High Performance Polyols from CO_2 at Low Cost

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Description of Most Recent Milestone:
In 2011, Novomer developed an enhanced version of its proprietary catalyst which is both more active than past versions and can be easily recovered and recycled. This discovery significantly improves the economics of Novomer's CO_2-based polyols, making them cost competitive or advantaged vs. virtually all petroleum-based polyols.

Eligibility: The nominated technology is eligible for the small business award as Novomer's annual sales in 2011 were less than $40 million.

Focus Area: The EPA award focus area which fits Novomer technology is the use of greener synthetic pathways.

Description of U.S. Component: Novomer is a U.S. company with commercial offices in Waltham, MA and R&D/manufacturing operations in Ithaca, NY and Rochester, NY.

Abstract:
The vast majority of Polyols used today in coatings, foams, adhesives, elastomers, and TPUs are derived exclusively from petrochemical raw materials. Novomer has developed a proprietary technology platform which transforms waste carbon dioxide (CO_2) into very precise, high performance polyols at a lower cost than either petroleum or natural oil-based polyols.

Novomer has developed a breakthrough catalyst which is over 500x more active and far more precise than past CO_2/epoxide catalysts. In 2011, Novomer modified this catalyst system so that it can be recovered and recycled with no loss of activity or selectivity. In addition, Novomer was the first to develop low molecular weight CO_2-based polyols using chain transfer agents and holds the foundational intellectual property for these materials globally. The combination of these innovations comprises Novomer's polyol technology platform.

The environmental and human health benefits of Novomer's CO_2-based polyol technology platform are considerable. As these polyols contain 40-50% CO_2 by weight, they have the potential to sequester 10 billion pounds of CO_2 per year in targeted polyol markets. More importantly, they enable the chemicals industry to eliminate 10 billion pounds per year of petroleum-based raw materials, a source reduction which impacts the full petrochemical value chain back to exploration and extraction. In addition, as Novomer polycarbonate polyols contain no BPA, they can potentially eliminate the use of BPA-containing resins in food contact coatings.

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The manufacturing process to create Novomer's CO_2-based polyols is a proven, low cost, synthetic chemistry-based technology. It can be completed in existing chemical industry infrastructure at mild reaction conditions with high (>90%) conversions in short timeframes. Thus, through the use of CO_2 as a raw material, Novomer's technology enables raw material costs to be cut nearly in half, yielding a significant cost advantage.

Novomer is commercializing these polyols in a number of markets. As part of a joint development effort with DSM, Novomer will introduce its first large scale commercial polyol product for coil coatings applications in 2012. In partnership with industry-leading polyol producers, formulators, and end users, additional polyol products are in development for footwear foams, rigid insulating foams, and polyurethane adhesives.

Contents of Full Nomination:
The following full report is structured in three sections: Novomer's innovative chemistry, environmental and human health benefits, and commercial applicability and impact.

SECTION 1: NOVOMER'S INNOVATIVE CHEMISTRY

Carbon Dioxide as a Chemical Feedstock

Carbon dioxide is a non-toxic, non-flammable and readily available raw material, but it has seen limited use to date due to its thermodynamic stability and low reactivity.

One promising potential use is in the copolymerization of epoxides (such as propylene oxide and ethylene oxide) and carbon dioxide to generate aliphatic polycarbonates (Figure 1). These materials contain up to 50% CO_2 by weight, directly incorporating it into the polymer backbone. To date, use of these polymers has focused on high molecular weight thermoplastic applications and has been limited due to high production costs and inconsistent quality – both largely the result of inefficient catalysts. Thus, they have enjoyed limited commercial success.

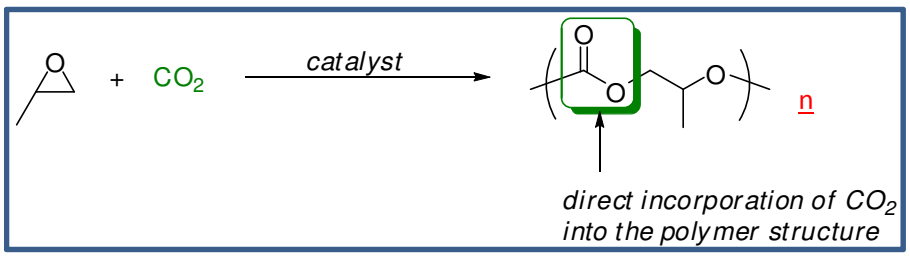

Figure 1: Direct incorporation of CO_2 into Novomer polymer backbone

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Novomer Catalyst System, Reactions, and Products

