Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.


Electronic Supplementary Information

for

# System-level feasibility analysis of a novel chemical looping combustion integrated with electrochemical $CO_2$ reduction

Nimish Pankhedkar [a], Rohan Sartape [b], Meenesh Singh [b], Ravindra Gudi [a,*], Pratim Biswas [c]

[a] Department of Chemical Engineering,
Indian Institute of Technology, Bombay,
Powai, Mumbai, 400 076, India.

[b] Department of Chemical Engineering,
University of Illinois Chicago, 929 W. Taylor St.,
Chicago, Illinois 60607, United States.

[c] Dept of Chemical, Environmental and Materials Engineering,
University of Miami,
Coral Gables, FL 33146, USA.

* To Whom Correspondence Must be Addressed: Ravindra Gudi, E-mail: ravigudi@iitb.ac.in

## S1. Reactions involved in modeling of in-situ gasification CLC

$$Coal \rightarrow Volatile\ Matter + Char\ (C) + H_2O + Ash$$

$$Char\ (C) + H_2O \rightarrow H_2 + CO$$

$$CO + Me_xO_y \rightarrow Me_xO_{y-1} + CO_2$$

$$H_2 + Me_xO_y \rightarrow Me_xO_{y-1} + H_2O$$

$$Me_xO_{y-1} + \frac{1}{2}O_2 \rightarrow Me_xO_y$$

$$Char\ (C) + CO_2 \rightarrow 2\ CO$$

$$CO + H_2O \rightarrow CO_2 + H_2$$

$$Char\ (C) + \frac{1}{2}O_2 \rightarrow CO$$

$$Char\ (C) + O_2 \rightarrow CO_2$$

$$Char\ (C) + 2\ H_2 \rightarrow CH_4$$

$$Char\ (C) + H_2O \rightarrow CO + 3\ H_2$$

The *RGIBBS* reactor module estimates the product composition based on the minimization of Gibbs Free energy of the system.

$$G^{total} = \sum_{i=1}^{N} n_i G_i^0 + R(T + 273.15) \sum_{i=1}^{N} n_i \ln\left(\frac{f_i}{f_i^0}\right)$$

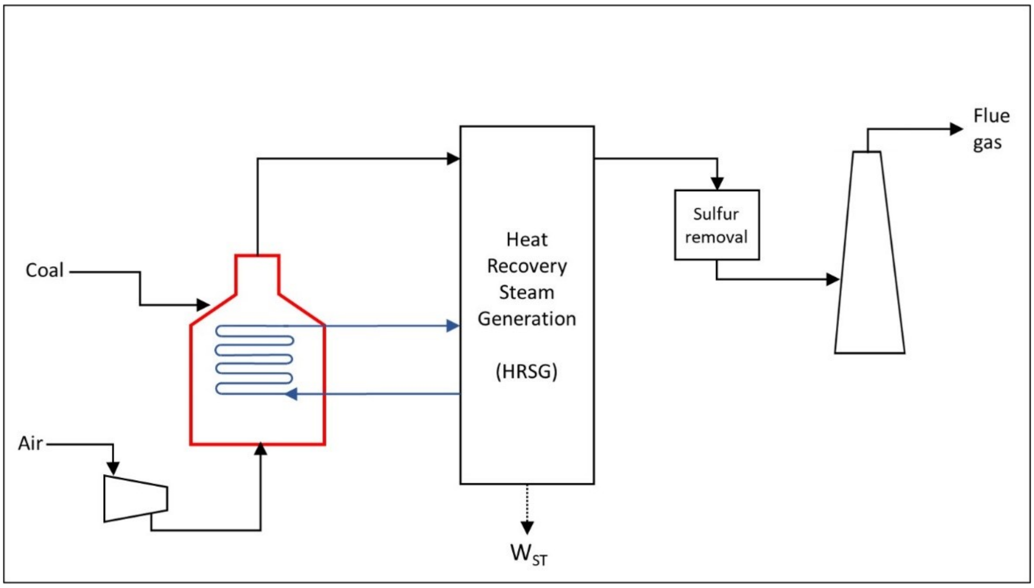
Where,

$G_i^0$: Gibbs free energy of species i under standard conditions

R: molar gas constant

$f_i, f_i^0$: fugacity of each species at standard operating conditions.

