

# TEA of the CO<sub>2</sub> Capture Process in SMR-CCS Applications

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## SMR-CCS Blue Hydrogen

Steam Methane Reforming (SMR) produces most of the hydrogen (H<sub>2</sub>) in the world and in the USA at 49% and 95%, respectively. The H<sub>2</sub> produced via SMR is called "grey hydrogen," when the CO<sub>2</sub> produced is released to the atmosphere. However, it is called "blue hydrogen," when most of the CO<sub>2</sub> produced is sent for carbon capture and storage (CCS) in geological formation. In the DOE/NETL SMR-CCS process flow diagram (Figure 1), the syngas is produced in a steam reformer and is shifted in a WGS reactor. The shifted fuel gas is cooled and then sent for CCS. The conditions and composition of this gas are given in Table 1.

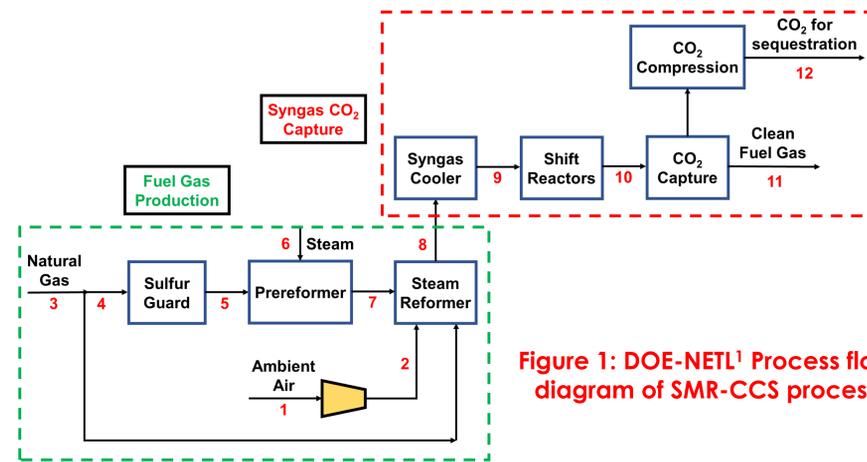


Figure 1: DOE-NETL<sup>1</sup> Process flow diagram of SMR-CCS process

Table 1: Shifted SMR fuel gas<sup>1</sup>

Pressure, bar	24.5	
Temperature, °C	204	
Molar flow rate, kmol/h	19,519	
Mass flow rate, kg/h	240,967	
Composition	Mol%	Mass%
H <sub>2</sub>	60.01	9.80
CH <sub>4</sub>	4.11	5.34
CO	0.40	0.91
CO <sub>2</sub>	15.17	54.07
H <sub>2</sub> O	20.00	29.18
N <sub>2</sub>	0.31	0.70
Total	100.00	100.00

Solvent Used: CASSH-1  
(Diethyl Sebacate)  
Hydrophobic and  
Non-corrosive

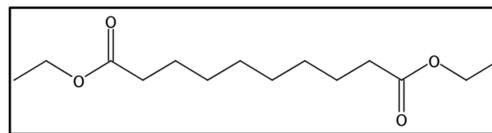


Figure 2: Chemical structure of CASSH-1

## PC-SAFT EOS in Aspen Plus V12.1

In this study, a physical solvent diethyl sebacate (DES) (Figure 2) was used for CO<sub>2</sub> capture. The physical properties of DES, including, density, viscosity, surface tension and heat capacity, were obtained and regressed in Aspen Plus V12.1. Also, the solubilities of CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub> in DES were measured and modeled using the PC-SAFT Equation-of-State (EOS) in Aspen Plus V12.1. The predicted solubility values were also validated against the experimental data in Figure 3.

