DE-FE0031869

Core-Shell Oxidative Aromatization Catalysts for Single Step Liquefaction of Distributed Shale Gas

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Project Partners: **West Virginia University, Lehigh University, Susteon Inc. and Shell**

DOE/NETL Project Manager: **Anthony Zammerilli**

08/27/2021

Outline

- Project Overview and Technology Background
- Technical Approach and Current Status
- Future development plan
- Summary

Project Overview

Period of Performance: 04/01/2020 - 06/30/2023 (two budget periods)

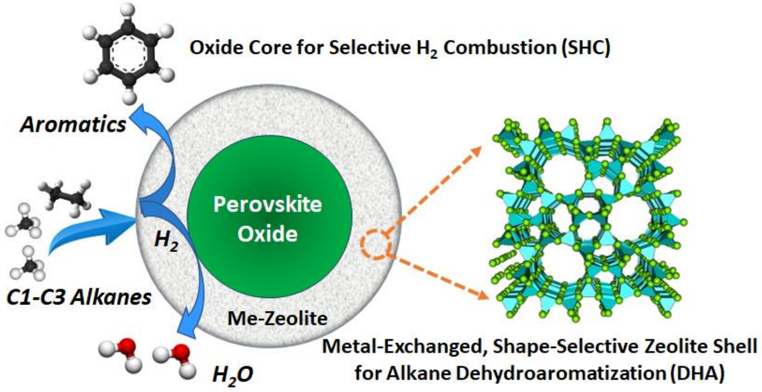
	DOE Funds	Cost Share
NC State Univ. *Dr. Fanxing Li*	***$359,940***	***$68,452***
Lehigh Univ. *Dr. Israel Wachs*	***$290,000***	***$80,268***
West Virginia Univ. *Dr. John Hu*	***$270,001***	***$67,500***
Susteon Inc. *Dr. Raghubir Gupta*	***$80,030***	***$15,000***
Shell (CS Only)	***$0***	***$25,000***
Total ($)	***$999,971***	***$256,220***

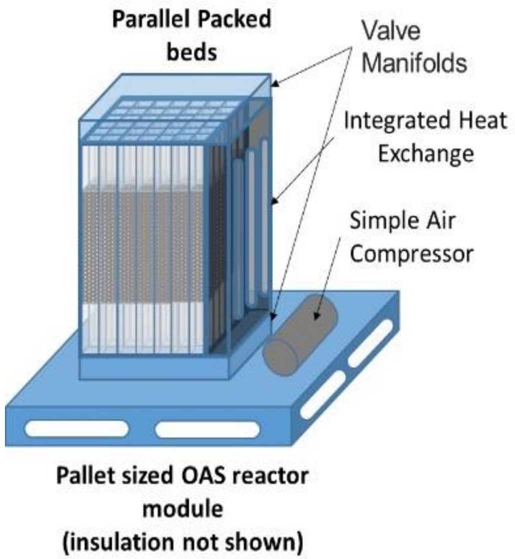
Project Objective: To design and demonstrate multifunctional catalysts to convert the light (dry) components of shale gas into liquid aromatic compounds and water in a modular oxidative aromatization system (OAS).

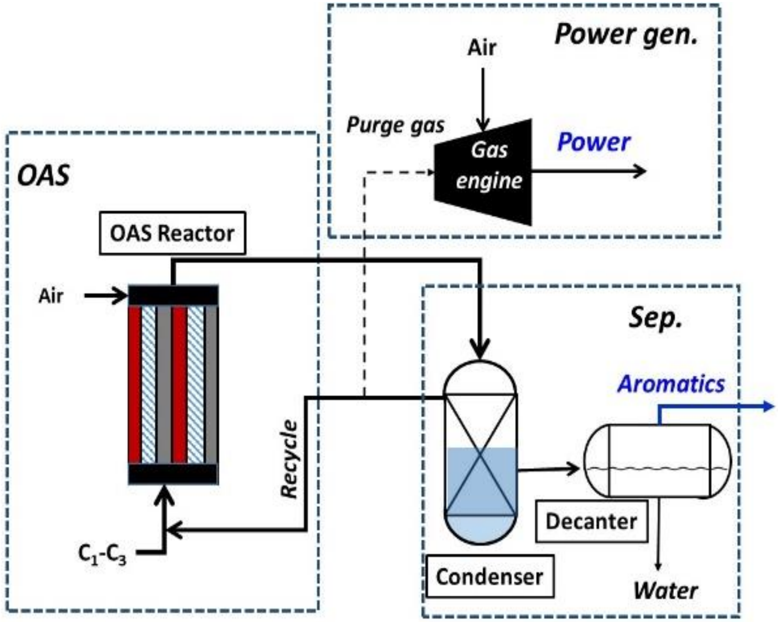
BP1 Go/No-Go: Report Dehydroaromatization (DHA)/ selective hydrogen combustion (SHC) physical mixture (or composite) with > 800 g/kgCat-hr aromatics productivity at <700 °C.

End of Project Goals: (1) Report SHC-DHA catalysts for 100 hours of continuous operation with >40% single pass aromatics yield and <5% deactivation; (2) Confirm 90% overall aromatics yield and 25% return on investment using refined process model.

Modular Oxidative Aromatization System (OAS)

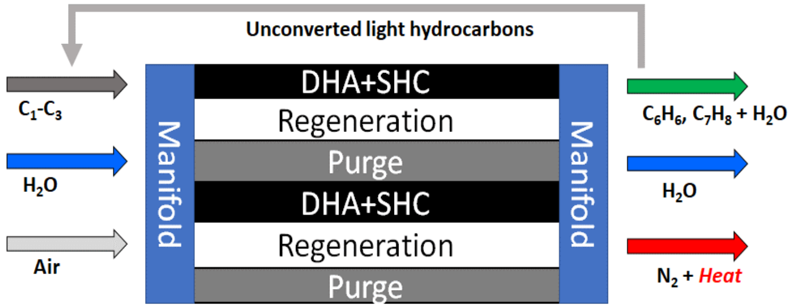






Cyclic operation in two steps:

- **DHA+SHC:** $6CH_4 + 9[O] \rightarrow C_6H_6 + 9H_2O$
- **Regeneration:** $O_2 \rightarrow 2[O] + \text{heat}$
- Steam purge between steps, also prevents CO_x accumulation;

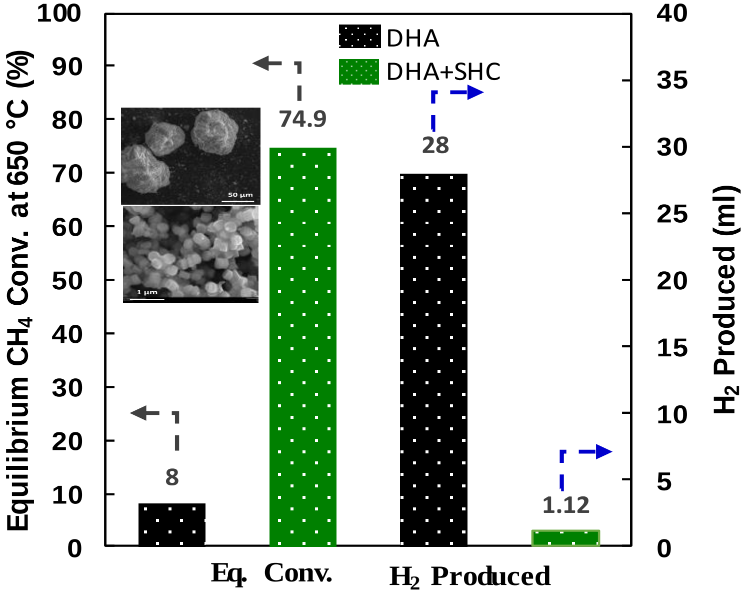


Conventional methane and ethane dehydroaromatization (DHA) is both highly endothermic and equilibrium limited.

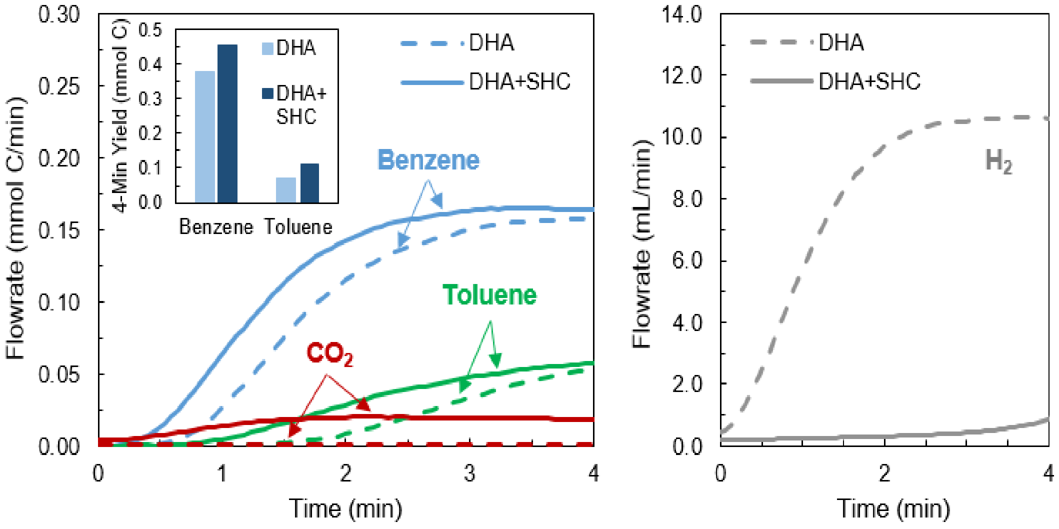
$$6CH_4 \leftrightarrow C_6H_6 + 9H_2 \qquad (\Delta H = 722\ \text{kJ/mol})$$

Integrating a zeolite catalyst shell on a perovskite oxide-based selective hydrogen combustion core can: (a) facilitate autothermal operation; (b) eliminate equilibrium limitation; (c) inhibit coke formation; (d) allow modular conversion of C1-C3 alkanes to aromatics in a greatly simplified process.

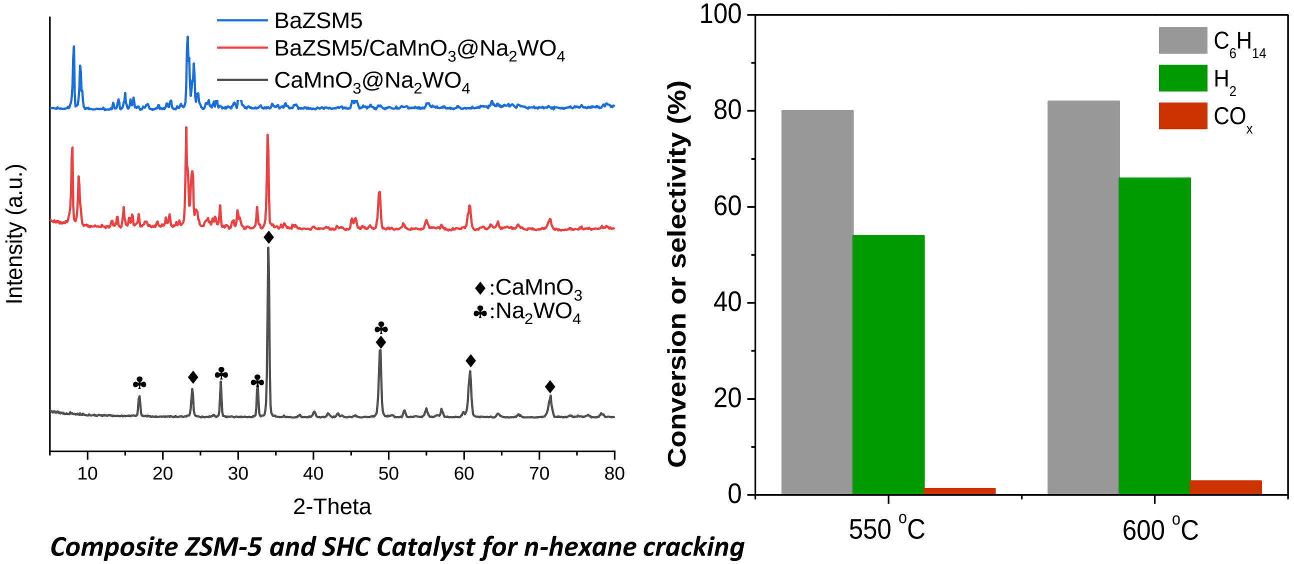
Preliminary Data for the OAS Concept



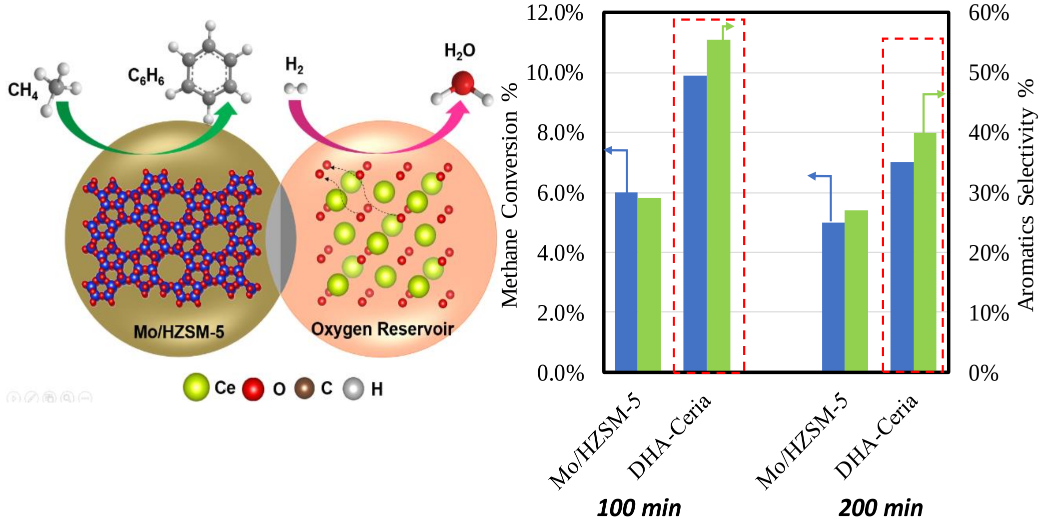
H_2 combustion can lead to 10-fold increase in equilibrium aromatic yield.



