Pressurized Chemical Looping for Direct Reduced Iron Production: Carbon Neutral Process Configuration and Performance

Supplementary Data

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Table S1. Base – M stream table. Stream numbers correspond to Figure 1(a).

Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0
Temperature (°C)	25	25	25	25	25	54	750	54	25	-10
Pressure (kPaa)	400	400	400	400	101.3	132.3	127.3	132.3	300	200
Molar Flow (kgmole/h)	3391	1778	0	1613	16675	10934	10934	5741	288	2266
Mass Flow (t/h)	56.6	29.7	0.0	26.9	481.1	315.4	315.4	165.6	9.2	340.6
Species Mole fraction										
CH_4	0.9594	0.9594	0.9594	0.9594	0	0	0	0	0	0
H_2O	0	0	0	0	0	0	0	0	0	0
CO	0	0	0	0	0	0	0	0	0	0
CO_2	0.0073	0.0073	0.0073	0.0073	0	0	0	0	0	0
O_2	0	0	0	0	0.2100	0.2100	0.2100	0.2100	0.9900	0
H_2	0	0	0	0	0	0	0	0	0	0
N_2	0.0169	0.0169	0.0169	0.0169	0.7900	0.7900	0.7900	0.7900	0.0100	0
C_2H_6	0.0160	0.0160	0.0160	0.0160	0	0	0	0	0	0
C_3H_8	0.0004	0.0004	0.0004	0.0004	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0.9098
FeO	0	0	0	0	0	0	0	0	0	0
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0	0	0.0902

Stream Number	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Vapour Fraction	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (°C)	50	285	51	51	51	51	155	500	925	957
Pressure (kPaa)	150	142	122	122	122	122	300	280	220	200
Molar Flow (kgmole/h)	4730	17953	16083	1613	5267	9202	9202	10980	14960	16875
Mass Flow (t/h)	250.0	319.8	286.1	28.7	93.7	163.7	163.7	193.4	193.4	229.5
Species Mole fraction										
CH_4	0	0.0300	0.0335	0.0335	0.0335	0.0335	0.0335	0.1834	0.0055	0.0909
H_2O	0	0.2000	0.1070	0.1070	0.1070	0.1070	0.1070	0.0897	0.0299	0.0426
CO	0	0.1900	0.2121	0.2121	0.2121	0.2121	0.2121	0.1777	0.3606	0.3197
CO_2	0	0.1600	0.1786	0.1786	0.1786	0.1786	0.1786	0.1509	0.0136	0.0216
O_2	0	0	0	0	0	0	0	0	0	0
H_2	0	0.4000	0.4465	0.4465	0.4465	0.4465	0.4465	0.3742	0.5746	0.5094
N_2	0	0.0200	0.0223	0.0223	0.0223	0.0223	0.0223	0.0214	0.0157	0.0157
C_2H_6	0	0	0	0	0	0	0	0.0026	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0
FeO	0.0550	0	0	0	0	0	0	0	0	0
Fe	0.8122	0	0	0	0	0	0	0	0	0
C	0.0881	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0.0446	0	0	0	0	0	0	0	0	0

Stream Number	**21**	**22**	**23**	**24**	**25**	**26**
Vapour Fraction	1.0	1.0	1.0	1.0	0.0	1.0
Temperature (°C)	1125	542	327	334	51	41
Pressure (kPaa)	112	102	97	101	122	200
Molar Flow (kgmole/h)	14467	20207	20207	20207	1870	3785
Mass Flow (t/h)	409.2	574.8	574.8	574.8	33.7	58.7
Species Mole fraction						
CH_4	0	0	0	0	0	0.7590
H_2O	0.2259	0.1617	0.1617	0.1617	0.9999	0.0320
CO	0	0	0	0	0	0.0430
CO_2	0.1544	0.1106	0.1106	0.1106	0.0001	0.0240
O_2	0.0144	0.0700	0.0700	0.0700	0	0
H_2	0	0	0	0	0	0.1342
N_2	0.6052	0.6577	0.6577	0.6577	0	0.0078
C_2H_6	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0
FeO	0	0	0	0	0	0
Fe	0	0	0	0	0	0
C	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0

Table S2. Base – E stream table. Stream numbers correspond to Figure 1(b).

Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
Temperature (°C)	25	25	25	500	25	25	25	67	500	880
Pressure (kPaa)	1025	1025	1025	1005	1025	101	750	661	1005	945
Molar Flow (kgmole/h)	3141	1557	652	652	395	12142	172	2333	1557	6593
Mass Flow (t/h)	51.5	25.6	10.7	10.7	6.5	350.3	5.5	351.1	25.6	69.2
Species Mole fraction										
CH_4	0.9758	0.9758	0.9758	0.9758	0.9758	0	0	0	0.9758	0.0321
H_2O	0	0	0	0	0	0	0	0	0	0.139
CO	0	0	0	0	0	0	0	0	0	0.1691
CO_2	0.0073	0.0073	0.0073	0.0073	0.0073	0	0	0	0.0073	0.0311
O_2	0	0	0	0	0	0.2100	0.9900	0	0	0
H_2	0	0	0	0	0	0	0	0	0	0.6247
N_2	0.0169	0.0169	0.0169	0.0169	0.0169	0.7900	0.0100	0	0.0169	0.0040
C_2H_6	0	0	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0.9063	0	0
FeO	0	0	0	0	0	0	0	0.0320	0	0
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0.0617	0	0

Stream Number	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (°C)	370	470	67	66	426	900	962	412	158	50
Pressure (kPaa)	885	885	825	805	765	745	725	661	641	621
Molar Flow (kgmole/h)	6593	6593	6593	6458	18125	18125	18692	20439	20439	12971
Mass Flow (t/h)	69.2	69.2	69.2	66.8	180.7	180.7	192.7	293.7	293.7	168.5
Species Mole fraction										
CH_4	0.0321	0.0321	0.0321	0.0327	0.0691	0.0691	0.0831	0.0586	0.0586	0.0803
H_2O	0.139	0.0538	0.0538	0.034	0.0212	0.0212	0.0296	0.2847	0.2847	0.0204
CO	0.1691	0.0839	0.0839	0.0856	0.11669	0.11669	0.1619	0.1391	0.1391	0.1907
CO_2	0.0311	0.1164	0.1164	0.1188	0.0469	0.0469	0.0502	0.0728	0.0728	0.0988
O_2	0	0	0	0	0	0	0	0	0	0
H_2	0.6247	0.7099	0.7099	0.7248	0.6830	0.6830	0.6623	0.4333	0.4333	0.5938
N_2	0.0040	0.0040	0.0040	0.0041	0.0129	0.0129	0.0129	0.0117	0.0117	0.016
C_2H_6	0	0	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0
FeO	0	0	0	0	0	0	0	0	0	0
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0	0	0

Stream Number	**21**	**22**	**23**	**24**	**25**	**26**	**27[a]**	**28**	**29**	**30**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (°C)	50	109	55	45	1125	106	26	96	600	350
Pressure (kPaa)	621	1000	980	180	161	121	990	181	161	161
Molar Flow (kgmole/h)	1942	12971	11668	1268	6957	6957	536	6365	6365	5777
Mass Flow (t/h)	25.2	168.5	113.9	53.9	191.9	191.9	8.7	183.6	183.6	166.7
Species Mole fraction										
CH_4	0.0803	0.0803	0.0892	0.0006	0	0	0.9758	0	0	0
H_2O	0.0204	0.0204	0.0141	0.054	0.2162	0.2162	0	0	0	0
CO	0.1907	0.1907	0.2119	0.0004	0	0	0	0	0	0
CO_2	0.0988	0.0988	0.0071	0.9433	0.1032	0.1032	0.0073	0	0	0
O_2	0	0	0	0	0.0201	0.0201	0	0.2100	0.2100	0.2100
H_2	0.5938	0.5938	0.6599	0.0016	0	0	0	0	0	0
N_2	0.0160	0.0160	0.0178	0	0.6605	0.6605	0.0169	0.7900	0.7900	0.7900
C_2H_6	0	0	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0
FeO	0	0	0	0	0	0	0	0	0	0
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0	0	0

[a]Composition from Zugliano et al was simplified to replace higher hydrocarbons as CH_4.