The *RYIELD* reactor module utilizes the ultimate and proximate analysis details to estimate the yields of the components.




S2. Conventional processes considered for relative analysis

*Figure S1 Schematic flow diagram for a conventional coal fired power plant*

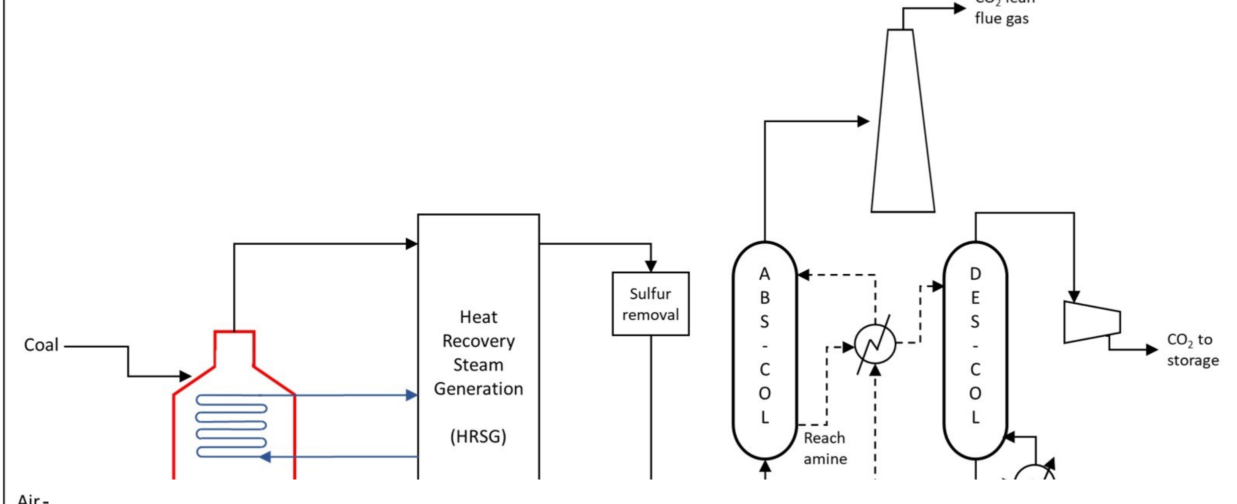



*Figure S2 Schematic flow diagram for a conventional coal fired power with amine -based $CO_2$ capture (CPCFPP+CCS)*

