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# **Thermodynamic Performance Evaluation of Supercritical**

2 CO<sub>2</sub> Closed Brayton Cycles for Coal-fired Power

Generation with Solvent-based CO<sub>2</sub> Capture 4

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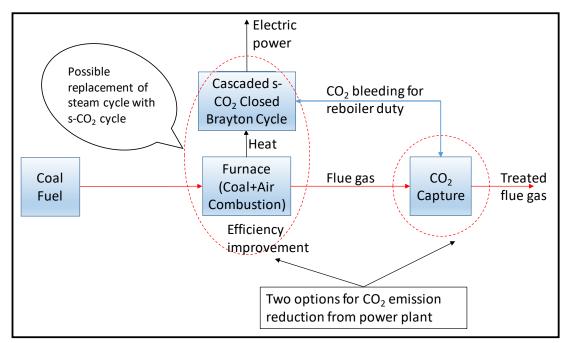
# 11 Abstract

12 Power generation from coal-fired power plants represents a major source of CO<sub>2</sub> emission into 13 the atmosphere. Efficiency improvement and integration of carbon capture and storage (CCS) facilities have been recommended for reducing the amount of CO<sub>2</sub> emissions. The focus of 14 15 this work was to evaluate the thermodynamic performance of s-CO<sub>2</sub> Brayton cycles coupled 16 to coal-fired furnace and integrated with 90% post-combustion CO<sub>2</sub> capture. The modification 17 of the s-CO<sub>2</sub> power plant for effective utilisation of the sensible heat in the flue gas was 18 examined. Three bottoming s-CO<sub>2</sub> cycle layouts were investigated, which included a newly 19 proposed single recuperator recompression cycle. The performances of the coal-fired s-CO<sub>2</sub> 20 power plant with and without carbon capture were compared. Results for a 290 bar and 593 21  ${}^{0}C$  power cycle without CO<sub>2</sub> capture showed that the configuration with single recuperator recompression cycle as bottoming cycle has the highest plant net efficiency of 42.96% (Higher 22 23 Heating Value). Without  $CO_2$  capture, the efficiencies of the coal-fired s- $CO_2$  cycle plants 24 were about 3.34-3.86% higher than the steam plant and about 0.68-1.31% higher with CO<sub>2</sub> 25 capture. The findings so far underscored the promising potential of cascaded s-CO<sub>2</sub> power

26 cycles for coal-fired power plant application.

- 27
- 28 29 30 31 32 33 34 35
- 36

# 37 Graphical abstract



38

# 39 Keywords

- 40 Coal-fired power plant;
- 41 Supercritical CO<sub>2</sub> Brayton cycle;
- 42 Carbon capture;
- 43 Chemical absorption;
- 44 Process modelling/simulation;
- 45

### 46 Highlights

- Supercritical CO<sub>2</sub> cycle was investigated for coal-fired power plant application
- Three s-CO<sub>2</sub> cycles were investigated as possible bottoming cycle options
- Integration of coal-fired plant with post-combustion CO<sub>2</sub> capture was studied
- Thermodynamic analysis and performance comparison were performed
- 51

# 52 Nomenclature and Units

#### 53 Abbreviations

CCS	carbon capture and storage
ESP	electrostatic precipitator
FD	forced draft
FGD	flue gas desulfurization

HP	high-pressure
HHV	higher heating value
HTR	high temperature recuperator
ID	Induced draft
LP	low-pressure
LTR	low temperature recuperator
MC	main compressor
MEA	monoethanolamine
PA	primary air
PCC	post-combustion CO <sub>2</sub> capture
PSD	particle size distribution
RC	recompression compressor
s-CO <sub>2</sub>	supercritical carbon dioxide
TTD	terminal temperature difference
USC	ultra-supercritical

54

# 55 Symbols

$C_i$	Concentration of the ith component (mol/m <sup>3</sup> )
Ĕ	Activation energy (J/mol)
HHV	Higher heating value (J/kg)
k	Pre-exponential factor
'n	Mass flow rate (kg/s)
n	Temperature exponent
Ν	Number of components
Р	Power (watt or $J/s$ )
Q	Heat transferred (watt or J/s)
r	Rate of reaction
R	Universal gas constant
Т	Temperature (K)
$\alpha_i$	Exponent of the ith component
η	Efficiency
π	Product operator
Σ	Sum operator

56

# 57 Subscripts

aux	auxiliary
С	Compressor
elec	Electrical
gen	Generator
HP	High pressure
i	Component index
LP	Low pressure
MC	Main compressor
RC	Recompression compressor
Т	Turbine

# 59 **1** Introduction

## 60 1.1 Background

61 Coal-fired power plants are still playing a significant role in meeting world energy demands 62 and it is expected to remain a key component of the global energy mix into the future due to 63 its reliability, security of fuel supply, cheap fuel and competitive cost of electricity [1, 2]. 64 However, one prime concern about continued use of fossil fuels like coal is the emission of 65  $CO_2$  to the atmosphere. Therefore, reducing  $CO_2$  emissions from coal-fired power has become a policy focus in many countries. Two options that have been identified for mitigating  $CO_2$ 66 67 emissions from fossil fuel power plants are CCS (carbon capture and storage) and efficiency 68 improvement. Post-combustion  $CO_2$  capture (PCC) by chemical absorption with solvent is currently the most preferred CCS option [3, 4]. Efficiency improvement usually requires 69 70 increased main steam temperature and pressure. Hence, the state-of-the-art technology for 71 coal-fired power generation, the ultra-supercritical (USC) steam plant, now operates at a steam pressure up to 300 bar and temperature up to 600 °C with reheat [5]. However, CCS systems 72 73 and efficiency improvement have their limitations. Integration of PCC system with fossil fuel 74 power plants leads to significant efficiency penalty and increased cost of electricity generation. 75 Also, lack of advanced materials to withstand harsh operating conditions limits further 76 improvement in efficiency.

77 In this paper, to improve the efficiency of coal-fired power plants, supercritical carbon dioxide 78 (s-CO<sub>2</sub>) Brayton cycle is considered as an alternative to the conventional steam Rankine cycle. 79 Additionally, CO<sub>2</sub> capture is facilitated by integrating an aqueous monoethanolamine (MEA)-80 based PCC system with the s-CO<sub>2</sub> cycle power plant. S-CO<sub>2</sub> Brayton cycle has been found to 81 have higher cycle efficiency than steam Rankine cycle and other gas Brayton cycles in the 82 temperature range typically encountered in pulverised coal-fired power plant (450 °C to 650 83  $^{0}$ C) [6-10]. Other potential benefits of s-CO<sub>2</sub> cycle compared to steam cycle include [6, 11-84 19]:

- Smaller size of the components
- Less complex system layout
- Less risk of corrosion and scaling and no formation of water droplets that could damage the turbine blades [10, 20]
- Reduced water consumption [14, 19]

### 90 1.2 Review of s-CO<sub>2</sub> power cycle

A CO<sub>2</sub> closed Brayton cycle was originally patented by Sulzer in 1950 [21]. Later in the 1960s, 91 Feher [10, 22], Angelino [12, 23] and Dekhtiarev [24] all investigated s-CO<sub>2</sub> power cycle. 92 93 Feher identified CO<sub>2</sub> as a suitable working fluid due to its unique properties such as low critical 94 pressure, good thermal stability at temperature of interest, inertness, availability of property 95 data, and abundant, non-toxic and inexpensive [10]. Angelino concluded that s-CO<sub>2</sub> power 96 cycle has the potential to perform better than reheat steam cycle on account of efficiency, 97 simplicity and compactness [12]. Dekhtiarev [24] studied condensing reheated s-CO<sub>2</sub> cycles 98 as a good alternative to steam cycle for fossil fuel plant [25]. According to recent 99 comprehensive reviews by Olumayegun et al. [26], Ahn et al. [19], Crespi et al. [27] and Li et 100 al. [28], s-CO<sub>2</sub> power cycles are currently being widely investigated as power conversion system for application in nuclear, fossil, concentrated solar power, biomass, and waste heat 101 102 recovery systems because of its advantages [8, 11, 15, 17, 20, 29-31].

103 Dostal [11] contributed to renewed interest in  $s-CO_2$  power cycle for nuclear reactor 104 application by providing a detailed analysis based on thermodynamic performance and cost. 105 The study showed that  $s-CO_2$  cycle achieved higher thermal efficiency and reduced cost of 106 power plant compared to steam cycle at 550 °C turbine inlet temperature. Studies by Pharm et 107 al.[8] concluded that the s-CO<sub>2</sub> recompression cycle in condensing mode is the most fitting 108 configuration for pressurised water reactor (PWR) and sodium-cooled fast reactor (SFR) application. The use of mixture of CO<sub>2</sub> with additive gases to improve the performance of s-109 110  $CO_2$  cycle of a nuclear reactor was investigated by Hu et al. [17]. Even though s-CO<sub>2</sub> cycle is usually viewed to provide superior thermodynamic performance than steam cycle only in the 111 medium to high-temperature range (greater than 450 °C), Santini et al. [25] investigated the 112 113 adoption of s-CO<sub>2</sub> cycle for a far lower temperature (about 260 °C) of an existing PWR. The 114 results indicated that a reheated recompression s-CO<sub>2</sub> cycle achieved a net cycle efficiency of 115 about 34% compared to 33.5% of the existing steam cycle and the plant footprint was 10 times 116 smaller than the steam cycle plant.

117 For concentrated solar power (CSP), Chacartegui et al. [32] investigated two stand-alone s-118  $CO_2$  cycle configurations and a combined cycle (comprising a topping s-CO<sub>2</sub> cycle and a bottoming Organic Rankine Cycle (ORC)) as an alternative to the conventional steam cycle. 119 Preliminary results from the study showed that the s-CO<sub>2</sub> cycles could provide both efficiency 120 121 and cost benefits. Al-Sulaiman and Atif [33] compared the performance of five different s-122 CO<sub>2</sub> Brayton cycle configurations for CSP application and the recompression cycle was found 123 to give the best efficiency. Recompression and partial cooling cycles were compared by Neises 124 and Turchi [29] for CSP, highlighting the potential reduction in cost and improvement of CSP 125 receiver efficiency with the partial cooling cycle. Recently, Wang et al. [34] reviewed and 126 compared the main s-CO<sub>2</sub> cycle configurations integrated with molten salt solar power towers 127 having both the main heater and a reheater.