Effect of SHC redox catalyst on DHA in a sequential bed configuration



Composite ZSM-5 and SHC Catalyst for n-hexane cracking



Dudek, et al. AIChE Journal, 2018. 64(8): 3141-3150

Zhang and Jiang, Chemical Communications 2018, 54(73): 10343-10346

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Technical Approach

BP1 (Month 1-18): SHC, DHA, and SHC-DHA catalyst optimizations and preliminary design/TEA.

Task 2 (Q1-Q4). SHC redox catalyst optimization (NCSU) and DHA catalyst optimization (WVU and Lehigh)

Milestone 2.1: SHC catalyst screening, Q1
Milestone 2.3.1: DHA catalyst screening, Q3
Milestone 2.3.2: DHA catalyst characterization, Q3

Task 3 (Q4-Q6). SHC-DHA catalyst development (NCSU, Lehigh, and WVU)

Milestone 3.1: SHC-DHA catalyst screening, Q5
Milestone 3.2: G0/No-go, Q6

Task 4 (Q3-Q6). Process design, optimization and simulation (Susteon)

Milestone 4.0: Process Model, Q4

BP2 (Month 19-36): SHC@DHA catalyst optimization, OAS demonstration, and detailed TEA.

Task 5 (Q7-Q10). SHC@DHA catalyst optimization (NCSU, Lehigh, and WVU)

Milestone 5.1: Core-shell synthesis/screening, Q8
Milestone 5.2 : Core-shell synthesis scale-up, Q10

Task 6 (Q8-Q12). Long term OAS demonstration

Milestone 6.1: Modular test unit commissioning, Q9
Milestone 6.2: Long-term OAS testing, Q11
Milestone 6.3: Post testing characterization, Q12

Task 7 (Q9-Q12). Process scale-up, comprehensive TEA, and commercialization plan development (Susteon)

Milestone 7.0: Final TEA, Q12

Success Criteria

BP1:

Report DHA/SHC physical mixture (or composite) with > 800 g/kgCat-hr aromatics productivity.

BP2 (End of Project Goals):

Report selected SHC-DHA catalyst for 100 hours of continuous operation with >40% single pass aromatics yield and <5% deactivation;

Confirm 90% overall aromatics yield and 25% return on investment using refined process model. Develop commercialization roadmap with TEA and LCA for the OAS system.

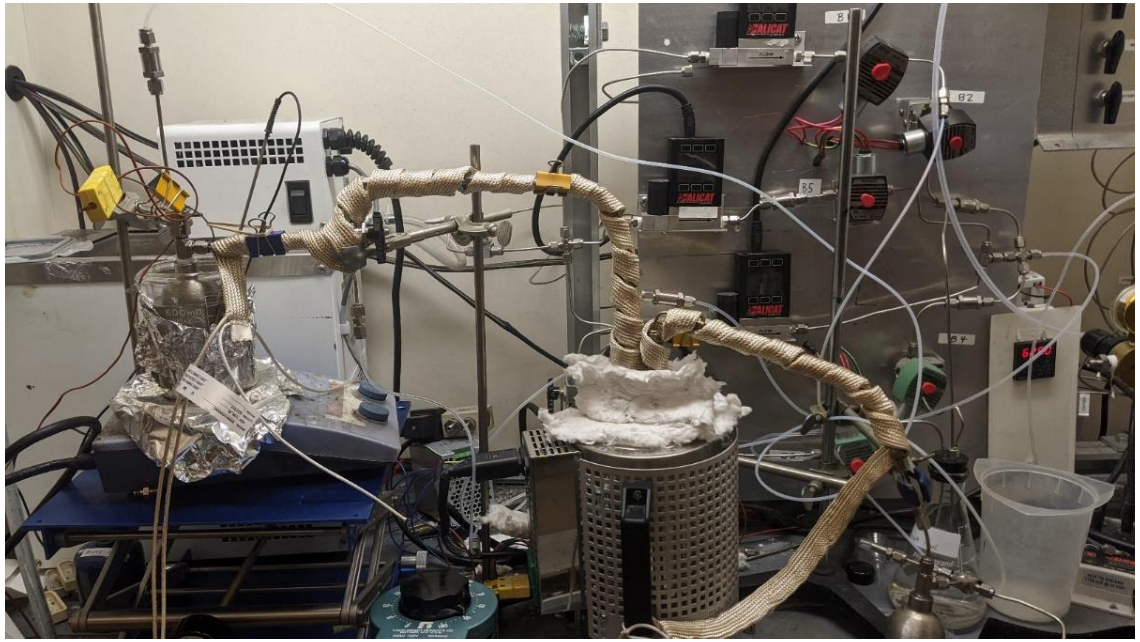
Risk Mitigation

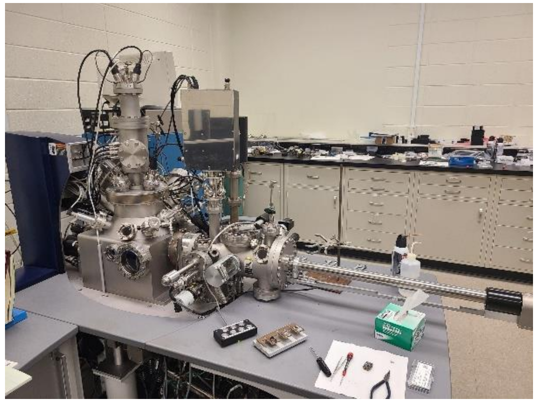
Cost/Schedule Risks:	**Probability**	**Impact**	**Overall**	**Mitigation Strategy**
Delayed/Extended negotiations	Med	Low	Low	Facilities are in place for rapid ramp up
Technical/Scope Risks:				
Insufficient DHA or SCH catalyst performance	Low	High	Med	Develop large library catalytic of materials and approaches; rationalized catalyst design based on molecular insights
Compatibility issues between DHA and SHC catalyst				
Management, Planning, and Oversight Risks:				
Delayed personnel ramp-up	Low	Low	Low	Sufficient personnel are in place and/or quickly filled (e.g. Ph.D. students) for the project.

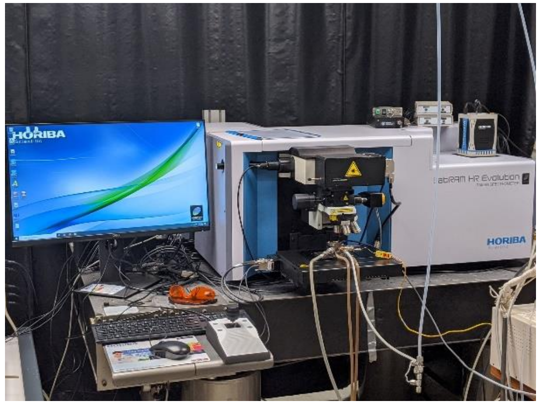
Synthesis Apparatus: CEM Microwave Synthesizer

- The zeolite synthesis is being optimized using the new CEM MW synthesizer
- This will allow for shorter synthesis times and increased zeolite yields in comparison to the previous synthesis methods (conventional hydrothermal autoclaves and solid-state crystallization)
- Uses the same solution preparation as the original conventional hydrothermal autoclave method
- Two solutions are prepped and stirred for 4 hours before being placed in the two Teflon vessels with small stir bars
- The vessels are then placed in the CEM MW and run according to a temp/time matrix that was developed to find the optimal process conditions (still in the process of this)

Catalyst Testing and Characterizations







Summary of Project Progress – DHA %Mo & Carburization Study

- The goal of this study was to identify three or more selective DHA catalyst which have an 80% selectivity to aromatics and >500 g/kgCat-hr aromatic productivity.
- Four different Mo-loaded catalysts were prepared via incipient wetness impregnation of SAR 23 commercial ZSM-5 and pretreated three different ways.
  - Mo-Loading: 2.5%, 4%, 6% and 10%
  - Carburization: None, CH_4/H_2 carburization, and a CH_4 carburization
- 0.3g loaded into quartz reactor tube and heated to 700°C and held for four hours TOS
- At 700°C the production rate was not acquired
- Further testing of the 6% - CH4/H2 carb. was performed

Table 1: Mo-Loading and Carburization Study at 700°C

Mo-Loaded ZSM-5 Catalysts (wt. %) and Carburization Method	Methane Conversion (%)	Selectivity to Aromatics (%)	Total Aromatic Production Rate (g/kgCat-hr)
2.5%Mo – no carb	12.8	84.3	333
2.5%Mo – CH_4/H_2	12.2	85.2	312
2.5%Mo – CH_4	10.0	84.1	245
4%Mo – no carb	15.4	86.2	427
4%Mo – CH_4/H_2	12.5	85.5	321
4%Mo – CH_4	7.3	85.5	269
6%Mo – no carb	15.5	84.7	380
6%Mo – CH_4/H_2	13.5	87.1	413
6%Mo – CH_4	13.0	86.2	340
10%Mo – no carb	25.6	80.6	305
10%Mo – CH_4/H_2	20.0	87.4	444
10%Mo – CH_4	11.3	85.7	292

Summary of Project Progress – Selectivity & Aromatic Prod. Study

- The 6%Mo – CH4/H2 carb. catalyst showed a better TOS stability in conversion than the other catalysts and was investigated further at different temperatures 700°C, 750°C, and 800°C
- At 750 and 800°C, the catalyst was able to successfully meet the goal proposed
- The reaction at 800°C shows the highest methane conversion and aromatic production however has a slight decrease in selectivity and rapid deactivation due to coke formation

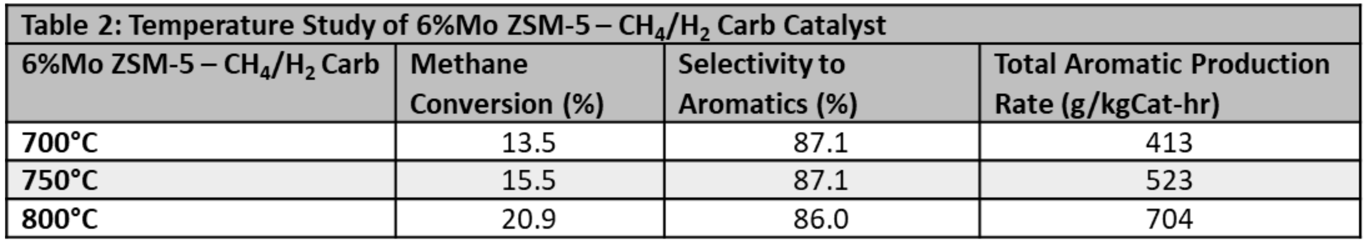


Table 2: Temperature Study of 6%Mo ZSM-5 – CH_4/H_2 Carb Catalyst

6%Mo ZSM-5 – CH_4/H_2 Carb	Methane Conversion (%)	Selectivity to Aromatics (%)	Total Aromatic Production Rate (g/kgCat-hr)
700°C	13.5	87.1	413
750°C	15.5	87.1	523
800°C	20.9	86.0	704

