

# TECHBRIEF

## HYDROPHOBIC ALKYL-ESTER PHYSICAL SOLVENTS FOR CO<sub>2</sub> REMOVAL FROM H<sub>2</sub> PRODUCED FROM SYNTHESIS GAS

### OPPORTUNITY:

The invention is a family of hydrophobic, low viscosity, low vapor pressure physical solvents with molecular structures consisting of two or more alkyl-ester functional groups on a central hydrocarbon chain. These solvents have been shown to possess high carbon dioxide (CO<sub>2</sub>) solubility and absorption selectivity, which make them well suited for the removal of CO<sub>2</sub> from hydrogen (H<sub>2</sub>) produced from synthesis gas. This technology is available for licensing and/or further collaborative research from the U.S. Department of Energy's National Energy Technology Laboratory.

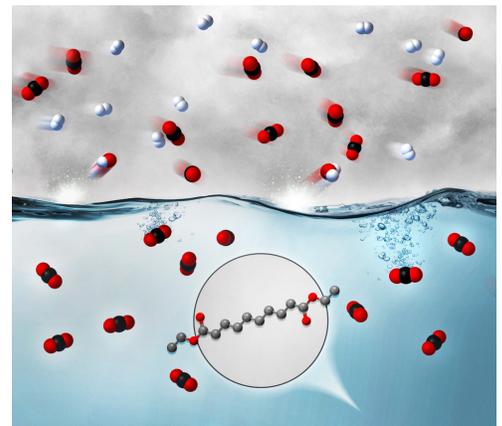
### CHALLENGE:

Future integrated gasification combined cycle (IGCC) power plants and steam methane reforming (SMR) chemical plants have the potential to reduce the cost of CO<sub>2</sub> capture. These power and chemical plants generate high-pressure CO<sub>2</sub> gas streams from the in-situ water gas shift reaction when producing H<sub>2</sub> used to power the electrical turbines. A variety of methods have been proposed to capture CO<sub>2</sub>, including solvent, sorbent, and membrane technologies, with continuous solvent looping systems currently considered to be the most advanced. Precombustion capture of CO<sub>2</sub> is typically accomplished using physical solvents.

State-of-the-art precombustion CO<sub>2</sub> capture processes predominantly employ hydrophilic physical solvents. Current commercial physical solvents touted for IGCC CO<sub>2</sub> capture were developed for removing acid gases from raw natural gas streams. Therefore, they were designed to remove significant amounts of water from the process gas. As such, the focus was on the purification of the process gas with less concern for generation of high-purity CO<sub>2</sub> streams suitable for pipeline transmission and sequestration. While water removal is important for natural gas pipeline applications, it is not favorable for applications in which the fuel stream is directly combusted on-site, as would be encountered in IGCC systems.

### OVERVIEW:

Researchers at NETL have developed a family of hydrophobic, low viscosity, low vapor pressure physical solvents with molecular structures consisting of two or more alkyl-ester functional groups on a central hydrocarbon chain. These solvents have been shown to possess high CO<sub>2</sub> solubilities at high CO<sub>2</sub> partial pressures (such as ~ 25 bar) and high CO<sub>2</sub>/H<sub>2</sub> absorption selectivity and are well suited for the removal of CO<sub>2</sub> from H<sub>2</sub> produced from synthesis gas. The NETL-developed solvents offer attractive properties for applications involving CO<sub>2</sub> capture from high humidity H<sub>2</sub> gas streams containing elevated partial pressures of CO<sub>2</sub>, particularly in IGCC processes. The rare combination of low toxicity, high CO<sub>2</sub> capacity, high selectivity, and low water affinity of these solvents provide opportunities for more efficient, cost-effective and environmentally friendly CO<sub>2</sub> mitigation.



(continued)



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**ADVANTAGES:**

- The CO<sub>2</sub> absorption of the solvents listed in the invention compare favorably to currently used solvents such as Selexol, Purisol and Fluor Solvent.
- The solvents listed in the invention exhibit a greatly reduced tendency to absorb water, which imparts advantages in reduced cost and complexity when used in gasification systems.
- This solvent family exhibits excellent CO<sub>2</sub> absorption and good CO<sub>2</sub>/H<sub>2</sub> selectivity.
- Solvents listed in the invention are non-toxic and are non-corrosive.
- The solvents are prepared from common chemical reagents easily sourced in large quantities at relatively low cost.
- The tri-esters and tetra-esters reported in this work were all prepared in high yields (>85%).

**APPLICATIONS:**

Applications of Hydrophobic Alkyl-Ester Physical Solvents include:

- Pre-combustion CO<sub>2</sub> separation and capture at IGCC power facilities
- CO<sub>2</sub> removal during generation of H<sub>2</sub> from reformed natural gas or from syngas
- Adjusting CO<sub>2</sub>/H<sub>2</sub> ratio for coal and biomass to liquids
- The removal of CO<sub>2</sub> from syngas for coal and biomass to ammonia/fertilizer
- Natural gas sweetening

**PATENT STATUS:**

U.S. Patent Pending (provisional patent application)

Filed: 07/19/2021

Title: Hydrophobic Alkyl-Ester Physical Solvents for CO<sub>2</sub> Removal from H<sub>2</sub> Produced from Synthesis Gas

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NETL Reference No: 20N-25