Kick-off meeting

Cooperative Agreement Number: DE FE0029570

Low temperature process utilizing nano-engineered catalyst for olefin production from coal derived flue gas

Principal Investigator: Amit Goyal
Co-Principal Investigator: Jadid Samad
DOE FPM: Sai Gollakota

6/9/2017

Meeting Agenda

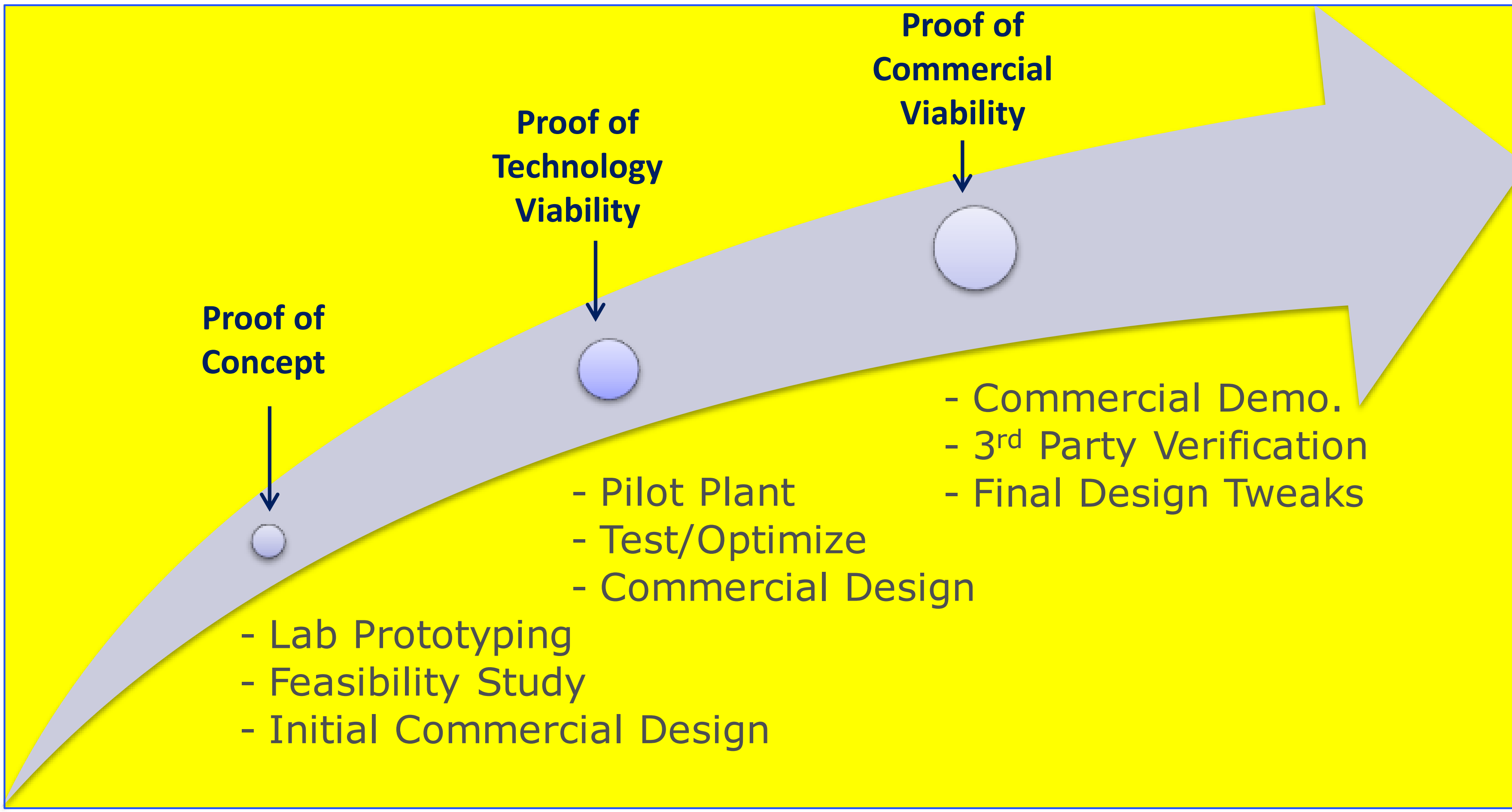
❑ Attendee introductions	9:00-9:15 AM
❑ Project overview	9:15-9:45 AM
❑ Project structure	9:45-10:15 AM
▪ Project schedule and task summary	
▪ Task description and Progress/plans	
❑ Open discussion	10:15-11:00 AM

