Field-Scale Testing of the Thermocatalytic Ethylene Production Process Using Ethane and Actual Coal-Fired Flue Gas CO_2

DE-FE0031713

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SOUTHERN RESEARCH

Founded in 1941

Team ~ 400
Divisions - 4

Private 501(c)(3) non-profit

Discovered 7 FDA approved Cancer drugs

Sustainable Chemistry and Catalysis – New Processes and catalysts for production of chemicals/fuels

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. Department of Energy

Carbon Utilization Virtual Project Review Meeting
October 21-22, 2020

TECHNOLOGY BACKGROUND

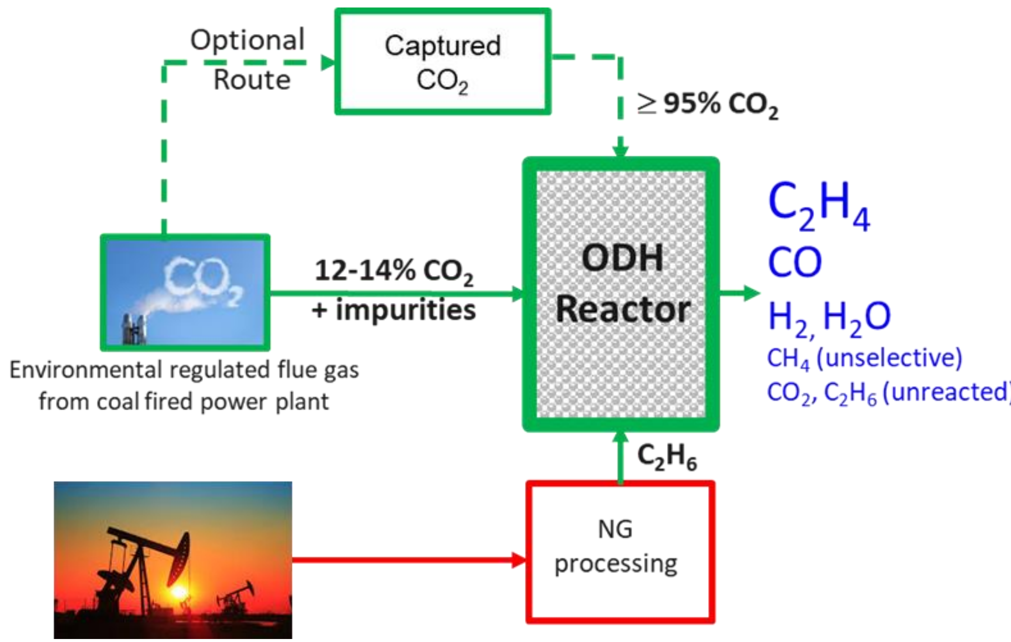
Summary

Thermo-catalytic ethylene production using ethane and CO_2 *(CO_2 ODH)*

Oxidative dehydrogenation (ODH): $C_2H_6 + CO_2 = C_2H_4 + CO + H_2O$

Advantages over *commercial steam cracking (SOA)*-

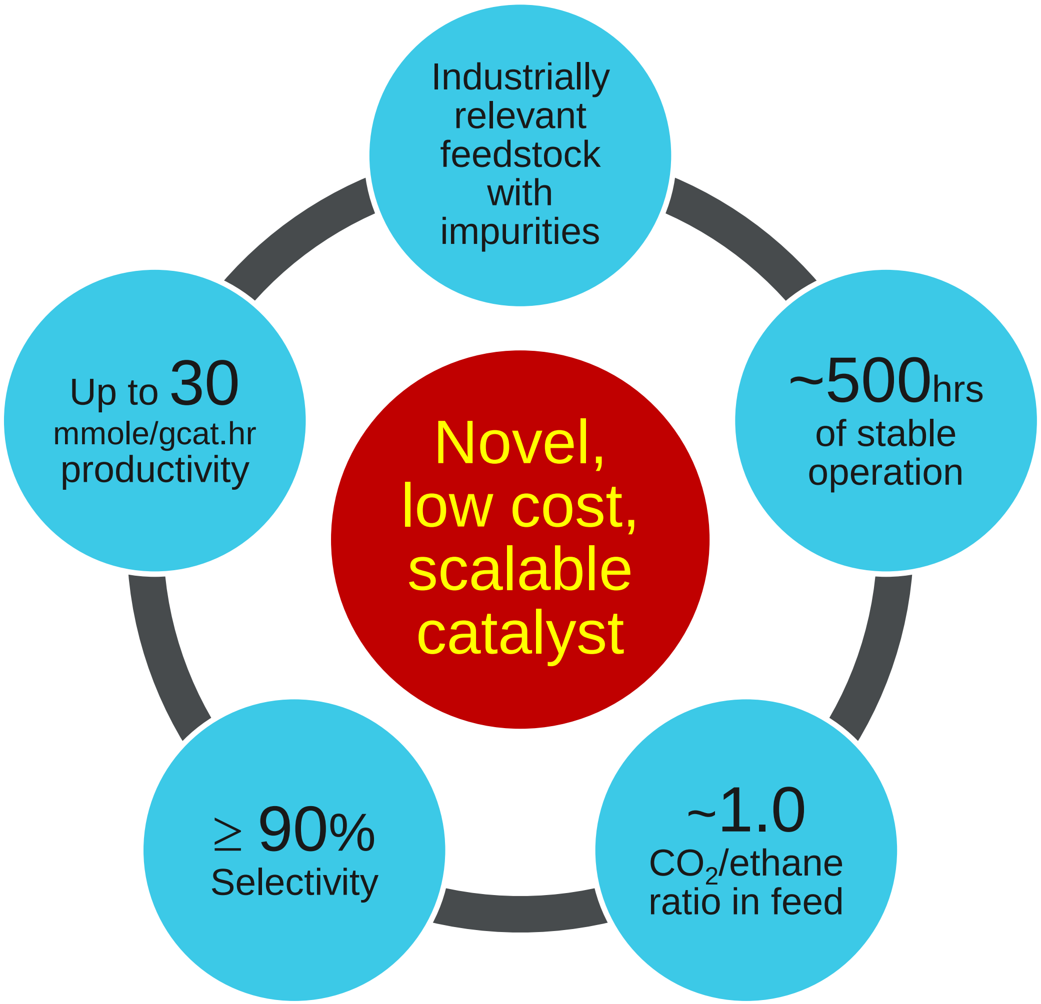
- ✓ At least **150°C** lower operating temperature
- ✓ Catalytic process that **utilizes CO_2** and **eliminates** use of **H_2O and external reductants (e.g., H_2) or strong oxidant (e.g., O_2)**
- ✓ Process adaptable to different CO_2 streams with impurities
- ✓ Reduced process footprint due to high reaction selectivity
- ✓ Co-production of CO-rich syngas
- ✓ With co-product utilization, production cost can be lowered to SOTA cost
- ✓ **50%** or more overall GHG emission reduction via direct CO_2 conversion



