

CLEAR ADVANTAGE

Finding smarter, more efficient routes to existing products is a main driver of innovation and technology programmes. In pursuing this agenda Shell technologists have developed advantaged process chemistry with the potential to create a more sustainable route to producing diphenyl carbonate, a key raw material for polycarbonates used in everything from space helmets and laptop computers to car headlights and mobile phones.



New process technology offers more sustainable route to polycarbonates production



The high optical clarity of polycarbonate makes it ideally suited to automotive glazing applications.

Polycarbonate (PC) is the largest volume engineering thermoplastic and has enjoyed strong demand growth due to its combination of technical performance characteristics. These properties include strength, light weight, thermal stability and, most importantly for some applications, excellent polymer clarity.

Global demand for PC in 2009 was around 3 million tonnes – larger than the market for nylon – and is growing at 5-7% per year. The main applications are optical media, automotive components, electronics and sheeting/film.

While demand from optical media applications has slowed due to sales of CDs, DVDs etc reaching a plateau, automotive glazing offers strong growth opportunities. PC is already used in headlamp and tailgate lenses, roof modules and fixed side windows in cars and trucks. It has also replaced glass on windscreens for motorcycles due to its light weight and safety factors.

Development of scratch-resistant multi-layer polycarbonates is expected to drive its wider application in automotive glazing. PC offers important weight savings over glass as well as more design options and easier handling within automotive production processes.

THE PHOSGENE ISSUE

Historically, most polycarbonate production has been based on reacting phosgene with bisphenol A (BPA) to produce the polymer (so-called interfacial or solution polycarbonate). However, this chemistry is inefficient and has some significant environmental drawbacks.

Phosgene is toxic and requires stringent exposure management and controls. The phosgene-based process is also complex and energy intensive, involving the use of carbon monoxide, caustic soda and a chlorinated solvent, which has its own health and safety issues.

During the reaction process the chlorine is converted to sodium chloride which then has to be removed from the finished polymer in an additional washing stage in order to achieve the material's optical clarity. Disposal of the waste salt presents another issue.

Increasing environmental restrictions have added impetus to the search for alternative, safer and more sustainable process technology. Replacing phosgene with diphenyl carbonate (DPC) in the initial polymer synthesis has been the key to this.

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Garo Vaporciyan - Principal Scientist, Shell Global Solutions.

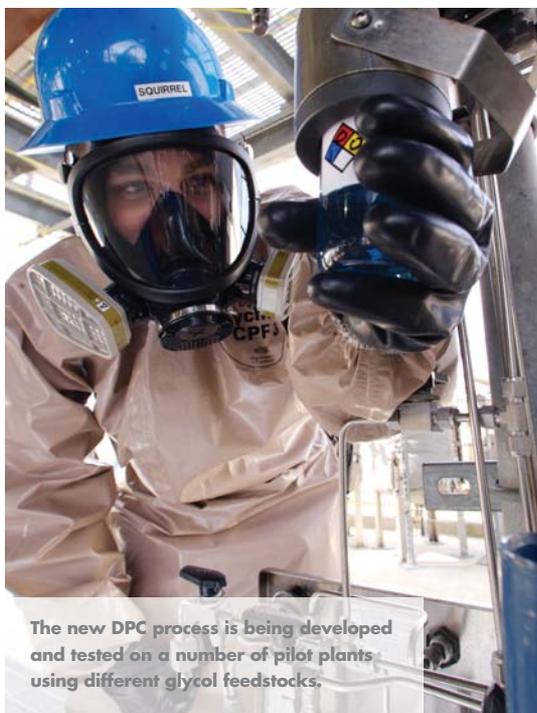
PC made by reacting DPC with the BPA is called melt-PC, because the process does not require a solvent and is performed neat – in the melt.

Existing routes for making DPC have not, however, fully addressed all the critical manufacturing issues. Although the melt-PC process eliminates phosgene, chlorine and solvents from the polymer production, a large percentage of producers continue to use phosgene in the production of DPC, via reaction with phenol.

Over the years, polycarbonate players have also explored and developed a number of phosgene-free routes to DPC but these are still capital and energy intensive.

