

Sustainable Aromatics Manufacturing from Methane via Oxidative Coupling and Aromatization

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at

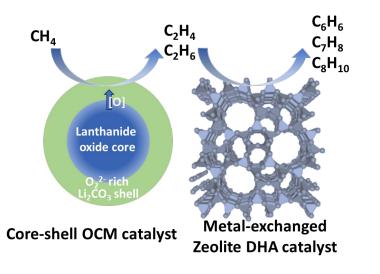
NETL Carbon Management Research Project Review Meeting August 8th, 2024





Technology characteristics





$$2CH_{4}+MO_{x} \rightarrow C_{2}H_{6} + H_{2}O + MO_{x-1}$$

$$2CH_{4}+2MO_{x} \rightarrow C_{2}H_{4} + 2H_{2}O + 2MO_{x-1}$$

$$3C_{2}H_{4} \leftarrow \rightarrow C_{6}H_{6} + 3H_{2}$$

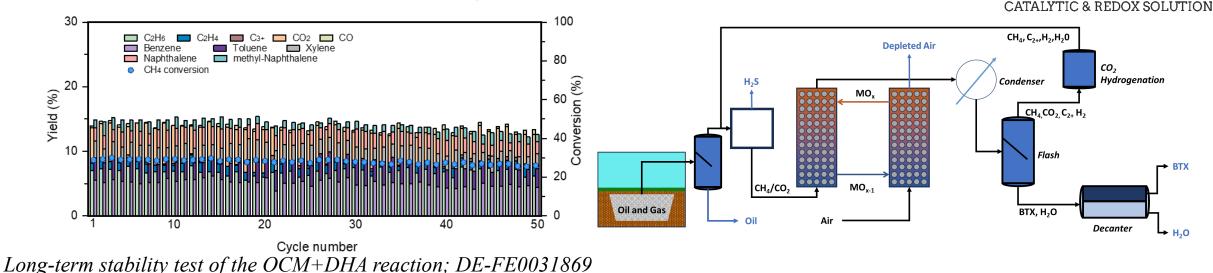
$$MO_{x-1}+Air \rightarrow MO_{x}+N_{2}$$

- Reaction 1a Reaction 1b Reaction 2
- Reaction 3

- Stranded methane is converted into aromatics (BTX) in a 2-steps
 - CL-OCM(Rxn. 1 a&b): Methane is oxidatively coupled over a chemical looping catalyst to form ethane or ethylene
 - DHA(Rxn. 2): The C_2 products are reacted over a zeolite to form aromatics
- To close the chemical looping mass balance the CL-OCM catalyst is regenerated in air (Rxn 3)
- The OCM/regeneration steps provide heat allowing for autothermal operation.
- The hydrogen byproduct can be used to hydrogenate CO₂ to improve ultimate yields
- The feasibility of the chemical looping OC-DHA catalyst was recently validated in DOE-NETL funded project and NCSU and WVU (DE-FE0031869: PM Anthony Zammerilli)



Technology advantages



- 1. Simplified feedstock preparation; The OC-DHA redox catalyst will simultaneously convert C_1 - C_3 components in shale or bio/land fill gas.
- 2. Increased single pass yield and productivity; existing DHA is limited by thermodynamics with 8% single pass CH₄ conversion at 650 °C vs 75% CH₄ conversion for CL-OCM within a single pass. Aromatic yields of ~15% have been demonstrated;
- 3. Simplified product separation and recycle scheme; OC-DHA results in an easy-to-separate product slate consisting of liquids (aromatics and water) and gas (gaseous alkanes and alkenes with small amount of CO_x and unconverted H_2).
- 4. High robustness; The cyclic process periodically regenerates the catalysts.



Planned project approach



- Process Modeling and Techno Economic Analysis
 - The preliminary ASPEN+ model will be evaluated and refined. Literature review and stakeholder outreach will be used to update TEA parameters.
 - The cost of a commercial-scale DHA plant will be estimated and the potential ROI will be estimated.
- Life Cycle Analysis
 - Process modeling will be used to update the cradle-to-gate GHG emissions by using International Standards Organization (ISO) 14040/14044 standards.
- Experimental Process Data Collection and TEA/LCADriven Experimental Validation
 - Previous experimental data will be evaluated for completeness and used as the basis for process modeling.
 - A limited amount of experimental data will be collected in cases where there are gaps in available data/conditions.
- EH&S Risk Assessment, Gap Analysis, and Project Planning
 - A high-level screening hazardous operations review will be done by the project team to identify potential hazards in the conceptual plant and develop mitigation strategies.
 - Based upon the conceptual plant design, TEA, LCA, and stakeholder outreach will be conducted to identify remaining gaps that need to be addressed in phase 2 and beyond.
 - These gaps will be integrated into project planning and detailed scope of work for phase 2.



