Conversion of CO_2 to Alkyl Carbonates Using Ethylene Oxide as Feedstock (DE-SC0013233)

Integrated Process of CO_2 Capture and Conversion to Chemicals: Technology Challenges & Opportunities

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U.S. Department of Energy
National Energy Technology Laboratory
Carbon Management and Natural Gas & Oil Research Project Review Meeting
Virtual Meetings August 2 through August 31, 2021

Project Overview

- **Project Started in 2014 with ERA, Alberta Round 1 Grant**
- **SBIR Funding**: $2,140,781 : total Phase I, II and IIb
- **Overall Project Performance Dates**:

  SBIR Phase I: 02/17/2015 - 11/16/2015

  SBIR Phase II: 06/10/2016 - 06/10/2018

  SBIR Phase IIb: 05/27/2019 - 08/27/2021
- **Project Participants**:

  Michigan State University (MSU)

  Illinois Sustainability Technology Center (UIUC/ISTC)

  Gas Technology Institute (GTI)

  Air Liquide Advanced Separation (ALAS)

  Unitel Technologies, Inc.

Project Overview

Overall Project Objectives

SBIR Phase I and Phase II: Development of heat-integrated reactive distillation (HIRD) for conversion of captured CO_2 to Dimethyl Carbonate (DMC)

SBIR Phase IIb: Advancing Phase II process development to an integrated process of capture and conversion of CO_2 to alkyl carbonates.

Technology Background

Challenges for Carbon-to-Chemical (C2C)

Technical

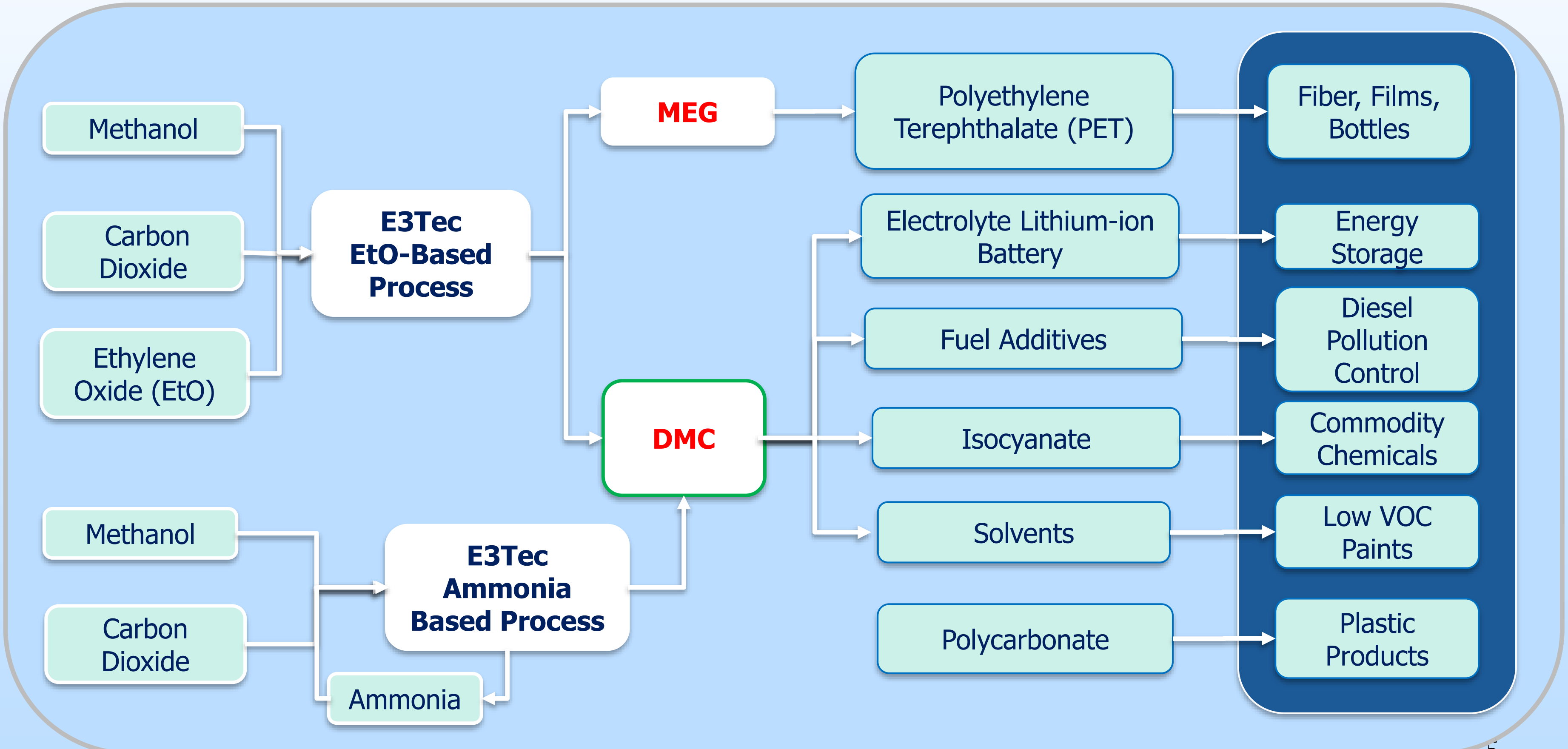
- Unsuitable process technologies developed for petrochemicals
- Lack of credible techno-economic merits of C2C technology
- Uncertain market analysis for long-term demands of C2C chemicals
- Nascent stage of technologies for conversion of CO_2 to Chemicals