### References

[1] COMPARISON OF COMMERCIAL, STATE OF THE ART, FOSSIL BASED HYDROGEN PRODUCTION TECHNOLOGIES, April 12, 2022. DOE/NETL-2022/3241

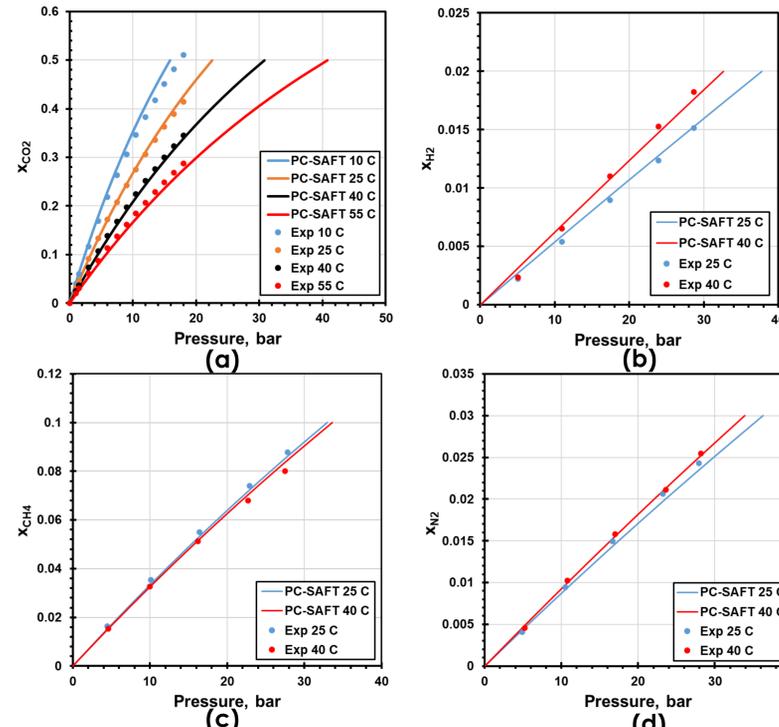


Figure 3: Gas solubility validation against experimental results

The objective of this study is to design a novel process in Aspen Plus V12.1 packed with a structured packing (Mellapak 250Y) for CO<sub>2</sub> capture from fuel gas streams of an SMR-CCS process using a DES in a counter-current fixed-bed absorber. The specific area of this packing (a) is 256 m<sup>2</sup>. The schematic of the novel CO<sub>2</sub> capture process is shown in Figure 4.

The constraints imposed on the process were: (1) no flooding in the absorber and the packing height (H) to the absorber diameter (D) ratio (H/D) is ≥ 6, (2) the CO<sub>2</sub> capture efficiency is ≥ 97 mol%, and (3) the CO<sub>2</sub> stream intended for sequestration has a water content of < 600 ppm, and a fuel gas (CH<sub>4</sub>, H<sub>2</sub>, and CO) content of < 0.5 mol%. The solvent flow rate and CO<sub>2</sub> absorber dimensions were varied to meet the process constraints. The process hydraulics (pressure drop, liquid holdup, and flooding) and mass transfer characteristics (liquid-side (k<sub>L</sub>) and gas-side (k<sub>G</sub>) mass transfer coefficients, and the normalized specific packing wetted area (a<sub>w</sub>/a) were obtained. Also, a detailed techno-economic analysis (TEA) of the CO<sub>2</sub> capture process in terms of the capital expenditure (CAPEX), operating expenditure (OPEX) and levelized cost of CO<sub>2</sub> captured (LCOC) was performed. The LCOC was calculated as follows:

$$LCOC = \left( \frac{f_{CR}}{f_c} \right) \sum (CAPEX_{2020} / \dot{m}_{CO_2} + OPEX_{2020} / \dot{m}_{CO_2})$$

$$f_{CR} = \frac{i(1+i)^N}{(1+i)^N - 1}$$

f<sub>CR</sub> = Capital recovery factor, 1/year  
f<sub>c</sub> = Capacity factor = 0.8  
m<sub>CO<sub>2</sub></sub> = CO<sub>2</sub> captured, 4,793 ton/h  
N = project lifetime, 30 year  
i = discount rate = 10%/year  
CAPEX = capital expenditure, \$  
OPEX = operating expenditure, \$/year

Parameter	Value	
	2019	2023
Cost of electricity	\$50/MWh	\$83.3/MWh
Cost of steam	\$6.46/ton	\$6.21/ton
CEPCI*	590	800.7
i	10%/year	
N	30 years	
f <sub>c</sub>	0.8	
f <sub>O&amp;M</sub>	4% of the Total CAPEX, \$/year	
f <sub>CR</sub>	0.10608	