Laboratory Scale √

Field Scale - ongoing

Nano-Engineered Catalyst



Validation Using Two Relevant CO_2 Concentrations:

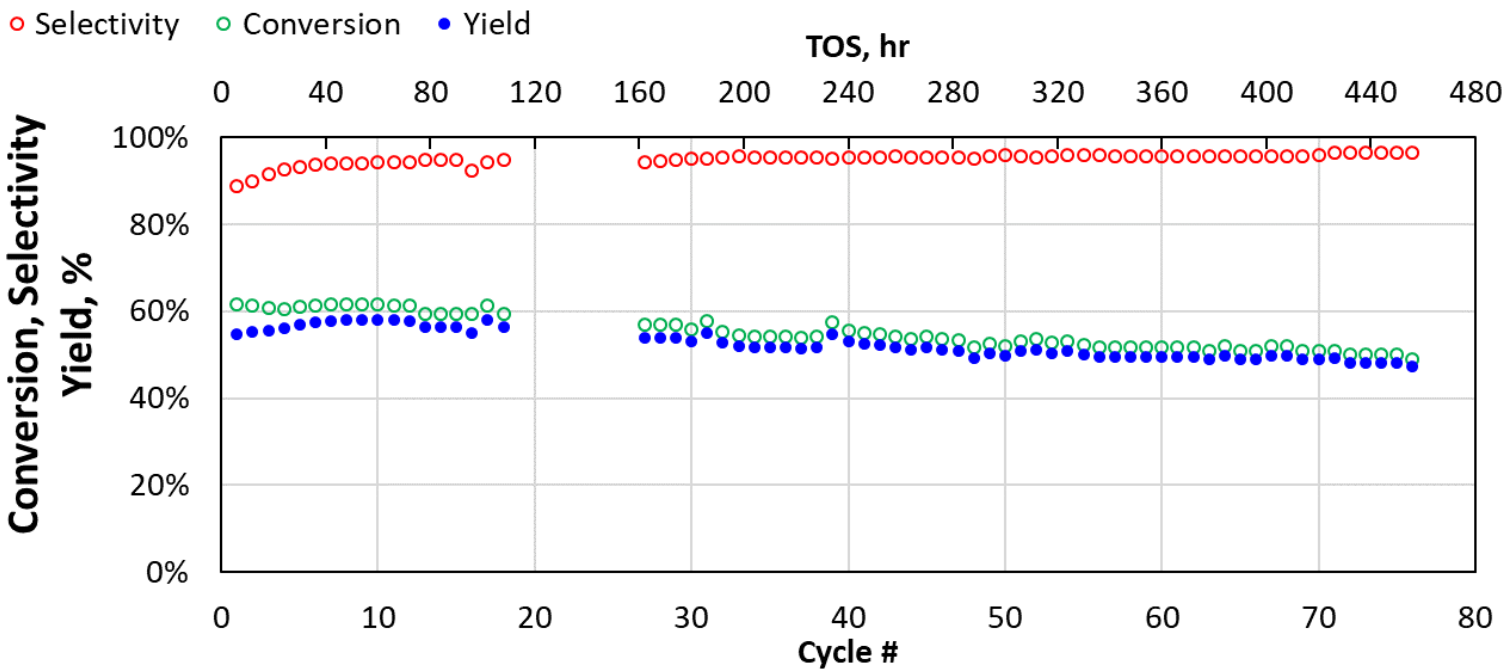
DFG: Environmentally Regulated Flue Gas (**12-14% CO_2, balance N_2 + impurities**)

CAP: Captured CO_2 (**>95% CO_2, balance N_2**)