- Additional promotors were added to the Mo catalyst and the same reaction test was performed at 750°C

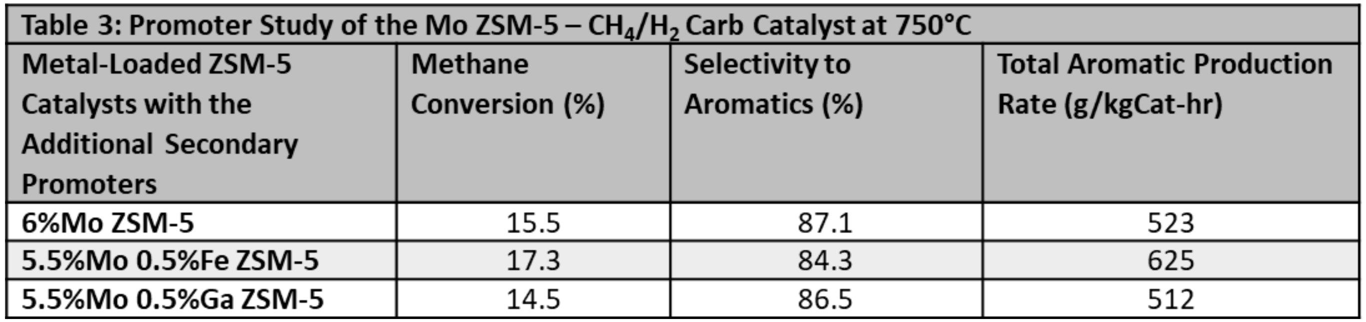


Table 3: Promoter Study of the Mo ZSM-5 – CH_4/H_2 Carb Catalyst at 750°C

Metal-Loaded ZSM-5 Catalysts with the Additional Secondary Promoters	Methane Conversion (%)	Selectivity to Aromatics (%)	Total Aromatic Production Rate (g/kgCat-hr)
6%Mo ZSM-5	15.5	87.1	523
5.5%Mo 0.5%Fe ZSM-5	17.3	84.3	625
5.5%Mo 0.5%Ga ZSM-5	14.5	86.5	512

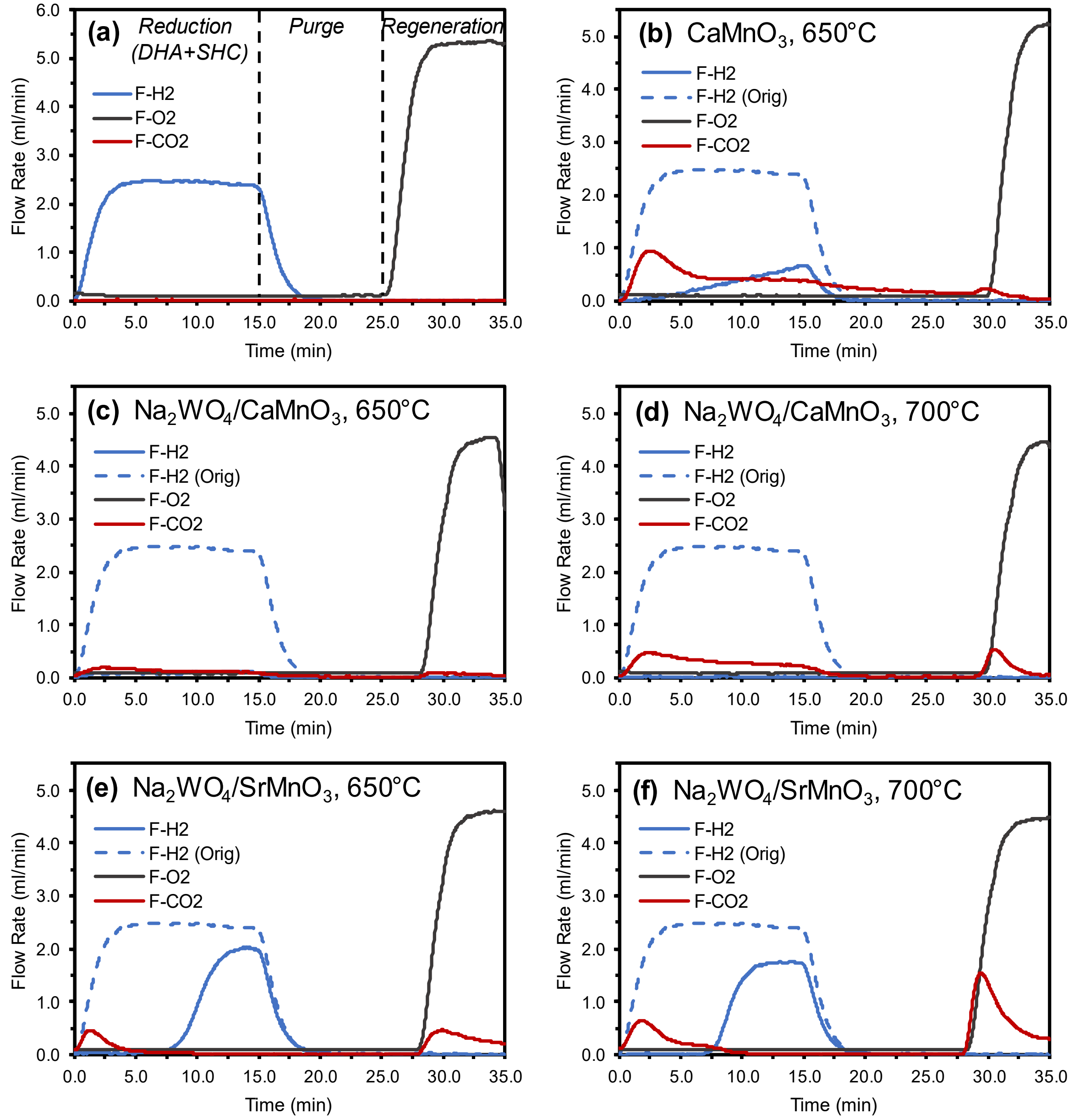
Summary of Project Progress – SHA Selectivity & Aromatic Prod. Study

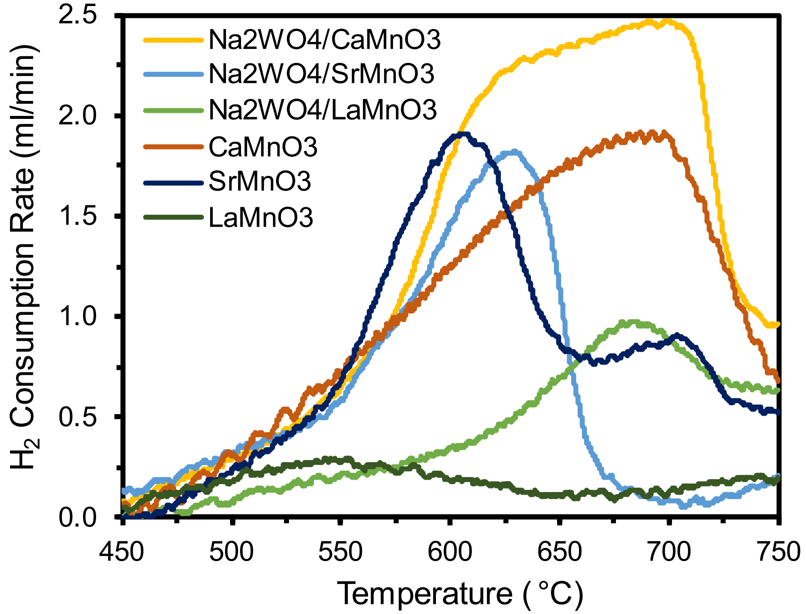
- A similar investigation was performed using 30% ethane, 4%Mo ZSM-5 at different reaction conditions (temperature, GHSV, and grams loaded)
- The production rate to aromatics was met by all the reactions performed at 650°C, however the large product distribution of ethane DHA makes the selectivity parameter hard to meet
- Additional testing of carburized catalysts CH_4 and CH_4/H_2 showed no improvement over the 0.3 grams reaction at 650°C

Table 4: Ethane Study of 4%Mo ZSM-5 Under Different Reaction Conditions

Grams Loaded (grams)	GHSV (mL/hr/gram catalyst)	Temperature (°C)	Ethane Conversion (%)	Selectivity to Aromatics (%)	Production Rate to Aromatics (g/kgCat-hr)
0.2	9000	650	40.6	28.8	608.5
0.2	6000	650	55.2	30.4	501.2
0.3	6000	650	57.2	30.8	520.0
0.3	6000	625	45.5	30.0	451.3
0.3	6000	600	34.4	28.3	336.9

Summary of Project Progress - SHC



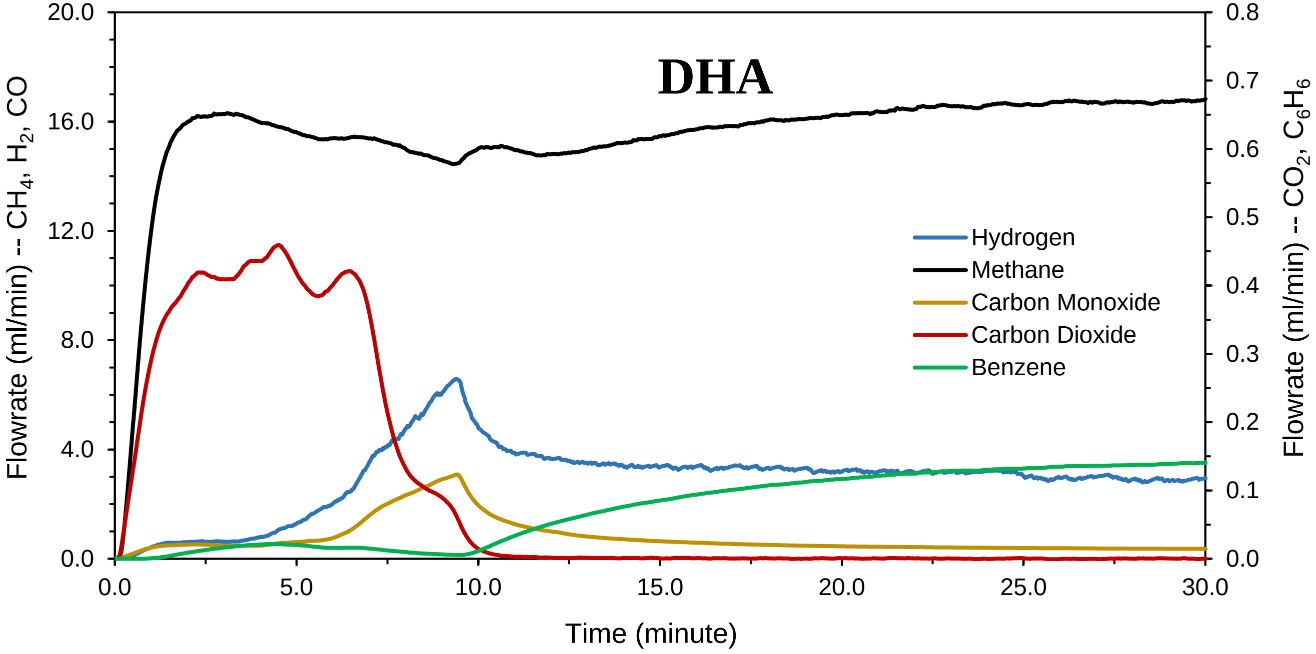


Sample	T (°C)	Total H_2 Combustion	Selectivity w/o Coke	Selectivity w/ Coke
CaMnO$_3$	650	1.40 mmol	70.4%	N/A
Na$_2$WO$_4$/CaMnO$_3$	650	1.55 mmol	89.7%	N/A
Na$_2$WO$_4$/CaMnO$_3$	700	1.60 mmol	79.6%	75.1%
Na$_2$WO$_4$/SrMnO$_3$	650	1.16 mmol	90.2%	76.9%
Na$_2$WO$_4$/SrMnO$_3$	700	1.15 mmol	82.5%	60.6%

Co-feed of 1:1 H_2/C_6H_6 on 500 mg of redox catalyst particles. Selectivity based on oxygen distribution basis; 75% oxygen distribution selectivity corresponds to 97.8% selectivity (H_2 combusted v.s. C_6H_6 combusted).

Summary of Project Progress – DHA + SHC Composite Bed

0.7 g 3% Mo/HZSM-5 + 0.1 g $Na_2WO_4/CaMnO_3$



- DHA bed starts to work only when the SHC bed is fully consumed of active lattice oxygen.