Introduction to Southern Research

Southern Research Institute

- Established in 1941 in Birmingham, Alabama as an independent, 501-(c)-3 center for scientific research and development.
- A proven team of 450 technologists across 5 U.S. states organized into three divisions:
  - Engineering, Energy and Environment (E&E)
  - Drug discovery
  - Drug development (pre-clinical)
- Funding 71% Federal and 29% commercial.
- Discovered 7 FDA-approved cancer drugs and evaluated half of all the FDA-approved oncology drugs.
- Worked with NASA since the 1960s.
- Operating the state of Alabama's first solar and energy research centers.
- Helped develop a crucial HIV treatment.
- Developing sustainable energy and manufacturing processes.

Full Pathway to Technology Commercialization



Operating locations

1. Corp Offices & Drug Research - Birmingham, AL
2. Advanced Energy Technologies - Durham, NC
3. Engineering Research Center - Birmingham, AL
4. Engineering/Flight Ops Support - Ellington Field, TX
5. Program Management/Engineering - Huntsville, AL
6. Infectious Disease Research Labs - Frederick, MD
7. National Carbon Capture Center - Wilsonville, AL
8. Water Research Center - Cartersville, GA

Birmingham research centers

Combustion Research Facility
Southeastern Solar Research Center
Energy Storage Research Center

Regional research centers

National Carbon Capture Center, Wilsonville, AL
Water Research Center Cartersville, GA
Clean Technology Development Center Durham, NC

Energy and Environment (E&E)

LOW CARBON ENERGY SYSTEMS

- carbon capture
- emissions control
- waste heat to power
- biomass to energy
- photovoltaics
- energy storage
- Gen IV nuclear

WATER TREATMENT

- management of industrial brines and waste waters
- engineered biology for contaminant removal from watersheds
- water quality monitoring

SUSTAINABLE CHEMISTRY

- catalyst and process development for cost competitive conversion of bio-derived raw materials to fuels and chemicals
- chemical process intensification

RESOURCE RECOVERY

- “mining” valuable metals (e.g., Li, Ge, Gd, Zn) from industrial wastes
- nutrient recovery from agriculture waste streams

INTENSIVE FOOD PRODUCTION

- development of food protein production using engineered aquatic plant systems
- combined carbon capture, water treatment and food production

Energy and Environment (E&E)

Technology Evaluation

- Independent lab and field validation of new processes and equipment
- Modeling, Aspen-based process simulation, Techno-economic evaluation and life-cycle assessment

Lab, Bench, and Pilot-plant facilities

- Lab to pilot-scale testing of chemical and thermal processes
- Catalyst and sorbent preparation, testing, and scale up
- Chemical, structural and spectroscopic characterization

Technology Development

- Novel catalysts and sorbents that solve critical energy and sustainability problems
- Catalyst and sorbent-related intellectual property creation in diverse fields

Recent Technology Innovations

DOE/NETL funded:

- Sulfur-tolerant high temperature reforming catalyst (Patent application) – **DE-FE0012054**
- Combined CO_2 capture and water-gas shift reaction process – **DE-FE0026388**
- Selective gas to liquids for diesel or jet fuel production – **DE-FE0024083, DE-FE0010231**

Other major projects:

- Conversion of biomass sugars to platform chemicals and carbon fiber (2 patent applications)
- CO_2 Sorbents for thermochemical energy storage (Patent application)
- Biomass/Biomass-Coal down draft gasification
- Mild liquefaction process for biomass to diesel
- Germanium recovery from flue gas pond ash

Project overview

- Goals/objectives
- Proposal summary
- Relevance
- Chemistry of process
- Comparison with state of art processes
- Project budget and participant roles
- Major milestones and deliverables
- Success criteria

Goals/objectives

- Large volumes of CO_2 emission from fossil fuel based power plants, significant portion of which are often released to the atmosphere.
- CO_2 to chemical possible yet energy intensive (and hence cost prohibitive) due to low energy state of CO_2 molecule.
- Current commercial utilization of CO_2 is very small compared to total emission.
- Research needs to reduce energy demand, low cost materials/process designs, integration with coal-fired power plant.
- The project seeks to develop a technology that can utilize CO_2 from coal-fired power plants to reduce the emissions and create valuable products to offset the cost of Carbon Capture and Storage (CCS).

