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Tech Transfer Hub

Council of Scientific and Industrial Research
National Chemical Laboratory

Match Maker/ Renewable Chemicals & Materials/ 9 Apr 2021

Bio-derived ‘drop-in’ replacement for di-isocyanates in polyurethane production

Lead Inventor: Dr Prakash Wadgaonkar

Organization: CSIR-NCL, Pune

TechEx.in Case Manager: Devanshi Patel (devanshi@venturecenter.co.in)

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The Opportunity

- The market of polyurethanes made from bio-based monomers is growing fast. Bio-based polyurethane market is ~ 50 m$ and is growing at 9-10%. Global polyurethane market is ~ 60-70 b$.
- Many options available for bio-derived polyols/diols. Not too many options for bio-derived di-isocyanates. (Global MDI market ~ 30b$)
- This technology provides a ‘drop-in’ substitute di-isocyanates (comparable to MDI) derived from lignin as raw material
- Lignin is abundantly available - mostly waste of the paper and pulp industry.
- Approx. 100 million tons of lignin produced per year (2015), as a by product
  - Most of these are burnt for heat
  - Only 2% lignin are utilized for commercial applications

Who should be interested and why?

Who?	Why?
PU manufacturers	• PU will have higher bio-derived content
MDI/ Diisocyanate manufacturers	• Addition of a bio-derived diisocyanate to their product portfolio
Manufacturers of specialty chemicals from Lignin	• New additions to product portfolio • Higher value products
Biorefineries	• Lignin value chain

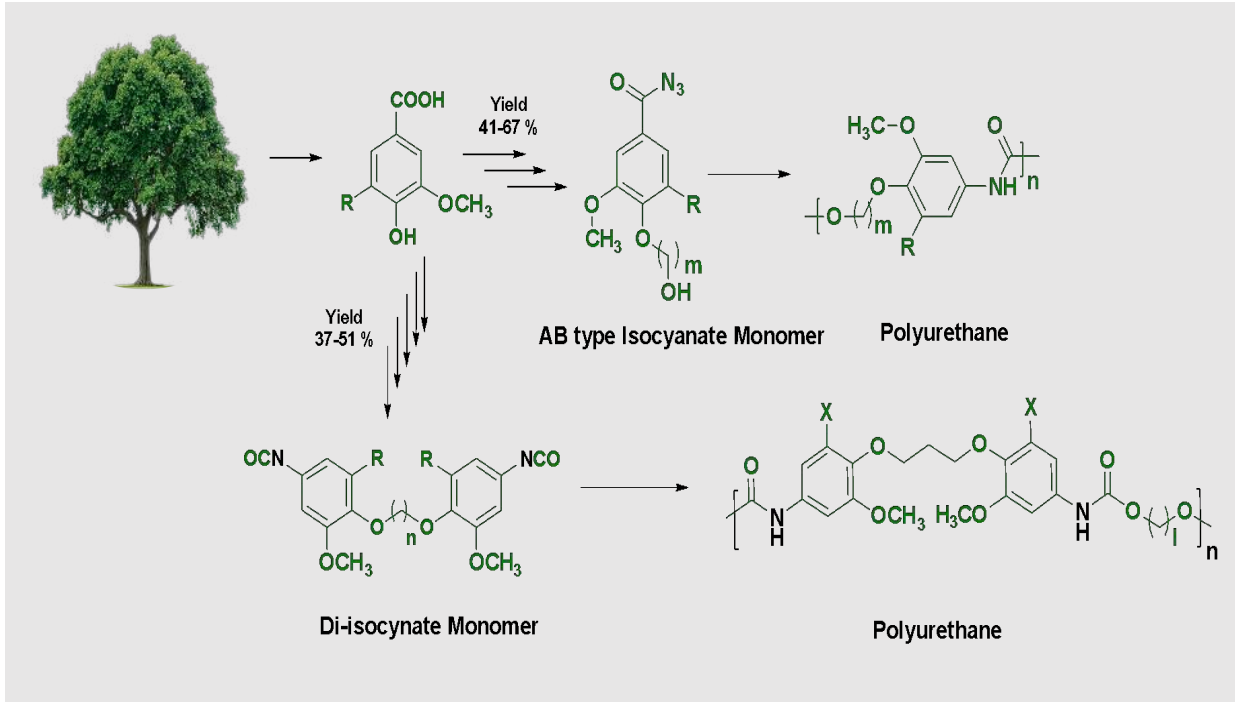
About the technology: bio-based aromatic diisocyanates

Technology features:

- Starting materials: Lignin-derived phenolic acids: vanillic and syringic acids
- Diisocyanate produced: New aromatic diisocyanates synthesized in overall high yields
- Carbon-neutral monomers
- Colorless liquid to solid
- Lower vapor pressure, advantages of handling and processing
- Equivalent in reactivity to MDI