Catalyst addresses key commercialization issues

Laboratory Scale Results

Long Term Stability: Direct Flue Gas (FG) Utilization



- **Cycle:** 5hr continuous run followed by 1hr air regeneration
- **Feed**: Ethane and simulated flue gas (CO_2 12.5%, 80ppm SO_2, 80ppm NO, Trace O_2 and balance N_2), CO_2:Ethane ~ 1.5
- **Productivity:** Up to 9 mmole/gcat.hr C_2H_4 production

CURRENT PROJECT PROGRESS AND SCOPE

Project Timeline

Task Name	Start	End	Resource
Task 1: Project management and reporting	Fri, 02/01/19	Sun, 01/31/21	SR
Task 2: Field scale preparation and testing	Fri, 02/01/19	Sun, 06/30/19	SR
Task 2.1: Catalyst scale up	Fri, 02/01/19	Sun, 03/31/19	SR
Task 2.2: Catalyst testing in a lab scale reactor	Mon, 04/01/19	Sun, 06/30/19	SR
Task 3 : Technology maturation plan	Mon, 07/01/19	Wed, 07/31/19	SR
Task 4: Procurement and integration of actual flue gas with skid	Thu, 08/01/19	Fri, 01/31/20	SR/NCCC
Task 4.1 Field scale skid preparation and transportation to the host site	Thu, 08/01/19	Mon, 09/30/19	SR
Task 4.2 Integration with the host site and commissioning of the skid	Tue, 10/01/19	Fri, 01/31/20	SR/NCCC
Task 4.3 Development of a baseline ASPEN simulation model	Mon, 09/30/19	Fri, 01/31/20	SR
Task 5: Continuous operation using actual flue gas	Sat, 02/01/20	Mon, 11/30/20	SR/NCCC
Task 6. Techno-economic and life cycle/ technology gap analysis	Tue, 12/01/20	Sun, 01/31/21	SR

Project Financial Overview

	Project duration: 2 years (02-01-2019 to 01-31-2021)	
	DOE funds	**Cost Share**
Total ($)	$1,499,442	$375,458
Total Cost Share %		20%

Baseline reporting Quarter	**Year 1**							
	01/1/2019 – 03/31/2019		04/1/2019 – 06/30/19		07/1/19 – 09/30/19		10/1/19 – 12/31/19	
	Q1	Cumulative Total	Q2	Cumulative Total	Q3	Cumulative Total	Q4	Cumulative Total
Federal Share	46235.4	46235.4	151157.3	197392.7	203707.9	401100.6	155258.0	556358.6
Non-Federal Share	4794.6	4794.6	6875.4	11670.0	25834.2	37504.2	18457.0	55961.1
Total Incurred	51030.0	51030.0	158032.7	209062.7	229542.1	438604.8	173714.9	612319.7

Baseline reporting Quarter	**Year 2**							
	01/1/2020 – 03/31/2020		04/1/2020 – 06/30/20		07/1/20 – 09/30/20		10/1/20 – 12/31/20	
	Q5	Cumulative Total	Q6	Cumulative Total	Q7	Cumulative Total	Q8	Cumulative Total
Federal Share	120293.6	676652.2	161492.0	838144.2				
Non-Federal Share	43469.0	99430.2	58662.7	158902.8				
Total Incurred	163762.6	776082.3	220154.7	997046.9				

Partners: ARTC (Catalyst consultant) **Host site:** NCCC

Technical Approach

- National Carbon Capture Center (NCCC), Wilsonville, AL (*Host site)*
- ~100x catalyst scale up
- Lab scale run using captured CO_2 (Pre-evaluation of scaled up catalyst)
- Total 2000-hr of total testing using **two actual** CO_2 streams (**DFG & CAP**)
- Technoeconomic and Lifecycle assessment (TEA/LCA)

Flow rates for different CO_2 test cases

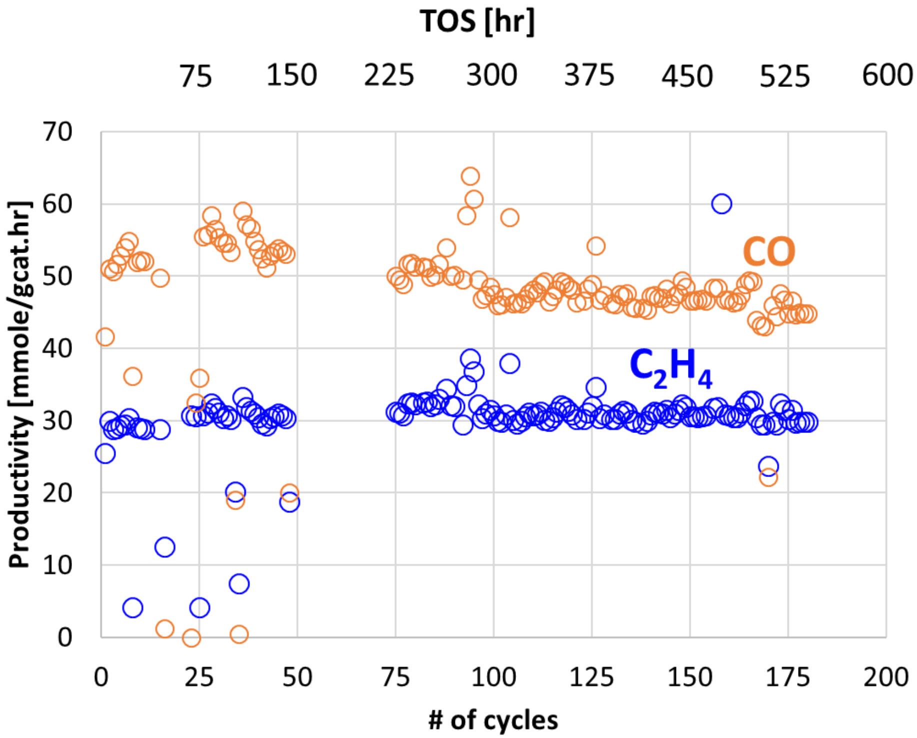
Test Case	Max. flow rate (L/min)				Ethane vol% in feed	Testing duration (hrs)
	Cap. CO_2	Flue gas	C_2H_6	Total Max.		
CAP	10	N/A	5	12	≥ 20%	1000
FG	N/A	12	1	12	≤ 10%	1000

