based on total diols in the feed) both produce higher pencil hardness, HB and F respectively, than the reference BPA polycarbonate, which in this study has a pencil hardness of B. A major focus here was to optimally tune the mechanical properties of the copolycarbonates and from this perspective the 70% isosorbide material was especially successful since it also demonstrated a higher Young's modulus and ultimate tensile strength than the BPA baseline.

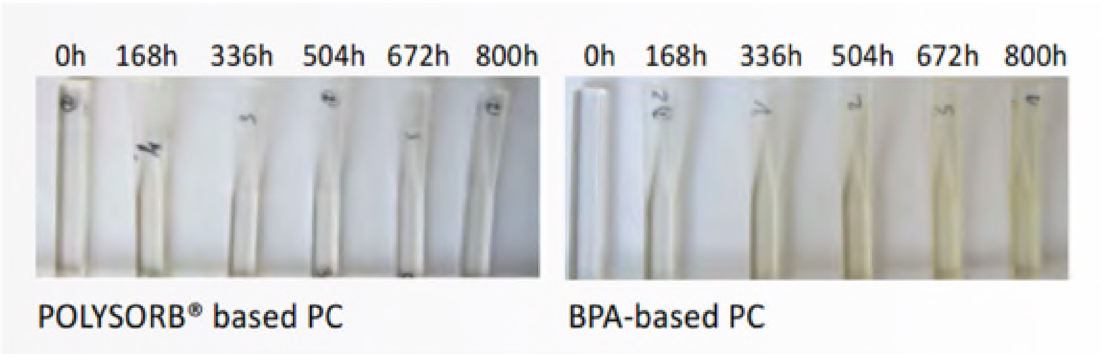
	$PI_{20}CC$	**$PI_{30}CC$**	**$PI_{50}CC$**	**$PI_{70}CC$**	**$PI_{85}CC$**	**BPA-PC**
Pencil hardness test	3B	2B	B	HB	F	BPA-PC
Contact angle(°)	84	85	87	84	81	86

Table 1: CHDM-isosorbide copolycarbonates with high isosorbide content also exhibit higher pencil hardness than BPA-based polycarbonate.

These two studies exhibit differences with respect to the scratch resistance of BPA-based polycarbonate, which could be attributed to test or coating preparation method, but both are internally consistent and illustrate how isosorbide inclusion produces polycarbonates with superior hardness/scratch resistance.

UV stability and resistance

Figure 5 shows data from assessments of the impact of isosorbide inclusion on the UV stability and resistance of polycarbonates. Response to UV is crucial for many potential applications from eyewear to greenhouse construction and exterior lighting. For these applications, yellowing, over the long-term, directly compromises performance. The data show that isosorbide-based polycarbonates exhibit significantly higher resistance to UV than BPA analogues, a result attributable to the removal of aromatic components of the polycarbonate. The images indicate minimal detectable yellowing after 800 hours with the isosorbide-based polycarbonate while the BPA-based material shows distinct coloration. The graph summarizes data measured using a Xenon weather meter for accelerated, precisely-controlled UV exposure testing (irradiation intensity 180 W/m^2; wavelength 300 – 400 nm; Black Plate Temperature (BPT) 53°C; humidity 53%). These results contrast the performance of conventional polycarbonates specified for general and outdoor use with the superior performance of isosorbide-based polycarbonate which exhibits stable UV resistance with minimal discoloration over the long term.