Goals/objectives (Contd.)

- This project falls under the purview of area of interest 3 of the FOA : **NOVEL PHYSICAL AND CHEMICAL PROCESSES FOR BENEFICIAL USE OF CARBON.** The objective is to–

"Demonstrate of innovative concepts for beneficial CO_2 use via novel physical and/or chemical conversion processes, which include high energy systems and nano-engineered catalysts that can transform CO_2 into valuable products and chemicals (i.e., carbon fibers or plastics) while significantly reducing the energy demand/over potential required for the conversion process"

- Novel approaches to breaking the bonds between carbon and oxygen to generate carbon monoxide (CO), oxygen (O_2), and/or elemental carbon that can be used as building blocks for the chemical industry.

- Early technology readiness levels, typically 2-3.

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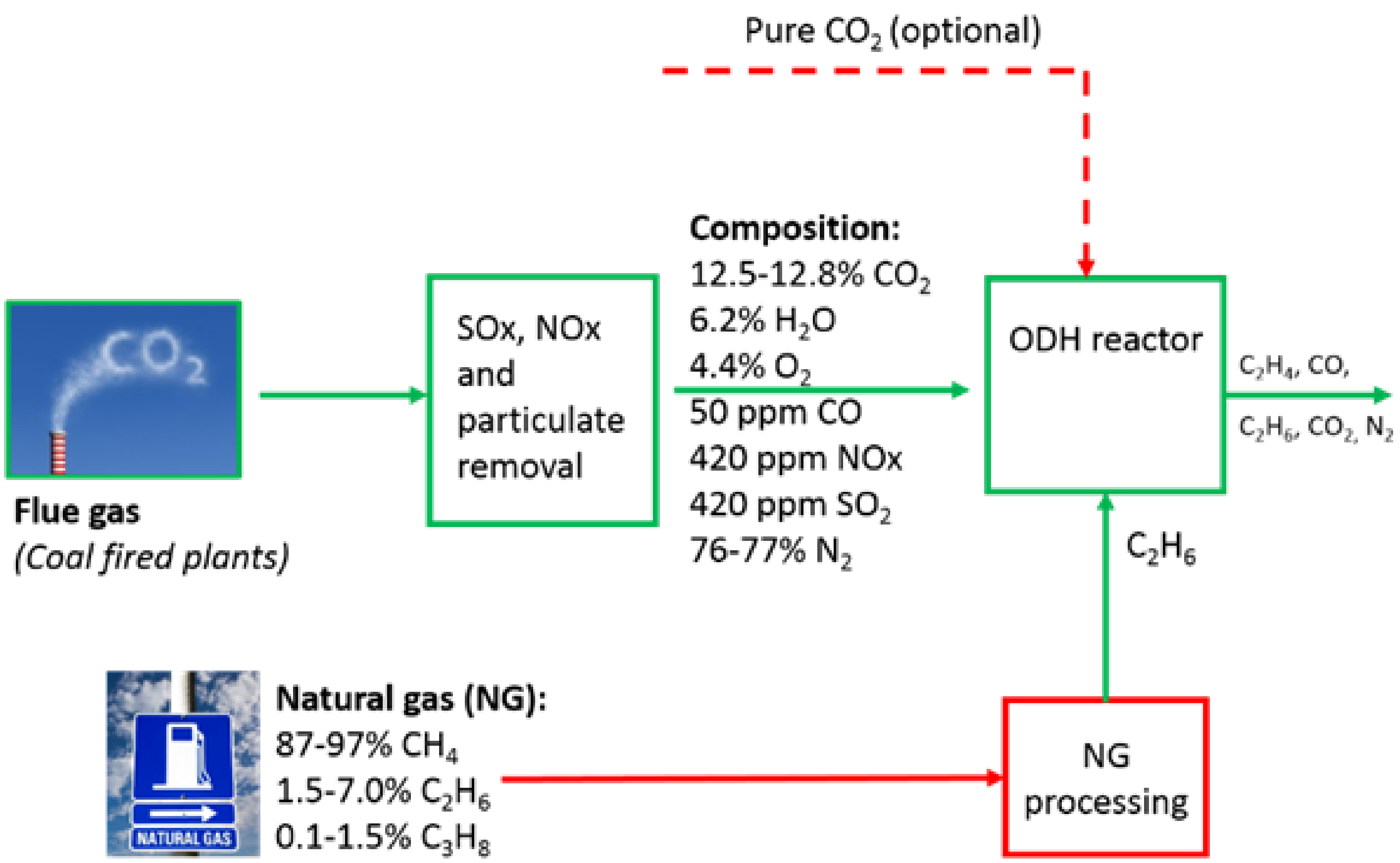
Proposal summary

