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1	Thermodynamic analysis and economic assessment of a carbon dioxide hydrate-		
2	based vapor compression refrigeration system using load shifting controls in		
3	summer		
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#### 14 Abstract

15The present work proposed a novel two-stage carbon dioxide hydrate-based vapor-16 compression refrigeration system. The proposed system applied pure carbon dioxide 17hydrate as the primary refrigerant and arranged both of hydrate formation and 18 dissociation at the low-pressure stage. The thermodynamic and economic models were 19 developed and then performances of the proposed system using load-levelling storage 20 and full storage operations were evaluated and compared with those of a conventional 21 carbon dioxide single-stage vapor-compression refrigeration system, which is treated 22 as the baseline and with no energy storage. The simulation results indicate that the 23 design capacity of the proposed system using full storage is the largest among the three 24 systems, but with lowest operation cost, and with the incentivization of electricity prices 25 ratio of on and off-peak this cost savings would raise significantly. Noted that the bill 26 structure reveals the load-levelling storage system saves most on the water consumption. 27 Due to the dominant expenditure on the two compressors, compare with the baseline

1, \*Corresponding author: Tel: +44 (0)121 414 5135 E-mail y.li.1@bham.ac.uk system, the initial capital cost of the full storage system was 75.5% higher, whereas that of the levelling-load storage system was only 21.5% higher. Finally, this paper discussed the economic feasibility on the initial capital cost for the proposed system and developed an indication map to predict the profit years in case of that the new system using load-levelling storage operation replaces the baseline system assuming a system lifetime of 15 years under different electricity prices ratios.

34

- 35 Keywords: Two-stage compression; Carbon dioxide hydrate; Cold energy storage;
- 36 Load shifting strategy; Thermo-economics
- 37

#### 38 Nomenclature

39	a	subcooling degree
40	Α	surface area (m <sup>2</sup> )
41	С	cost (£) or cycle of concentration of cooling tower
42	CFR	capital recovery factor
43	СОР	coefficient of performance
44	Ср	specific heat (J kg <sup>-1</sup> K <sup>-1</sup> )
45	d	diameter (m)
46	$D_{\rm c}$	fin collar outside diameter (m)
47	$D_{ m h}$	hydraulic diameter (m)
48	е	electricity tariff (pence kWh <sup>-1</sup> )
49	Ε	evaporation loss (kg s <sup>-1</sup> )
50	f	frequency (Hz) or friction factor
51	$F_{ m p}$	fin pitch (m)
52	GWP	global warming potential

53	h	enthalpy (J kg <sup>-1</sup> ) or heat transfer coefficient (W m <sup>-2</sup> K <sup>-1</sup> )
54	i	segment index
55	j	the Coburn factor
56	l	length (mm)
57	k	thermal conductivity (W m <sup>-1</sup> K <sup>-1</sup> )
58	LMTD	log mean temperature difference (K)
59	m	mass flow rate (kg s <sup>-1</sup> )
60	Ν	number of tube row
61	NTU	number of transfer unit
62	Nu	Nusselt number
63	ODP	ozone depletion potential
64	Р	pressure (kPa)
65	$P_1$	longitudinal tube pitch
66	Pr	Prandtl number
67	$P_{\rm t}$	transverse tube pitch
68	Q	heat transfer rate (W)
69	r	ratio of mass flow rate in high- and low-stages
70	Re	Reynolds number
71	Т	temperature (°C)
72	U	overall heat transfer coefficient (W $m^{-2} K^{-1}$ )
73	V	volume (m <sup>3</sup> )
74	W	power consumption (kW)
75	$X_{ m tt}$	Lockhart-Martinelli parameter
76		