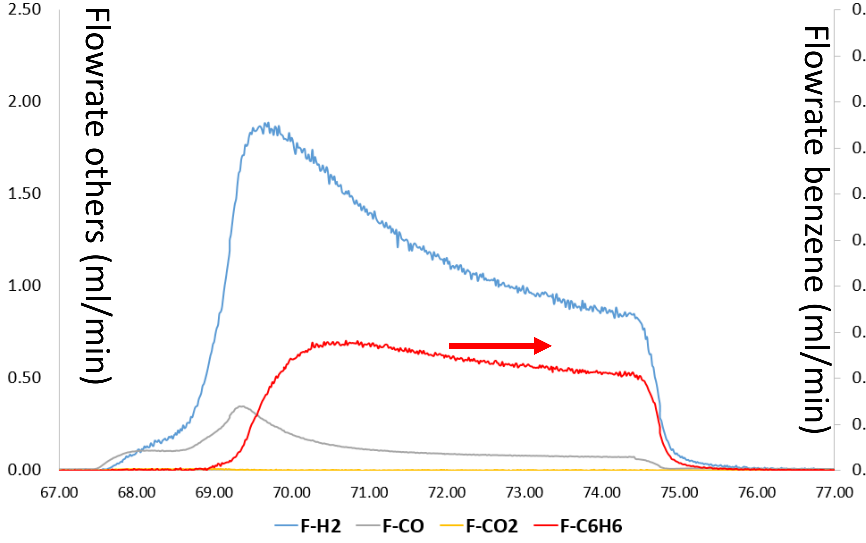
Other compositions tried:

Composition	Result
Pre-carburized DHA + NW/CMO	Failed.
DHA+NW/CMO (partially oxidized)	Failed.
Pre-carburized DHA + NW/CMO (partially oxidized)	Failed.

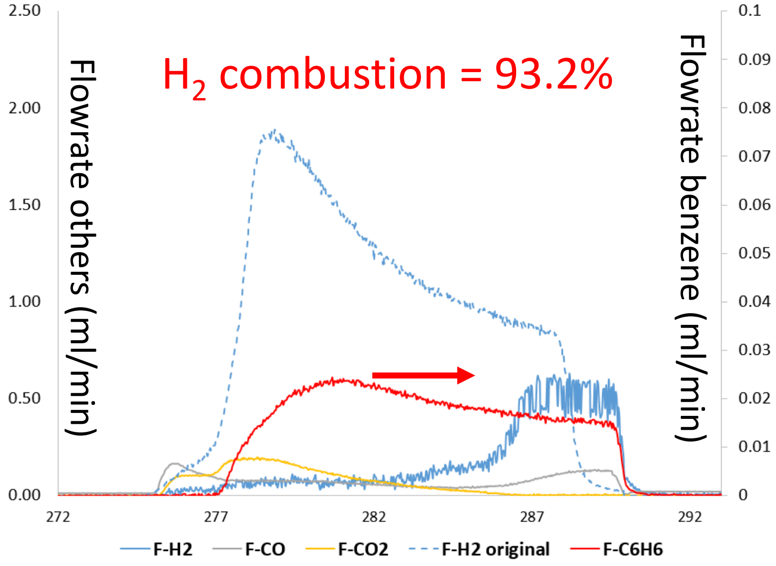
- **Water concentration in our study = ~6.2 Vol.%**
- **Water concentration in Chem. Comm. paper on Mo/ZSM5+CGO = <2.7 Vol.%**
  - **Note that CGO has poorer H_2 conversion ability than $Na_2WO_4/CaMnO_3$**

Summary of Project Progress – DHA + SHC 2-layer sequential bed

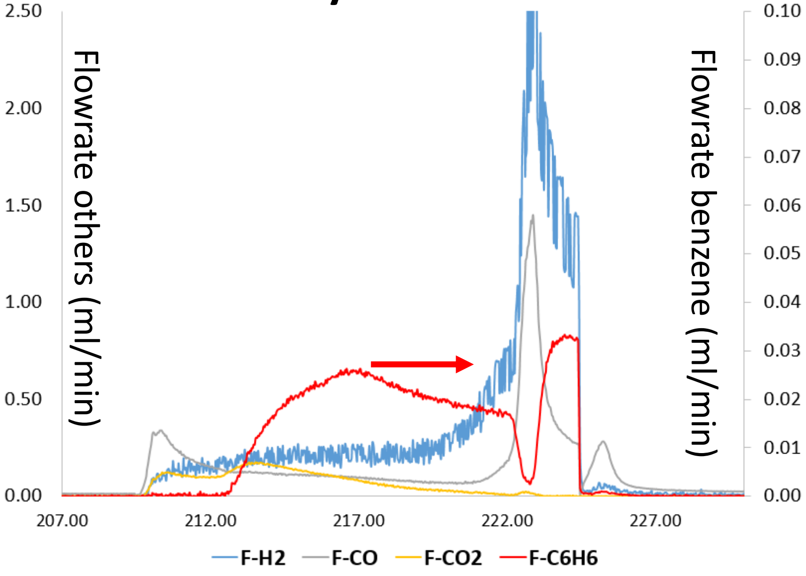
DHA
single bed



DHA+SHC
2-layer bed



DHA+SHC+DHA
3-layer bed

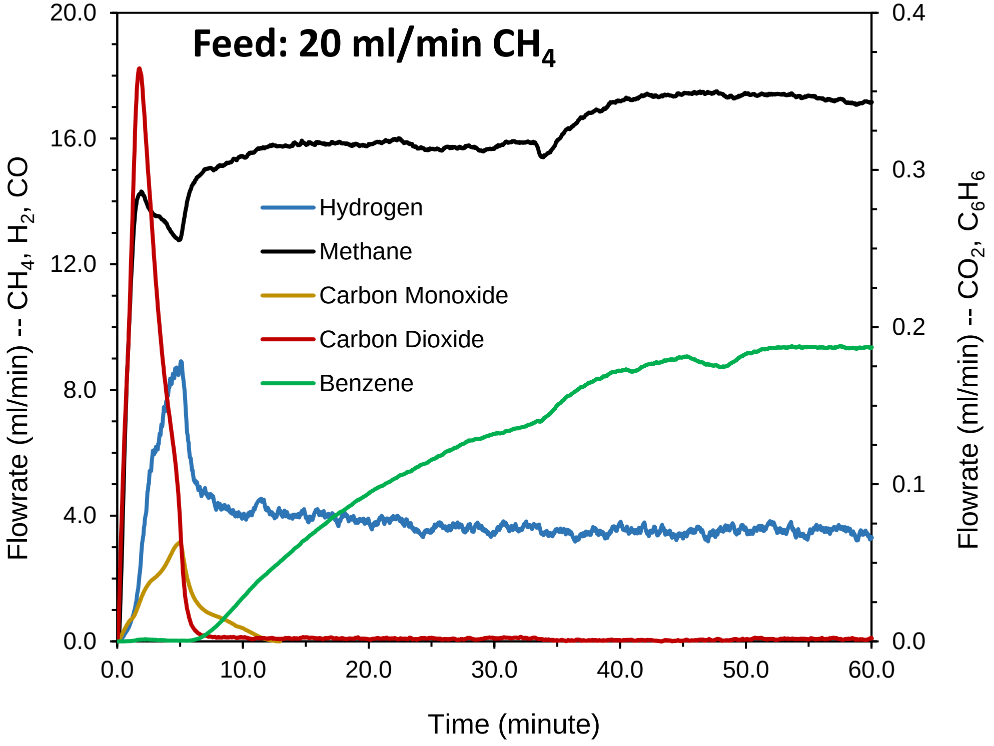


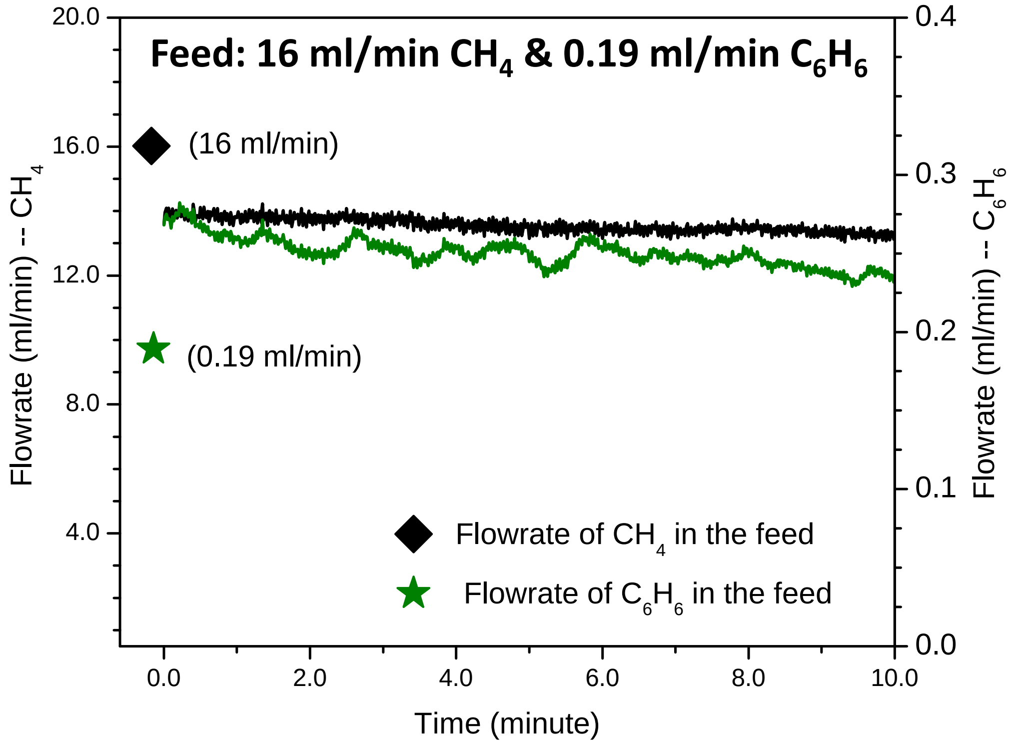
- $Na_2WO_4/CaMnO_3$ leads to H_2 combustion = 93.2%.
- CO by-product is also combusted into CO_2.
- Benzene formation rate is barely affected.

- H_2O formed in the SHC bed deactivates benzene formation from the 2nd DHA bed.
- 2nd DHA bed starts to form benzene only when the SHC bed is fully consumed of active lattice oxygen.

Summary of Project Progress – Alternative Approach

DHA → ***SHC*** → ***H_2O Removal*** → ***DHA***

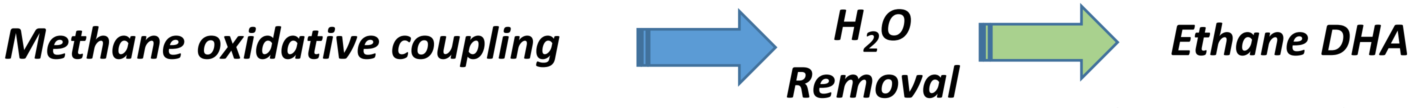




- Gas mixture simulating the product after H_2O removal was used as the feed for a second DHA step.
- Equivalently, the benzene yield in the alternative approach was ~40% more than a single DHA step.