- The process uses ethane and CO_2 to produce ethylene via oxidative dehydrogenation (ODH) pathway.
- Sourcing ethane from abundantly available and low priced natural gas and CO_2 from coal fired flue gas stream with partial removed impurities.
- Use of nano-engineered mixed oxide catalysts.
- Catalyst screening using pure ethane and pure CO_2.
- Catalyst stability and performance evaluation on the screened catalysts in presence of 'partially removed' flue gas impurities (SOx, NOx, H_2O, O_2).
- Produces ethylene and CO, two highly desirable platform chemicals which are proposed to be co- or separately processed.

Proposal summary (Contd.)



A commercial embodiment for the proposed ODH process

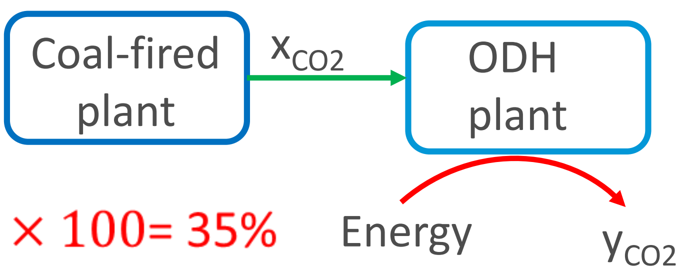
Relevance

- Ethylene is the highest producing petrochemical in the world (334 billion lb/year)[1]. U.S. produces ~20% of the worldwide ethylene[2].
- Ethane is abundantly available here in the U.S. due to the growth of shale gas. Currently a great deal of purified and separated ethane is readily available at an already lower cost (~$68 per metric ton).
- Globally, ethylene production is ranked as the second largest contributor of energy consumption (1% of world's total energy) and GHG emissions (180-200 million tons of CO_2 per year) in the global chemical industry[3,4].
- Coal based electric power sector in U.S. emitted 1241 million tons of CO_2 in 2016 alone[5].

[1]http://energy.globaldata.com/media-center/press-releases/oil-and-gas/us-and-china-driving-global-ethylene-capacity-to-record-208-million-tons-per-year-by-2017-says-globaldata. [2]Maffiaet al (2016). *Topics in Catalysis*: 1-7. [3]Ren et al *Energy* 31.4 (2006): 425-451. [4]Yao, Y. et al (2015). *Industrial & Engineering Chemistry Research*, *55*(12), 3493-3505. [5]https://www.eia.gov/tools/faqs/faq.php?id=77&t=11

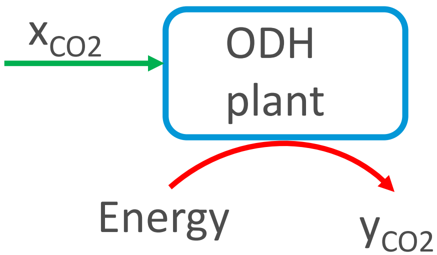
Relevance (Continued)

- Due to large scale of ethylene production, the scale of CO_2 consumption via proposed ODH would be significant.
- Initial estimates suggest a 1 million tons/year capacity ethylene plant operated in the proposed process next to a 200MW coal fired plant could potentially consume all CO_2 emitted from the power plant.
- A combined coal fired power plant and the proposed ODH plant can reduce 35% of the overall CO_2 emission **(Fig 1).**
- A stand alone ODH plant would consume 56% more CO_2 as a reactant than it would emit because of the energy requirement of the process **(Fig 2).**



$$\frac{y_{CO2}}{x_{CO2}} \times 100 = 35\%$$

Fig. 1



$$\frac{x_{CO2} - y_{CO2}}{y_{CO2}} \times 100 = 56\%$$

Fig. 2

Comparison with state of art

Two competing processes -

(1) Ethane steam cracking (SC) and

(2) Ethane oxidative dehydrogenation by O_2 (ODH(O_2))