Economic

- Uncertainty of imminent regulatory policy for carbon management
- Accounting costs associated with CO_2 capture, transportation, sequestration and monitoring
- Competitiveness of Green Chemicals versus petroleum derived chemicals
- Large investment in R&D leading to Demonstration for innovative C2C processes

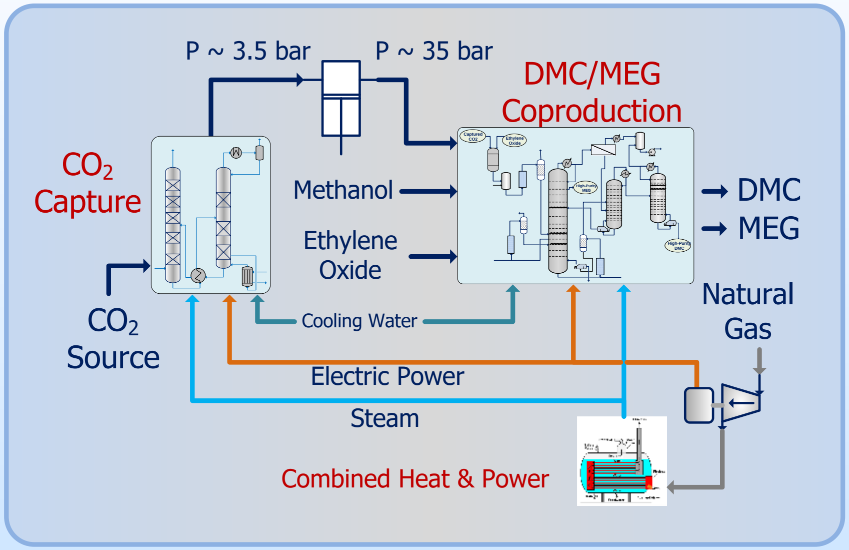
Technology Background

<u>Essential 1st Step</u>: C2C Opportunity Based on Supply Chain and Product Margin to Offset the Cost of CO_2 Capture and Sequestration