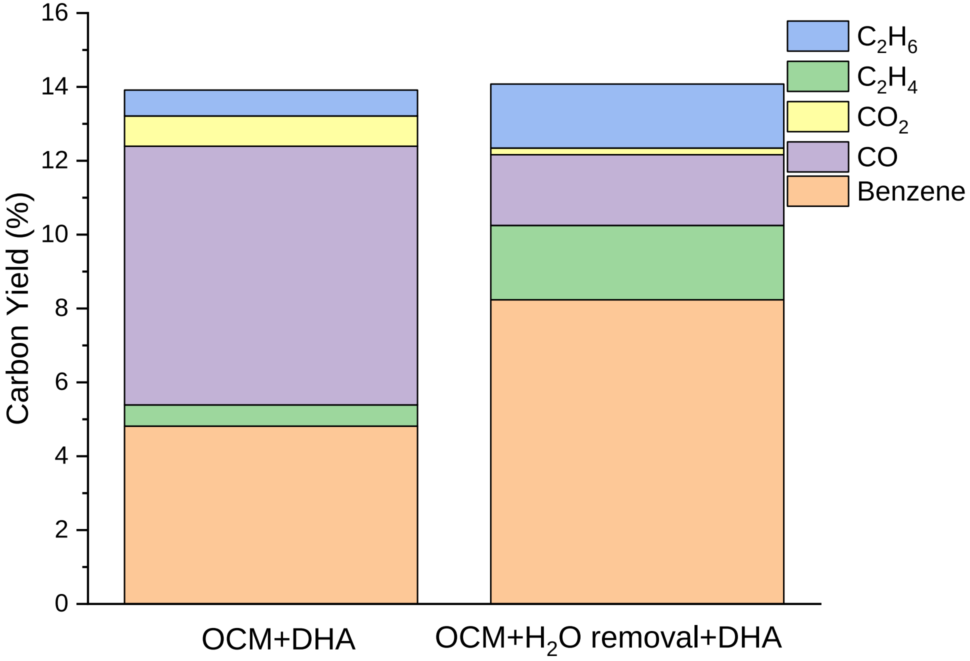
Summary of Project Progress – Alternative approach
OCM + H_2O removal+ DHA

Alternative approach flow diagram:



Methane oxidative coupling → ***H_2O Removal*** → ***Ethane DHA***

Ethane DHA catalyst: GaPt/ZSM5



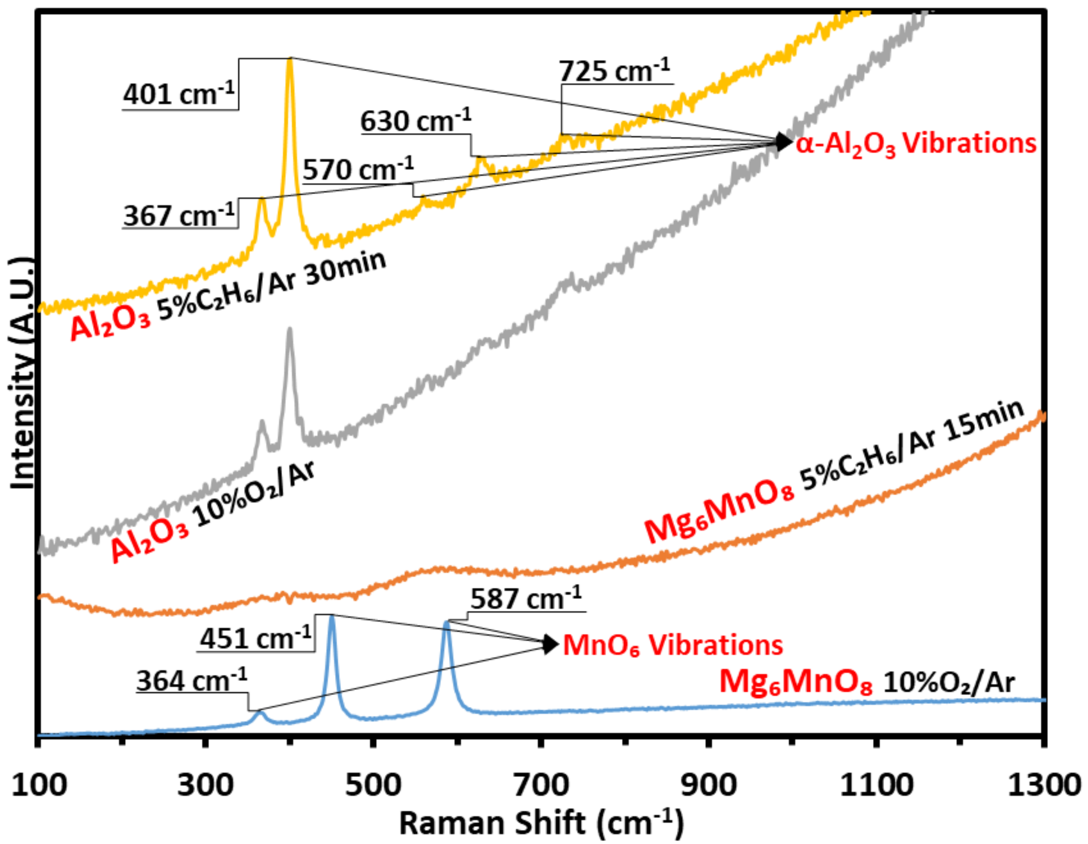
- This approach could achieve benzene yield ~8.2% at 700°C (total B+T up to 11%).
- H_2O and CO_2 leads to reforming reaction, forming CO.

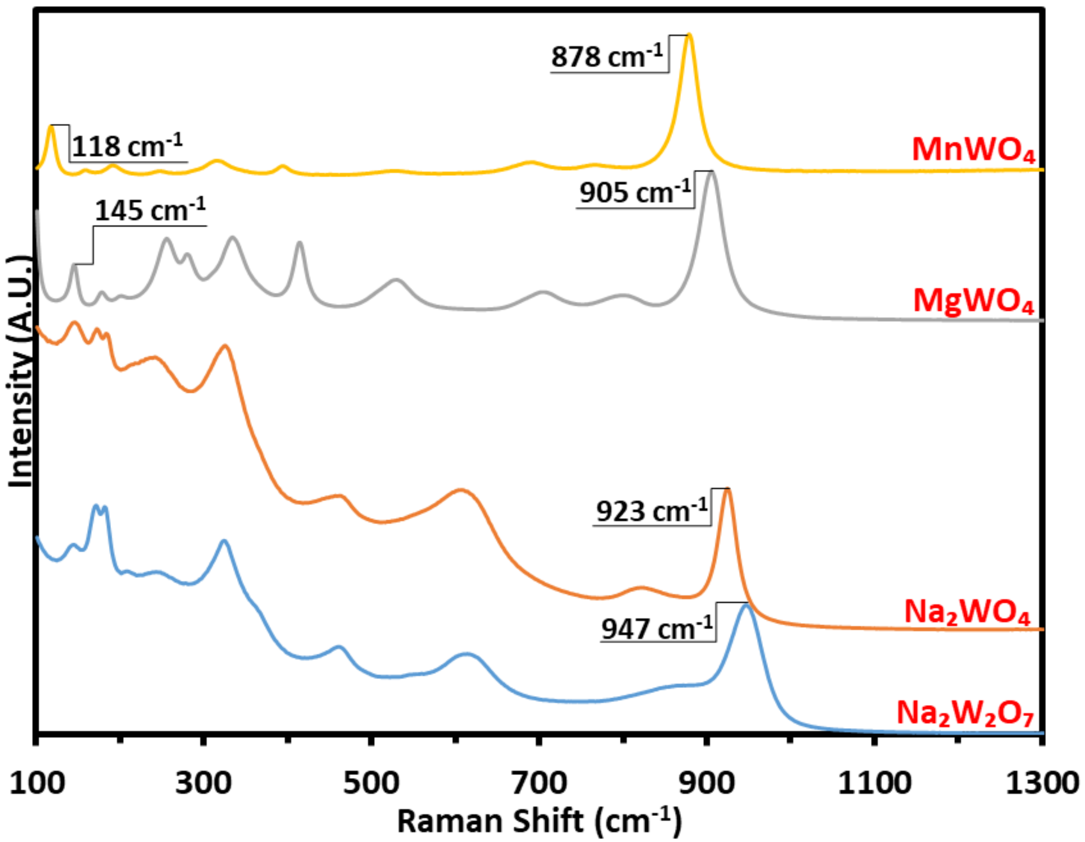
LEHIGH UNIVERSITY

In Situ Raman Characterization of SHC Catalysts

Metal Oxide Supports and Bulk Tungstate Reference Materials

- Spectra of the Mg_6MnO_8 mixed oxide support acquired under *in situ* oxidizing and reducing conditions (**left figure**) is dominated by distorted MnO_6 vibrations, which are reduced under a 5%C_2H_6/Ar flow.
- Conversely, the α-Al_2O_3 support remains stable even after 30 minutes under a 5%C_2H_6/Ar flow (**left figure**).
- The tungstate anion symmetric stretch vibration shifts from 947 to 878 cm^{-1} due to the interaction with the respective cations (**right figure**), enabling the identification of the tungstate species present in the catalyst using Raman.


Supports at 850°C under O_2 and C_2H_6

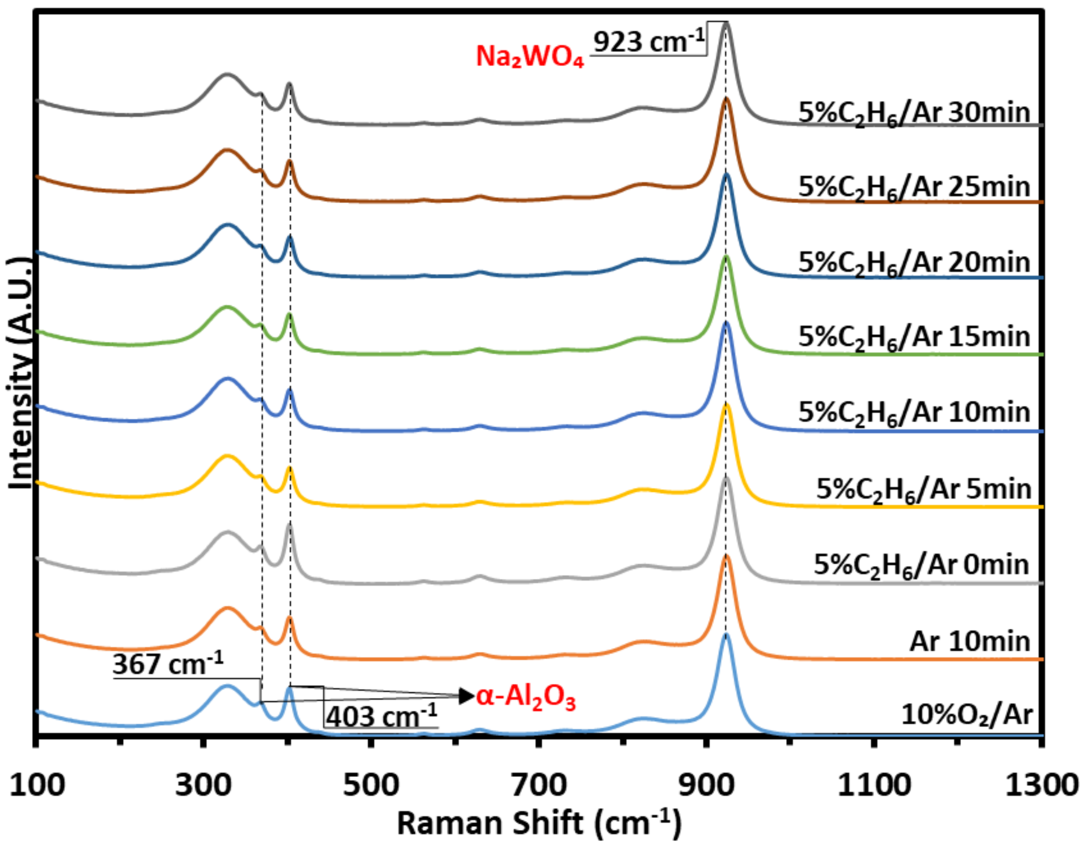

Bulk Tungstates at 850°C under 10%O_2/Ar

In Situ Raman Characterization of SHC Catalysts

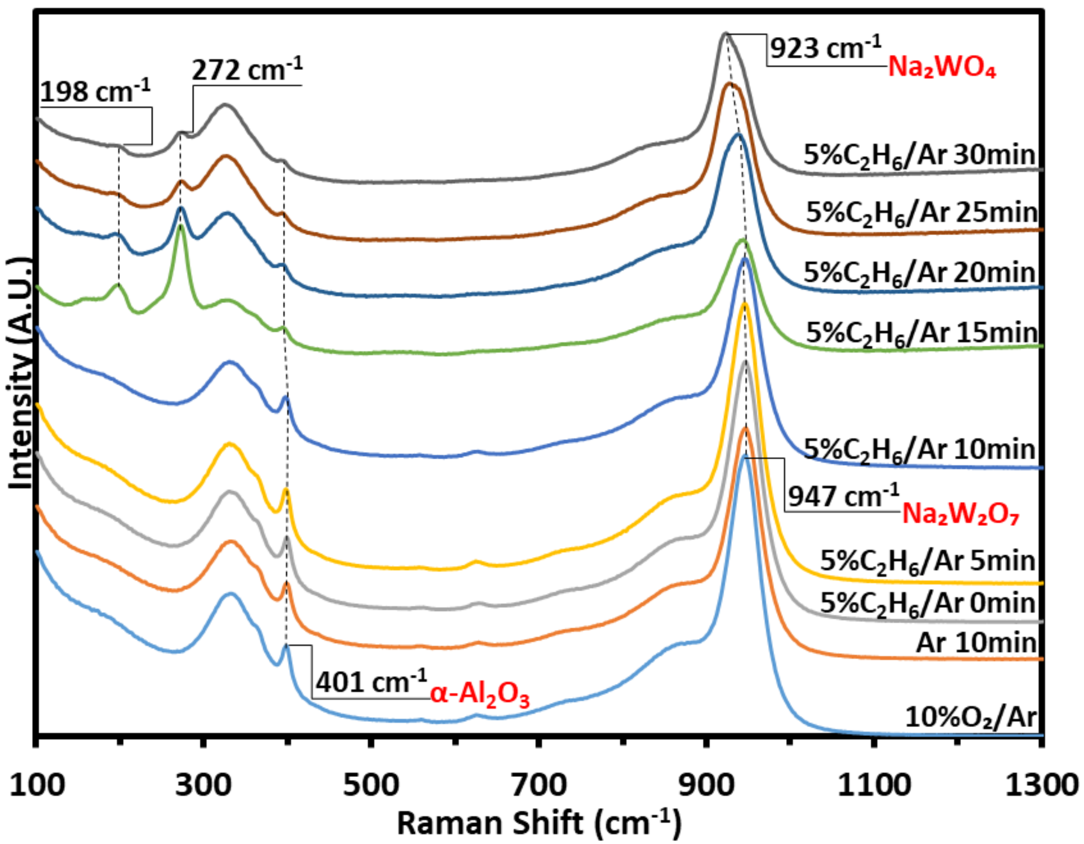
α-Al_2O_3 supported Tungsten Oxide SHC Catalysts