128 S-CO<sub>2</sub> cycles and the various configurations have also been investigated as bottoming cycles 129 for fuel cell [20] and gas turbine system [15] as well as an alternative power conversion system for other waste heat recovery processes [35, 36] and biomass plants [7]. Bae et al. [20] 130 investigated s-CO<sub>2</sub> cycle configurations comprising an s-CO<sub>2</sub> Brayton-steam Rankine cycle 131 132 cascade, a recompression cycle and two simple recuperated cycle (a supercritical and a trans-133 critical cycle) as bottoming cycles for molten carbonate fuel cell. Kim et al. [15] compared the 134 performance of nine s-CO<sub>2</sub> cycle layouts together with three newly developed concept as bottoming cycles for gas turbine plant. It was concluded that although the recompression cycle 135 136 has a good cycle efficiency, it is not suitable as a bottoming cycle due to its poor heat recovery 137 factor. Small to medium-scale biomass power plant employing either a simple recuperated or 138 a recompression s-CO<sub>2</sub> Brayton cycle as topping cycle and a simple recuperated s-CO<sub>2</sub> Brayton 139 cycle as bottoming cycle was studied by Manente and Lazzaretto [7]. Results of performance 140 optimisation showed that the cascaded s-CO<sub>2</sub> Brayton cycles plant could achieve about 10% 141 higher efficiency than existing biomass plant.

Various researchers have also proposed adaptation of s-CO<sub>2</sub> Brayton cycle as the main/topping 142 143 cycle for coal-based power plant. However, one problem of such application is the inefficient utilisation of the heat content of the flue gas [16, 30, 31]. Mecheri and Le Moullec [30] 144 145 investigated the performance of coal-fired s-CO<sub>2</sub> Brayton cycle by comparing the effects of 146 number of reheat and number of recompression, and the effects of advanced flue gas 147 economiser configurations. Heat utilisation was improved by transferring flue gas heat to a 148 fraction of cold CO<sub>2</sub> working fluid taken from the main compressor outlet as well as preheating 149 of combustion air. Results showed that the plant net efficiency was higher than that of 150 supercritical and USC steam plant by 5.3% and 2.4% respectively. Le Moullec [31] presented 151 a conceptual study of coal-fired s-CO<sub>2</sub> Brayton cycle integrated with 90% post-combustion 152 amine-based  $CO_2$  capture unit. Performance improvement entailed the use of double reheat configuration, cold CO<sub>2</sub> bleeding from two locations and two stages of combustion air 153 154 preheating. Technical and economic evaluation of the plant showed that 15% reduction in 155 levelised cost of electricity and 45% reduction in the cost of avoided CO<sub>2</sub> emission could be 156 achieved. Hanak and Manovic [16] proposed s-CO<sub>2</sub> cycle instead of the conventional steam 157 cycle for electricity generation from the high-grade heat of calcium looping process. Results

158 of retrofitting the calcium looping process with s-CO<sub>2</sub> recompression cycle indicated that a 159 gain in efficiency of about 1-2% over that of the steam cycle could be obtained.

#### 160 **1.3** Aim of this study and its novelties

The aim of this paper is to evaluate the thermodynamic performance of coal-fired s-CO<sub>2</sub> 161 Brayton cycle power plant that has been adapted for efficient utilisation of flue gas heat by 162 using a bottoming s-CO<sub>2</sub> Brayton cycle in conjunction with a main/topping s-CO<sub>2</sub> Brayton 163 cycle. So far, the use of s- $CO_2$  Brayton cycles as both topping cycle and bottoming cycle of a 164 165 coal-fired power plant has not been explored in the literature. In this study, a single reheat s- $CO_2$  recompression cycle was considered as the topping cycle while three simpler s- $CO_2$  cycle 166 were investigated as possible bottoming cycle for recovering the excess heat in the flue gas 167 168 exiting the furnace. The investigated bottoming cycle options are simple recuperated cycle, partial heating cycle and a newly proposed concept referred to as single recuperator 169 recompression cycle. Performance evaluation was performed both for s-CO<sub>2</sub> cycle plants 170 171 without  $CO_2$  capture and for plants with  $CO_2$  capture unit integrated. The performances of the 172 different coal-fired s-CO<sub>2</sub> cycle configurations were compared with reference to a supercritical steam cycle that was chosen as the benchmark. The most promising of the layouts was 173 174 determined and the effects of cycle parameters such as turbine inlet temperature, precooler outlet temperature/pressure and recuperator's minimum terminal temperature difference (TTD) 175 176 on the plant performance were investigated. The whole system comprising the coal-fired 177 furnace, the s-CO<sub>2</sub> cycles and the MEA-based PCC plant were modelled and simulated with 178 Aspen Plus software.

# **2** Process configurations and description

#### 180 2.1 Supercritical CO<sub>2</sub> closed Brayton cycle

181 A unique feature of  $CO_2$  as working fluid is that its critical pressure (7.3773 MPa) and 182 temperature (30.978 °C) are easily achievable. The properties of  $CO_2$  vary rapidly around the 183 critical point and the density is greatly increased. Hence, s- $CO_2$  cycles take advantage of the 184 increased density by operating the compressor inlet close to the critical point so that the 185 compression work is significantly reduced. The reduced compression work thus enables the 186 achievement of high thermodynamic efficiency.

187 The baseline closed Brayton cycle is the simple recuperated cycle. The layout and T-S diagram 188 of a simple recuperated s- $CO_2$  Brayton cycle are shown in Figure 1a. It consists of a heat 189 source (1-2), a turbine (2-3), a recuperator (3-4 & 6-1), a precooler (4-5) and a 190 compressor (5-6). Though the rapidly varying fluid properties around the critical point is a 191 feature that facilitates the reduced compression work of s-CO<sub>2</sub> cycle, it also prevents effective 192 heat transfer in the recuperator of simple recuperated s-CO<sub>2</sub> cycle. This is due to mismatch of 193 specific heat capacity between the high-pressure  $CO_2$  in the cold side and the low-pressure 194  $CO_2$  in the hot side of the recuperator. This could lead to temperature cross over in the 195 recuperator (the so-called "pinch point problem") and consequently, the cold stream cannot be 196 preheated high enough to achieve good recuperator effectiveness. Hence, it is difficult to 197 achieve high efficiency in simple recuperated s- $CO_2$  cycle even with the conventional methods 198 of enhancing efficiency such as reheating and intercooling because of the excessively low 199 effectiveness of the recuperator [37].

Other complex layouts have been suggested in the literature to minimise the detrimental effects of the differences in heat capacities [10-12, 15, 19, 38]. Of all the layouts, the recompression s- $CO_2$  cycle (Figure 1b) is generally considered the most promising with the highest thermodynamic efficiency and a relatively simpler configuration than most others [11]. A component count of the different layouts by Kim et al. [15] showed that only the simple recuperated (Figure 1a) and the partial heating cycle (Figure 1c) is simpler (fewer components) 206 than the recompression cycle. Hence, this study considered only the simple recuperated cycle,

207 the recompression cycle and the partial heating cycle. However, an additional new cycle concept referred to as single recuperator recompression s-CO<sub>2</sub> cycle (Figure 1d) was proposed. 208

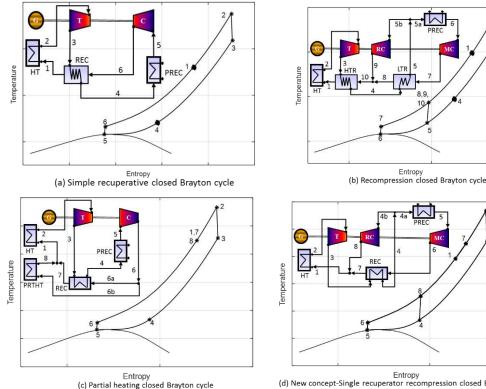
209 The newly proposed layout has one component less than the recompression cycle and just one

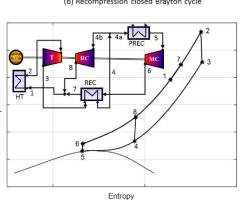
210 component more than the simple cycle. This configuration has been investigated previously in

211 an initial study by the authors [39]. Conboy et al. [40] suggested a similar but more complex

212 cycle layout for geothermal heat application.

213 In the recompression cycle (Figure 1b), the recuperator is separated into two: the hightemperature recuperator (HTR) and the low-temperature recuperator (LTR). The problem of 214 215 heat capacity mismatch is resolved by splitting the flow into two streams at point 5. The main stream is cooled in the precooler (point 5 to point 6) to the main compressor (MC) inlet 216 217 temperature. The second stream is compressed directly in the recompressing compressor (point 5 to point 9) and mixed with the main flow at the exit of the LTR cold stream (point 8) before 218 entering the cold side of the HTR (point 10). The flow split fraction can be adjusted to make 219 the heat capacity (i.e. the product of mass flow rates and specific heat capacity) of CO<sub>2</sub> on the 220 221 high-pressure side of the LTR the same as that of the low-pressure side  $CO_2$ . Hence, with an 222 optimal selection of flow split fraction, high recuperator effectiveness and consequently high 223 thermodynamic efficiency can be achieved. The layout, as well as T-S diagram of partial 224 heating cycle, is shown in Figure 1c. Matching of the heat capacities of the recuperator streams 225 is achieved by splitting the flow at the compressor outlet (point 6) after compressing the fluid 226 to the maximum cycle pressure in the compressor (point 5 to 6). The new concept, the single 227 recuperator recompression cycle is shown in Figure 1d. It is similar to the recompression cycle 228 except that the HTR was eliminated leaving only one recuperator. The flow is split into two 229 streams at point 4, just like the recompression cycle. This permits the advantage associated 230 with splitting the flow, that is, a balance of the heat capacity between the cold stream and the 231 hot stream of the recuperator.