Stream Number	**31**	**32**	**33**	**34**	**35**	**36**
Vapour Fraction	1.0	1.0	0.0	1.0	0.0	0.0
Temperature (°C)	1125	351	50	500	66	634
Pressure (kPaa)	141	101	621	1005	805	500
Molar Flow (kgmole/h)	7017	7017	3107	2419	135	4768
Mass Flow (t/h)	194.4	194.4	56.0	43.6	2.4	249.6
Species Mole fraction						
CH_4	0	0	0	0	0	0
H_2O	0.1814	0.1814	0.9998	0.9998	0.9998	0
CO	0	0	0	0	0	0
CO_2	0.0914	0.0914	0.0002	0.0002	0.0002	0
O_2	0.0091	0.0091	0	0	0	0
H_2	0	0	0	0	0	0
N_2	0.7181	0.7181	0	0	0	0
C_2H_6	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0
FeO	0	0	0	0	0	0.0545
Fe	0	0	0	0	0	0.8164
C	0	0	0	0	0	0.0994
Gangue (SiO_2)	0	0	0	0	0	0.0297

Table S3. PCL-DRI – M stream table. Stream numbers correspond to Figure 2(a).

Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0
Temperature (°C)	25	25	25	25	337	620	25	-10	50	285
Pressure (kPaa)	400	400	400	101.3	971.325	951.325	300	200	150	142
Molar Flow (kgmole/h)	3391	1778	1613	9271	9271	9271	288	2266	4730	17953
Mass Flow (t/h)	56.6	29.7	26.9	267.5	267.5	267.5	9.2	340.6	250.0	319.8
Species Mole fraction										
CH_4	0.9594	0.9594	0.9594	0	0	0	0	0	0	0.0300
H_2O	0	0	0	0	0	0	0	0	0	0.2000
CO	0	0	0	0	0	0	0	0	0	0.1900
CO_2	0.0073	0.0073	0.0073	0	0	0	0	0	0	0.1600
O_2	0	0	0	0.2100	0.2100	0.2100	0.9900	0	0	0
H_2	0	0	0	0	0	0	0	0	0	0.4000
N_2	0.0169	0.0169	0.0169	0.7900	0.7900	0.7900	0.0100	0	0	0.0200
C_2H_6	0.0160	0.0160	0.0160	0	0	0	0	0	0	0
C_3H_8	0.0004	0.0004	0.0004	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0.9098	0	0
FeO	0	0	0	0	0	0	0	0	0.0550	0
Fe	0	0	0	0	0	0	0	0	0.8122	0
C	0	0	0	0	0	0	0	0	0.0881	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0.0902	0.0446	0

Stream Number	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0
Temperature (°C)	51	155	155	243	342	950	600	528	77	77
Pressure (kPaa)	122	300	300	971	951	801	781	761	721	721
Molar Flow (kgmole/h)	14038	9202	4835	4835	4835	5095	5095	5095	2298	2797
Mass Flow (t/h)	249.7	163.7	86.0	86.0	86.0	145.3	145.3	145.3	94.8	50.5
Species Mole fraction										
CH_4	0.0335	0.0335	0.0335	0.0335	0.0335	0.0062	0.0062	0.0062	0.0138	0
H_2O	0.1070	0.1070	0.1070	0.1070	0.1070	0.5763	0.5763	0.5763	0.0622	0.9987
CO	0.2121	0.2121	0.2121	0.2121	0.2121	0	0	0	0	0
CO_2	0.1786	0.1786	0.1786	0.1786	0.1786	0.3963	0.3963	0.3963	0.8770	0.0013
O_2	0	0	0	0	0	0	0	0	0	0
H_2	0.4465	0.4465	0.4465	0.4465	0.4465	0	0	0	0	0
N_2	0.0223	0.0223	0.0223	0.0223	0.0223	0.0212	0.0212	0.0212	0.0470	0
C_2H_6	0	0	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0
FeO	0	0	0	0	0	0	0	0	0	0
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0	0	0