Actual CO_2 composition

	Actual Composition (vol%)
FG	14% CO_2, 4.5% O_2, 68.5% N_2+Ar, 13% H_2O, < 1ppm SO_2, ~ 50ppm NO
CAP	> 99.5% CO_2, balance N_2

Catalyst scale up and validation

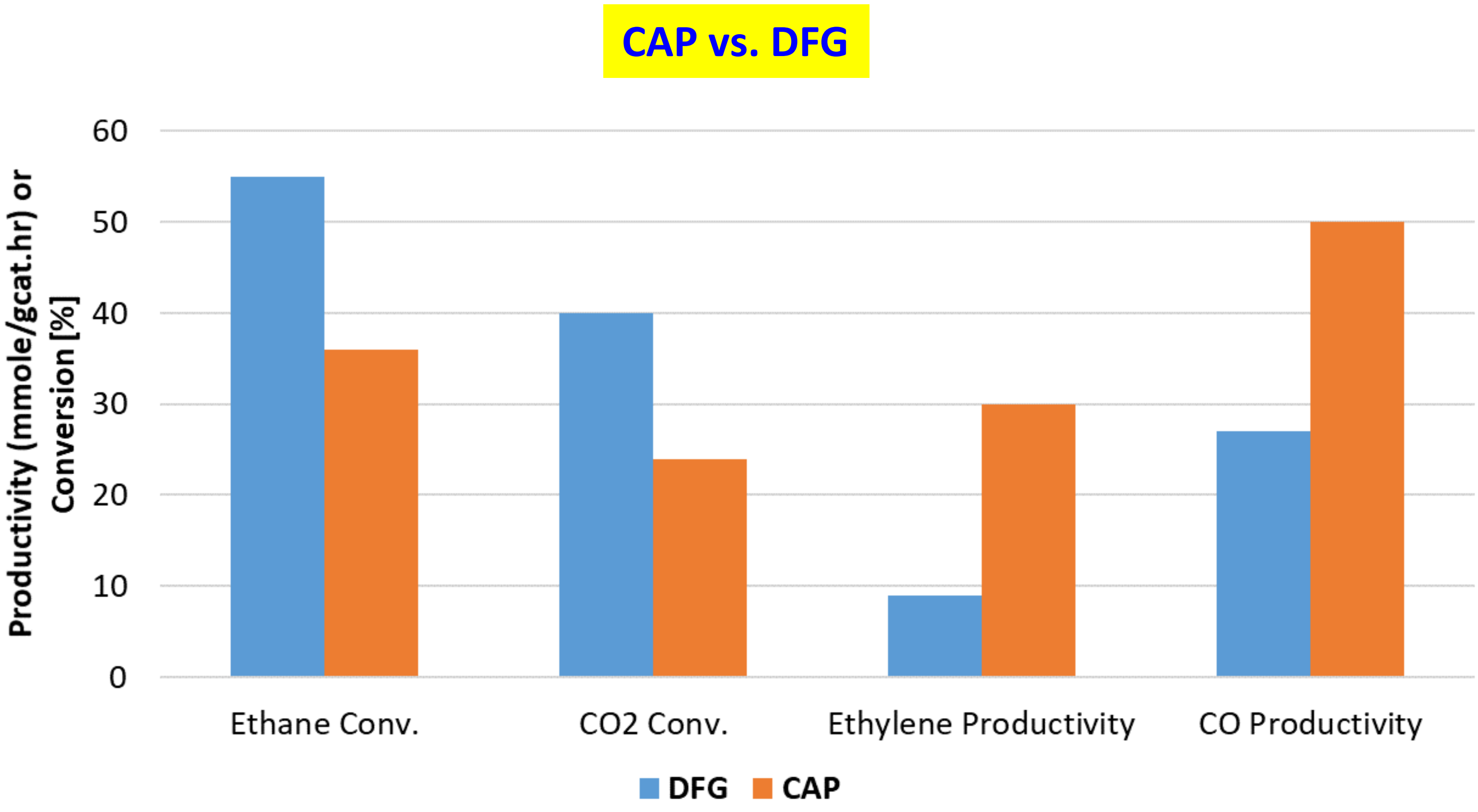
Long Term Stability: Captured CO_2 (CAP) Utilization