(d) New concept-Single recuperator recompression closed Brayton cycle

#### Figure 1 Layout and T-S diagrams of simple recuperative, recompression, partial heating and single recuperator recompression s-CO<sub>2</sub> closed Brayton cycles [18-20, 22]

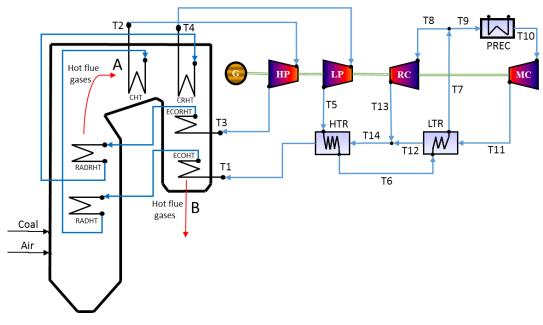
# 234 2.2 Supercritical CO<sub>2</sub> Brayton cycles for pulverised coal-fired 235 application

#### 236 2.2.1 Coal-fired furnace and the main s-CO<sub>2</sub> closed Brayton cycle

237 Integration of the main/topping s-CO<sub>2</sub> cycle with the coal-fired furnace is shown in Figure 2. 238 A recompression s-CO<sub>2</sub> cycle was adopted due to its superior performance when compared to 239 other s-CO<sub>2</sub> cycle layouts. The performance is further improved with a single stage of reheat. 240 Preheated CO<sub>2</sub> coming from the HTR entered the furnace at point T1 and exit at T2 after being 241 heated to the maximum cycle temperature. The hot working fluid is expanded in the high-242 pressure (HP) turbine and returned to the furnace at point T3 for reheating. The reheated CO<sub>2</sub> exiting the furnace at T4 is finally expanded in the LP turbine. During each pass through the 243 244 furnace, the CO<sub>2</sub> working fluid is heated in three steps: convective economiser 245 (ECOHT/ECORHT), radiant heater (RADHT/RADRHT) and final convective heater or 246 reheater (CHT/CRHT).

247 Radiant section of the furnace contains the two radiant heaters while the convective section 248 contains the four convective heaters. Approximately half of the heat transferred to the  $CO_2$  is 249 through radiation from the flame to the radiant heaters. Combustion products rise to the top of 250 the furnace and entered the convection zone at point A. The temperature of the hot flue gases 251 at A was maintained at 1010 °C so that it was below ash softening temperature [41]. As the 252 flue gases flow through the convective section, they are first used for final heating of  $CO_2$  to turbine inlet temperature in the convective heater and reheater. Then CO<sub>2</sub> leaving the HTR and 253 254 HP turbine are heated in the economisers to the radiant heaters inlet temperature. The flue 255 gases leave the furnace at point B. The CO<sub>2</sub> entering the furnace at T1 is at a higher temperature 256 (about 465 °C) than the usual feedwater temperature in conventional coal-fired steam boiler 257 (about 260 °C) [42]. This is due to the high level of recuperation in recompression cycle. 258 Consequently, the flue gases leave the furnace at relatively high temperature (about 495  $^{\circ}$ C) in 259 the coal-fired s-CO<sub>2</sub> cycle power plant.





262 Figure 2 Main single reheat recompression cycle integration with coal-fired furnace

#### 263 2.2.2 Utilisation of flue gases residual heat

264 A major drawback of coupling closed Brayton cycle to coal-fired furnace is the significant loss of heat through the hot flue gases leaving the furnace. If this exiting flue gases are not utilised, 265 it will represent the main cause of inefficiency in the power plant [41]. Several options exist 266 267 for utilising waste heat of flue gases. The first option is to use the flue gases to produce steam or hot water for industrial use or district heating in a combined heat and power (CHP) system. 268 In fact, some of the early-operated coal-fired closed Brayton cycle plants such as the 269 270 Oberhausen and Kashira plants were used to generate electricity as well as to produce heat for 271 district heating [43]. Secondly, the hot flue gases can be used to preheat part or all of the cycle working fluid prior to the main heat addition in the furnace. Mecheri and Le Moullec [30] 272 employed this option by transferring the flue gases heat to a fraction of CO<sub>2</sub> flow that is 273 extracted from the MC outlet. A third option is to add a bottoming cycle that uses the flue 274 275 gases high-grade heat to generate additional electrical power [7, 15]. For instance, Echogen 276 (USA) is in the process of commercialising s-CO<sub>2</sub> bottoming power cycle utilising waste heat 277 [44]. The final option is to use the flue gases to preheat the incoming combustion air. This is 278 a common practice in conventional coal-fired power plants.

279 In this study, the use of bottoming cycle in conjunction with combustion air preheating was 280 selected. In bottoming cycles, the net electric efficiency is a function of not just cycle 281 efficiency (ratio of net electric power produced to heat transferred to the cycle) but also of the heat recovery factor (ratio of recovered heat to available heat in the flue gas) [15]. Closed 282 Brayton s- $CO_2$  cycle has favourable cycle efficiency. However, when used as a bottoming 283 cycle, the heat recovery in the heater is limited by the high temperature of  $CO_2$  leaving the 284 285 recuperator [15]. However, the addition of air preheater downstream of the bottoming cycle will help to improve the plant's overall heat recovery factor. Recompression cycle was not 286 287 used as bottoming cycle in this study. Cycles with simpler layouts and better heat recovery 288 factor were favoured. Hence, the simple recuperated cycle, the partial heating cycle and the 289 newly proposed single recuperator recompression cycle were considered as bottoming cycles 290 in cascade with the main/topping single reheat recompression s-CO<sub>2</sub> cycle.

#### 291 2.2.3 Overall plant configurations and its integration with PCC

296

In this study, three coal-fired s-CO<sub>2</sub> cycle configurations (Figure 3, Figure 4 and Figure 5)
 representing three different bottoming cycle choices were investigated:

- Case A: the simple recuperated s-CO<sub>2</sub> cycle was selected as bottoming cycle as shown in Figure 3
  - Case B: shown in Figure 4, the bottoming cycle is the partial heating s-CO<sub>2</sub> cycle
- Case C: the new concept, the single recuperator recompression s-CO<sub>2</sub> cycle was used as the bottoming cycle (Figure 5)

299 In all the cases, the topping cycle remains the single reheat recompression  $s-CO_2$  cycle integrated with coal-fired furnace. Coal is pulverised to fine powder in the mill. Secondary air, 300 which is a large proportion of the incoming air, is sent to the forced draft (FD) fan while the 301 remaining incoming air goes to the primary air (PA) fan. Air from the PA fan and FD fan is 302 303 heated in the air preheater thereby recovering part of the remaining heat content of the flue gas exiting the bottoming cycle heater at point C. The heated primary air goes to the mill/pulveriser 304 305 for drying and conveying the pulverised coal to the burners in the furnace. The heated secondary air is also introduced into the burners, where the coal and the air are mixed and 306 307 combustion takes place. Heat released from the combustion is transferred to the  $CO_2$  working 308 fluid in the radiant and convective heaters.

The cooled flue gas leaving the air preheater passes through fabric filters or electrostatic precipitator (ESP) for particulate matters (majorly ash) removal. An induced draft (ID) fan

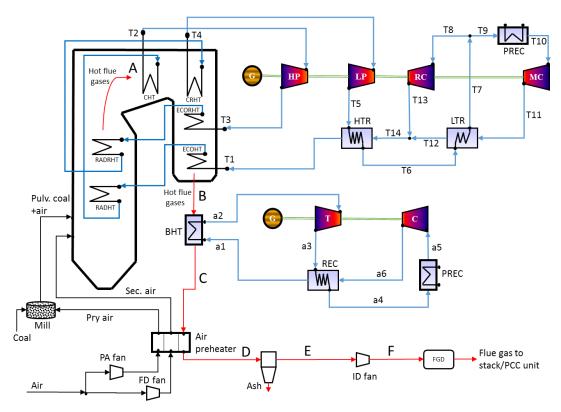
311 increases the flue gas pressure to provide suction to the flue gas in the furnace and for the flue

312 gas to pass through the flue gas desulfurization (FGD) unit. The cleaned flue gas leaving the 313 FGD unit is finally sent either to the PCC unit to remove the  $CO_2$  in the flue gases or directly

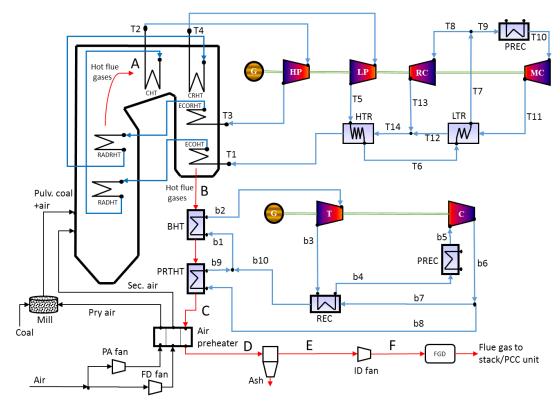
314 to the stack.

315 The s-CO<sub>2</sub> Brayton cycle will need to be altered when a PCC unit is added. In the conventional 316 coal-fired plant, low pressure saturated steam from steam turbine is used for solvent regeneration in the PCC unit. However, in the coal-fired s-CO<sub>2</sub> Brayton cycle plant, sensible 317 318 heat of the  $CO_2$  working fluid is used for solvent regeneration. Hence, each of the three cases 319 is integrated with the PCC unit as shown in Figure 6. Hot CO<sub>2</sub> from the HTR hot stream outlet 320 is conveyed to the reboiler of the PCC unit. The  $CO_2$  is then returned to the s- $CO_2$  cycle at the 321 LTR hot stream outlet after supplying the required reboiler duty. The flue gas from the power plant is stripped of its  $CO_2$  before being sent to the stack. A detailed description of the PCC 322 323 unit is provided in Section 4.

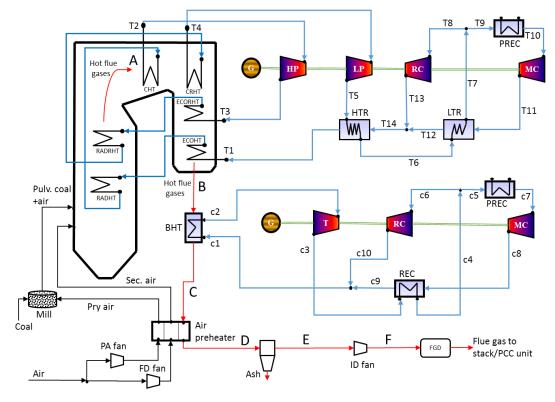




326 Figure 3 Case A - Simple recuperative bottoming cycle



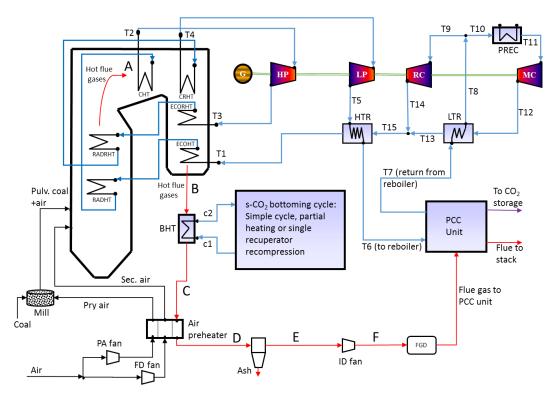
329 Figure 4 Case B - Partial heating bottoming cycle