Stream Number	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**
Vapour Fraction	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (°C)	51	67	425	170	925	957	41	51
Pressure (kPaa)	122	122	800	101	220	200	200	122.
Molar Flow (kgmole/h)	1870	4667	7419	7419	14960	16875	3785	2045
Mass Flow (t/h)	33.7	84.2	208.2	208.2	193.4	229.5	58.7	36.4
Species Mole fraction								
CH_4	0	0	0	0	0.0055	0.0909	0.7590	0.0335
H_2O	0.9999	0.9992	0	0	0.0299	0.0426	0.0320	0.1070
CO	0	0	0	0	0.3606	0.3197	0.0430	0.2121
CO_2	0.0001	0.0008	0	0	0.0136	0.0216	0.0240	0.1786
O_2	0	0	0.0127	0.0127	0	0	0	0
H_2	0	0	0	0	0.5746	0.5094	0.1342	0.4465
N_2	0	0	0.9873	0.9873	0.0157	0.0157	0.0078	0.0223
C_2H_6	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0
FeO	0	0	0	0	0	0	0	0
Fe	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0

Table S4. PCL-DRI – E stream table. Stream numbers correspond to Figure 2(b).

Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (°C)	25	25	420	500	880	370	470	67	67	900
Pressure (kPaa)	1000	1000	980	1005	945	905	905	845	845	785
Molar Flow (kgmole/h)	2817	395	2341	1560	6604	6604	6604	6604	6468	18155
Mass Flow (t/h)	46.2	6.5	31.8	25.7	69.3	69.3	69.3	69.3	66.9	181.0
Species Mole fraction										
CH_4	0.9758	0.9758	0.2312	0.9758	0.0321	0.0321	0.0321	0.0321	0.0327	0.0691
H_2O	0	0	0.0170	0	0.1390	0.1390	0.0537	0.0537	0.0338	0.0211
CO	0	0	0.1584	0	0.1691	0.1691	0.0839	0.0839	0.0856	0.1669
CO_2	0.0073	0.0073	0.0838	0.0073	0.0311	0.0311	0.1164	0.1164	0.1188	0.0469
O_2	0	0	0	0	0	0	0	0	0	0
H_2	0	0	0.4934	0	0.6247	0.6247	0.7100	0.7100	0.7249	0.6831
N_2	0.0169	0.0169	0.0162	0.0169	0.0040	0.0040	0.0040	3.99E-03	0.0041	0.0129
C_2H_6	0	0	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0
FeO	0	0	0	0	0	0	0	0	0	0
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0	0	0

Stream Number	**11**	**12**	**13[a]**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Vapour Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0
Temperature (°C)	962	25	26	25	25	339	550	950	17	67
Pressure (kPaa)	725	1025	990	750	101	971	951	801	101	661
Molar Flow (kgmole/h)	18723	395	536	172	8991	8991	8991	7199	7199	2333
Mass Flow (t/h)	193.0	6.5	8.7	5.5	259.4	259.4	259.4	202.0	202.0	351.1
Species Mole fraction										
CH_4	0.0830	0.9758	0.9758	0	0	0	0	0	0	0
H_2O	0.0296	0	0	0	0	0	0	0	0	0
CO	0.1619	0	0	0	0	0	0	0	0	0
CO_2	0.0502	0.0073	0.0073	0	0	0	0	0	0	0
O_2	0	0	0	0.9900	0.2100	0.2100	0.2100	0.0133	0.0133	0
H_2	0.6623	0	0	0	0	0	0	0	0	0
N_2	0.0130	0.0169	0.0169	0.0100	0.7900	0.7900	0.7900	0.9867	0.9867	0
C_2H_6	0	0	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0.9063
FeO	0	0	0	0	0	0	0	0	0	0.0320
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0	0	0.0617

[a]Composition from Zugliano et al was simplified to replace higher hydrocarbons as CH_4.

