

Comparative Investigation of Different CO₂ Capture Technologies for Coal to Ethylene Glycol Process

Yanqing Ma¹, Yitao Liao¹, Yi Su¹, Baojie Wang¹, Yong Yang², Dong Ji², Hongwei Li², Huairong Zhou² and Dongliang Wang^{2,*}

¹ Lanzhou Petrochemical Research Center, Petrochemical Research Institute, PetroChina, Lanzhou 730060, China; mayanqing@petrochina.com.cn (Y.M.); liaoyitao@petrochina.com.cn (Y.L.); suyi1@petrochina.com.cn (Y.S.); wangbaojie@petrochina.com.cn (B.W.)

² School of Petrochemical Engineering, Lanzhou University of Technology, Lanzhou 730050, China; yangy@lut.edu.cn (Y.Y.); jidong@lut.edu.cn (D.J.); lihw@lut.edu.cn (H.L.); zhouhr@lut.edu.cn (H.Z.)

* Correspondence: wangdl@lut.edu.cn; Tel.: 86-0931-7823215

Table S1. Main reactions take place in gasifier.

Reaction number	Reaction	Heat of reaction
R1	$C + 0.5O_2 \leftrightarrow CO$	-110.4 kJ/mol
R2	$C + O_2 \leftrightarrow CO_2$	-394.1 kJ/mol
R3	$C + H_2O \leftrightarrow CO + H_2$	+135.0 kJ/mol
R4	$C + 2H_2O \leftrightarrow CO_2 + 2H_2$	+96.6 kJ/mol
R5	$CO + 0.5O_2 \leftrightarrow CO_2$	-283.7 kJ/mol
R6	$H_2 + 0.5O_2 \leftrightarrow H_2O$	-242 kJ/mol
R7	$C + CO_2 \leftrightarrow 2CO$	+173.3 kJ/mol
R8	$CO + H_2O \leftrightarrow CO_2 + H_2$	-41.0 kJ/mol
R9	$C + 2H_2 \leftrightarrow CH_4$	+84.3 kJ/mol
R10	$CH_4 + H_2O \leftrightarrow CO + 3H_2$	+206 kJ/mol
R11	$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2$	+165 kJ/mol
R12	$CH_4 + 2O_2 \leftrightarrow CO_2 + H_2O$	-893.0 kJ/mol

Table S2. Key parameters for the simulation of four CO₂ capture technologies.

Technology	Equipment	Model	Operational parameters	Equipment	Model	Operational parameters
Rectisol	Lean cooler	Heater	$T_{out} = -58^\circ C, \Delta P = 0$	CO ₂ Flash1	Flash	$P = 1.38 \text{ MPa}, Q = 0$
	Acid gas Absorber	Radfrac	$N = 20, P = 5.5 \text{ MPa}$	H ₂ S con. column	Radfrac	$N = 20, P = 0.2 \text{ MPa}$
	SO ₂ Flash	Flash	$P = 0.69 \text{ MPa}, Q = 0$	H ₂ S	Radfrac	$N = 10, P = 0.3 \text{ MPa}$
MEA	Cooler	Heater	$T_{out} = 40^\circ C, \Delta P = 0$	Desorber	Radfrac	$N = 11, P = 0.19 \text{ MPa}$
	Absorber	Radfrac	$N = 11, P = 0.12 \text{ MPa}$	Lean cooler	Heater	$T_{out} = 40^\circ C, \Delta P = 0$
	Rich-pump	Pump	$P = 0.21 \text{ MPa}, \eta = 0.8$	Lean pump	Pump	$P = 0.21 \text{ MPa}, \eta = 0.8$
CAP	Heat exchanger	HeatX	$T_{cold} = 95^\circ C, \Delta P = 0$	Separator	Flash2	$T_{out} = 40^\circ C, \Delta P = 0$
	Contact cooler	Radfrac	$N = 5, P = 0.12 \text{ MPa}$	Rich-pump-2	Pump	$P = 0.14 \text{ MPa}, \eta = 0.8$
	Absorber	Radfrac	$N = 20, P = 0.12 \text{ MPa}$	Heat exchanger-2	HeatX	$\Delta T_{cold} = 5^\circ C, \Delta P = 0$
	Rich-pump-1	Pump	$P = 1.0 \text{ MPa}, \eta = 0.8$	Lean pump	Pump	$P = 0.14 \text{ MPa}, \eta = 0.8$
	Heat exchanger-1	HeatX	$\Delta T_{cold} = 5^\circ C, \Delta P = 0$	NH ₃ -desorber	Radfrac	$N = 5, P = 0.12 \text{ MPa}$
	Desorber	Radfrac	$P = 2.0 \text{ MPa}$	Cooler-2	Heater	$T_{out} = 40^\circ C, \Delta P = 0$
	Lean cooler-1	Heater	$T_{out} = 25^\circ C, \Delta P = 0$	Lean cooler-2	Heater	$T_{out} = 10^\circ C, \Delta P = 0$
DMC	Flash	Flash2	$T_{out} = 40^\circ C, \Delta P = 0$	Mixer	Mixer	Adiabatic mixing
	Absorber	Radfrac	$N = 10, P = 2.84 \text{ MPa}, \Delta P = 0.02 \text{ MPa}$	Heat exchanger	HeatX	$T_{lean} = 30^\circ C, \Delta P = 0$
	Flash	Flash2	$T_{out} = 30^\circ C, \Delta P = 0$	Lean MEA	-	35%

Table S3. Ratio factor of the components in the TCI.

Component	Capital Investment	RF
<i>I_{EI}</i>	equipment and installation cost	100
<i>I_{IE}</i>	instruments, piping and electrical	74
<i>I_{BL}</i>	buildings and land	51
<i>I_{ES}</i>	engineering and supervision	32
<i>I_{CCF}</i>	construction and contractor's fee expenses	42
<i>I_{WCC}</i>	working capital and contingency	76