C_2H_6 conversion 36%
C_2H_4 Selectivity 90%
CO_2 conversion 24%

- ❑ **Cycle** = 2.5hr continuous run followed by 1hr air regeneration
- ❑ **Feed:** Ethane and simulated captured CO_2 (95% CO_2, balance N_2); CO_2:ethane ~1.5
- ❑ Up to 30 mmole/gcat.hr C_2H_4 production

Performance Summary (Lab scale)



- Higher productivity in CAP (lower reactor volume and capital investment)
- Higher conversion in DFG

Field Scale Skid

- 52” x 76” skid enclosure to maintain Class I, Division 2 and industrial code standards
- Skid successfully transported to NCCC on February 25, 2020

Two cases: 1. Direct flue gas (DFG), 2. Captured CO_2 (CAP)

TECHNO-ECONOMIC ASSESSMENT

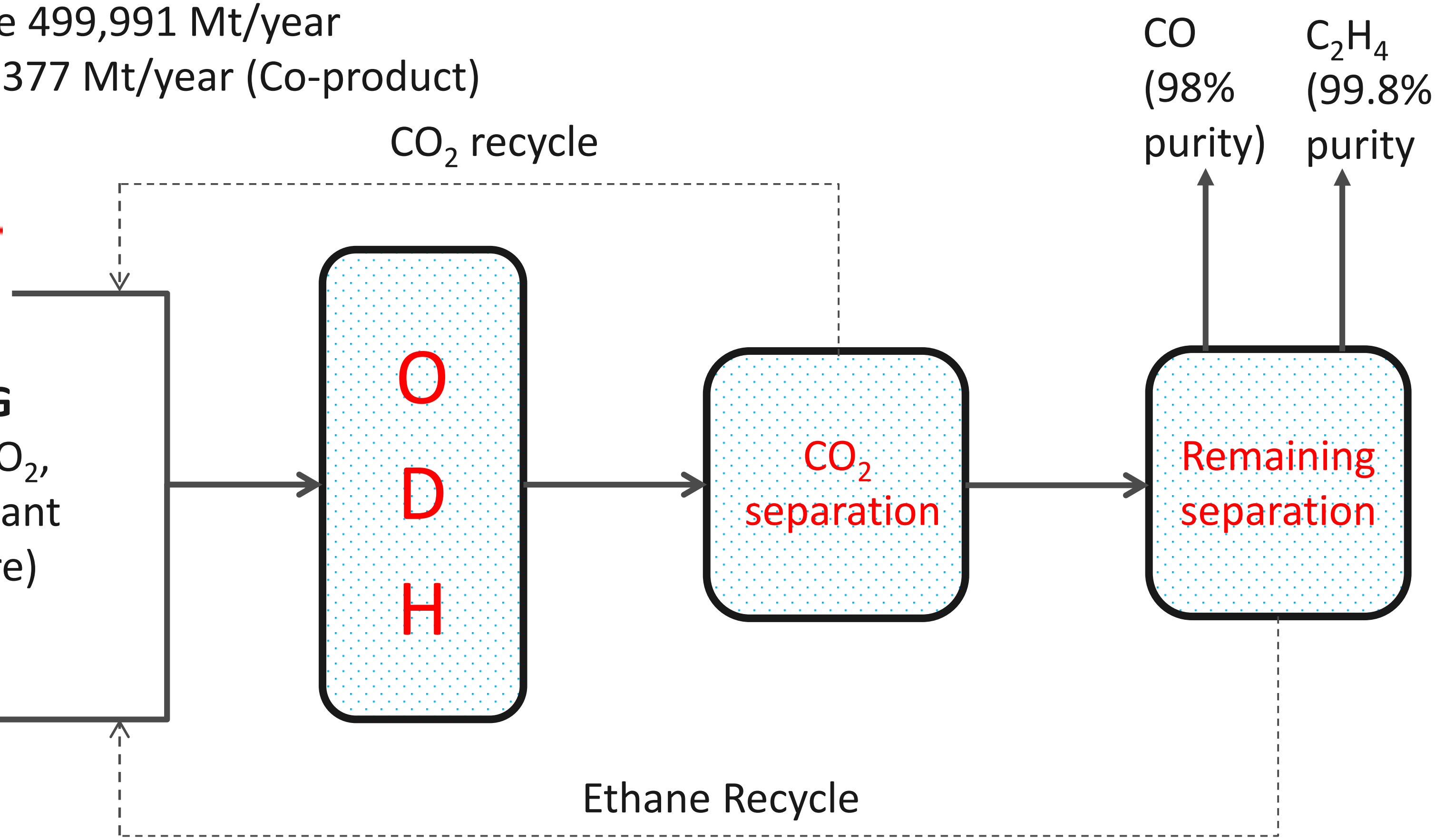
Material Balance

DFG

- **Projected plant capacity**
  - Ethylene 499,991 Mt/year
  - CO 772,377 Mt/year (Co-product)

