The post-WGS fuel gas in an IGCC power plant is at ~250°C and 800psi (5.5MPa), with a composition of 31 mol% CO₂, 43% H₂, 23% H₂O, and 3% of other gases such CO, COS, H₂S. The CO₂ partial pressure is about 250psi (1.7MPa). The dew point of the gas mixture is ~180°C. The conventional strategy for the removal of CO₂ from this stream is to cool the it to ~40°C; the water will begin to condense out of the stream at 180°C and the vast majority of the water will be removed as a liquid from this stream when cooled to 40°C. A very hydrophilic solvent, such as the Selenol solvent, which is rich in polyethylene glycol dimethylether (PEGDME) can then be used to remove the CO₂ from the hydrogen. The hydrogen can then be diluted with N₂ from the air separation prior to combustion.

This study considers an alternate means of removing the CO₂ from the post WGSR stream. Rather than cooling the stream and condensing the water prior to absorption of CO₂, the CO₂ is absorbed from the hot or warm, humid stream with a CO₂-selective hydrophobic solvent that absorbs little H₂ or H₂O vapor. In this case the H₂O would dilute the H₂ sent to combustion. Process modeling at NETL indicates that this minimization of fuel gas cooling and heat exchange equipment could increase the thermal efficiency of an IGCC by 1-3 % points.

Solvents such as Selexol that are rich in PEGDME cannot be used for such a process because PEGDME is completely miscible with water in all proportions and would therefore absorb both water vapor and CO₂. Our team is using PEGDME as a “control” and assessing the viability of the five hydrophobic solvents for this high temperature absorption process:

- **Polyethyenglycol dimethylether (PEGDME 250)** Extremely hydrophilic
- **Polydimethylsiloxane (PDMS 550)** Extremely hydrophobic, high thermal stability
- **PPGDME-B 430** PPGDME absorbs ~2wt% water at 25°C, but slowly forms rigid gels upon exposure to liquid water
- **PPGDME-L 650** PDMS 6000 + 2% Fe-siloxane high temperature stabilizer
- **Hybrid PDMS-PEGDME** (2,2,4-trimethyl-4-(trimethyloxyl)oxy)-3,8,11,14-tetraoxa-2,4-disilapentadecane

Designed by Nulwala of CMU-RUA to provide high CO₂ solubility of low H₂ solubility of PEGDME, while being hydrophobic.

CO₂-solvent bubble point pressure at 25°C. The lower bubble point curves correspond to the strongest CO₂ solvents (desirable). The solvents are all reasonable CO₂ solvents. PEGDME is the best CO₂ solvent. The PDMS 6000 + Fe solvent is the weakest of the CO₂ solvents primarily due to its high MW.

H₂-solvent bubble point pressure at 25°C. The higher bubble point curves correspond to the weakest H₂ solvent (desirable). PPGDME-L is the weakest H₂ solvent, PDMS 550 is the strongest H₂ solvent. In general H₂ exhibits its lowest solubility in linear (monomer) polymers due to smaller free volume.

H₂ solubility increases with increasing temperature (not shown in this plot to the left, but shown below) due to increased free volume of polymers at elevated T.

Solubility of CO₂ and H₂ in PDMS-PEGDME hybrid at various temperatures. Because CO₂ solubility decreases and H₂ solubility increases with T, the separation will be more difficult at higher T values. This occurs for all solvents.