- The *in situ* spectra of the 20%Na_2WO_4/Al_2O_3 catalyst (**left figure**) is dominated by Na_2WO_4 vibrations, with minor contribution from the α-Al_2O_3 support at 367 and 403 cm^{-1}. The acquired spectra suggest that the catalyst remains stable under reducing conditions.
- The *in situ* spectra of the 20%$Na_2W_2O_7/Al_2O_3$ catalyst (**right figure**) is initially dominated by $Na_2W_2O_7$ vibrations with a minor α-Al_2O_3 contribution at 403 cm^{-1}. However, over time under reducing conditions, the $W_2O_7^{2-}$ anion vibration shifts to lower wavenumbers indicative of WO_4^{2-} anions, and new unidentified vibrations rise at 198 and 272 cm^{-1}. These results suggest that the $Na_2W_2O_7$ melt phase on the α-Al_2O_3 support is not stable under reducing conditions and may transform partially to Na_2WO_4.

20%Na_2WO_4/Al_2O_3 Reduction at 850°C



20%$Na_2W_2O_7/Al_2O_3$ Reduction at 850°C

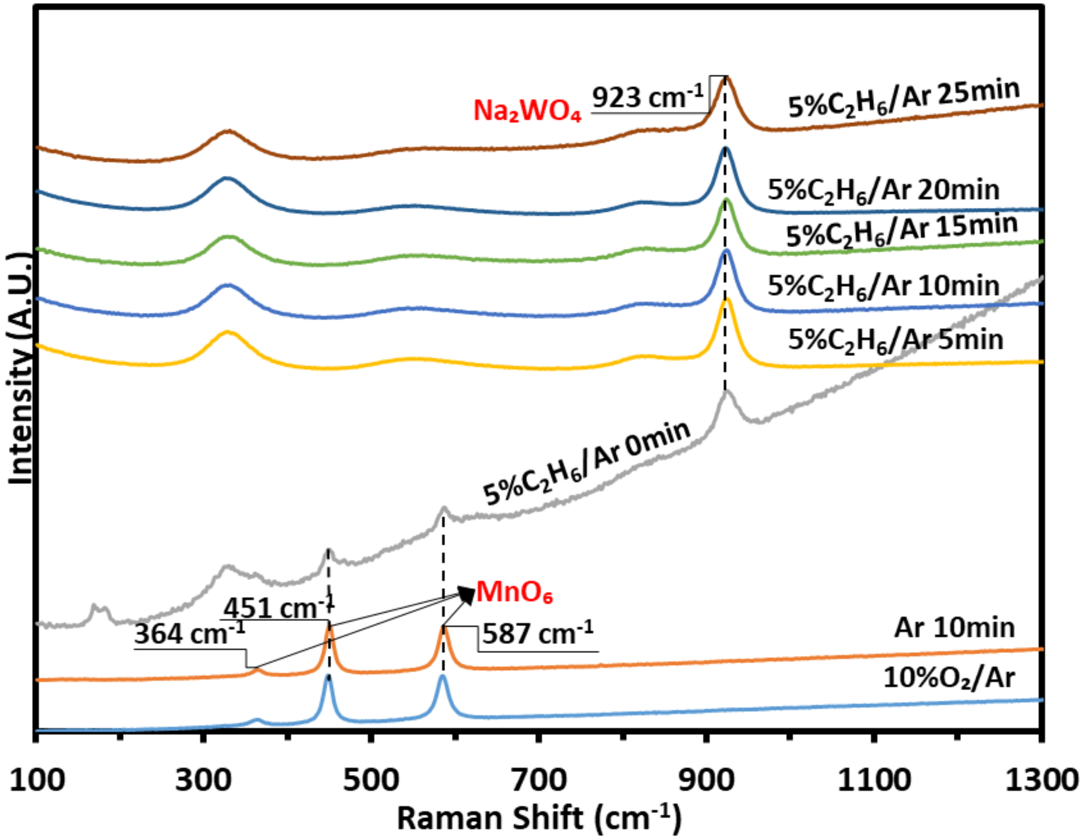


In Situ Raman Characterization of SHC Catalysts

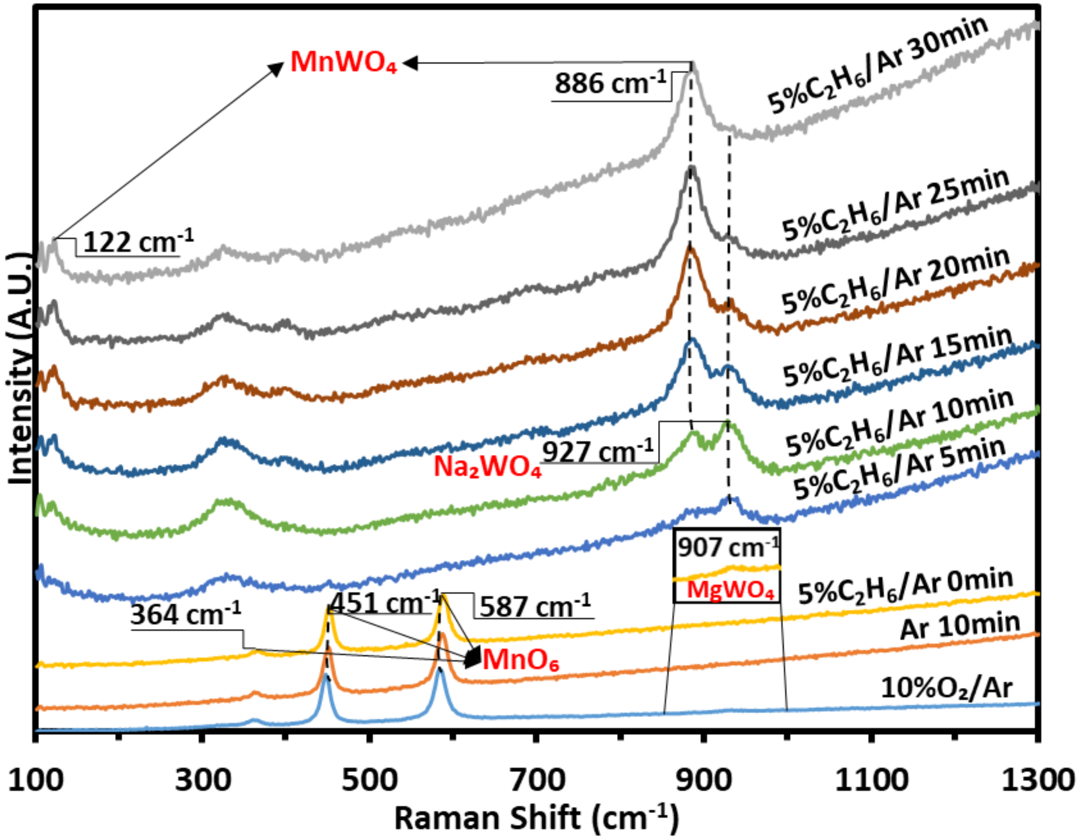
Mg_6MnO_8 supported Tungsten Oxide SHC Catalysts

- The *in situ* spectra of the $33\%Na_2WO_4/Mg_6MnO_8$ catalyst (**left figure**) is dominated by the Mg_6MnO_8 support under oxidative conditions. However, the support rapidly reduces under a $5\%C_2H_6/Ar$ flow, leaving only the sharp Na_2WO_4 vibrations visible.
- The $30\%Na_2W_2O_7/Mg_6MnO_8$ catalyst's *in situ* spectra (**right figure**) too is dominated by the Mg_6MnO_8 support vibration when oxidized, but exhibits a weak $MgWO_4$ vibration (907 cm^{-1}). Once exposed to reducing conditions the Mg_6MnO_8 and $MgWO_4$ vibrations rapidly decay, and vibrations at 927 (probably Na_2WO_4), 886 and 122 ($MnWO_4$) cm^{-1} become dominant. Over time the reducing environment transforms more and more of the Na_2WO_4 to $MnWO_4$, indicating a complex interaction between the tungstate and the Mg_6MnO_8 support during reaction.

$33\%Na_2WO_4/Mg_6MnO_8$ Reduction at 850°C



$30\%Na_2W_2O_7/Al_2O_3$ Reduction at 850°C



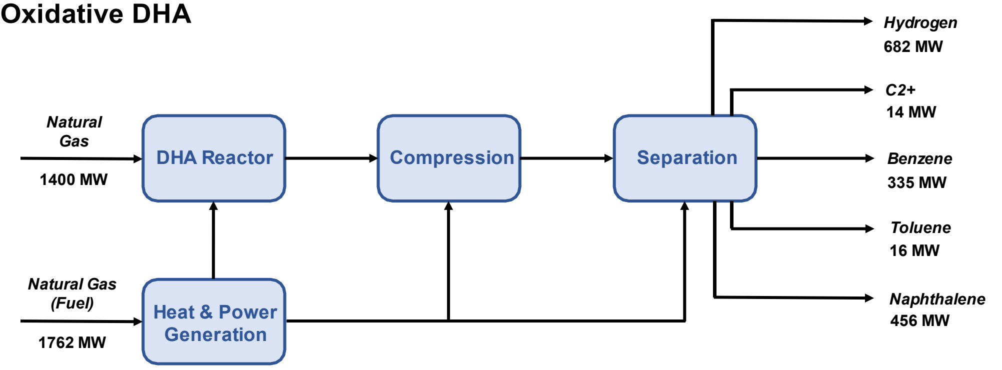
Energy Demand Comparison

Values in MW (unless otherwise noted)	Base Case	OAS 10%Y	OAS 20%Y	OAS 40%Y
NG for Heat (60% eff.)	1131.8	713.7	274.7	63.0
NG for Electricity (40% eff.)	655.5	344.9	0.0	-203.9
Fuel Requirement before Credits	1787.3	1058.5	274.7	63.0
Fuel NG Requirement after Credits	**1080.1**	**1026.1**	**233.1**	**-148.8**
Energy in Valuable Products	820.9	857.0	837.3	829.8
Net Energy Demand (Energy Lost) [d]	**1659.2**	**1569.1**	**750.8**	**352.0**
Aromatics Production Rate (kg/s)	18.8	19.4	19.0	18.8
Specific Net Energy Demand (MJ/kg)	88.3	80.9	39.6	18.7
% Reduction in Energy Demand	**--**	**8.4%**	**55.2%**	**78.8%**

* Aromatics production basis set at *19 kg/s*.