Resulting Polyurethanes:

- 100% bio-derived content, low carbon footprint
- Elastomers, foams, …etc
- High molecular weight
- Can be cast into transparent and flexible films

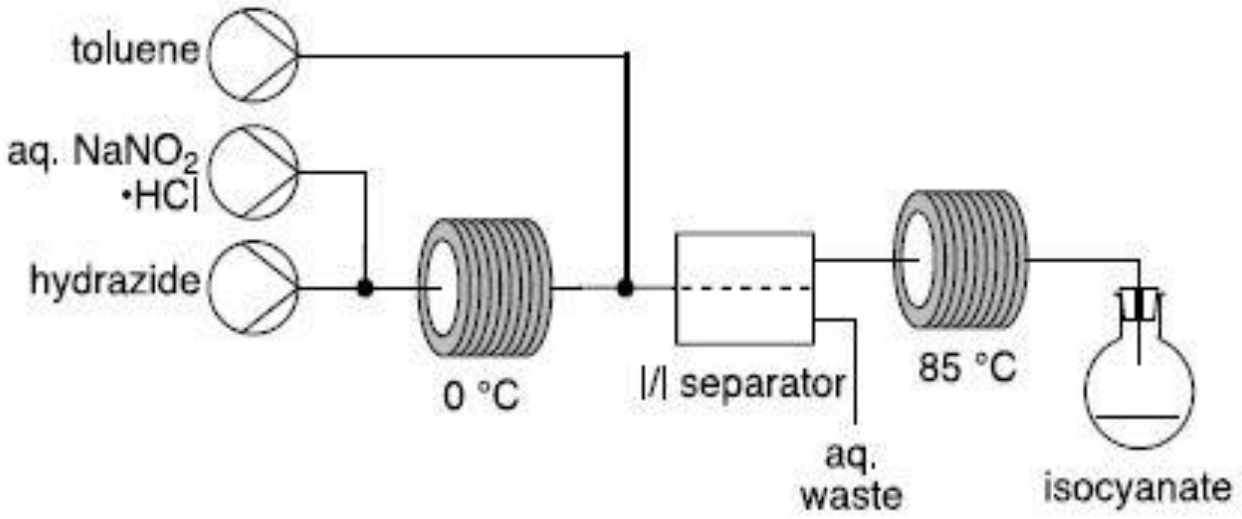


Curtius reaction can be done safely!

Preparation of Mono- and Diisocyanates in Flow from Renewable Carboxylic Acids

Thien An Phung Hai, Laurent J. S. De Backer, Nicholas D. P. Cosford, and Michael D. Burkart*

Org. Process Res. Dev. 2020, 24, 2342–2346



Flow chemistry diagram for the synthesis of isocyanates.

- Simple flow chemistry methodologies.
- The transformation is safe, scalable, and sustainable
- Amenable to distributed manufacturing processes.
- No need for capital-intensive phosgene generation and containment facilities

Current status

Technology status:

- Demonstrated at lab scale (upto 25 g synthesized)
- Patent protected

Patents:

- Priority document: IN 3866DE2014 (23 Dec 2014)
- Coverage: IN, US
- Granted: US9950996B2, IN346907

Publications:

- Poly(ether urethane)s from aromatic diisocyanates based on lignin-derived phenolic acids, Sachin S Kuhire, Samadhan S Nagane & Prakash P Wadgaonkar, Polym. Int., 66 (2017) 892–899. (Link)
- New poly(ether urethane)s based on lignin derived aromatic chemicals via A-B monomer approach: Synthesis and characterization , Sachin S.Kuhire, C.V.Avadhani and Prakash P.Wadgaonkar, Eur. Polym. J., 71, (2015), 547-557. (Link)
- Synthesis and characterization of partially bio-based polyimides based on biphenylene-containing diisocyanate derived from vanillic acid, Sachin S.Kuhire, Amol B.Ichake, Etienne Graub, Henri Cramail, Prakash P.Wadgaonkar, Eur. Polym. J. 109, (2018), 257-264. (Link)

Team & Organization

Lead Scientist: Dr Prakash P. Wadgaonkar
Emeritus Scientist, Polymers and Advanced Materials Laboratory,
Polymer Science and Engineering Division, CSIR-NCL

Expertise:
Sustainable and Green Chemistry (Monomers and Polymers)
Controlled Polymerization Methods
New Macromolecular Architectures and Structure-Property Co-relationships
High Performance Polymers, Thermosets,
Self- Healing Polymers, Specialty Polymer Applications

Awards/Honors:
Prof. M Santappa Award (2006);
Prof. Sukumar Maiti Award (2004);
CSIR Technology Award (2003);
Dunlop Award (1984).