331 Figure 5 Case C - Single recuperator recompression bottoming cycle

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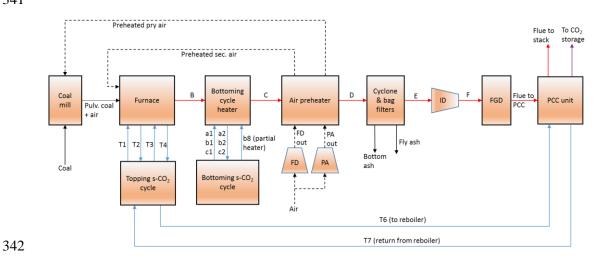
332

333 Figure 6 Integration of coal-fired s-CO<sub>2</sub> Brayton cycle with PCC unit

334

# 335 **3 Steady state modelling in Aspen Plus®**

A model of the three cases of coal-fired s-CO<sub>2</sub> cycle power plant with PCC was developed for performance comparison among the cases as well as comparison with a benchmark coal-fired supercritical power plant with 90% CO<sub>2</sub> capture. The benchmark plant was not modelled in this study but the performance results were obtained from Olaleye et al. [45]. A simplified block diagram of the modelled coal-fired s-CO<sub>2</sub> cycle power plant is shown in Figure 7



343 Figure 7 Simplified block diagram of the coal-fired s-CO<sub>2</sub> cycle power plant

# 344 3.1 Aspen Plus<sup>®</sup> software and thermo-physical property methods

The steady state models were implemented with Aspen Plus<sup>®</sup> V8.4 software to simulate the performance of the coal-fired s-CO<sub>2</sub> cycles power plants. The simulation environment is very flexible for describing the power plant components and connections. The plant components modelled include coal mill, fans, preheaters, pulverised coal-fired furnace, ash removal components, flue gas desulfurization and s-CO<sub>2</sub> cycle components like the external heat sources, turbine, compressor, recuperator and precooler. Description of the PCC structure and its modelling are left until the next section.

352 Concomitant with process simulation is the need for accurate physical property data and models [46]. Aspen Plus<sup>®</sup> contains extensive property calculation methods for the physical, 353 chemical and thermodynamic properties of different solid, liquid and gaseous substances. In 354 355 Aspen Plus®, coal and ash were modelled as nonconventional solids. The HCOALGEN and the DCOALIGT physical property models were used to calculate the enthalpy and density of 356 coal and ash [47]. Peng-Robinson equation of state with Boston Mathias modification (PR-357 BM) was used to estimate the properties of air and combustion products. For the s-CO<sub>2</sub> 358 properties, REFPROP property package in Aspen Plus® was used. REFPROP has been 359 reported to be accurate and widely applicable to a variety of pure fluid and mixtures [48, 49]. 360

#### 361 3.2 Coal combustion and furnace modelling

The coal type fired is the Illinois No 6 bituminous coal. Details of the ultimate and proximate analysis of the coal are given in Table 1. The higher heating value (HHV) of the coal was calculated from the ultimate analysis by using the Dulong and Petit formula [50]:

$$HHV \left(\frac{MJ}{kg}\right) = 33.83C + 144.45 \left(H - \frac{0}{8}\right) + 9.38S$$
(3.1)

Where C, H, O and S are mass fractions of carbon, hydrogen, oxygen and sulphur in coal respectively.

Incoming air was assumed to consist of nitrogen (76.8 wt.%) and oxygen (23.2 wt.%) at 15  $^{\circ}$ C 367 and 1.01 bar. Percent excess air supplied was specified to be 20%. A user-defined Fortran 368 369 subroutine calculator was implemented to calculate the flow rate of air required for combustion 370 based on the specified percent excess air, the coal flow rate and the coal characteristic. About 371 23.5% of the incoming air was sent to the PA fan while the rest was sent to the FD fan as 372 secondary air. By specifying the isentropic efficiencies of the fan, the inlet conditions and the 373 discharge pressure, Aspen Plus<sup>®</sup> determined the power required by the fans. Coal is dried with 374 preheated PA and grounded to fine powder in the coal mill. Volatile matter may be distilled 375 off from the coal in addition to moisture if the temperature of the PA is too high, which may 376 lead to fire hazard [50]. Therefore, the primary air was only preheated to about 215 °C so that 377 after drying the coal the temperature at pulveriser outlet was within the allowable pulveriser 378 outlet temperature of 75 °C.

379 The drying process was modelled with RStoic block. Wet coal and hot PA streams were fed 380 to the RStoic block. The block was used to model drying by converting a portion of the coal to form water. The outlet, which is a stream of dried coal and moist air, is fed to the pulverising 381 382 mill. The milling process was modelled with a combination of crusher and screen. The crusher 383 was modelled by specifying the outlet particle size distribution (PSD) of coal. The screen block was used to separate the coarse material from the fine material. The coarse portion was 384 returned to the crusher for further grinding. The PSD of the pulverised coal was specified such 385 that about 70% of coal will pass through a 200-mesh screen and less than 1.3% retained on the 386 387 50 mesh. The pulverised coal is then conveyed with the PA to the furnace.

388 In the furnace, the pulverised coal and PA are mixed with the heated secondary air for 389 combustion. A sequence of RYield and RGibbs Aspen Plus<sup>®</sup> built-in reactor models were used to simulate combustion of coal. RGibbs models chemical equilibrium and phase equilibrium by minimising the Gibbs free energy of the system. Therefore, there was no need to specify the reaction stoichiometry, only a list of possible products may be specified. However, Gibbs free energy can only be calculated for conventional components. Since coal was specified as a nonconventional component, it was first decomposed into its constituent elements by the RYield block. A calculator block was used to determine the actual yield distribution based on the inlet coal attributes. The products of the decomposition together with the heat of reaction

associated with the decomposition was then passed to the RGibbs block.

398 During combustion, the chemical energy in the coal is converted to heat energy, which is 399 transferred to the CO<sub>2</sub> working fluid. Heat radiation from the centre of the flame and absorption of the radiant heat by the working fluid were modelled with HEATER blocks. The radiant heat 400 401 was divided in the ratio 0.65/0.35 between the main radiant heater and the reheat radiant heater. 402 The exit of the radiant heat source corresponds to the top of the furnace and entrance to the 403 convective zone where the flue gases temperature was maintained at 1010 °C. Convective heaters in this zone comprising of two final CO<sub>2</sub> heaters and two economisers were modelled 404 405 with HEATX blocks with flue gases as the hot stream and  $CO_2$  as the cold stream. For a given 406 coal flow rate, a design specification was defined in Aspen Plus® to determine the topping cycle CO<sub>2</sub> flow rate required to cool the flue gases such that a 30 °C minimum temperature 407 difference was maintained between the flue gases leaving the furnace at point B and CO<sub>2</sub> 408 409 entering the furnace at point T1.

410

Parameter	Weight %			
Proximate Analysis (as received)				
Moisture	11.12			
Ash	9.70			
Volatile matter	34.99			
Fixed carbon	44.19			
Total	100			
Ultimate Analysis (as received)				
Moisture	11.12			
Carbon	63.75			
Hydrogen	4.50			
Nitrogen	1.25			
Chlorine	0.29			
Sulphur	2.51			
Ash	9.70			
Oxygen	6.88			
Total	100			

411 Table 1 Proximate and ultimate analysis of Illinois No 6 coal [42]

412

### 413 3.3 Modelling of s-CO<sub>2</sub> closed Brayton cycles

The topping and bottoming s-CO<sub>2</sub> cycles have the same maximum cycle pressure of 290 bar corresponding to the maximum cycle pressure of the benchmark supercritical steam turbine cycle [45]. Similarly, the topping cycle HP and LP turbines inlet temperature were fixed at 593  $^{\circ}$ C. Both topping and bottoming cycles' compressor inlet temperature and pressure were fixed just above the critical point at 31  $^{\circ}$ C and 76 bar. The bottoming cycle' turbine inlet temperature was fixed at 465  $^{\circ}$ C, which is 30  $^{\circ}$ C below the flue gas temperature entering the bottoming cycle heater. The values of recuperator's minimum TTD, compressor and turbine 421 isentropic efficiencies, and heat exchanger pressure losses were selected based on values 422 reported in literature. Hence, a minimum TTD of 10°C was specified for the recuperators [30]. 423 Main compressor, recompression compressor and turbine isentropic efficiencies were 90%, 424 89% and 93% respectively [30]. Heat exchanger relative pressure losses were fixed at 0.5% [15]. For cycles with split flows, the split fractions could be independently adjusted to obtain 425

optimum cycle efficiency. 426

427 Compressors and turbines were simulated in Aspen Plus<sup>®</sup> with COMPR block. Aspen Plus<sup>®</sup> 428 calculates the power required (or delivered) based on the inlet conditions, discharge pressure 429 and efficiency. Recuperators were modelled with HEATX block while precoolers were modelled with HEATER blocks. In the bottoming cycle, design specification was used to 430 431 determine the needed  $CO_2$  flow rate based on a minimum temperature difference of 30  $^{\circ}C$ 432 between the flue gas leaving the bottoming cycle heater and the  $CO_2$  entering the heater.

#### 3.4 Preheater, ash removal and flue gas desulfurization 433

Air preheater was modelled with MHeatX block, which represents heat transfer between the 434

435 hot flue gases leaving the bottoming cycle heater and two cold streams (i.e. PA and SA). Outlet

436 specifications must be given for two of the three streams. PA and flue gas outlet temperatures were specified. Flue gas outlet temperature of 116 °C specified for the benchmark steam plant 437

- 438 was assumed. Then, an overall energy balance determines the unspecified outlet temperature
- 439 of the secondary air.
- Ash removal from the flue gas was modelled with cyclone and bag filter blocks. 20% of ash 440
- 441 was removed as bottom ash by the cyclone while the remaining 80% was removed as fly ash
- by bag filters. The ash-free flue gas is pushed through the FGD unit by ID fan. The power 442
- 443 required by the fan was determined based on its discharge pressure and isentropic efficiency.
- 444 The FGD removed sulphur oxide in the flue gas before entering the PCC unit.