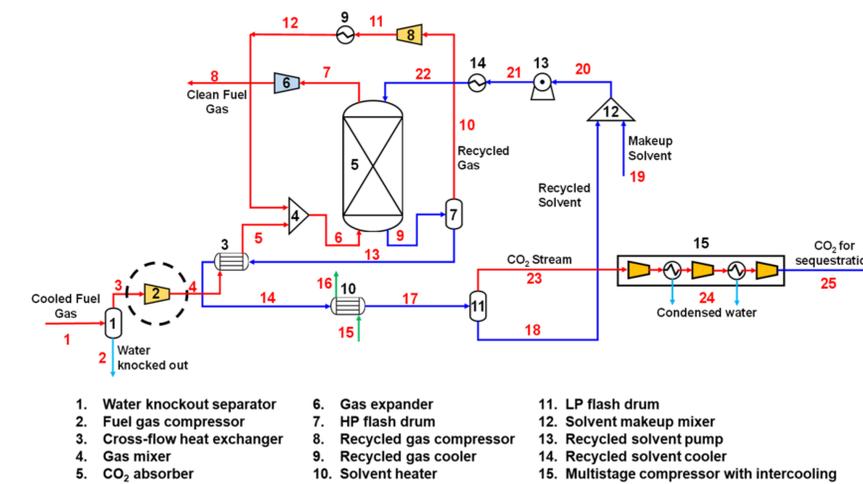


Figure 4: Schematic of CO<sub>2</sub> capture process

The process began with knocking off the water vapor from the shifted fuel gas stream using a water separator at 38 °C and 24.5 bar. To increase the CO<sub>2</sub> partial pressure in the shifted fuel gas stream, a compressor was used to boost the total pressure of the water-free fuel gas from 24.5 bar to different discharge pressures (49 bar, 61 bar, 73.5 bar, 97 bar, 98 bar, 99 bar, 110 bar, and 122.5 bar). Hence, the effects of the gas compression ratio on the process hydraulics, mass transfer, and TEA (CAPEX, OPEX, and LCOC) were investigated at 2019 and 2023 (Figure 5).

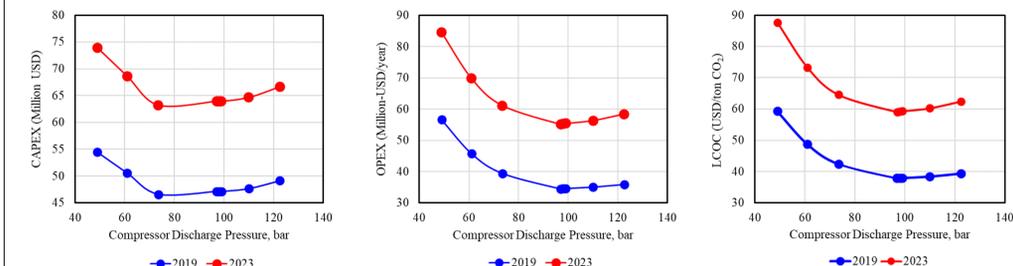


Figure 5: CAPEX, OPEX, and LCOC of different compressor discharge pressures in 2019 and 2023

### Concluding Remarks:

(1) In 2023, the lowest LCOC was 59.04 USD per ton of CO<sub>2</sub> captured at a compressor discharge pressure of 97 bar, and the corresponding CAPEX and OPEX values were 63.97 million USD and OPEX of 55.10 million USD per year, respectively; (2) At 97 bar, the total pressure drop was 12 mbar, and the average liquid-phase holdup was 27.8%; (3) The average k<sub>L</sub>, k<sub>G</sub>, and a<sub>w</sub>/a were 2.15E-4 s<sup>-1</sup>, 1.86E-2 s<sup>-1</sup>, and 63.4%, respectively; and (4) The mass transfer data indicating that the process was mainly controlled by (k<sub>L</sub>) since the liquid-side resistance to mass transfer (1/k<sub>L</sub>) is much greater than that of the gas-side resistance (1/k<sub>G</sub>).

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### Disclaimer:

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