856 Mt/hr FG
(124.5 Mt/hr CO_2,
160 MW coal plant
with no capture)

110 Mt/hr
Ethane

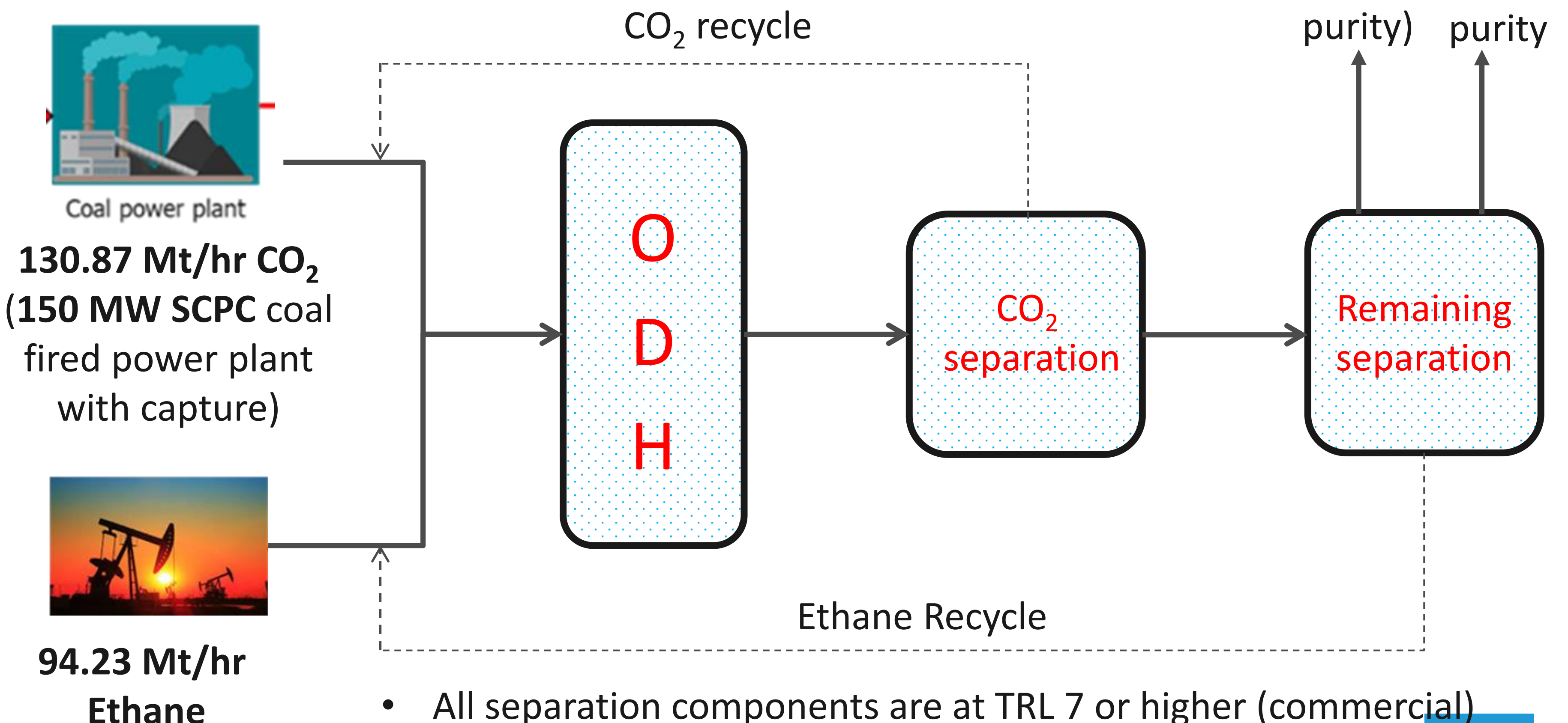


- All separation components are at TRL 7 or higher (commercial)

Material Balance

CAP

- **Projected plant capacity**
  - Ethylene 500,000 Mt/year
  - CO 879,142 Mt/year (Co-product)



- All separation components are at TRL 7 or higher (commercial)

Pricing of Materials/Chemicals

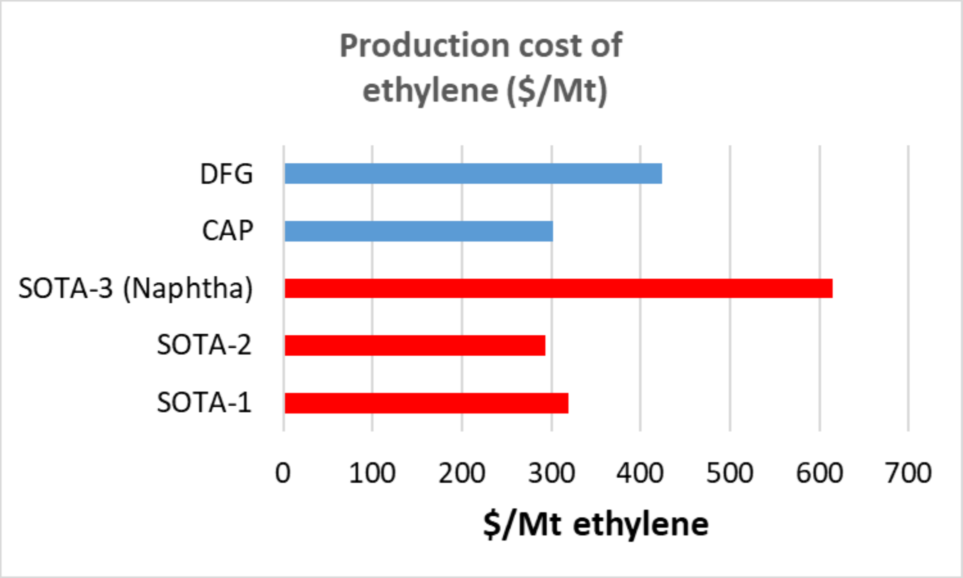
Material	Role	$/unit
Ethane	Raw material	$150/Mt
Flue gas	Raw material	$0.0/Mt
Captured CO_2	Raw material	$40/Mt
Natural gas	Utility	$3.1/ 10^3ft3
Steam	Utility	$3.0/klb