Aspects	SC	ODH (O_2)	ODH (CO_2)
Commercialization status	Commercial	Research	Research
Reactants except hydrocarbons	Steam	Air /O_2	CO_2
Exothermocity	Lowest	Highest	Intermediate
Operating Temperature	750-900°C	<500°C	<700°C
CO_2 emission	+	+	- (consumption)
Major by-product(s)	C_1-C_4 alkanes/olefins	CO_2	CO
Selectivity to Ethylene	80% (yield)	Up to 90%.	>90%
Catalyst	Steam	Expensive mixed oxides	Low cost mixed oxides.
Chemical safety risk	Low	Highest	Lowest

Project budget and participant roles

DOE/NETL Share: $ 799,442 (80%) **Southern Research:** $200,418 (20%)

Project duration: 2 years April 1, 2017-March 31, 2019

	Budget Period 1		Budget Period 2		Total Project	
	4/1/2017-3/31/2018		4/1/2018-3/31/2019			
DOE Share	$ 398,617.00	80%	$ 400,825.00	80%	$ 799,442.00	80%
Cost Share	$ 100,209.00	20%	$ 100,209.00	20%	$ 200,418.00	20%
Total Cost	$ 498,826.00		$ 501,034.00		$ 999,860.00	

Participants and Roles

Southern Research: Lab-scale reactor system design and commissioning, Product analysis, Catalysis Synthesis and Characterization, Catalyst Deactivation studies, Reports and deliverables.

Petrochemical consultant: Guidance on catalyst design, testing and industrial requirements for integration with utility and petrochemical sectors especially with respect to easy retrofits and early adoption opportunities.

Partner Company: Guidance on flue gas characteristics, composition, heat integration with coal fired plant and opportunities to use other CO_2 streams within plant.

Major milestones and deliverables

BP	Task/ Subtask	Milestone Description	Planned Completion	Verification Method
1	1	Updated Project Management Plan	5/31/2017	PMP file
1	1	Kickoff Meeting	6/7/2017	Presentation file
1	2	Catalyst identified for >60% yield of ethylene from ethane	12/31/2017	Letter Report to DOE
1	2	Go/No-Go Decision Point: At least two catalyst prepared and tested for acceptable level of performance ≥60% yield	3/30/2018	Letter Report to DOE
2	4	Complete impact of impurities on the catalyst activity	9/30/2018	Letter Report to DOE
2	4	Technical Decision Point: Identify levels of impurities acceptable and assess impact of impurity removal on process economics	9/28/2018	Letter Report to DOE
2	5	Complete long term stability tests	2/30/2019	Letter Report to DOE
2	6	Technical Decision Point: TEA and LCA assessment to calculate ethylene production cost and net CO_2 reduction	3/30/2019	Letter Report to DOE
2	1	Draft Final Report	6/30/2019	Report file to DOE