#### 3.5 Performance calculation 445

- MS Excel<sup>TM</sup> spreadsheets were used to carry out the performance calculations. Therefore, the 446 MS Excel<sup>TM</sup> was linked with Aspen Plus<sup>®</sup> to access simulation results. 447
- Two important performance indicators are the furnace (or heat recovery) efficiency and the 448 cycle efficiency. The furnace efficiency is an indication of the ability of the power cycle to 449 receive the heat available in the heat source while cycle efficiency indicates the ability to 450 convert the received heat into electrical power [7]. The furnace efficiency,  $\eta_{furnace}$  is 451 452 calculated by taking the total amount of heat transferred to the s-CO<sub>2</sub> cycles and dividing it by 453 the coal fuel power supplied to the plant.

$$\eta_{furnace} = \frac{(Q_{cycle})_{top} + (Q_{cycle})_{bottom}}{\dot{m}_{coal}(HHV)}$$
(3.2)

Where  $(Q_{cvcle})_{top}$  is the sum of the heat transferred to the topping s-CO<sub>2</sub> cycle through the 454 economisers, radiant heaters and final convective heater/reheater,  $(Q_{cvcle})_{bottom}$  is the heat 455 input from flue gases to the bottoming s-CO<sub>2</sub> cycle,  $\dot{m}_{coal}$  is the mass flow rate of coal and 456 HHV is the higher heating value of the supplied coal. 457

Cycle efficiency,  $\eta_{cycle}$ , is calculated by taking the electrical power output of the cycle and 458 dividing by the heat transferred to the cycle. Hence, cycle efficiency for the toping 459 460 cycle,  $(\eta_{cycle})_{ton}$ , is

$$(\eta_{cycle})_{top} = \frac{(P_{elec})_{top}}{(Q_{cycle})_{top}}$$
(3.3)

Where  $(P_{elec})_{top}$  is the topping cycle electrical power output given as: 461

$$(P_{elec})_{top} = \left[ \left( \sum_{T} P_{T} \right)_{top} - \left( \sum_{T} P_{C} \right)_{top} \right] \eta_{gen}$$

$$= (P_{HP} + P_{LP} - P_{MC} - P_{RC}) \eta_{gen}$$

$$(3.4)$$

462  $(\sum P_T)_{top}$  is the sum of topping cycle turbine power,  $(\sum P_C)_{top}$  is the sum of topping cycle 463 compressor power,  $P_{HP}$  is the HP turbine power,  $P_{LP}$  is the LP turbine power,  $P_{MC}$  is the main 464 compressor power,  $P_{RC}$  is the RC power and  $\eta_{gen}$  is the electrical generator efficiency.

465 Cycle efficiency for the bottoming cycle is

$$(\eta_{cycle})_{bottom} = \frac{(P_{elec})_{bottom}}{(Q_{cycle})_{bottom}} = \frac{[(\Sigma P_T)_{bottom} - (\Sigma P_C)_{bottom}]\eta_{gen}}{(Q_{cycle})_{bottom}}$$
(3.5)

466 Where  $(P_{elec})_{bottom}$  is the bottoming cycle electrical power output,  $(\sum P_T)_{bottom}$  is the sum 467 of bottoming cycle turbine power and  $(\sum P_C)_{bottom}$  is the sum of bottoming cycle compressor 468 power.

469 The overall cycle efficiency,  $\eta_{overall cycle}$  is the ratio of the total electrical power output from 470 the cycles,  $(P_{elec})_{total}$  to the total heat transferred to the cycles,  $(Q_{cycle})_{total}$ .

$$\eta_{overall \, cycle} = \frac{(P_{elec})_{total}}{(Q_{cycle})_{total}} = \frac{(P_{elec})_{top} + (P_{elec})_{bottom}}{(Q_{cycle})_{top} + (Q_{cycle})_{bottom}}$$
(3.6)

471

472 The net power output of the plant,  $P_{net}$  is the total or gross power output from the topping and 473 bottoming cycles,  $(P_{elec})_{total}$  minus the auxiliary power consumption,  $P_{aux}$  in pumps, fans,

bottoming cycles,  $(P_{elec})_{total}$  minus the auxiliary power consumption,  $P_{aux}$  in pumps, fans, coal mill etc.:

$$P_{net} = (P_{elec})_{total} - P_{aux} \tag{3.7}$$

475

476 The plant net efficiency,  $\eta_{net}$  is defined as the ratio of the net power output to the coal fuel 477 energy input to the plant:

$$\eta_{net} = \frac{P_{net}}{\dot{m}_{coal}(HHV)} \tag{3.8}$$

478

The three cases in this study with different bottoming cycle options will present different cycle
efficiencies and furnace efficiencies. Therefore, the overall impact of the choice of power plant
configurations on the plant net efficiency can only be determined through performance
calculations and comparison among the cases.

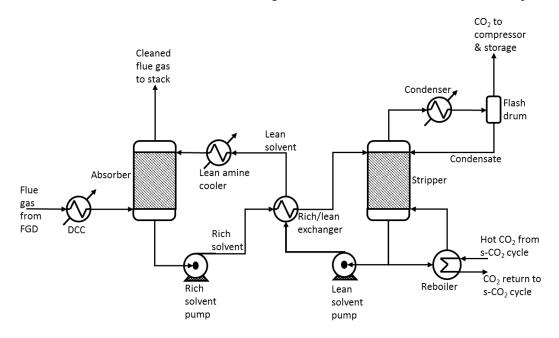
# 483 **4** Solvent-based post-combustion CO<sub>2</sub> capture

This section discusses the PCC, which is based on chemical absorption through MEA solvent.
Benefits of MEA-based PCC include (1) high separation selectivity; (2) It operates at atmospheric conditions; (3) Experimental/pilot plant data are available.

#### 487 4.1 Description of MEA-based CO<sub>2</sub> capture process

Figure 8 shows a simplified process flow diagram for a typical chemical absorption CO<sub>2</sub>
capture process. The main components are absorber, stripper with a reboiler and a condenser
attached, direct contact cooler (DCC), rich MEA pump, lean MEA pump, lean/rich cross heat
exchanger and lean MEA cooler.

492 Flue gas from the power plant's FGD unit is first cooled in the DCC to a suitable temperature 493 for absorption (about 40 °C). The cooled flue gases are introduced into the absorber at the bottom while the lean MEA solvent solution enters the absorber at the top. The flue gases flow 494 495 upward while the MEA solvent solution flows down under gravity through the absorber 496 (packed column). Chemical absorption of  $CO_2$  in the flue gases by the MEA solvent takes 497 place during the counter-current flow in the absorber. Treated flue gases leave the absorber at 498 the top. Rich MEA solvent (i.e. with higher loading of  $CO_2$ ) leaves the absorber at the bottom. 499 Its pressure is then increased by the rich MEA pump and heated in the lean/rich cross heat 500 exchanger before entering the stripper at the top. In the stripper column, the rich MEA solvent 501 is stripped of the CO<sub>2</sub> by the application of heat energy in the reboiler. The water vapour and CO<sub>2</sub> mixture released in the stripper is sent to the stripper condenser, which cools the mixture 502 503 thereby turning most of the water vapour to liquid water. The condensed water and  $CO_2$  are separated in the flash drum. The condensed water is returned back to the stripper while the 504 separated CO<sub>2</sub> leaves the stripper at the top. The resulting lean MEA solvent (i.e. with lower 505 loading of  $CO_2$ ) exits the stripper at the bottom. The lean MEA solvent leaving the stripper is 506 507 used to heat the rich MEA solvent in the cross heat exchanger and the temperature is further 508 reduced in the lean MEA cooler before being returned to the absorber column at the top.



509

510 Figure 8 Simplified process flow diagram for MEA-based post-combustion CO<sub>2</sub> capture unit 511 [3]

### 512 4.2 Rate-based simulation of the CO<sub>2</sub> capture system in Aspen

### 513 Plus®

The MEA-based PCC was simulated in Aspen Plus® to determine the performance. The 514 515 simulation was based on the parameters reported for the benchmark supercritical steam plant's PCC unit, which was validated with data from University of Kaiserslautern pilot plant by 516 Olaleye et al. [45]. The PCC used a 30 wt.% MEA solution as solvent. The temperature of the 517 518 flue gas and the lean MEA entering the absorber was 40 °C. Absorber operating pressure was 1.013 bar. The rich MEA solution was heated up to  $106 \, {}^{0}$ C in the cross heat exchanger. The 519 stripper was operating at a pressure of 1.9 bar and the reboiler temperature was maintained at 520 about 120 °C to avoid thermal degradation of the amine solvent. In Aspen Plus<sup>®</sup>, RadFrac 521 522 block was used to model the absorber and the stripper. Koch FLEXIPAC<sup>®</sup> 1Y structured 523 packing was selected for the absorber and stripper. Previously, the MEA-based PCC model has been validated and scaled up to match the flue gas flow rate of the supercritical power plant by Olaleye et al. [45]. For the plant with 1402 MW of heat input, the design of the absorber and stripper arrived at four absorber columns with a diameter of 5.41m each and three stripper column with a diameter of 4.62m each in order to maintain the columns diameters within the structural limit. Fifteen equilibrium stages were required for each of the absorber and the stripper column.

Modelling of the absorber and stripper in Aspen Plus<sup>®</sup> was through the use of rate-based models. Rate-based model provides a rigorous and good prediction of the simulation over a wide range of operating conditions unlike the traditional equilibrium-stage modelling approach [51]. The Electrolyte Non-Random-Two-Liquid (ElecNRTL) activity coefficient property package was selected to accurately predict the ionisation equilibrium and the heats of solution of the MEA-CO<sub>2</sub>-H<sub>2</sub>O system. The solution chemistry of the MEA-based chemical absorption process can be represented by the following equilibrium reactions (R1-R5) [52]:

 $2H_20 \leftrightarrow 0H^- + H_30^+$ Water dissociation: **R**1 538  $CO_2 + 2H_2O \leftrightarrow HCO_3^- + H_3O^+$ CO<sub>2</sub> hydrolysis: R2 539  $HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{2-}$ Bicarbonate dissociation: R3 540  $MEACOO^- + H_2O \leftrightarrow MEA + HCO_3^-$ Carbamate hydrolysis: R4 541  $MEAH^+ + H_2O \leftrightarrow MEA + H_3O^+$ MEA protonation: R5 542

543 Reaction models for the absorber and stripper consist of three equilibrium rate-based 544 controlled reactions, R1, R3 and R5, in conjunction with the following kinetic rate-based 545 controlled reactions (R6-R9) [52]:

546	Bicarbonate formation (forward):	$CO_2 + OH^- \rightarrow HCO_3^-$	R6
547	Bicarbonate formation (reverse):	$HCO_3^- \rightarrow CO_2 + OH^-$	R7
548	Carbamate formation (forward):	$MEA + CO_2 + H_2O \rightarrow MEACOO^- + H_3O^+$	R8
5.40	Carbamate formation (reverse):	$MEACOO^- + H_3O^+ \rightarrow MEA + CO_2 + H_2O$	R9