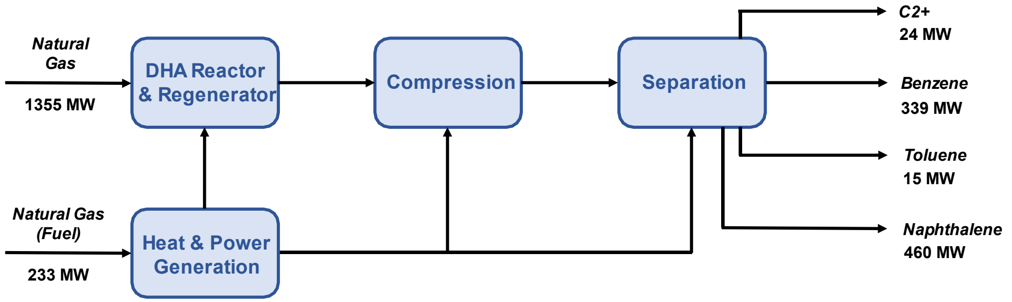
- The principal reductions in net energy input come from:
  - Reduction in overall process flowrate and resulting impacts on pre-heating, compression, and refrigeration duties
  - Simplified downstream separation requirements (particularly H_2/CH_4 cryogenic separation
- OAS technology enables modular operation
  - Non-oxidative DHA requires large scale demonstration due to H_2/CH_4 separation requirement
  - OAS able to economically produce Aromatics at **50 bbl/day scale**

Base Case:
Non-Oxidative DHA



Net Energy Input = 1659 MW
= 88.3 MJ/kg aromatics

Oxidative Aromatization System (OAS): 20% Yield

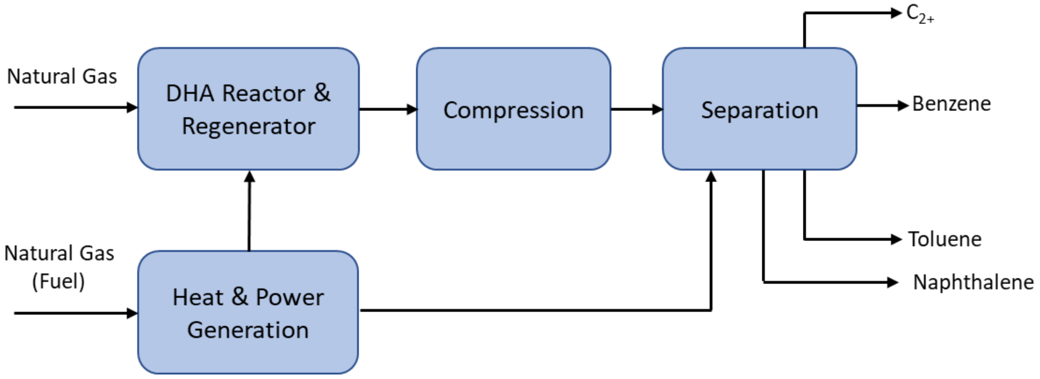


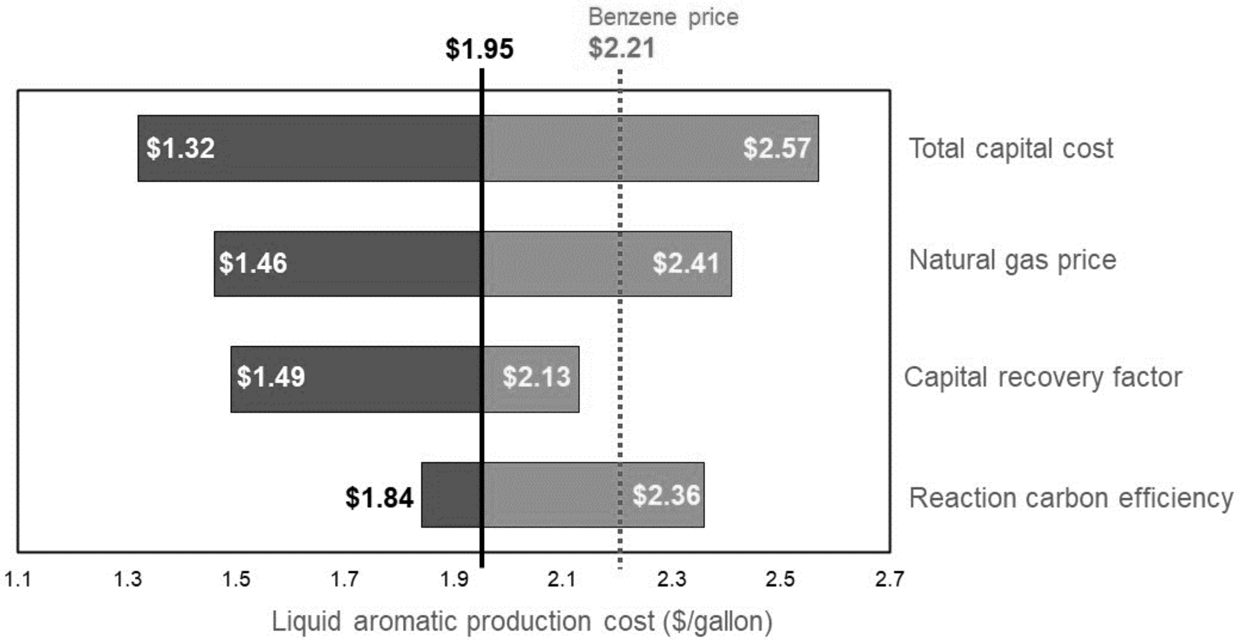
Net Energy Input = 751 MW
= 39.6 MJ/kg aromatics

Preliminary Economics: 50 bbl/day Modular Plant

- NCSU Oxidative Aromatization System (OAS) achieves a breakeven liquid aromatic production cost of $1.95/gal compared to a market price of $2.21/gal
- Capital expenditure and yield efficiency identified as major factors in final product cost
- Improving the reactor design can reduce the aromatic costs to <$1.50/gal

Parameter	**Units**	**Low**	**Base**	**High**
Total capital cost	$/bbl/day	50,000	100,000	150,000
Natural gas price	$/MMBTU	0	3	5
Capital recovery factor	%	6	12.4	15
Reaction carbon efficiency	%	50	80	95





Outline

- Project Overview and Technology Background
- Technical Approach and Current Status
- Future development plan
- Summary

Plans for Future Development

Future work within the project:

- SHC and DHA catalyst optimizations;
- Optimization of the process scheme guided by TEA;
- Long-term OAS demonstration and post demonstration characterization;
- Finalization of TEA and scale-up roadmap.

Future work beyond the project:

- Further scale up testing (up to 1000 cuft/day);
- Detailed catalyst cost and scalability study;
- Detailed system design and costing;
- Demonstration and commercialization with industrial partner(s).

Summary Slide

Various ZSM based DHA catalysts have been developed, meeting the 500 g/kgCat-hr and 80% aromatics selectivity target;

Effective SHC redox catalysts have been developed, demonstrating >200 mol/kgCat-hr activity and >80% selectivity at 700 °C;

Efficient hydrogen combustion resulted in high steam concentration, eliminating the active sites on the DHA catalyst;

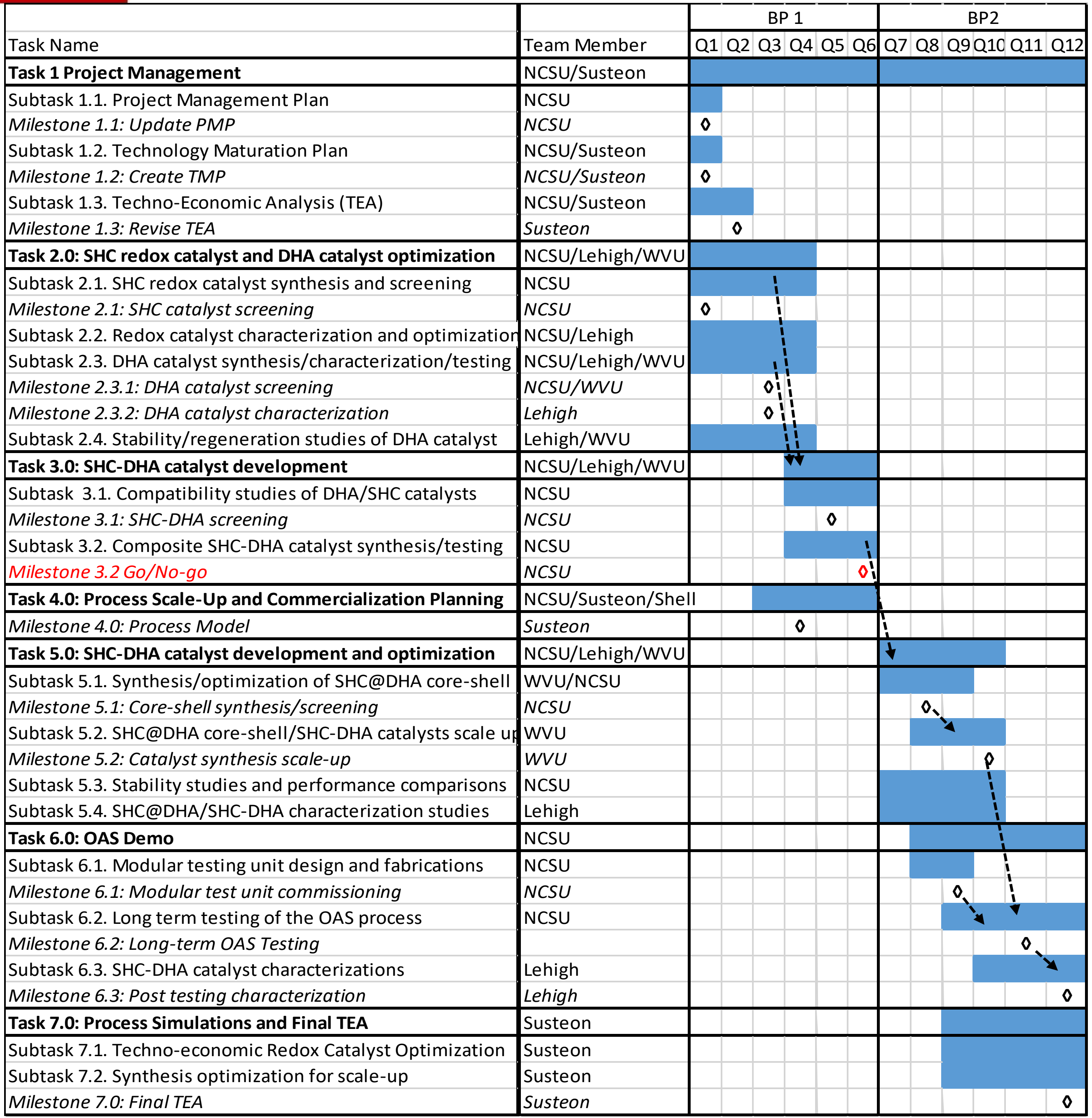
Alterative schemes for methane DHA have been developed, showing excellent aromatics yields;

In-situ characterization of the catalysts generated mechanistic insights;

TEA indicates that the proposed OAS technology has excellent potential for energy savings and emission reduction.

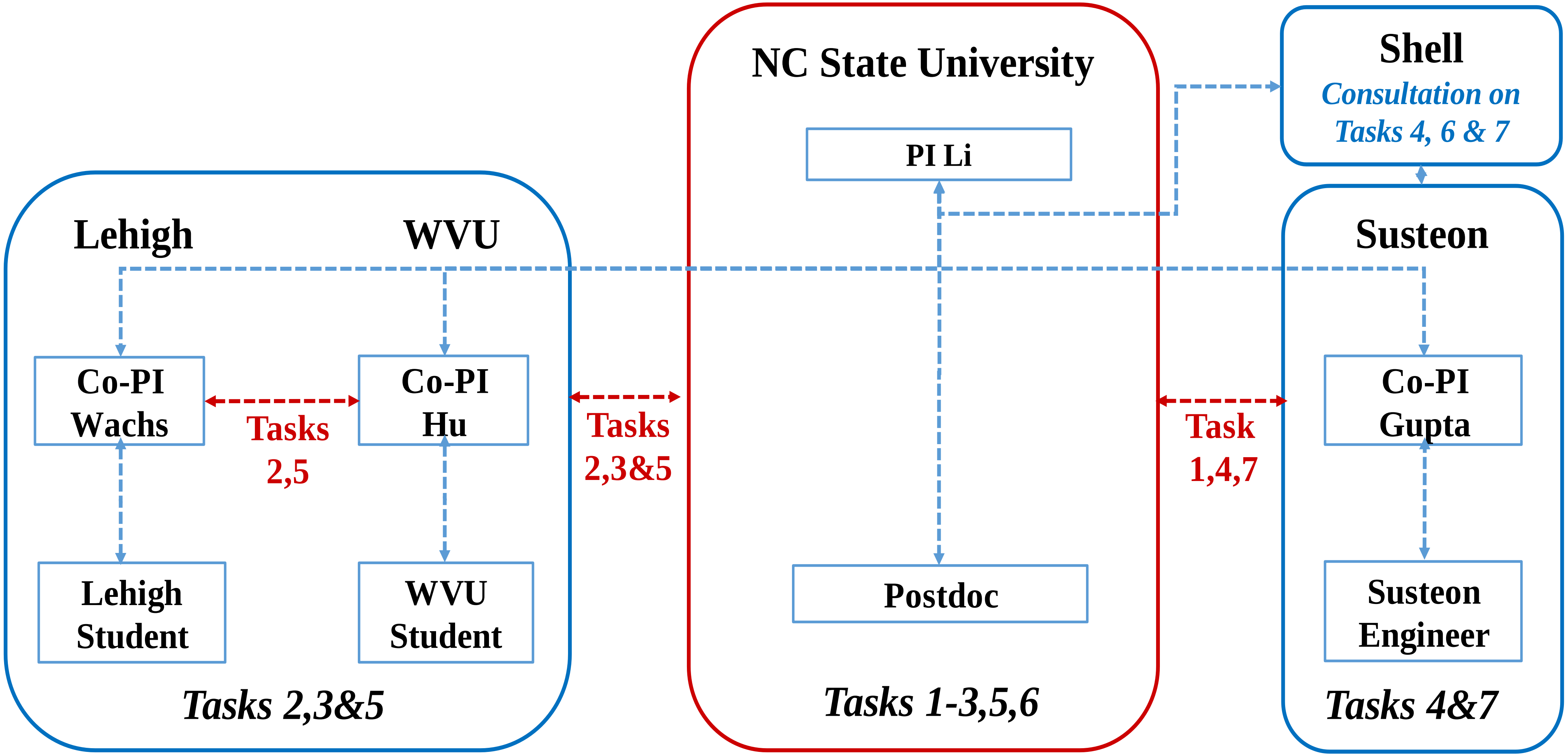
Thanks for the support!
Questions or suggestions?