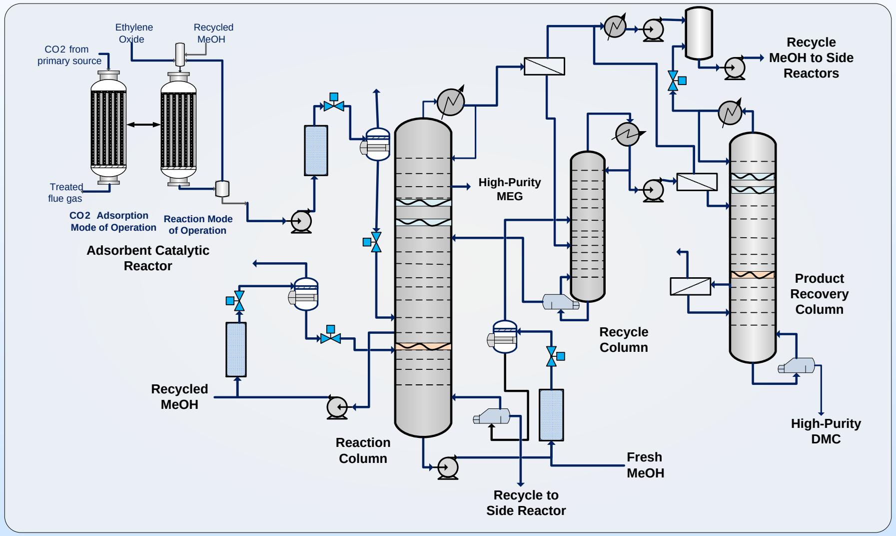


Technology Background

Solution: Integrated Process of CO_2 Capture and Conversion to DMC



Conversion of Captured CO_2 to DMC using Trickle-Bed Reactor



CO_2 Capture from Primary Sources and Conversion to DMC using Adsorbent Catalytic Reactor

Method of direct conversion of CO_2 to alkyl carbonates using ethylene oxide as feedstock
US Patent, 2021

Technology Background

CO_2

↓

DMC & MEG

↓

Alkyl Carbonates & Derived Chemicals

Technology Background

E3Tec

Ethylene & Propylene Oxide Based DMC Process

Direct Conversion by Eliminating Ethylene Carbonate Process

SBIR Phase I and SBIR Phase II

$CH_2O\text{-}CO\text{-}OCH_2 + 2\ CH_3OH \rightleftharpoons CH_3O\text{-}CO\text{-}OCH_3 + HOCH_2\text{-}CH_2OH$

Ethylene Carbonate + Methanol ⇌ Dimethyl Carbonate + Mono-Ethylene Glycol

SBIR Phase IIb Sequential

$CH_2\text{-}O\text{-}CH2 + CO_2 + 2\ CH_3OH \rightleftharpoons CH_3O\text{-}CO\text{-}OCH_3 + HOCH_2\text{-}CH_2OH$

Ethylene Oxide + Methanol ⇌ Dimethyl Carbonate + Mono-Ethylene Glycol

$CH_3\text{-}CH\text{-}O\text{-}CH2 + CO_2 + 2\ CH_3OH \rightleftharpoons CH_3O\text{-}CO\text{-}OCH_3 + HOCH_2\text{-}CH\text{-}OH\text{-}CH_3$

Propylene Oxide + Methanol ⇌ Dimethyl Carbonate + Propylene Glycol

Technology Background

Green Technology Merits

High-Purity Products and 9x Reduction in carbon-footprint compared to commercial DMC processes

C-footprint Analysis*, kg CO_2 / kg DMC	**E3Tec Process**	**Syngas-Based Process**
CO_2 Consumption[+]	-0.51	NA
CO_2 Emission Inside Battery Limits (ISBL)	0.58	1.29
Methanol from Commercial Process	0.39	0.47
Ethylene Oxide from Commercial Process	0.31	NA
Total CO_2 Emissions	1.28	1.76
Offsetting CO_2 Emissions of Coproduction of MEG	-0.58	NA
Net CO_2 Emissions	**0.19**	**1.76**

* Ethylene-oxide based DMC process; [+]Captured CO_2 with 90%+ purity

Technology Background

Techno-Economic Analysis

Commercially profitable to syngas-based DMC process

Economic Parameters	E^3Tec Process	Syngas-Based Process
DMC Capacity, kTA	57	57
MEG Capacity, kTA	40	NA
Capital Cost (CAPEX), $MM	$198	$219
Cost of Production, $/tonne DMC*	$488	$685
Levelized Cost of DMC, %	15% lower	
DMC Quality	99.9%	90% to 95%