Shell technologists, working in the USA and the Netherlands, have developed an alternative process for making DPC without phosgene, which is expected to be significant in terms of both its cost and CO₂ footprint.

“We have been looking at the underlying technology behind DPC for more than 10 years,” explains Garo Vaporciyan, a Principal Scientist



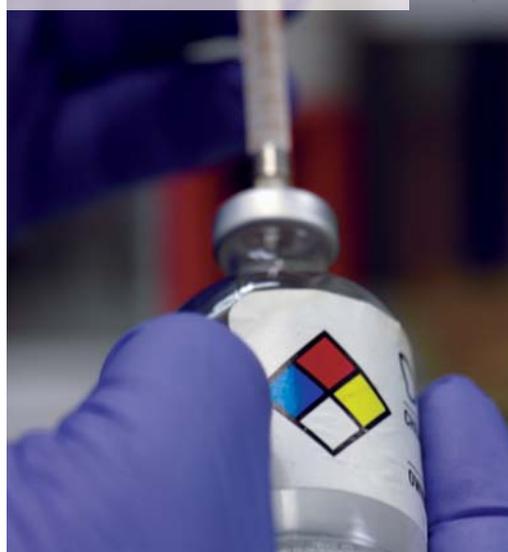
The new DPC process is being developed and tested on a number of pilot plants using different glycol feedstocks.

One of the process development facilities at the Shell/CR&L laboratories in Houston.





Phosgene-free DPC has the potential to become a significant intermediate for the polycarbonates value chain.



with Shell Global Solutions, who first recognised the opportunity and is leading its development.

"As polycarbonate has transitioned from a specialty polymer to more of a commodity, its relevance to Shell Chemicals has increased," he says. "Today, DPC produced via a phosgene-free route has potential to become a significant intermediate and fits well with Shell Chemical's strategy, portfolio and customer base."

Shell is already a major supplier of phenol and acetone to the polycarbonate sector, for use in making BPA. "DPC would enhance Shell's value proposition as a major supplier to these customers, especially because Shell is not a polycarbonate player, and so does not compete with its customers," says Vaporciyan.

MULTI-STAGE REACTION

Shell's process is based on a multi-stage reaction involving carbon dioxide, phenol and either propylene oxide (PO) or ethylene oxide (EO), and produces DPC as well as a glycol co-product.

"The reaction conditions involved are relatively mild and so can take place in one continuous

process, which translates into a significant economic advantage," says Vaporciyan.

"Thanks to efficient catalysts we are also able to achieve very high conversion rates in a single pass. The catalysts used in the reactions have over 99% selectivity, which delivers impressive yields."

All of the feedstocks involved in the process, as well as the glycol co-products, are already in the Shell portfolio. As well as providing a new route to DPC, it also offers an additional source of glycols.

Development of the DPC process was initiated through the Shell "GameChanger" programme, which fosters the development of new products or processes and provides support to bring them to market. Specifically, it looks for ideas and sustainable solutions that address a demand or significant problem in the energy or petrochemicals industry - with potential to 'change the game'.

The DPC chemistry is also one that fits well with Shell manufacturing competencies. "The essential conversion of epoxide to glycol at the heart of the process is similar to reactions happening every day in our MPG (mono propylene glycol) and MEG (mono ethylene glycol) manufacturing operations.

"We drew on this production expertise, and especially detailed knowledge of the epoxide reaction, to explore all the potential catalyst options and optimise the process."

The DPC process has been tested using both PO and EO as the primary feedstock. "We were able to adapt existing pilot plants very easily to run the new process, which gives a good indication of the simplicity of the assets that would be involved in a full-scale plant," says Vaporciyan.

He says results to date have delivered on every aspect of the process, including high conversion rates and minimal byproduct formation. As part of the development process, samples of the DPC have been provided to customers for evaluation.

While Shell has filed a number of patents for the process, it is still considering options for how it could be applied commercially. "A number of parties have expressed interest in the technology because it has potential to be a 'gamechanger' for both existing players and new entrants in the polycarbonates industry," says Vaporciyan.

"It would significantly strengthen Shell's position in the polycarbonates value chain and help to enhance and develop supply relationships."

For more information on DPC visit:
www.shell.com/chemicals/dpc