Ref:

1) Ethane price: http://marketrealist.com/2016/05/ethane-prices-fell-4-week-rally-impact-mlps/.
2) Natural gas: eia.gov
3) Steam: How to calculate true steam cost. US DOE. EERE

Cost of Production

Cost type	DFG	CAP
Total permanent investment[1]	$ 811,635,823	$ 410,602,298
Capital depreciation[2]	$ 35,987,442	$ 18,008,872
Annual operating Cost	$ 503,249,579	$ 398,058,669
Total production cost (annual)[3]	$ 539,237,021	$ 416,067,542
Ethylene production cost	**$0.424/kg**	**$0.302/kg**



TEA comparison

Production cost in CAP case is similar to the lowest SOTA[4] case

[1] Includes 25% contingency, 4% (of TDC) land and 10% (of TDC) start-up
[2] 20-year straight
[3] Includes capital depreciation, fixed and variable operating cost

[4] Yang, M., & You, F. (2017). Industrial & Engineering Chemistry Research, 56(14), 4038-4051.

Two cases: 1. Direct flue gas (DFG), 2. Captured CO_2 (CAP)

LIFE-CYCLE ASSESSMENT (LCA)

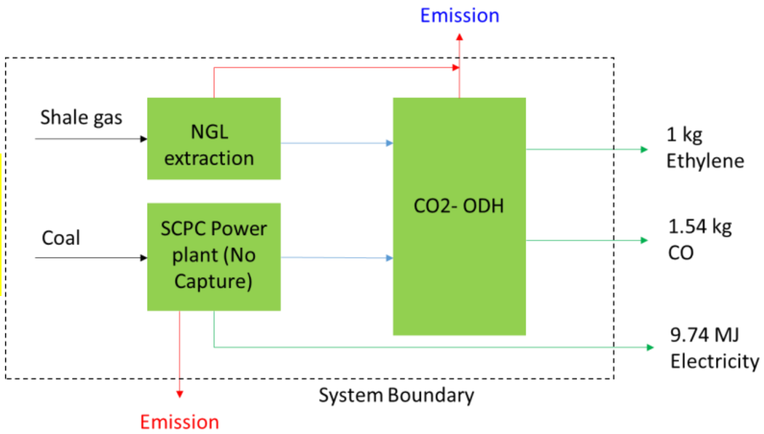
Database Libraries

Following database libraries were used in openLCA–

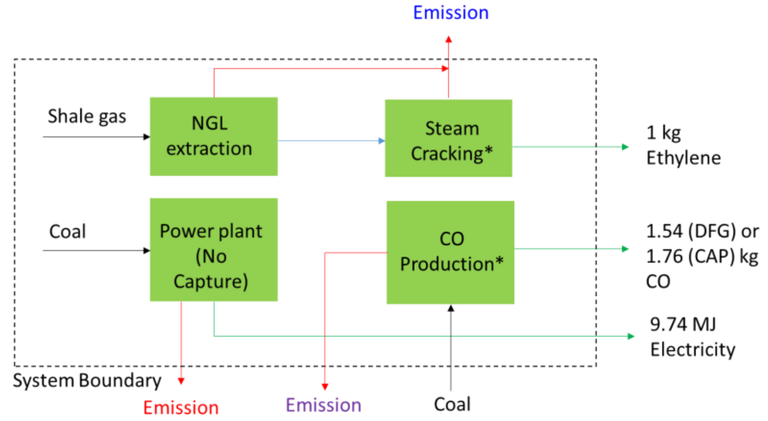
- Power plants - *NETL process library*
- *Ethylene, materials, production, organic compound, at plant, kg* (lcacommons.gov)
- *Carbon monoxide, at plant* (lcacommons.gov)
- PI generated laboratory scale data