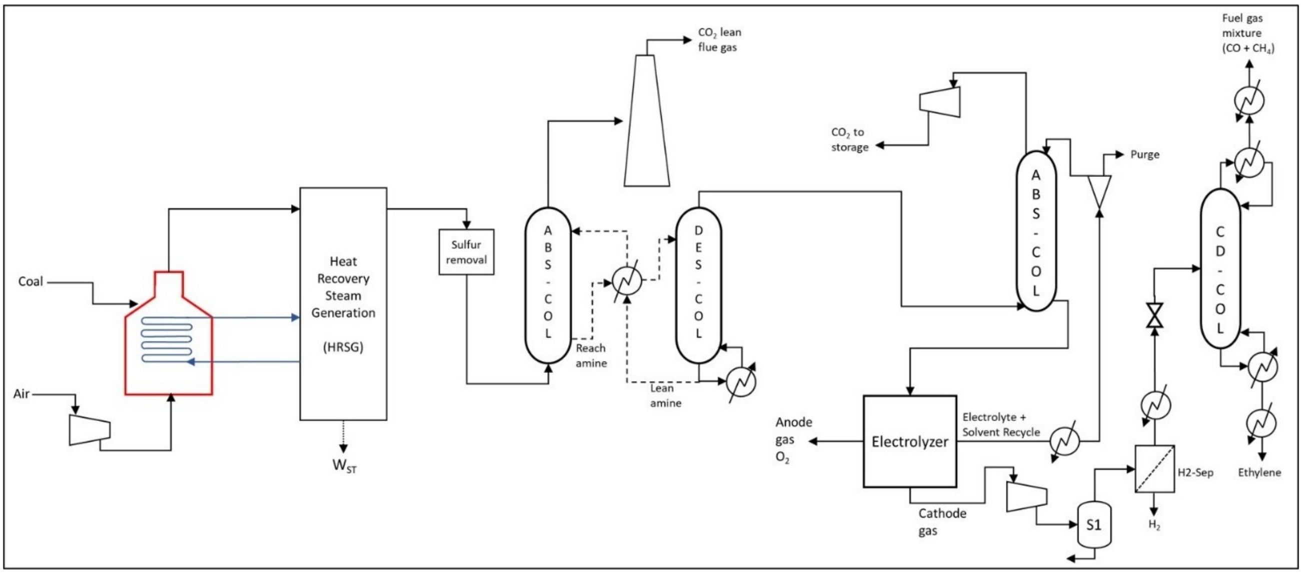



*Figure S3 Schematic flow diagram for a conventional coal fired power with amine based $CO_2$ capture followed by $CO_2$ electroreduction (CPCFPP+CCS+CO2ER)*

## S3. Details for Economic analysis

*Table S1 Parameters for CAPEX calculation [48,49,55]*

| | |
|---|---|
| *Direct Cost Components (DC)* | |
| Purchased Equipment (PE) | |
| Delivered purchase equipment (DPE) | 110% of PE |
| Purchased Equipment Installation | 20% of PE |
| I&C | 15% of PE |
| Piping | 7% of PE |
| Electrical systems | 10% of PE |
| Buildings | 15% of PE |
| Land & Yard Improvements | 10% of DPE |
| *Indirect cost components (IC)* | |
| Engineering and Construction | 30% of DPE |
| Management | |
| Contingencies | 12% of DPE |

| | |
|---|---|
| *FCI* | DC + IC |
| *Working Capital (WC)* | 75% of FCI |
| **TCI** | **FCI + WC** |

*Table S2 CAPEX Estimation details [48,49,55]*

| **CEPCI (2001) = 397** | | |
|---|---|---|
| **Heat Exchangers** | $\log_{10} C_p{}^{\circ} = K_1 + K_2 \log_{10}(A) + K_3[\log_{10}(A)]^2$ where,<br>A = Heat transfer area ($m^2$) | $K_1$ = 4.1884<br>$K_2$ = -0.2503<br>$K_3$ = 0.1974 |
| **Turbine** | $\log_{10} C_p{}^{\circ} = K_1 + K_2 \log_{10}(A) + K_3[\log_{10}(A)]^2$<br>where,<br>A = Power (kW) | $K_1$ = -21.7702<br>$K_2$ = 13.2175<br>$K_3$ = -1.5279 |
| **Compressor** | $\log_{10} C_p{}^{\circ} = K_1 + K_2 \log_{10}(A) + K_3[\log_{10}(A)]^2$<br>where,<br>A = Power (kW) | $K_1$ = 2.2897<br>$K_2$ = 1.3604<br>$K_3$ = -0.1027 |

*S3-c: Estimation of metal oxide requirement:*

The oxygen carrier loading has been estimated based on the typical residence time in the CLC reactors (Fluidized bed type). It has been reported in Mantripragada et. al., 2012, Wolf et. al., 2005, and Naqvi et. al., 2005 that the residence times in AR and FR are around 4s and 60s respectively, and the same have been considered for estimating the metal oxide inventory. Furthermore, as suggested by Mantripragada et. al., 2012, a degradation rate of '0.027 % / hr' has been utilized to estimate the make-up oxygen carrier. This rate is based on the lifetime of the metal oxide particles observed during the experimental tests performed by Abad et. al., 2009 and Mattison et. al. 2007.Assumptions: Residence time in AR = 4 s, Residence time in FR = 60 s, Degradation rate = 0.0272 %/hr [50]

$$Solid\ inventory = (Flow\ of\ OC\ \times Residence\ time) \times Excess\ factor$$

$$\therefore Total\ Solid\ inventory = 4.24\ \ tonnes$$

$$Make\ up\ OC = Total\ Solid\ inventory\ \times Degradation\ rat \times Annual\ operating\ hours$$

$$Makeup\ OC = \ 9.24\ tonnes/year$$