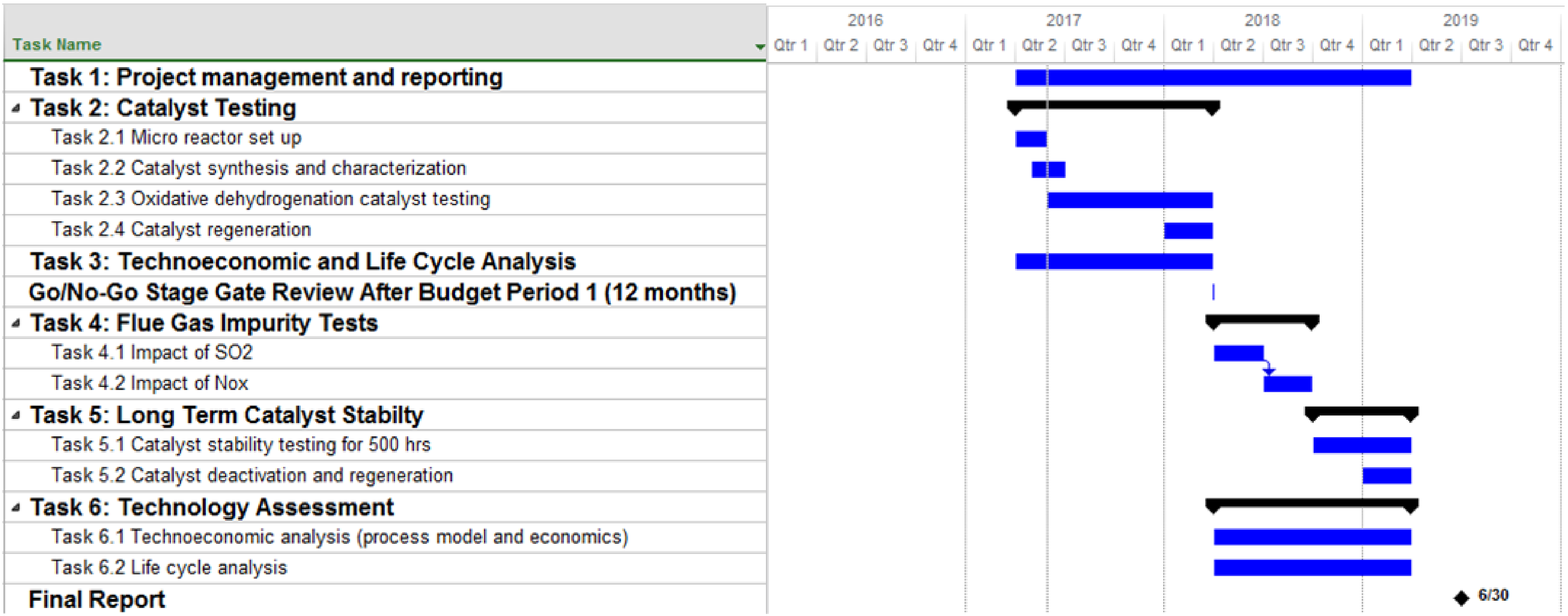
Success criteria

Decision Point	Date	Success Criteria
Go/No-Go Decision Point: At least two catalyst prepared and tested for acceptable level of performance	3/30/2018	Two catalysts with ≥60%yield of olefin demonstrated
Technical Decision Point: Identify levels of impurities acceptable and assess impact of impurity removal on process economics	9/28/2018	Level of SO_2 and NO_X that are acceptable for catalyst without deactivation determined. Feed will contain up to 400 ppm of SO_2 and NOx for testing.
Technical Decision Point: TEA and LCA assessment to calculate ethylene production cost and net CO_2 reduction	3/30/2019	Final cost of ethylene compared with conventional ethylene production and lower then $1/kg. CO_2 consumption determined and integrated with coal-fired power plant to demonstrate net benefit.

Project structure

- Project schedule and task summary
- Task description and Progress/plans

Project schedule and task summary



Task description and Progress/plans

Start of Budget Period (BP) 1

Task 1: Project management and reporting

- Revised Project Management Plan (PMP) upon award; updated periodically as necessary
- Regular updates to/discussions with project participants for coordination/scheduling
- ***Kick-Off Meeting upon award***; additional Project Review Meetings as appropriate
- Quarterly Technical, Financial, and Other Reports to DOE/NETL per FARC
- Papers at national conferences.
- Final Technical/Scientific Report