System Boundary

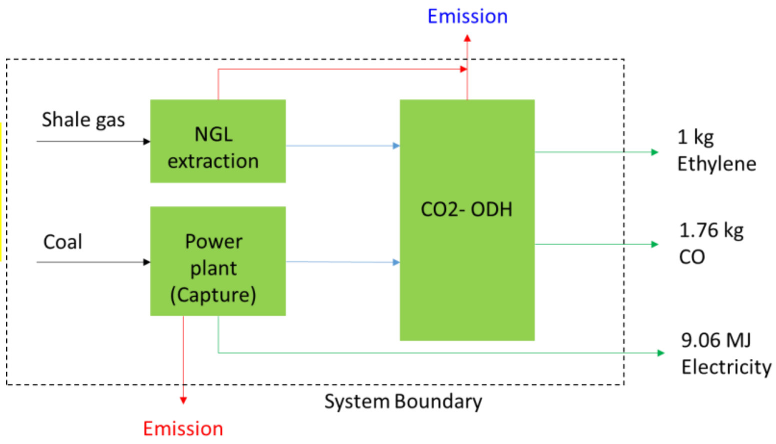
DFG



SOTA-Baseline

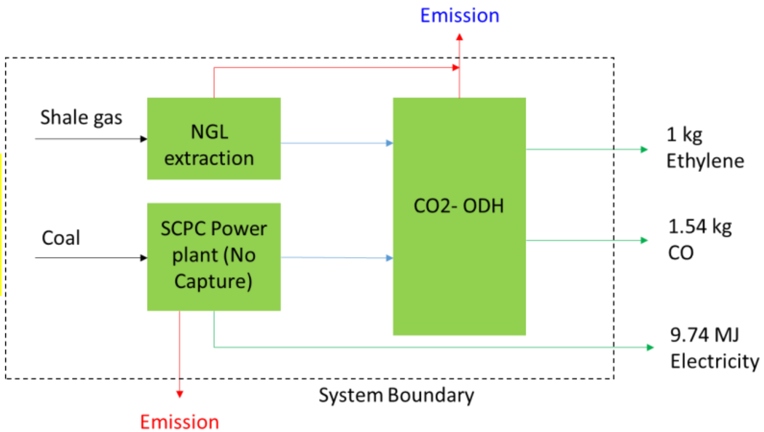


CAP

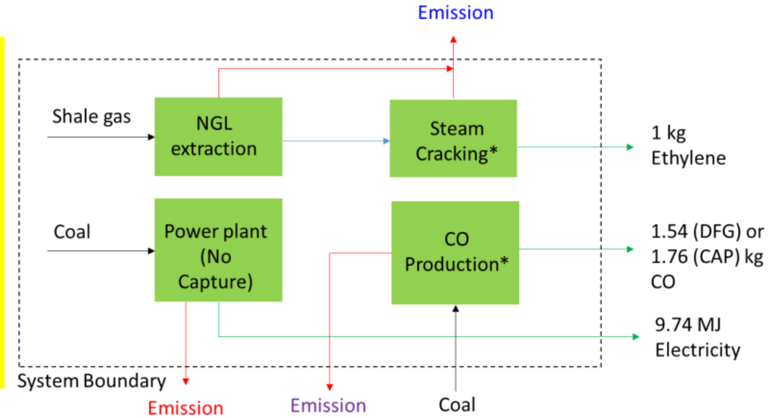


LCA Summary

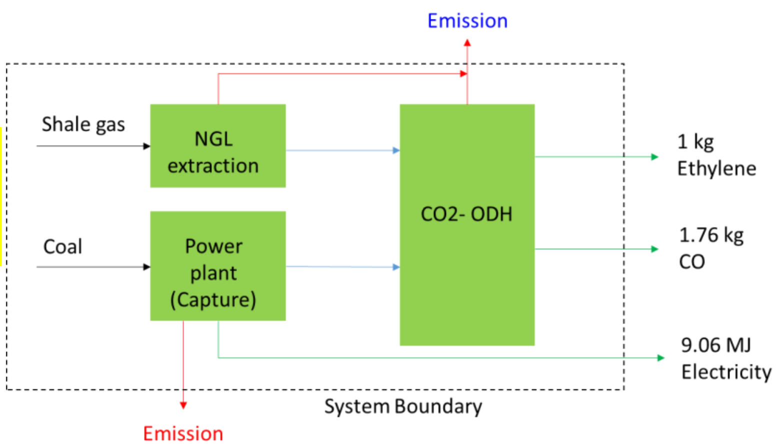
DFG



SOTA-Baseline

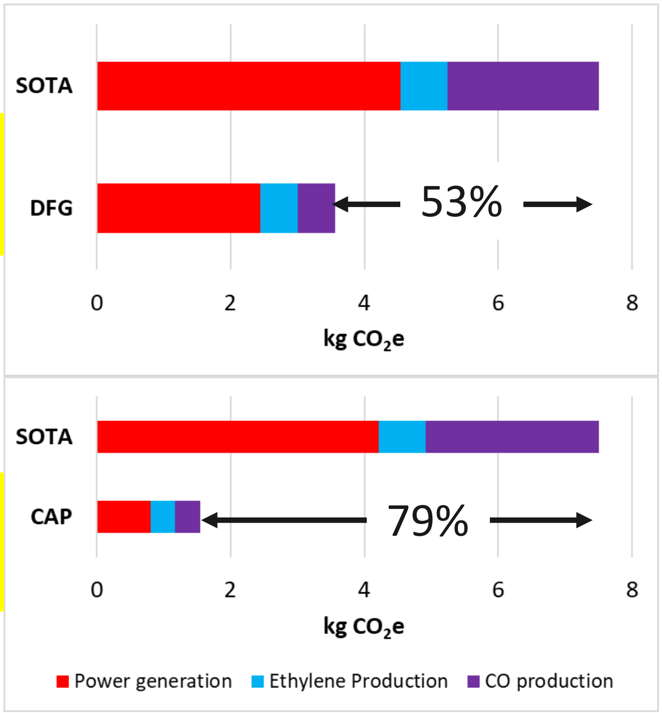


CAP



DFG

CAP



- 53 (DFG) – 79 (CAP)% reduction in CO_2 emission compared to SOTA baseline

Future Plans

- **Complete ongoing project**
  - Complete a cumulative 2000-hr testing on field scale
  - Update TEA/LCA

- **Recommendations for future research include -**
  - Other sources of real CO_2 wastes: Concentration/Purity
  - Product processing and separation
  - Process scale up with separation
  - Co-product utilization

Acknowledgement

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Thank you!

Questions/Comments?