PhDs Guided: 23;
RA/Post-doc's Trained: >50
Publications:215 (h-Index: 35)
International Patents: 24

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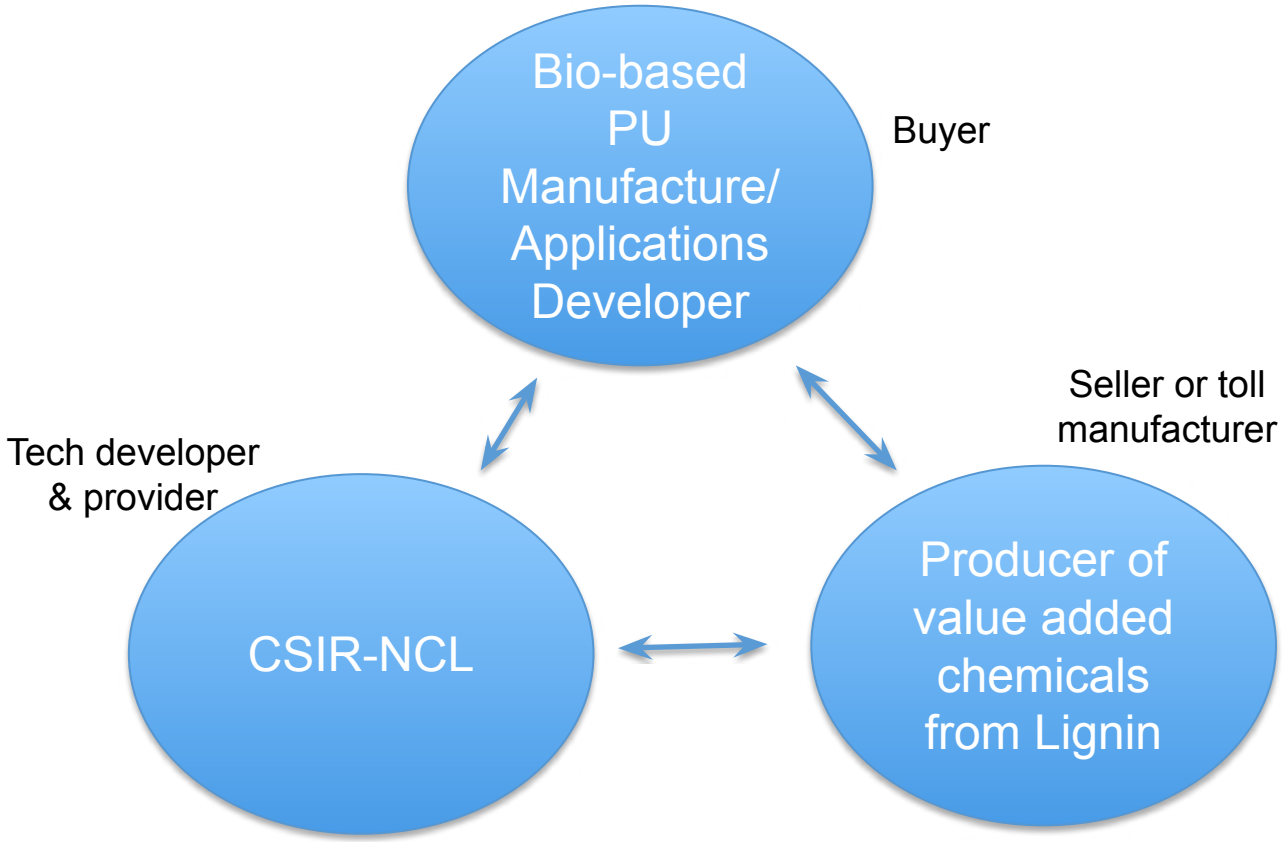
- NCL is a constituent lab of the CSIR, India
- Attractive models of engagement and flexible terms for IP
- Publicly funded non-profit R&D lab & DSIR recognized SIRO => R&D project sponsors can claim tax benefits; Eligible for CSR support
- Key assets and strengths
  - Team strength: Strong expertise in small organic molecule (monomers) and polymer synthesis
  - Well equipped wet chemistry labs and facilities for polymer synthesis (polycondensation chemistries, melt reactors, SSP reactors, anionic polymerization)
  - State-of-the- art analytical facilities for characterization of polymers
  - Process engineering lab, flow synthesis facilities
  - Pilot plant facility: Proof-of-concept (gm scale) to Kg scale synthesis
  - Track record of technology transfer and working with both Indian and multinational companies:

Next Steps

- Optimize molecular structure of di-isocyanate monomer for application
- Scale-up in partnership with industrial partner



Seeking Industrial partners interested in:

- Licensing technology knowhow with patents
- Sponsoring further technology advancement and scale-up
- Utilizing the chemistry skills for other projects
- Collaborative development
- Licensing of patents

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References > Market data

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2. https://www.imarcgroup.com/isocyanates-market
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