CO₂ as building block for the chemical industry

United Nations Climate Change Conference, Bonn, Germany
Dr. Angelina Prokofyeva, Bayer Technology Services
Dr. Christoph Gürtler, Bayer MaterialScience
Raw materials – CO₂ as alternative carbon source

Variety of chemical products

> 40.000
Chemical products

~ 400
Bulk chemicals and key intermediates

~ 40
Basic chemicals

4
Raw materials

CO₂ as alternative carbon source

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New raw material CO$_2$
Motivation for its chemical use

Sustainability

• Resource efficiency
  • Saving scarce fossil fuels
  • Broadening raw material base
• Climate protection
  • Using CO$_2$
  • Avoiding CO$_2$ emissions

Value creation

• Market needs
  • Comply with growing desire for sustainable products
• Profitability and competitiveness
  • Improved products and processes

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Only small amounts of the anthropogenic CO₂ can be utilized in a chemical way - adequate innovation in catalysis might offer great potential
Strategies for CO\(_2\) conversion and utilization

**Existing**
- Urea (80 m. t/a)
- Methanol (2 m. t/a)
- Cyclic carbonate (0.04 m. t/a)
- Salicylic acid (0.025 m. t/a)

**Emerging**
- CO\(_2\) based polymers
- Dry reforming
- CO\(_2\) hydrogenation to formic acid
- Fuels (DME) etc., Intermediates
- ....

**Exploratory**
- Isocyanates
- Organic carbonates
- Lactone synthesis
- Carboxylic acids
- ....

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Industrial application of epoxide/CO₂ chemistry for carbonate syntheses

C₃O₂

Cyclcic carbonate

Alternating aliphatic polycarbonate

Polyether polycarbonate polyol

- Green solvent
- Synthesis of dimethyl carbonate
  - High molecular weight
  - Binders for ceramics
  - Biodegradable/compostable polymers
- Low molecular weight
- Terminal OH-functionalities yields polyols for polyurethanes synthesis

- Selectivity is strongly influenced by the catalyst / competing reaction
- Up to 43 wt% incorporation of CO₂ (R = CH₃) possible
- Homogenous and heterogeneous catalyst suitable

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Research Case CO₂ – Break-through at Bayer

1969 - 2008
Basic research

Lab success: Dream Reactions

2009

Implementation: Dream Production

2010

Dream Polymers

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Dream Production – From power plant to polyurethane

- Scrubbing and supply of CO₂
- Process development and conversion of CO₂
- Production and testing of polyurethanes with CO₂

Fundamental research

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Scientific breakthrough
Special catalyst found after 40 years

Success of close cooperation between Bayer and the CAT Catalytic Center in Aachen, Germany.

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Dream Production –
Covering the value chain

Bayer Technology Services

Construction and operation of a pilot-plant

Samples

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Dream Production –
Covering the value chain

Slab stock plant for CO$_2$-PET testing in foams
Target product polyurethanes – Allrounder among plastics

\[ \text{Polyol} + \text{Isocyanate} \rightarrow \text{Polyurethane} \]
Foam quality evaluation results
Very good foam properties achievable

- CO₂ based polyurethanes can be used for many applications
- Properties on the same level or even better than conventional polyurethanes

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New technology works
But is it sustainable?
Complex LCA by RWTH University – All aspects covered

Environmental factor

Environmental effect

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Impacts on Climate Change

kg CO₂-eq / kg polyol

Conventional polyol

- epoxide
- epoxide
- starter
- utilities & others *

* includes process steam, electricity, cooling water, catalyst etc.

N. von der Assen and A. Bardow (2013). Oral presentation, ICCDU XII, Alexandria, VA, USA
Impacts on Climate Change

- kg CO₂-eq / kg polyol
  - Conventional polyol
    - epoxide
    - raw material replacement
    - starter
    - utilities & others*
  - CO₂-based polyol
    - epoxide
    - CO₂

* includes process steam, electricity, cooling water, catalyst etc.

Niklas von der Assen and André Bardow
*Green Chem.*, 2014, 16, 3272-3280

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Dream Production
From research to commercial use

- Following successful research phase, commercial use of the new process and the production of the first CO$_2$-based polyols for sale.
- Construction of a production line at the Dormagen site with an annual capacity of 5,000 metric tons.
- Investment volume of EUR 15 million
- Planned start of production early 2016
Thank you for your attention!
✓ It works
✓ Very good foam properties achieved
✓ Improved CO$_2$ footprint
CO$_2$-based polyols:
Balance between value creation and market acceptance

CO$_2$

Viscosity
Effect of CO$_2$ in polyols
Carbonate groups contribute to increased viscosity

- Viscosity strongly depends on functionality and CO$_2$ content
- Polyols can be designed according to application requirements
- CO$_2$-based polyols show viscosity properties in the range between polyether and polyester grades
Thermal foam stability
CO₂-based foam show good performance

Thermal stability test* for PUR slabstock:
• Identical onset temperature and mass loss
• No difference in thermal sensitivity

Conclusion:
• CO₂ is chemically fixed inside the polyurethane backbone
• Thermal foam stability matches that of conventional polyols

* TGA: Thermo-Gravimetric Analysis (heating rate: 10 K/min)
New CO$_2$-based polyols for flex-foam
Comfort materials count for ~36% of the PU market

Global slabstock polyol market 2012*

- Conv. Polyol: ~2.8 Mio. t
- HR Polyol: 4%
- All Filled Polyols: 18%
- Other Polyols: 9%
- Global slabstock: 69%*

* Estimate based on IAL studies

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