The core of Novomer's technology platform is a highly selective (>98%) cobalt-based complex that is over 500 times more active than past zinc-based catalysts for epoxide/ CO_2 copolymerization. Building upon the work of Coates[1] et al. who demonstrated cobalt salen complexes in combination with co-catalysts have good activity and excellent selectivity for the copolymerization of propylene oxide and CO_2, Novomer has tethered the co-catalyst directly to the salen ligand and thereby developed a family of proprietary unimolecular cobalt catalysts with much higher activity[2]. These unimolecular catalysts maximize CO_2 incorporation and yield very precise, high performance polymers with perfectly alternating CO_2-epoxide backbones, 90+% head-to-tail linkages, and polydispersity indices of ~1.1. In addition to improving the performance of the resulting polymers, these catalysts allow Novomer to conduct polymerizations using orders of magnitude less catalyst. In 2011, Novomer achieved another breakthrough which enables efficient catalyst recovery and reuse with commonly used, inexpensive resin bed technology. These advances significantly reduce the production costs of CO_2-based polyols, making them at least cost competitive – and in most cases cost advantaged – with respect to virtually all petroleum-based polyols.

	Zinc-based catalysts	Mengxi group	Novomer 2010	Novomer 2011
Activity (g polymer / g metal*h)	29	20-24	3,000	6,000
Productivity (g polymer / g metal)	860	570	25,000	30,000
Selectivity	95%	N/R	>98%	>98%
Recyclable?	-	-	-	Yes

Figure 2: Novomer vs. Competing CO_2 Catalyst Systems

Due to the Novomer catalyst's high productivity and ease of recycle, a commercial scale 50,000 ton/year polyol plant would produce less than a few hundred kilograms per year of cobalt waste. Unreacted epoxide is recycled and spent resins are regenerated; there are no other significant waste streams or byproducts. Reaction parameters are a mild 100-300 psi and 40-60 degrees C, enabling the Novomer process to be completed in existing chemicals industry assets with low operating costs.

Novomer originally developed high molecular weight polymers between ~45,000 and >250,000 g/mol for thermoplastic applications. Recently, Novomer developed and obtained the global foundational intellectual property[3] on the use of chain transfer

[1] J. Am. Chem. Soc. 2005, 127, 10869-10878, can be found at http://pubs.acs.org/doi/abs/10.1021/ja051744l
[2] WO 2010/022388, can be found at http://www.wipo.int/patentscope/search/en/WO2010022388
[3] WO2010/28362A1, can be found at http://www.wipo.int/pctdb/en/wo.jsp?WO=2010028362

technology to produce CO_2-based polyols with low molecular weights (<1,000 to ~10,000 g/mol). Novomer has proven the ability to design and produce tailored polypropylene carbonate (PPC) and polyethylene carbonate (PEC) polyols with very specific molecular weights, degrees of branching, and hydroxyl functionalities. This highly flexible polyol technology platform can thus be applied to a wide range of thermoset applications including coatings, foams, adhesives, elastomers, and TPUs.

Common characteristics of all Novomer CO_2-based polyols

- **Molecular weights**: from ~500 g/mol up to 10,000+ g/mol, precisely controlled to PDIs of ~1.1
- **Structures:** Linear polymers (diols) or branched structures of 3, 4, 6, or greater functionality.
- **% Carbonate linkages:** 100%; no ether linkages present in polymer backbone
- **OH Number:** Varies; ~45-70 for low Mw diols (observed); can be as low as 10 or above 100
- **Type of Hydroxyls:** PEC polyols have primary hydroxyls, PEC polyols have secondary hydroxyls
- **Residual catalyst:** None (removed from polyol). No trace metals to within detection limits
- **Other analytical:** 100% OH groups (no unsaturation), acid number <0.1, water white in color

Figure 3: Typical properties of Novomer PEC & PPC polyols

Patents, Publications, and Recognition

Novomer has a very strong intellectual property position with 15 patents granted and more than 100 pending covering the catalyst, catalyst use, finished product composition of matter, and select end applications.

Novomer has raised ~$30 million in private funding from top-tier venture capital firms and was awarded a $20.2 million grant from the U.S. Department of Energy's "Innovative Concepts for the Beneficial Reuse of Carbon Dioxide" program. In 2011, Novomer was awarded the ICIS "Innovation with Best Environmental Benefit" for its polyol technology platform.