*Includes cost of 60 $/Tonne CO_2 @ 90%+ purity; MEG @ market cost

Technical Approach/Project Scope

Project Success Criteria

- Development of validated design methodology for scale-up from prototype lab testing to commercial-scale plant
- Advancing conversion of CO_2 to DMC from TRL-5 of *Laboratory Testing of Semi-Integrated System* to TRL-7 of *Integrated Pilot System Demonstration*
- Justification of techno-economic merits of conversion of CO_2 to DMC

Project Risks and Mitigation Strategy

- Project Risks: Key technical challenge is to demonstrate synthesis of high-purity (99.9%) DMC by utilization of CO_2 from primary sources
- Mitigation Strategy: Reduce technical uncertainty by integrated technology demonstration unit for industry acceptance

Technical Approach/Project Scope

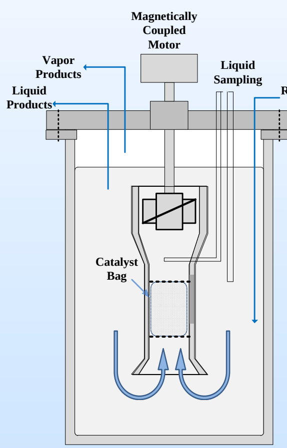
Work Plan

1. Prototype tests for validation of the ASPEN Plus® process scale-up methodology
2. Qualification of catalysts for direct conversion of CO_2 from primary sources to chemical intermediate for further conversion to dimethyl carbonate with HIRD process
3. Comparative analysis of C-footprint based LCA and TEA for a) Captured CO_2; b) Integrated CO_2 Capture and Conversion and c) syngas based DMC
4. Design of Technology Demonstration Unit

Progress and Current Status of Project

Test Units in Phase I, II and II-Sequential

Adsorbent Catalytic Reactor (ACR) Test Unit



Patented Differential Kinetic Test Unit (DKTU)

10-meter Reactive Distillation Columns Integrated with Side Reactors

Progress and Current Status of Project

Aspen Plus® Scale Up Design Methodology

Scale Up to Scale Down

Integrated ASPEN Plus® Process Model

Validated ASPEN Plus® Process Model

Differential Kinetic Test Unit

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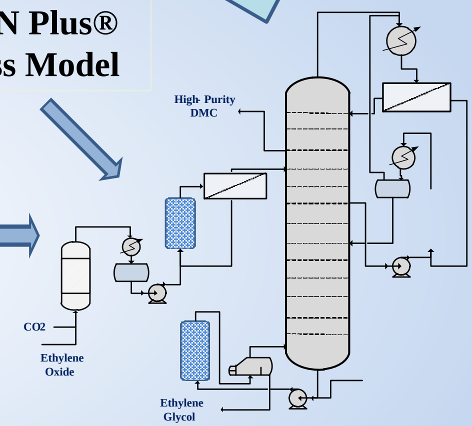
Integrated Pilot-Scale Test Unit



Commercial Unit

Scale Down to Scale Up

SBIR Phase IIb Technical Approach/Project Scope

Accomplishment of Milestones

1. Developed validated ASPEN Plus® scale-up model based on prototype test data
2. Developed adsorbent catalytic reactor for direct conversion of CO_2 from primary sources
3. Demonstrated favorable economics based on a detailed market analysis
4. C-footprint model interlinked with ASPEN Plus® exemplified that CO_2 emissions would be significantly lower compared to commercial syngas DMC process
5. Designed a demo unit and developed industry contacts for the next phase of the project

Progress and Current Status of Project

Synergistic efforts

a. <u>CO_2 capture technology</u>: E3Tec evaluated 2nd generation CO_2 capture technologies for synergistic efforts for implementing C2C technology in the near term

a. <u>Co-product formations</u>: DMC and Glycol are platform chemicals for production of valuable higher alkyl carbonates and consumer products. This multi-faceted technology would be adopted by large chemical manufactures with green agenda of C2C.