- 549
- 550 The kinetic reaction rates, r, are described in Aspen Plus<sup>®</sup> by the power law expression:

$$r = kT^{n} exp\left(-\frac{E}{RT}\right) \prod_{i=1}^{N} C_{i}^{a_{i}}$$

$$\tag{4.1}$$

# 552 5 Results and discussion

#### 553 5.1 Verification of the s-CO<sub>2</sub> Brayton cycle model

The suitability of the Aspen Plus<sup>®</sup> model for simulating the performances of supercritical CO<sub>2</sub> Brayton cycles was investigated. An s-CO<sub>2</sub> recompression Brayton cycle (Figure 1b) was modelled for verifying the calculation. Independent results of numerical model reported by Dostal et al. [53] were compared with the Aspen Plus<sup>®</sup> simulation results. The input parameters were:

- Maximum cycle pressure 200 bar
- Turbine inlet temperature 550 °C
- Precooler outlet temperature 32 °C
- Precooler outlet pressure 76.92 bar
- Mass flow rate 3176.4 kg/s
- MC pressure ratio 2.6
- Split flow fraction 0.41
- Turbine isentropic efficiency 90 %
- Main and recompression compressors efficiency 89 %
- 568 Comparison of the main simulation results against literature value is presented in Table 2. The
- 569 maximum relative deviation is about 2.51%. The small differences in the result can be 570 attributed to uncertainties in the pressure loss specifications and the round-off error in the input
- 570 parameters. Otherwise, the simulation results agreed well with the literature values.
- 572 Table 2 Validation of s-CO<sub>2</sub> Brayton cycle model against literature value

			Relative
Parameters	Literature value [54]	Simulation value	difference
Turbine outlet temperature	440.29 °C	440.29 °C	0%
MC outlet temperature	61.1 <sup>o</sup> C	61.11 °C	0.02%
RC inlet temperature	69.59 °C	71.34 <sup>o</sup> C	2.51%
RC outlet temperature	157.99 °C	160.25 °C	1.43%
Heater inlet temperature	396.54 °C	397.38 °C	0.21%
Thermal power	600 MWt	596.76 MWt	0.54%
Turbine work	383.71 MW	383.72 MW	0.003%
MC work	38.59 MW	38.57 MW	0.05%
RC work	74.84 MW	75.84 MW	1.34%
Net work output	270.28 MW	269.31 MW	0.36%
HTR duty	985.51 MW	977.49 MW	0.81%
LTR duty	398.8 MW	398.0 MW	0.2%
Precooler duty	328.38 MW	328.11 MW	0.08%
Cycle efficiency	45.05%	45.13 %	0.08%

573

#### 574 5.2 Baseline boundary conditions and design point parameters

575 The boundary conditions and parameters such as coal mass flow rate, combustion air 576 conditions, percent excess air, flue gas stack temperature, maximum cycle pressure and 577 turbines inlet temperature were selected based on the information published for the 578 supercritical reheat steam cycle [45]. This will ensure a fair comparison between the 579 performances of the s-CO<sub>2</sub> cycle plants and the conventional supercritical steam plant. Other 580 conditions and parameters like pressure losses and specifications of heat exchangers were 581 selected based on similar studies of  $s-CO_2$  power cycle reported in the literature [15, 30]. A 582 summary of the baseline boundary conditions and design point parameters is given in Table 3.

#### 583 Table 3 Boundary conditions and design parameters

Parameter/variable	Value
Coal feed $(^{0}C/bar/(kg/s))$	15/1.01/51.82
Air ( <sup>0</sup> C/bar)	15/1.01
Excess air (%)	20
Maximum cycle pressure (bar)	290
HP & LP turbines inlet temperature ( <sup>0</sup> C)	593
Compressor inlet pressure (bar)	76
Compressor inlet temperature ( <sup>0</sup> C)	31
Gas-CO <sub>2</sub> TTD ( $^{0}$ C)	30
Preheater hot outlet temperature ( <sup>0</sup> C)	116
Recuperator TTD ( <sup>0</sup> C)	10
Turbine isentropic efficiency (%)	93
MC isentropic efficiency (%)	90
Recompression compressor isentropic efficiency (%)	89
Fan isentropic efficiency (%)	80
Generator efficiency (%)	98.4
Ash distribution, fly/bottom ash (%)	80/20

<sup>584</sup> 

# 585 5.3 Performance comparisons among Cases A, B and C of the 586 coal-fired s-CO<sub>2</sub> Brayton cycle power plants

587 The flow split fraction (i.e. the fraction of the total flow that goes through the precooler/main 588 compressor) should be adjusted such that the differences in the heat capacities between the hot 589 streams and the cold streams in recuperators are minimised. This will improve heat transfer in 590 the recuperators and thereby maximised cycle efficiency. Figure 9 shows the cycle efficiencies 591 as a function of the flow split fractions. The optimum flow split fraction was found to be about 592 0.65 for the topping cycle while it was about 0.71 for the single recuperator recompression 593 bottoming cycle.

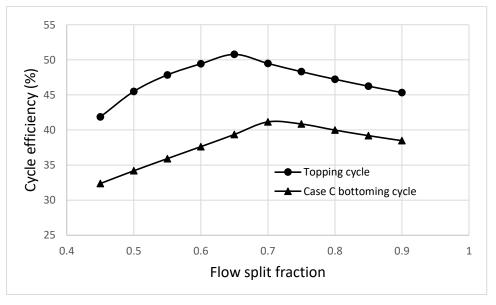


Figure 9 Cycle efficiencies of the topping cycle and Case C bottoming cycle as a function ofthe flow split fractions

597 In order to highlight the impact of integrating the coal-fired s-CO<sub>2</sub> power plants with the PCC 598 unit, the performances of the power plants without carbon capture were first determined based the optimum flow split fractions, and the baseline boundary conditions and design parameters 599 600 presented above. Table 4 shows the pressure, temperature and mass flow for the plants' main points. The stream nomenclature is based on Figure 3, Figure 4 and Figure 5. This was then 601 602 followed by simulation and performance evaluation of the whole power plants, incorporating 603 the PCC unit. The distribution of the fuel combustion heat energy among the different  $s-CO_2$ 604 heaters is shown in Figure 10. About 50% of the input heat energy was transferred by radiation 605 to the s-CO<sub>2</sub> working fluid in the radiant heaters. The Case A and Case B bottoming cycles 606 were able to recover about 12% of the total heat input, which otherwise would have been lost through the exhaust flue gas. In Case C, only about 9% was recovered but the unrecovered 607 608 heat was utilised for preheating the secondary air to higher temperature level (258 °C) than Case A (177 °C) and Case B (165 °C). This then leads to higher heat transfer in the furnace for 609 610 Case C. For the three cases, the heat losses were about 12%, that is, a furnace efficiency of approximately 88%. This value of furnace efficiency is comparable to the boiler efficiency 611 612 obtainable in coal-fired steam power plants. Hence, the addition of the bottoming cycles and the combustion air preheaters enables efficient utilisation of the furnace heat. 613

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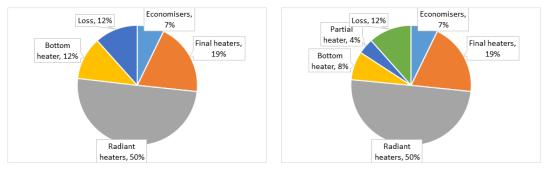
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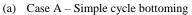
Table 4 Summary of the main stream values for the three cases calculated with baselineboundary conditions and design parameters

		Case A			Case B			Case C		
Stream	P (bar)	T ( <sup>0</sup> C)	m (kg/s)	P (bar)	T ( <sup>0</sup> C)	m (kg/s)	P (bar)	$T(^{0}C)$	m (kg/s)	
Coal	1.01	15	51.82	1.01	15	51.82	1.01	15	51.82	
Air	1.01	15	540.88	1.01	15	540.88	1.01	15	540.88	
Pry air	1.1	215	127.11	1.1	215	127.11	1.1	215	127.11	
Sec. air	1.1	177.23	413.77	1.1	164.59	413.77	1.1	257.82	413.77	
Pulv.Coal+air	1.09	75.28	178.93	1.09	75.28	178.93	1.09	75.28	178.93	
А	1.09	1010	592.7	1.09	1010	592.7	1.09	1010	592.7	
В	1.01	496	592.7	1.01	496	592.7	1.01	496	592.7	
С	1.01	253.26	592.7	1.01	244.86	592.7	1.01	306.70	592.7	
D	1.01	116	592.7	1.01	116	592.7	1.01	116	592.7	
Flue to stack	1.01	56.67	585.08	1.01	56.67	585.08	1.01	56.67	585.08	
T1	287.12	466	4052.52	287.12	466	4038.78	287.12	466	4163.13	
T2	282.82	593	4052.52	282.82	593	4038.78	282.82	593	4163.13	
T3	147.72	507.64	4052.52	147.72	507.64	4038.78	147.72	507.64	4163.13	
T4	145.51	593	4052.52	145.51	593	4038.78	145.51	593	4163.13	
a1,b1,c1	288.55	223.26	511.12	288.70	305.71	526.35	288.55	276.70	523.38	
a2,b2,c2	287.25	466	511.12	287.25	466	526.35	287.25	466	523.38	
b8	-	-	-	290	69.70	152.64	-	-	-	

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(b) Case B – Partial heating bottoming

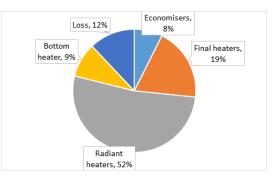




Figure 10 Distribution of the input heat value among the different heaters

622 Table 5 shows the performance result of the PCC unit that was integrated with the coal-fired 623 s-CO<sub>2</sub> Brayton cycle power plants. Integration of the PCC to the plants penalised the net 624 efficiency through (1) bleeding of  $CO_2$  for solvent regeneration in reboiler, which resulted in lower cycle efficiency (2) additional auxiliary loads associated with the PCC units. Table 6 is 625 626 a summary of the performance results for the three cases both without the PCC unit and with 627 the PCC unit integrated. Interestingly, Case C (i.e. the single recuperator recompression 628 bottoming cycle layout) gave the best overall plant net efficiency with or without PCC even 629 though the bottoming cycle recovered the least amount of heat and thus produced the least 630 power. The superior performance of Case C is due to better efficiency of the bottoming cycle. In contrast, Kim et al. [15] concluded that power produced by bottoming cycle is a more 631 632 important factor than the efficiency of bottoming cycle in determining the overall plant performance and therefore, did not recommend recompression cycle for bottoming cycle 633 634 application despite having the best cycle efficiency. However, unlike our study, Kim et al. 635 compared the performances of various s-CO<sub>2</sub> bottoming cycles without a downstream air 636 preheater.