Appendix: Project Schedule



		BP 1						BP2					
Task Name	Team Member	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12
Task 1 Project Management	NCSU/Susteon	■	■	■	■	■	■	■	■	■	■	■	■
Subtask 1.1. Project Management Plan	NCSU	■											
Milestone 1.1: Update PMP	*NCSU*	◊											
Subtask 1.2. Technology Maturation Plan	NCSU/Susteon	■											
Milestone 1.2: Create TMP	*NCSU/Susteon*	◊											
Subtask 1.3. Techno-Economic Analysis (TEA)	NCSU/Susteon	■	■										
Milestone 1.3: Revise TEA	*Susteon*		◊										
Task 2.0: SHC redox catalyst and DHA catalyst optimization	NCSU/Lehigh/WVU	■	■	■	■								
Subtask 2.1. SHC redox catalyst synthesis and screening	NCSU	■	■	■	■								
Milestone 2.1: SHC catalyst screening	*NCSU*	◊											
Subtask 2.2. Redox catalyst characterization and optimization	NCSU/Lehigh	■	■	■	■								
Subtask 2.3. DHA catalyst synthesis/characterization/testing	NCSU/Lehigh/WVU	■	■	■	■								
Milestone 2.3.1: DHA catalyst screening	*NCSU/WVU*			◊									
Milestone 2.3.2: DHA catalyst characterization	*Lehigh*			◊									
Subtask 2.4. Stability/regeneration studies of DHA catalyst	Lehigh/WVU	■	■	■	■								
Task 3.0: SHC-DHA catalyst development	NCSU/Lehigh/WVU				■	■	■						
Subtask 3.1. Compatibility studies of DHA/SHC catalysts	NCSU				■	■	■						
Milestone 3.1: SHC-DHA screening	*NCSU*					◊							
Subtask 3.2. Composite SHC-DHA catalyst synthesis/testing	NCSU				■	■	■						
Milestone 3.2 Go/No-go	*NCSU*						◊						
Task 4.0: Process Scale-Up and Commercialization Planning	NCSU/Susteon/Shell			■	■	■	■						
Milestone 4.0: Process Model	*Susteon*				◊								
Task 5.0: SHC-DHA catalyst development and optimization	NCSU/Lehigh/WVU							■	■	■	■		
Subtask 5.1. Synthesis/optimization of SHC@DHA core-shell	WVU/NCSU							■	■	■			
Milestone 5.1: Core-shell synthesis/screening	*NCSU*								◊				
Subtask 5.2. SHC@DHA core-shell/SHC-DHA catalysts scale up	WVU								■	■	■		
Milestone 5.2: Catalyst synthesis scale-up	*WVU*										◊		
Subtask 5.3. Stability studies and performance comparisons	NCSU							■	■	■	■		
Subtask 5.4. SHC@DHA/SHC-DHA characterization studies	Lehigh							■	■	■	■		
Task 6.0: OAS Demo	NCSU								■	■	■	■	■
Subtask 6.1. Modular testing unit design and fabrications	NCSU								■	■			
Milestone 6.1: Modular test unit commissioning	*NCSU*									◊			
Subtask 6.2. Long term testing of the OAS process	NCSU									■	■	■	■
Milestone 6.2: Long-term OAS Testing												◊	
Subtask 6.3. SHC-DHA catalyst characterizations	Lehigh										■	■	■
Milestone 6.3: Post testing characterization	*Lehigh*												◊
Task 7.0: Process Simulations and Final TEA	Susteon									■	■	■	■
Subtask 7.1. Techno-economic Redox Catalyst Optimization	Susteon									■	■	■	■
Subtask 7.2. Synthesis optimization for scale-up	Susteon									■	■	■	■
Milestone 7.0: Final TEA	*Susteon*												◊

Appendix: Project Organizational Structure



NC State University

PI Li

Postdoc

Tasks 1-3,5,6

Shell

Consultation on Tasks 4, 6 & 7

Lehigh

WVU

Co-PI Wachs

Co-PI Hu

Tasks 2,5

Lehigh Student

WVU Student

Tasks 2,3&5

Tasks 2,3&5

Task 1,4,7

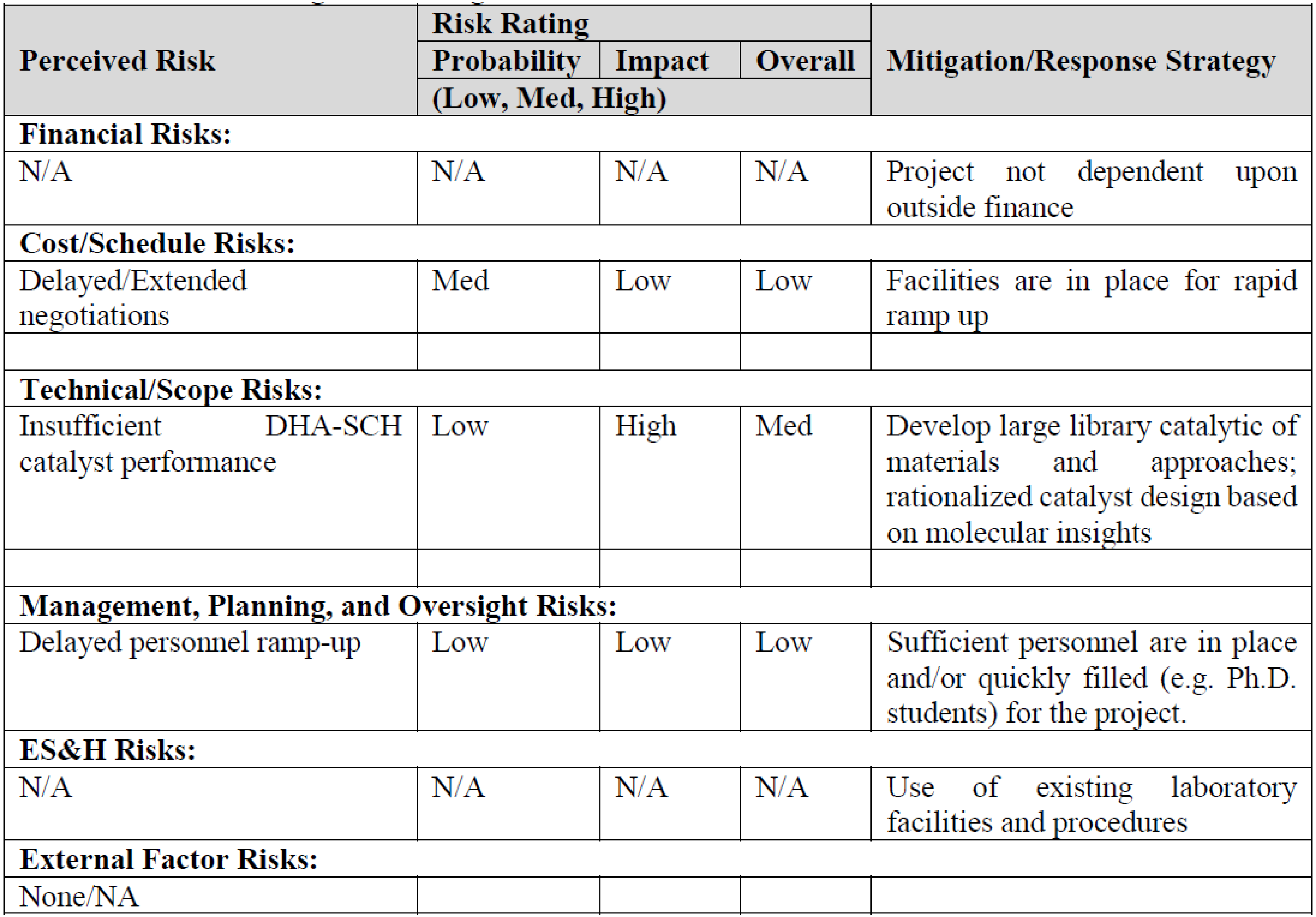
Susteon

Co-PI Gupta

Susteon Engineer

Tasks 4&7

Risk Management



Perceived Risk	**Risk Rating**			**Mitigation/Response Strategy**
	Probability	**Impact**	**Overall**	
	(Low, Med, High)			
Financial Risks:				
N/A	N/A	N/A	N/A	Project not dependent upon outside finance
Cost/Schedule Risks:				
Delayed/Extended negotiations	Med	Low	Low	Facilities are in place for rapid ramp up
Technical/Scope Risks:				
Insufficient DHA-SCH catalyst performance	Low	High	Med	Develop large library catalytic of materials and approaches; rationalized catalyst design based on molecular insights
Management, Planning, and Oversight Risks:				
Delayed personnel ramp-up	Low	Low	Low	Sufficient personnel are in place and/or quickly filled (e.g. Ph.D. students) for the project.
ES&H Risks:				
N/A	N/A	N/A	N/A	Use of existing laboratory facilities and procedures
External Factor Risks:				
None/NA				

Milestones

Task#	Milestone Title & Description	Due	Verification method
1.1	Update PMP	BP1-Q1	Submit updated PMP
1.2	Create TMP	BP1-Q1	Submit TMP
2.1	SHC Catalyst Screening: Report 4 SHC redox catalysts with hydrogen combustion activity of 200 mol/kgCat-hr and 80% selectivity at 700 °C.	BP 1-Q1	Report reaction data in Q-Report
1.3	Revise TEA	BP1-Q2	Submit Revised TEA
2.3.1	DHA Cat. Screening: Report 3 or more DHA catalysts with > 500 g/kgCat-hr aromatics productivity and > 80% selectivity at <700 °C	BP1-Q3	Report reaction data in Q-Report
2.3.2	DHA Cat. Characterization: Identify DHA catalysts phases and structures under reaction conditions.	BP1-Q3	Report data for 2 DHA catalyst.
4.0	Process Model: Report ASPEN models for a base case (non-oxidative DHA) reactor and OAS showing >50% reduction in net energy demand	BP1-Q4	Report energy demand for OAS vs. base-case
3.1.	SHC-DHA Screening: Report 3 or more physical mixtures (or composite) catalysts with > 20% single pass aromatics yield.	BP2-Q5	Report reaction data in Q-Report
3.2.	***Go/No-go:*** *Report DHA-SHC composite with > 800 g/kgCat-hr aromatics productivity at < 700 °C.*	BP1-Q6	Report reaction data in Q-Report
5.1	Core-shell Synthesis/Screening: Report three or more SHC@DHA (or composite) catalysts with > 30% single pass aromatics yield.	BP2-Q8	Report reaction data in Q-Report
6.1	Modular test unit commissioning: Report >50 ml/day aromatic productivity using >10 g physically mixed DHA-SHC catalyst bed at < 700 °C	BP2-Q9	Report reaction data in Q-Report
5.2	Catalyst synthesis scale-up: Prepare 20+ gram batch of DHA@SCH core-shall (or composite) catalyst for long-term testing	BP2-Q10	Report activity data of large batch catalyst
6.2	***Long-Term OAS Testing:*** Report selected SHC-DHA catalyst for 100 hours of continuous operation with >40% single pass aromatics yield and <5% deactivation, showing >200 ml/day aromatics productivity at 650 °C.	BP2-Q11	Report reaction data in Q-Report
6.3	Post testing characterization: Determine phase and surface properties of the catalyst after the long-term stability test.	BP2-Q12	Report Characterization in final report
7.0	***Final TEA:*** Confirm 90% overall aromatics yield and 25% return on investment using refined process model. Develop commercialization roadmap with TEA and LCA for the OAS system.	BP2-Q12	Report final TEA at end of project