Plans for future testing/development/ commercialization

Plans for Next Phase

Technology Demonstration Unit Leading to Commercialization

- Integration of 1 tonne/day technology demonstration unit with to validate techno-economic merits
- Strategic alliance with industry partners for commercial-scale pilot plant with 10 to 20 tonne/day or pre-commercial DMC plant

R&D Efforts

- Development of the adsorbent catalytic reactor with improved catalysts and CO_2 adsorbents
- Application of the HIRD equipped with side reactors and membrane separations to CO_2 conversion to other specialty chemicals

Summary Slide

Key Findings, Lessons Learned, and Future Plans

- Important to evaluate the thermodynamics of conversion of CO_2 to specialty chemicals before pursuing significant process development
- SBIR project will be completed in August 2021 and the future-plan focuses on ***Technology Demonstration Unit*** for validation of the techno-economic merits leading to commercialization
- E3Tec is seeking industry participation for Technology Demonstration Unit

"Take-Away" Message

DMC is an ideal platform chemical for CO_2 utilization based on expanding market demands of alkyl carbonates for lithium-ion batteries, expanding use of polycarbonates and its use in consumer products such as polyurethane

Acknowledgements

Financial and Technical Supports

Ethylene-Oxide Based Process Development of DMC Synthesis

Supported by the DOE SBIR Phase I, Phase II and Phase IIb Grants under DOE Contract No. DE-SC0013233.

Ammonia-Based Process Development of DMC Synthesis

Supported by the CCEMC-Alberta (now ERA) Round-1 Grand Challenge.

DOE NETL

Andy Aurelio, DOE Program Manager

Appendix

- Organization Chart
- Gantt Chart

Organization Chart

E3Tec Service, LLC
Project Manager (PM) and PI
C.B. Panchal

Project Team
PM, PI, Co-Investigators

Advisory Panel
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Dr. Arun Muley

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Co-Investigator
C.B. Panchal

Technical Staff
CB Panchal
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Dennis Miller
Kruti Goyal
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Howard Meyer

ISTC
Co-Investigator
B.K. Sharma

Technical Staff
B. K. Sharma
Kevin O'Brien
Vinod Patel
Post Doc

Unitel
Co-Investigator
Ravi Randhava

Gantt Chart – SBIR Phase IIb

ID	Task Name
1	**Milestones**
2	**Budget Perios 1**
3	**Performance model of the reactor**
4	**ASPEN Plus process analysis of the integrated process**
5	**Budget Period 2**
6	**TEA of the integrated process**
7	**LCA of the integrated process**
8	**Design of Technology Demonstration Unit**
9	**Process Analysis**
10	ASPEN Plus analysis of EtO and ammonia based processes
11	Documentation of PFD and equipment list
12	Comparative process analysis
13	Validation of the ASPEN Plus design model
14	**Qualification of Catalysts for Direct Conversion of CO2**
15	Characterization of catalyst effectiveness
16	Merit Analysis to qualify catalyst(s)
17	Determination of kinetic parameters of qualified catalyst(s)
18	**Performance of Adsorbent Catalytic Reactor (ACR)**
19	Performance tests of membrane reactor
20	Performance tests of adsorbent catalytic reactor
21	Development of performance model for theadsorbent catalytic reactor
22	Incorporation of the performance model in to ASPEN Plus process model
23	**TEA of the Integrated Process**
24	Estimation of CAPEX and OPEX
25	ProForma analysis to estimate IRR and NPV
26	TEA merit analysis of the integrated process vs. separate CO2 capture and conversion processes
27	Risk Register Management (RRM) matrix analysis
28	**LCA of the Integrated Process**
29	C-footprint analysis and comparison with separate CO2 capture and conversion processes
30	Update of the global market demands of DMC and its derived products
31	Global CO2 abatement potentials with timeline
32	**Design of Integrated Pilot Plant Test Unit**
33	ASPEN Plus process design
34	Estimation of capital and operating costs
35	**Implementation Plan for Integrated Test Unit**
36	Development of business plan
37	Implementation schedule
38	**Project Management and Reporting**