SECTION 2: ENVIRONMENTAL AND HUMAN HEALTH BENEFITS

Sequestering CO_2 in a Useful Product

Novomer's CO_2-based polyols are significantly more environmentally responsible than existing products as they put CO_2 to productive use. In specific targeted applications within coatings, foams, adhesives, and elastomers, Novomer polyols have the potential to sequester over 10 billion pounds of CO_2 and avoid the use of 10 billion pounds of petroleum-based raw materials per year. These figures are based on a carbon LCA conducted with the help of Deloitte (formerly ClearCarbon) using ISO 14040 methodology, which shows that Novomer polyols have a carbon footprint of

approximately 1.1-1.2 kg CO_2 equivalents emitted/kg polyol product. This is a significant reduction compared to epoxies, acrylics, and existing polyols used in coatings, foams, adhesives, and other polyurethane applications.

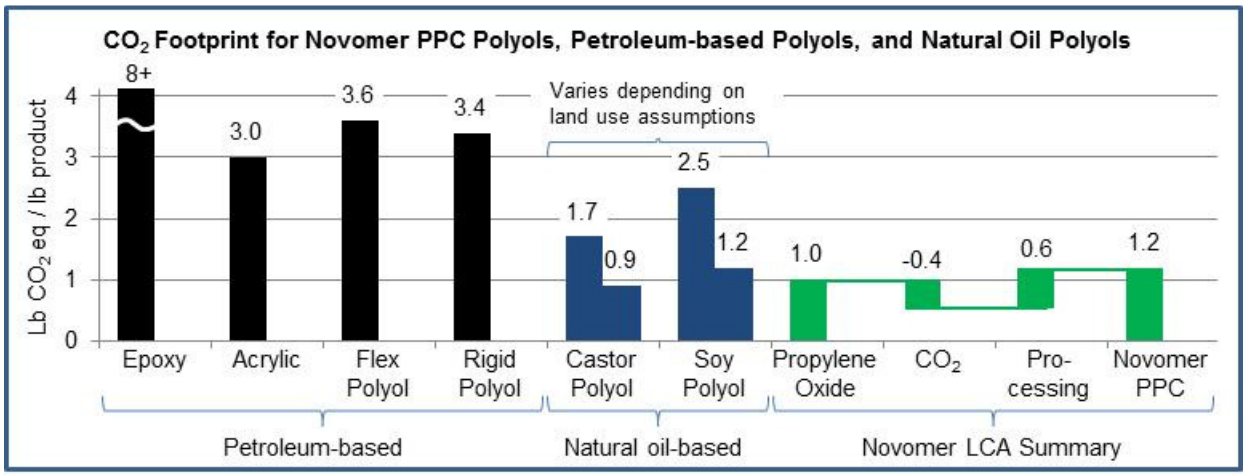

Figure 4: Novomer Carbon LCA Calculations & Comparison to Existing Products[4]

Novomer's life cycle analysis is highly transparent as there are no agricultural processes to consider. For biomass-based renewable materials such as the natural oil polyols shown in Figure 4 above, key assumptions on prior land use, irrigation requirements, and biomass transportation have a major impact on their LCA. In Novomer's case, all LCA inputs and assumptions are taken either from well-understood existing molecules such as propylene oxide and carbon dioxide or directly from Novomer's pilot and demonstration scale manufacturing facilities.

With the support of the U.S. Department of Energy, Novomer is constructing its first commercial manufacturing facility in Orangeburg, SC. This plant will sequester approximately 500,000 lbs/year of CO_2 and enable the coatings industry to avoid the use of 500,000 lbs/year of petroleum-based raw materials starting in 2012.

Eliminating Bisphenol-A (BPA) in Food Contact Applications

Novomer's products are free of Bisphenol-A, a chemical used in the production of conventional polycarbonate plastics and epoxy resins. Despite being a known endocrine disruptor and coming under increasing scrutiny as a potential human health hazard, 6-8+ billion pounds of BPA are still produced annually. Novomer's polyol technology has the potential to completely eliminate BPA with sustainable CO_2-based polymers in critical food contact coating applications.

[4] Sources: Franklin Associates, European Plastics Association, Stanford Soy Biohybrid Foam LCA, National Institute of Standards & Technology, Novomer LCA

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SECTION 3: APPLICABILITY & IMPACT

Novomer sustainable polyols are uniquely positioned to have a major impact on coatings, foams, adhesives, and related thermoset chemistries due to their compelling combination of low cost and high performance.

Low cost CO_2-based polyols, even as compared to existing commodity polyols

Novomer polymers can be manufactured at equivalent or lower costs than current petroleum-based products at any oil price and without external subsidies or a carbon tax. This represents a major advantage as clean technology development is often stifled by the high degree of risk around future oil prices. This is achieved by reducing expensive petroleum-derived raw materials by 40-50% and replacing them with far less expensive CO_2 using Novomer's cost-effective catalyst system. The traditional polyol shown in the cost comparison below is a standard 3000 Mw polyether polyol commonly used in resilient molded foam applications.