637 For a fixed coal fuel input, the plant overall performance depends on auxiliary loads, cycle 638 efficiency and furnace efficiency. The cycle efficiency is majorly determined by the choice of 639 cycle layout/configuration. Furnace efficiency, on the other hand, can be improved by heat 640 recovery in the bottoming cycle and preheating of combustion air. In summary, the cycle 641 layouts, the bottoming cycle heat recovery, the level of air preheating and the auxiliary loads 642 will determine the plant net efficiency. Hence, for plants with similar auxiliary loads, plant net 643 efficiency will be maximised by configurations with high cycle efficiency, good heat recovery 644 in bottoming cycle and high level of air preheating. Unfortunately, good heat recovery in the bottoming cycle cannot be achieved simultaneously with a high level of air preheating. For 645 instance, good heat recovery in the bottoming cycles of Case A and Case B meant that the 646 647 temperature of the flue gas entering the air preheater was relatively low, limiting the amount 648 of air preheating possible. On the other hand, Case C with the least heat recovery (or produced

- 649 power) in bottoming cycle gave the highest air preheating duty (Table 6). Therefore, the poor
- heat recovery was somewhat compensated for by the added air preheater.
- 651
- 652

653	Table 5 Parameters and	performance resul	ts of the PCC unit
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Parameter	Value
CO <sub>2</sub> removal percentage	90%
Flue gas absorber inlet temperature	40 °C
Lean solvent absorber inlet temperature	40 °C
MEA concentration	30 wt.%
Absorber operating pressure	1.013 bar
Stripper operating pressure	1.9 bar
Lean solvent loading	0.29 mol CO <sub>2</sub> /mol MEA
Rich solvent loading	0.53 mol CO <sub>2</sub> /mol MEA
Reboiler temperature	120 °C
Condenser temperature	31.98 <sup>o</sup> C
Condenser duty	1.13 GJ/ton CO <sub>2</sub>
Solvent circulation rate	18 m <sup>3</sup> /ton CO <sub>2</sub>
Reboiler duty	3.4 GJ/ton CO <sub>2</sub>

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Table 6 Comparison of plant performances with and without post-combustion  $CO_2$  capture (PCC) for Case A (simple recuperative cycle as bottoming cycle), Case B (partial heating cycle

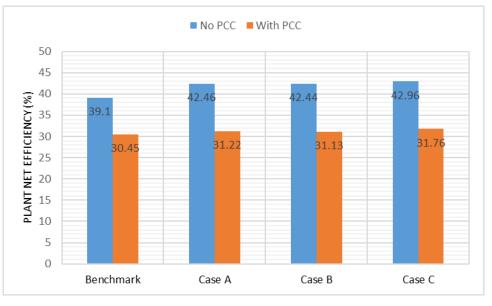
as bottoming cycle) and Case C (single recuperator recompression cycle as bottoming cycle)

	Cas	Case A		Case B		Case C	
Parameter	No PCC	With PCC	No PCC	With PCC	No PCC	With PCC	
HHV, MJ/kg	27.05	27.05	27.05	27.05	27.05	27.05	
Input heat value, MJ	1401.87	1401.87	1401.87	1401.87	1401.87	1401.87	
Heat transferred to top cycle, MW	1077.49	1103.16	1072.8	1095.63	1106.01	1131.81	
Heat transferred to bottom cycle, MW	161.46	161.46	167.03	149.57	126.75	106.56	
Furnace efficiency, %	88.38	88.74	88.44	88.82	87.94	88.34	
Preheater duty, MW	92.61	59.80	87.18	51.15	127.43	96.14	
Top gross electric power, MWe	545.40	401.98	543.31	398.08	560	416.32	
Bottom gross electric power, MWe	60.17	46.39	61.96	48.95	52.61	39.58	
Top cycle efficiency, %	50.62	36.44	50.64	36.33	50.63	36.78	
Bottom cycle efficiency, %	37.27	32.94	37.10	32.73	41.51	37.14	
Overall cycle efficiency, %	48.88	36.04	48.82	35.90	49.69	36.81	
Auxiliaries power, MW	10.38	10.7	10.38	10.7	10.39	10.7	
Net electric power, MWe	595.19	437.67	594.90	436.33	602.22	445.19	
CO2 specific emission, kg CO2/MWh	714.69	98.05	715.04	98.35	706.35	96.39	
Specific work output, kWh/m <sup>3</sup>	5.28	5.24	5.26	5.23	5.16	5.10	
Overall plant net efficiency, %	42.46	31.22	42.44	31.13	42.96	31.76	

661 In Figure 11, the performances of the coal-fired  $s-CO_2$  Brayton cycle power plants were 662 compared with the state-of-the-art supercritical reheat steam power plant [51]. The  $s-CO_2$ Brayton cycle power plants, without CO<sub>2</sub> capture, was found to be about 3.34 - 3.86% more 663 664 efficient than the steam power plant. When the power plants were integrated with the PCC unit, the plant net efficiencies of the s-CO<sub>2</sub> power plants were about 0.68 - 1.31% above the 665 steam plant's efficiency. Although the s-CO<sub>2</sub> Brayton cycle plants with CO<sub>2</sub> capture gave 666 higher efficiency than steam cycle plant, the s-CO<sub>2</sub> cycle suffered more efficiency penalty 667 (about 11.2%) than the steam plant (about 8.65%). This is probably due to the use of sensible 668 669 heat of s-CO<sub>2</sub> working fluid to meet reboiler thermal requirement instead of low pressure 670 condensing steam, as is usually the case in steam turbine power plant.

671 A comparison of the specific work output (i.e. the ratio of the generated power to the 672 volumetric flow rate of the working fluid) of each cycle can give an indication of the relative size of plants and by extension the relative capital cost [20, 54]. Table 6 shows that the specific 673 674 work outputs in all the three cases were comparable (approximately 5 kWh/m<sup>3</sup>). Case C shows a slightly lower specific work output but the difference is not considered significant. The 675 specific work output of the s-CO<sub>2</sub> cycle is over 30 times more than that of the steam cycle. 676 677 Therefore, the s-CO2 cycle plant has the potential to be significantly smaller than the steam 678 cycle plant. This is in good agreement with previous findings in the literature on the 679 compactness of s-CO<sub>2</sub> cycle in comparison with steam cycle [11-13, 43].





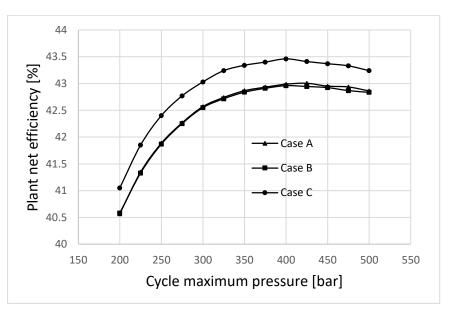
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Figure 11 Comparison of the overall plant net efficiency of Case A (simple recuperative cycle
as bottoming cycle), Case B (partial heating cycle as bottoming cycle) and Case C (single
recuperator recompression cycle as bottoming cycle) with the supercritical steam plant (from
Olaleye et al. [45]) as the benchmark

686 In this study, the cycle maximum pressure has been selected to match the maximum pressure in the steam cycle. However, a common feature of Brayton cycle is that there is an optimum 687 pressure ratio (or cycle maximum pressure in our case) at which the efficiency has a peak 688 value. Hence, the effect of cycle maximum pressure on plant performance was investigated by 689 varying the pressure from 200 bar to 500 bar while the compressor inlet pressure was kept 690 691 constant. Figure 12 shows the plant net efficiency as a function of cycle maximum pressure for the three configurations. Case C was found to maintain the best efficiency over the whole 692 693 pressure range. Maximum efficiency occurred at an optimum pressure of about 400 bar.

694 Currently, the choice of such a high pressure might not be feasible due to mechanical design 695 considerations such as the maximum pressure limit of heat exchangers, turbomachinery seal solutions to prevent leakage and the need to avoid excessively small compressor blades. 696 697 However, the USC steam plant with a maximum pressure of 350 bar and a turbine inlet temperature of 700 °C is expected to come into operation between 2020 and 2030 [31]. If the 698 699 s-CO<sub>2</sub> cycle is operated at such maximum pressure (i.e. 350 bar), a net efficiency gain up to 700 4.24% above the current efficiency of steam turbine plant can be achieved without a corresponding increase in turbine inlet temperature to 700 °C as planned. Hence, the s-CO<sub>2</sub> 701 702 plant has the advantage of increased efficiency at a lower temperature.

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704

Figure 12 Plant net efficiency as a function cycle maximum pressure from 200 bar to 500 bar
for the three configurations (Case A – simple recuperative cycle as bottoming cycle, Case B –
partial heating cycle as bottoming cycle and Case C – single recuperator recompression cycle
as bottoming cycle)

#### 5.4 Choice of configuration and parametric study

In this study, the performance comparison was carried out for three potential s-CO<sub>2</sub> cycle 710 711 configurations. The cycles were adapted for efficient utilisation of furnace heat similar to 712 boiler heat utilisation in conventional steam turbine plant, albeit with bottoming cycles added. 713 Operating conditions (290 bar, 593 °C and single reheat) were chosen to match the current 714 supercritical steam cycle conditions. Hence, current experience with material technology for 715 pulverised coal-fired boiler and steam turbine could be applied to the development of the coalfired s-CO<sub>2</sub> Brayton cycle power plant. The overall net efficiency of Case C option without 716 717 CO<sub>2</sub> capture was 0.5% and 0.52% over the efficiency of Case A and Case B respectively. With 718 CO<sub>2</sub> capture, the efficiency gains were 0.54% and 0.63% above the efficiency of Case A and 719 Case B respectively. Therefore, of the three alternative configurations considered, Case C 720 (with single recuperator recompression cycle as the bottoming cycle) is more attractive due to its better performance. It is also expected to be of similar size as the other two configurations 721 722 considering the relative value of the specific work output and the component count. When 723 compared with steam cycle plant, the net efficiency of Case C was higher than the efficiency 724 of steam cycle plant by about 3.86% and 1.31% without CO<sub>2</sub> capture and with CO<sub>2</sub> capture 725 respectively.