77 Greek symbols

78	α	heat transfer coefficient (W $m^{-2} K^{-1}$ )
79	ε	effectiveness
80	Δ	difference
81	η	efficiency
82	μ	dynamic viscosity (kg m <sup>-1</sup> s <sup>-1</sup> )
83	ρ	density (kg m <sup>-3</sup> )
84	σ	surface tension (N m <sup>-1</sup> )
85	$\phi$	relative humidity
86	χ	vapor quality
87	ω	capacity flow ratio
88		
89	Subscripts	
90	a	air
91	atm	atmospheric
92	b	bulk
93	b_down	blow-down
94	cap	capital
95	ct	cooling tower
96	comp	compressor
97	db	dry-bulb
98	dec	carbon dioxide hydrate decomposer
99	diff	difference
100	Е	electricity
101	eval	expansion valve
102	evap	evaporator

103	ex	exit
104	f	film temperature
105	fic	fictitious
106	gc	gas cooler
107	Н	high-stage
108	hyd	hydrate
109	i	inner
110	Ι	intermediate-stage
111	in	inlet
112	isen	isentropic
113	1	liquid
114	L	low-stage
115	m_up	make-up
116	min	minimum
117	mix	mixture
118	nom	nominal
119	0	outer
120	out	outlet
121	op	operation
122	r	ratio
123	rev	revolution
124	sat	saturation
125	su	supply
126	tot	total
127	V	vapor

128	V	vapor
129	vol	volumetric
130	W	water
131	wb	wet-bulb
132		
133	Acronyms	
134	CHB-VCRS	carbon dioxide hydrate-based vapor-compression refrigeration
135	system	
136	CTES	cold thermal energy storage
137	FS	full storage
138	LS	load-levelling storage
139	PCM	phase change material
140	SC-VCRS	single-stage carbon dioxide vapor-compression refrigeration system
141	VCRS	vapor-compression refrigeration system

#### 143 **1. Introduction**

144 Nowadays, fossil fuel, as the most important energy source, generates around 70-145 80% of the total world electricity. The continuous and excessive combustion of fossil fuel already causes a series of serious environmental problems, such as global warming 146 147 and climate change. This situation deteriorates with the significant rising in electricity 148 consumption. Coulomb et al. [1] pointed it out that more than 17% of total electric 149 demands is from the air-conditioning and refrigeration sector, whereas a considerable 150 portion of which is consumed during the peak-load hours. Under such a background, 151the development of high-efficiency refrigeration system and peak-load shift methods matched will effectively save the additional fossil fuel used to generate electricity which
in turn, helps to reduce carbon emissions and minimize environmental impact.

154 Advanced refrigeration system incorporating cold thermal energy storage (CTES) 155technology is one of the most promising options. The CTES is one of effective manners 156 dealing with peak-load shift. Mosaffa et al. [2] developed an air conditioning system consisting of a combination of latent heat thermal storage and vapor-compression 157 158refrigeration. It produces and stores the cooling capacity during nighttime, and utilizes 159the stored cooling capacity for air conditioning during daytime, which significantly 160 reduces the electricity demand during the peak-load period. During the cold storing 161 process in this combined system, the air in duct as the secondary refrigerant is extracted 162 heat by the primary refrigerant (1,1,1,2-tetrafluoroethane (HFC-134a)) of the vapor-163 compression refrigeration system (VCRS), and then cools down and stores cold energy 164 into the phase change materials (PCMs). As a process of indirect cooling, such a 165 refrigeration system requires additional components and generates extra exergy losses. 166 Therefore, a substance, which could be both the primary refrigerant and PCM would be 167 viable in developing a high-efficiency and economic refrigeration system incorporating 168 CTES.

169 As for one method of solution, refrigerant gas hydrate could be the one. Clathrate 170 hydrates are crystalline solid consisting of water molecular cavities and refrigerant gas 171guested molecules. The research on refrigerant gas hydrates applied to CTES systems 172 started in the 1980s [3] since the thermodynamic properties are suitable for refrigeration 173applications (high dissociation enthalpy, low pressure and wide temperature range). For 174instance, the studies of Mori and Mori [4] focused on the injection of a refrigerant fluid 175(trichlorofluoromethane (CFC-11), chlorodifluoromethane (HCFC-22) and HFC-134a) 176 into water stored in a direct-contact crystallizer and form clathrates during cold storing,