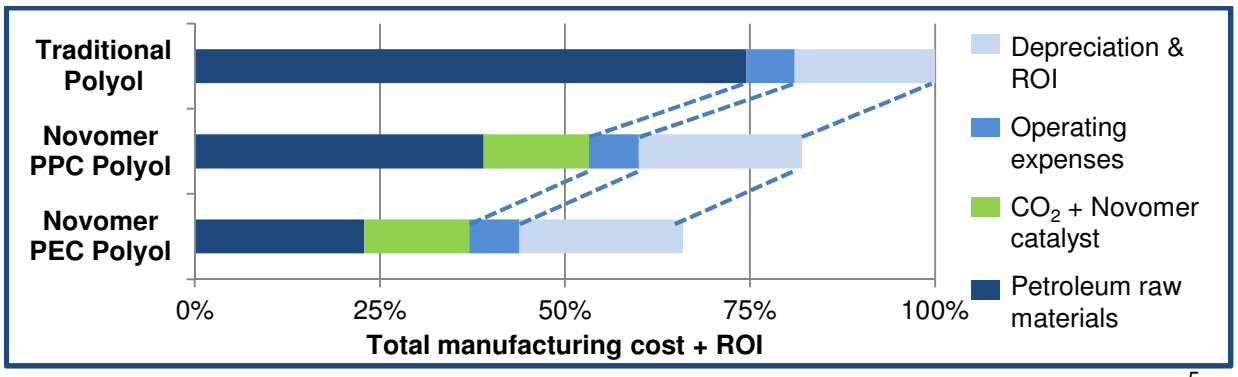

Figure 5: Novomer Polyol vs. Petroleum-based Polyol Manufacturing Costs[5]

High performance polyols for coatings

Novomer has been working with DSM (an $8 billion Dutch chemical company) under a joint development agreement since January 2010 to develop PPC polyols for coating resins. In this application, Novomer polyols have shown an exceptional combination of hardness and flexibility which leads to highly durable surface finishes. After extensive testing, DSM introduced Novomer-based coating resins to its customers with very positive feedback. The first product is currently being qualified with DSM's customers with initial commercial demand expected in 2012. See Figure 6 for demand projections for Novomer PPC polyols into coatings applications.

[5] 2004 Nexant "Polyether Polyols" report, adjusted for inflation and November 2011 raw material costs

Demand projections for Coil Coatings (tons)				
2012	2013	2014	2015	2016
25-50	100-300	300-600	600-1,200	1,500-5,000

Figure 6: Demand Projections for First PPC Coil Coatings Product

This demand will be supplied by the Orangeburg, South Carolina facility. This several hundred ton/year plant will be complete by mid-2012. Novomer's manufacturing partner for this facility is Albemarle, a multi-billion dollar U.S. fine chemical manufacturer.

High performance polyols for foams and adhesives

In 2011, Novomer completed early stage testing of its polyols in flexible and rigid foams applications. PPC polyols have been shown to have compelling processing and end-product performance in rigid insulating foam formulations. In specialty footwear foam applications, PEC polyols have yielded improved performance vs. standard petroleum based-polyols, particularly in terms of abrasion resistance.

	Weight Change (%)			Thickness Change (%)		
Cycles	1000	2000	3000	1000	2000	3000
Petroleum-based Control Polyol	0.59%	0.60%	0.62%	0.20%	0.60%	0.80%
Novomer CO_2-based PEC Polyol	0.03%	0.04%	0.07%	0.22%	0.44%	0.67%

Figure 7: Footwear Foam Abrasion Resistance Test Results

Novomer is currently in discussions with several major polyol producers, polyurethane systems houses, and end users on joint development agreements for rigid and flexible foams. Novomer is also exploring the performance of its polyols in adhesives, PU elastomer, and advanced surfactant applications.

SUMMARY

Novomer's groundbreaking catalyst system and innovative application of chain transfer technology have created a polyol platform that is well-positioned to compete with both petroleum-based and existing natural oil-based polyols. Novomer polyols have a significant sustainability advantage vs. existing materials, supported by a highly transparent LCA. Novomer polyols are also BPA free. In addition to their environmental benefits, Novomer polyols are also low cost relative to virtually all petroleum-based polyols and have demonstrated unique performance characteristics in a wide range of markets. Thus, Novomer polyols are poised to profoundly impact the world of thermoset chemistry in a positive, environmentally friendly way.