726 Cycle efficiency is known to depend on the turbine inlet temperature, precooler outlet/main

compressor inlet temperature and the recuperator minimum TTD. Hence, a parametric study

was performed to investigate the effects of these parameters on the net efficiency of the chosen

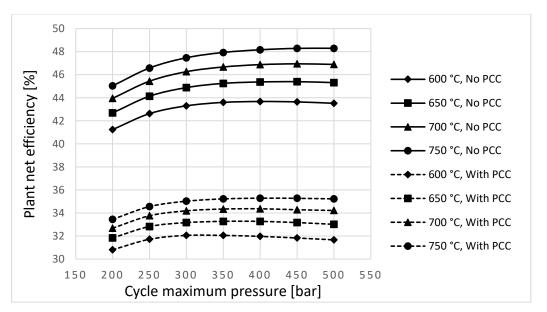
729 coal-fired s-CO<sub>2</sub> cycle power plant.

#### 730 5.4.1 Effect of turbine inlet operation conditions

Figure 13 shows the effect of changes in turbine inlet temperature on the cycle performance for the single recuperator recompression bottoming cycle configuration without PCC unit and with PCC unit integrated. The figure was produced by varying the cycle maximum pressure from 200 bar to 500 bar for four different selection of turbine inlet temperatures (600 °C, 650 °C, 700 °C and 750 °C). The cycle performance was calculated with the flow split fraction that gave the maximum efficiency for each data point while other cycle parameters were maintained at the baseline condition.

738 The results showed that the plant net efficiency increased with the rise in turbine inlet 739 temperature. Also for each selection of turbine inlet temperature, there is an optimum cycle 740 maximum pressure. The optimum cycle maximum pressure increase with an increase of turbine inlet temperature. With no PCC and at a turbine inlet temperature of  $600 \, {}^{\circ}$ C, the 741 742 optimum cycle maximum pressure was about 400 bar, while at 650 °C, the optimum cycle 743 maximum cycle pressure increased to about 450 bar and the trend continued with increase in 744 turbine inlet temperature. At the operating conditions of the next USC steam turbine power plant (700  $^{\circ}$ C and 350 bar), the efficiency of the s-CO<sub>2</sub> cycle power plant is about 46.67%. 745 This corresponds to about 7.57% above the efficiency of the conventional supercritical steam 746 747 plant.





749

Figure 13 Plant net efficiency as a function of cycle maximum pressure at different turbine
inlet temperature for the single recuperator recompression bottoming cycle configuration (i.e.
Case C) with no carbon capture and with carbon capture integrated

From the foregoing, the adoption of the s- $CO_2$  cycle for coal-fired power plant application is promising. The s- $CO_2$  cycle achieved higher efficiency than steam cycle plant at similar operating conditions. Even for the advanced USC steam plant that is expected to achieve efficiency around 47%, this will be done with two or more reheat stages, three or more turbine modules and series of feedwater heaters. However, with potentially smaller footprint and less complex configuration, similar efficiency can be achieved with coal-fired s-CO<sub>2</sub> Brayton cycle
 power plant investigated in this study.

#### 760 5.4.2 Effect of precooler outlet/main compressor inlet operating conditions

The selection of precooler outlet temperature (or main compressor inlet temperature) is based 761 762 on the ambient or heat sink temperature, which depends on location as well as the type of cooling (wet cooling or dry cooling). The effect of precooler outlet operating conditions on 763 cycle performance was investigated by varying the precooler outlet pressure from 60 bar to 764 110 bar for four selections of precooler outlet temperature (31, 34, 37 and 40  $^{\circ}$ C). In order to 765 766 keep the cycle supercritical at all times, only values of precooler outlet temperature above  $CO_2$ 767 critical temperature was considered. The cycle efficiency was optimised with the flow split 768 fraction while other parameters were fixed at the baseline value. Figure 14 shows the plant net 769 efficiency as a function of precooler outlet temperature and pressure.

770 The plant net efficiency decreases with rise in precooler outlet temperature. However, for each 771 precooler outlet temperature, there is a corresponding pseudo-critical pressure at which the 772 plant efficiency is maximum. For instance, the highest plant net efficiency for a precooler outlet temperature of 31 °C was achieved at a precooler outlet pressure of 76 bar. However, 773 when the precooler outlet temperature was increased to 34 °C, the optimum precooler outlet 774 775 pressure also increased to 81 bar. This trend continued with increase in precooler outlet 776 temperature. This is due to rapid rise of the density of the CO<sub>2</sub> working around the pseudocritical pressures associated with the selected temperatures as shown in Figure 15. The 777 increased density results in reduced compressor work and hence increased net work output or 778 779 efficiency.



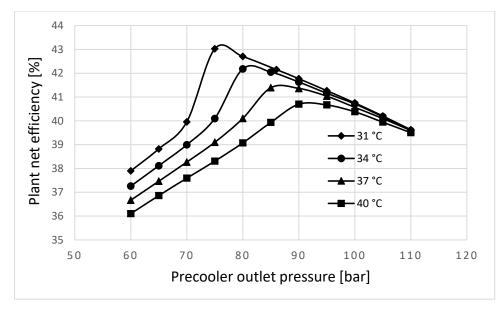


Figure 14 Effect of precooler outlet temperature on plant net efficiency of the single
recuperator recompression bottoming cycle configuration with no carbon capture with
precooler outlet pressure varying from 60 bar to 110 bar

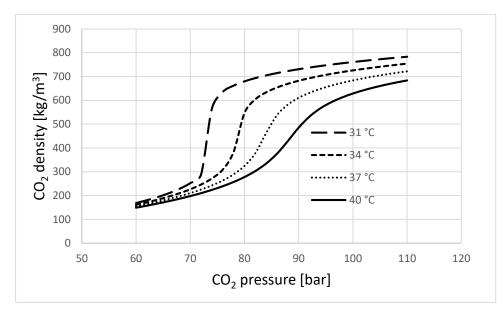


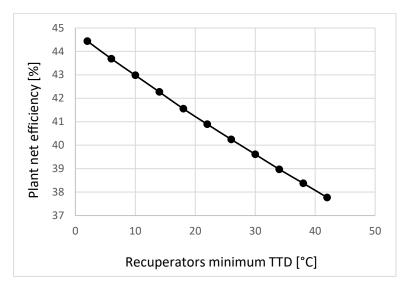


Figure 15 Plot of CO<sub>2</sub> pressure against density in the critical region showing the rapid rise in density at pseudo-critical pressures corresponding to different CO<sub>2</sub> temperatures

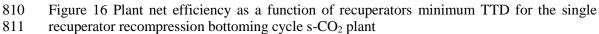
#### 5.4.3 Effect of minimum terminal temperature difference of the recuperators

789 The minimum TTD of the recuperators is considered to be the smallest temperature difference 790 between the hot and the cold stream at either hot inlet/cold outlet end or cold inlet/hot outlet 791 end of the heat exchanger. Supercritical CO<sub>2</sub> recuperator is known to have pinch-point problem 792 in which the smallest temperature difference occurs somewhere along the heat exchanger and 793 not at the terminals [30]. The occurrence of pinch-point along the recuperator can be avoided 794 by using recompression cycle and adjusting the flow split fractions to balance the heat 795 capacities of the hot and cold stream. Therefore, minimum TTD will be the same as pinch-796 point temperature difference if the pinch-point is located at the terminal of the recuperators.

797 The selection of recuperator TTD or pinch-point temperature difference will influence the 798 cycle efficiency and size of the recuperator [30]. Previous studies showed that the recuperator 799 constituted the largest percentage of the size of closed Brayton cycle plant [17, 55]. For the 800 coal-fired s-CO<sub>2</sub> cycle plant with single recuperator recompression bottoming cycle, the effect of the recuperators' minimum TTD on the plant net efficiency is shown in Figure 16. The plant 801 802 net efficiency decreased with increasing minimum TTD of the recuperators. For every 1°C 803 increase in minimum TTD, the net efficiency was reduced by approximately 0.17%. Hence, 804 improved plant performance can be achieved by reducing the TTD between the hot and cold stream. This is because reducing the TTD will improve the effectiveness of the recuperator, 805 806 and thus the plant performance. However, this will be at the cost of increased size of 807 recuperator because more heat transfer area will be required.







# 812 6 Conclusions

813 In this paper, s-CO<sub>2</sub> Brayton cycle has been proposed as a potential replacement for steam 814 Rankine cycle of coal-fired power plant with solvent-based post-combustion CO<sub>2</sub> capture. 815 Performance evaluation shows that the s-CO<sub>2</sub> Brayton cycle can be adapted for efficient utilisation of furnace and flue gases heat by using a topping s-CO<sub>2</sub> cycle and a bottoming s-816 817  $CO_2$  cycle in addition to combustion air preheating. The coal-fired s-CO<sub>2</sub> cycle is able to 818 achieve furnace efficiency of about 88% in the three cases, which is comparable to the boiler 819 efficiency of the conventional supercritical steam plant. The plant net efficiency of the s-CO<sub>2</sub> Brayton cycle plant without  $CO_2$  capture is about 3.34-3.86% more than that of the 820 supercritical steam plant. With CO<sub>2</sub> capture, the coal-fired s-CO<sub>2</sub> cycle suffers an efficiency 821 penalty of about 11.2%, which is more than the efficiency penalty of the reference supercritical 822 823 steam cycle plant (8.65%). Nevertheless, the plant net efficiency of the s-CO<sub>2</sub> cycle plant is still about 0.68-1.31% more than that of the supercritical steam cycle with PCC. For the three 824 825 investigated cases, Case C (newly proposed bottoming cycle) is the most attractive 826 configuration as it gives the highest plant net efficiency either without or with CO<sub>2</sub> capture. 827 Also, comparison of the specific work outputs indicates that the size of the new concept is not 828 expected to be significantly larger than those of Case A and Case B.

829 Taken together, these findings suggest that cascaded s-CO<sub>2</sub> Brayton cycle is a promising power 830 conversion system for coal-fired power plant application. The current study is conceptual in 831 nature. Nevertheless, it provides considerable insight into the thermodynamic performance of s-CO<sub>2</sub> Brayton cycle adapted for coal-fired power plant, employing a topping reheat 832 recompression s-CO2 cycle and different options of bottoming s-CO<sub>2</sub> cycles. Operating 833 834 conditions have been chosen to be similar to conditions obtainable in the current supercritical 835 steam boiler so that the current experience with boiler material technology can be applied to 836 the s-CO<sub>2</sub> furnace. Therefore, future development efforts can be focused on the s-CO<sub>2</sub> Brayton 837 cycles.

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