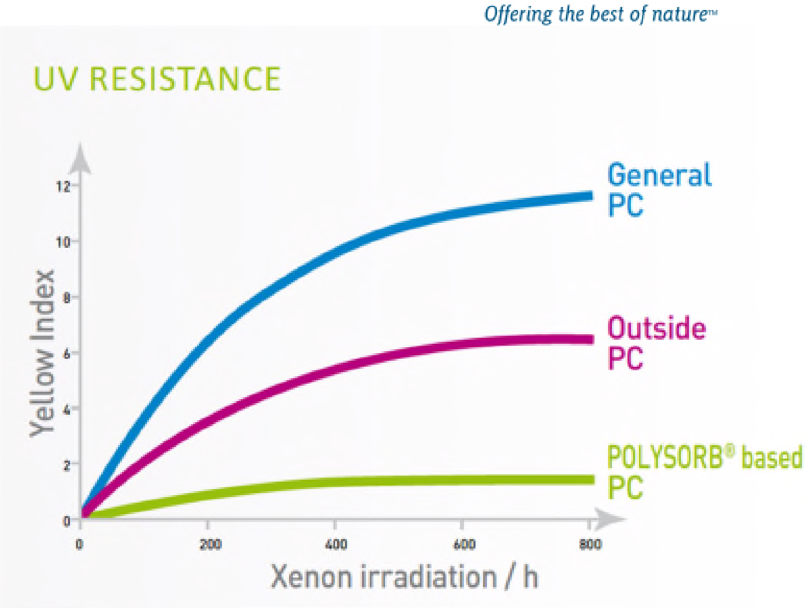
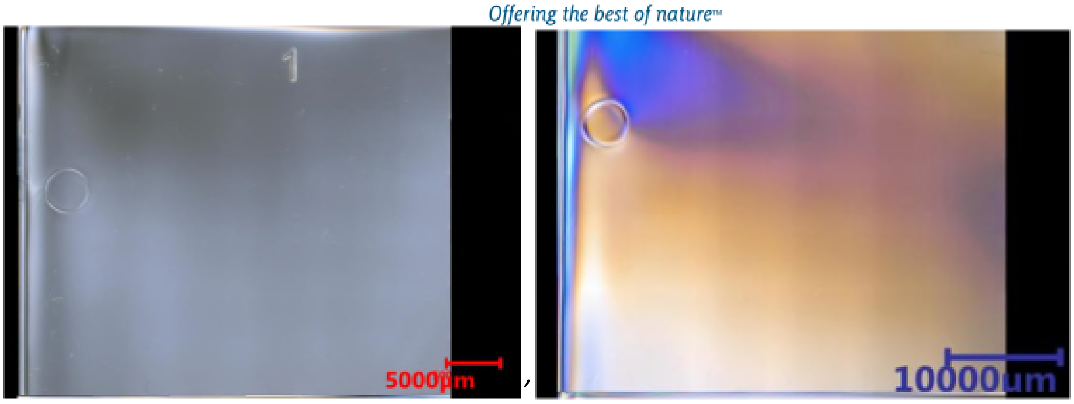


Figure 5: Isosorbide-based polycarbonate exhibits superior UV stability and resistance compared with BPA-based polycarbonates, increasing its suitability for a wide range of applications.

Optical properties/Birefringence

Figure 6 shows data comparing the optical properties of isosorbide and BPA-polycarbonates, including images of injection molded plates of polycarbonate under a polarized light microscope from an assessment of birefringence. Materials that exhibit birefringence are optically anisotropic, with a refractive index that depends on the polarization and propagation direction of the incident light. The results show that the isosorbide-based polycarbonate exhibits minimal birefringence relative to the BPA-based analogue.

The tabulated data provides further evidence of the improvements accessible by substituting BPA for isosorbide. With a lower refractive index, higher Abbe number and higher light transmittance, POLYSORB®-based polycarbonate shows a substantially improved set of optical properties relative to BPA-based alternatives. In fact, these data position isosorbide-based polycarbonate close to PMMA with respect to these important parameters. In combination, these properties, notably the low optical birefringence and high Abbe number, indicate that the polymer will result in minimal light dispersion reducing the likelihood of optically disturbing color fringes on the periphery of a product.



	POLYSORB® based PC	Usual PC	PMMA
Refractive index	1.500	1.584	1.491
Abbe number	64	32	55
Light transmittance	92%	90%	92%

Figure 6: Isosorbide-based polycarbonates (left) exhibit far lower birefringence, lower refractive index, higher Abbe number and better light transmittance than BPA-based polycarbonates (right) making them more suitable for screens, lights and other optical applications.

In conclusion

Using isosorbide in place of BPA enables the production of polycarbonates with a better performance, health and environmental profile. POLYSORB® is a highly consistent, high purity isosorbide, produced at commercial scale by Roquette, that enables polycarbonate producers to capitalize on this potential. The data presented here helps to illustrate what is feasible and show how the inclusion of isosorbide can support the development of polycarbonates that answer more successfully to both new and evolving applications than conventional engineering polymers.

Isosorbide-based polycarbonates in real life: Car navigation (left) and touchscreen (mobile phone and tablet - right) with high image quality (high transparency/low birefringence) and high scratch resistance. Headlamps (middle) with excellent light transmittance and high UV/scratch resistance.

Find out more about POLYSORB® and how you could use it to make better polycarbonates.

ROQUETTE
Offering the best of nature™

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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. 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.

In collaboration with customers who are also passionate about the ongoing food revolution, Roquette contributes to developing a whole new gastronomy that meets consumers' demands. In the pharma sector, Roquette offers solutions that play a critical role in medical treatments that cure and save lives.

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.

Founded in 1933, Roquette is a family-owned company which operates in more than 100 countries, has a turnover of around 3.5 billion euros, and employs 8,360 people worldwide. For more information, visit www.roquette.com.