Stream Number	**21**	**22**	**23**	**24**	**25**	**26**	**27[a]**	**28**	**29**	**30**
Vapour Fraction	1.0	0.6	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (°C)	916	132	77	412	158	50	109	109	55	45
Pressure (kPaa)	801	721	701	661	641	621	1000	1000	980	180
Molar Flow (kgmole/h)	3370	3370	1220	20470	20470	14942	1947	12997	11687	1270
Mass Flow (t/h)	89.2	89.2	50.3	294.1	294.1	194.4	25.3	169.1	114.1	54.0
Species Mole fraction										
CH_4	0.0079	0.0079	0.0219	0.0586	0.0586	0.0803	0.0803	0.0803	0.0892	0.0006
H_2O	0.6599	0.6599	0.0624	0.2847	0.2847	0.0204	0.0204	0.0204	0.0141	0.0540
CO	0	0	0	0.1391	0.1391	0.1906	0.1906	0.1906	0.2119	0.0004
CO_2	0.3209	0.3209	0.8846	0.0728	0.0728	0.0993	0.0993	0.0993	0.0071	0.9434
O_2	0	0	0	0	0	0	0	0	0	0
H_2	0	0	0	0.4333	0.4332	0.5934	0.5934	0.5934	0.6599	0.0016
N_2	0.0112	0.0112	0.0310	0.0117	0.0117	0.0160	0.0160	0.0160	0.0178	0
C_2H_6	0	0	0	0	0	0	0	0	0	0
C_3H_8	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0	0	0	0	0	0	0	0	0	0
FeO	0	0	0	0	0	0	0	0	0	0
Fe	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
Gangue (SiO_2)	0	0	0	0	0	0	0	0	0	0

Stream Number	**31**	**32**	**33**	**34**	**35**
Vapour Fraction	0.0	0.0	1.0	0.0	0.0
Temperature (°C)	77	50	500	67	634
Pressure (kPaa)	701	621	1005	845	500
Molar Flow (kgmole/h)	2151	3106	2423	136	4768
Mass Flow (t/h)	38.8	56.0	43.7	2.5	249.6
Species Mole fraction					
CH_4	0	0	0	0	0
H_2O	0.9987	0.9998	0.9998	0.9997	0
CO	0	0	0	0	0
CO_2	0.0013	0.0002	0.0002	0.0002	0
O_2	0	0	0	0	0
H_2	0	0	0	0	0
N_2	0	0	0	0	0
C_2H_6	0	0	0	0	0
C_3H_8	0	0	0	0	0
Fe_2O_3	0	0	0	0	0
FeO	0	0	0	0	0.0545
Fe	0	0	0	0	0.8164
C	0	0	0	0	0.0994
Gangue (SiO_2)	0	0	0	0	0.0297

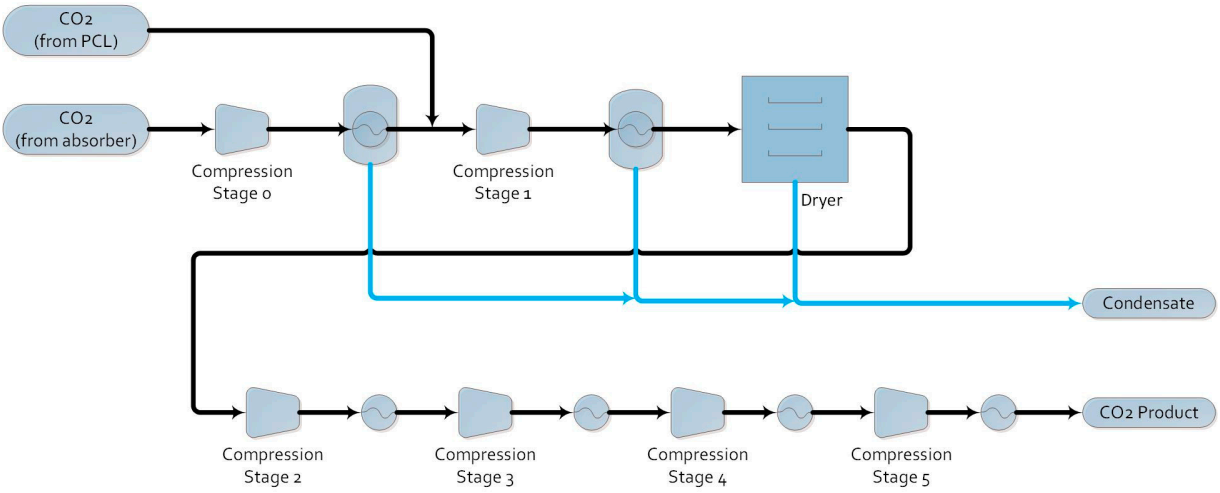


Figure S1. Process flow diagram of CO_2 compression and drying.