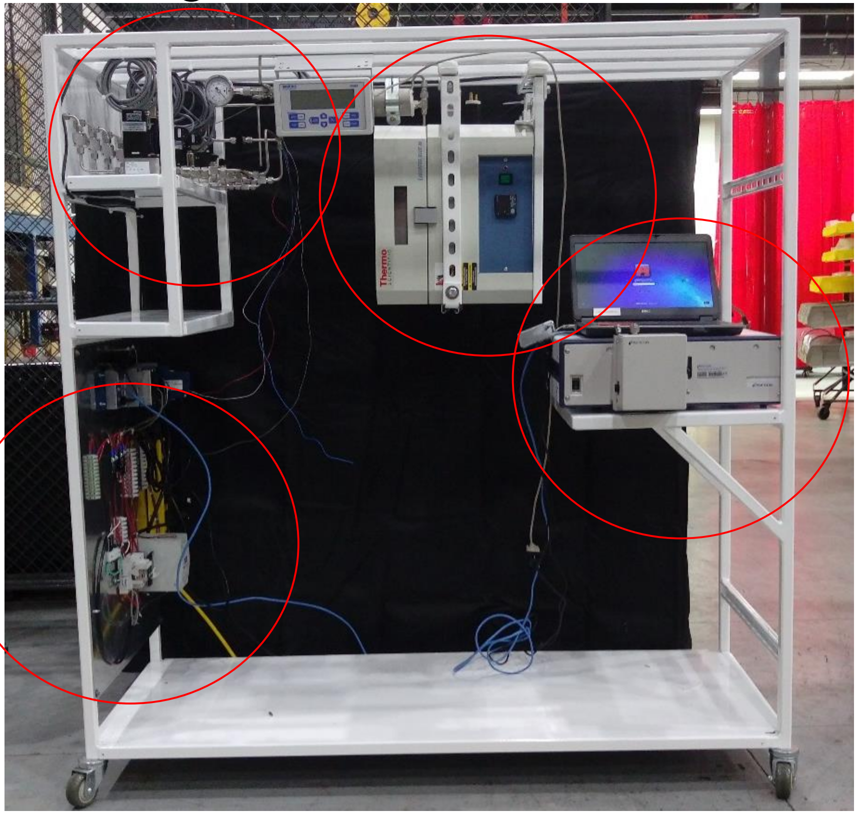
Task description and Progress/plans

Task 2: Catalyst testing

Task 2.1 Microreactor setup (Contd.)

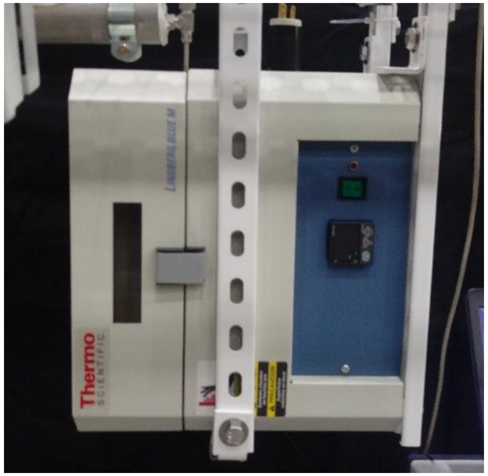
① 5 separate gas lines

② COM system



① ② ③ ④

Photograph of skid



③ Reactor furnace

④ Inficon Micro GC (Representative)

Task description and Progress/plans

Task 2: Catalyst testing

Task 2.2 Catalyst synthesis and characterization

- Catalyst formulation

Functionality	ID
Redox	**RD**
Acid-base	$\mathbf{A_xB_y}$
Ethane activation	**EA**
Ethylene selectivity	**ES**

- Careful balance of each functionality important.
  - Study catalytic performance using one component at a time.

Task description and Progress/plans

Task 2: Catalyst testing

Task 2.2 Catalyst synthesis and characterization (Contd.)

- Following characterization tools will be used –
  - BET – Surface area and pore size distribution
  - XRD – Oxide phase
  - Temperature programmed reduction/oxidation/desorption (TPR/TPO/TPD)
    - Acid-base sites
    - Redox function
  - Thermogravimetric analysis (TGA)
    - Coking on spent catalyst (Catalyst deactivation)

Task description and Progress/plans

Task 2: Catalyst testing

Task 2.3 Oxidative dehydrogenation catalyst testing

- As the reactor skid is being fabricated and readied for operation, a series of catalysts were synthesized and tested in an in-house, smaller scale catalyst testing apparatus.
  - Rapid catalyst screening
  - Onset temperatures of reactants (ethane and CO_2)
  - Qualitative comparison of catalytic performance

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Task description and Progress/plans

Task 2: Catalyst testing

Task 2.4 Catalyst regeneration

- Catalyst deactivation.
- Coking (TGA analysis).
- Regeneration scheme.
  - Process condition (Temperature)
  - Gas flow (Air/CO_2)

Task description and Progress/plans

Task 3: Techno-economic lifecycle analysis

- Preliminary techno-economic analysis (TEA) and life cycle analysis (LCA).
- Initial conceptual design.
- These results will serve as a starting point and help guide the BP2 and the design of full commercial embodiment.

End of Budget Period (BP) 1

Task description and Progress/plans

Task 4: Flue gas impurity tests

- Screened catalysts exposed to flue gas impurities. Their compositions will be representative of flue gas compositions:
  - O_2
  - H_2O
  - SOx
  - NOx

Task 5: Long term stability

- Catalytic run for up to 500hrs using simulated gas stream containing flue gas impurities.

Task description and Progress/plans

Task 6: Technology assessment

- Techno-economic analysis
- Life cycle analysis
- Technology gap analysis
  - Identify major/critical components for the proposed process
  - Performance, Cost, Emissions, Market, and Safety Metric advantages
  - R&D gaps and TRL levels
  - Potential vendors for commercial equipment
- Recommended flue gas composition
- Recommended catalyst composition

Thank you for your attention