177later the clathrate melted to produce chilled water. This process was not a continuous 178 and enclosed cycle. Recently, Ogawa et al. [5] proposed a novel conceptual design of a 179 refrigeration system using, refrigerant gas hydrates as the primary refrigerant. The 180 novel system can provide superior performance.. Different from a conventional VCRS, 181 evaporation and condensation are replaced by hydrate dissociation and formation. 182 Between those, a multiphase (guest gas and liquid water) compression occur in this 183 hydrate-based system. One of the notable hydrate properties is that the heat of 184 formation/dissociation is generally several times as large as the latent heat of the 185 conventional refrigerants. For instance, the enthalpy of dissociation of carbon dioxide 186  $(CO_2)$  hydrate is reported to be 80 kJ mol<sup>-1</sup> [6], whereas CO<sub>2</sub> enthalpy of evaporation is 187 only 18 kJ mol<sup>-1</sup> [7]. There are two basic principles of selection of the hydrate-forming guest refrigerant gas. One is that the environment-friendly gases are preferred. The 188 189 other is that the formation/dissociation pressure should be relatively low (less than 5 190 MPa) at the temperature of the application scenarios, usually between the range of 278-191 303 K [8].

192 Only a few publications reported the research on the hydrate-based refrigeration 193 system. Ogawa et al. [5] proposed the conceptual design and developed a numerical 194 modelling of an innovative hydrate-based refrigeration cycle using the hydrate of 195 difluoromethane (HFC-32)/cyclopentane (CP) guest pair. 0.03/1.67 MPa and 7.5/27 °C 196 were the design conditions at the low and high stages. The coefficient of performance 197 (COP) of the system reached as high as 8.0. A laboratory-scale prototype system was 198 constructed and steadily operated for two hours. Zhang et al. [9] conducted the 199 comparison of three types of hydrate-based refrigeration systems using Aspen Plus. 200 One is multiphase compression cycle and the other two are vapor compression cycles. 201 Two-group conditions of (0.336/2.988 MPa and 293.0/305.9 K) and (0.206/2.051 MPa 202 and 293.3/306.2 K) were selected for the two hydrates of methyl fluoride (HFC-41)/CP 203 and HFC-41/monofluo cyclopentane (FCP), respectively. Their results demonstrated 204 that the highest COP was 8.01-8.97, which was 2-4 times of those of the conventional 205 vapor-compression refrigeration system. Matsuura et al. [7] developed a 206 thermodynamic model to clarify the dominant factor to influence COP. 287 K and 297 207 K were set as the low and high temperatures for dissociation and formation. 0.139-0.234 208 MPa and 0.787-1.733 MPa are the pressure variation ranges at the low and high stages. 209 The maximum COP values of the three hydrate-based systems including HFC-210 32/CP/water, Kr/CP/water and HFC-41/CP/water were 18.22, 18.66 and 14.03, 211 respectively. Their calculated results revealed that the dissociation heat of the hydrates 212 and the enthalpy change of guest gas were the dominant factors. HFC-32 and HFC-41 213 have no ozone depletion potential (ODP), but considerable global warming potential 214 (GWP). Kr is the natural gas but only 0.000114 vol.% of the atmosphere. Thus, as an 215 ideal guest refrigerant gas forming the hydrate with attractive properties include no 216 ODP, very low GWP, non-flammable, non-toxic and low-cost is desired. CO<sub>2</sub> is then 217 becoming one of the popular guest gases. Xie et al. [10] had made their efforts to 218 develop a mixed CO<sub>2</sub> hydrate-based vapor-compression refrigeration system (CHB-219 VCRS). Normally, pure CO<sub>2</sub> hydrate is formed under high pressure and low 220 temperature [11]. They used tetrahydrofuran (THF) as the thermodynamics promoter 221 to alleviate the equilibrium formation pressure. 0.25/3.0 MPa and 280/292 K were 222 chosen as the design conditions. The simulated results showed that the COP of the 223 system was obtained as high as 6.8, and would be decreased by 30 % when the 224 formation temperature only raised by 5 K.

All refrigerant hydrate-based refrigeration systems are actually CTES systems. The formation heat exchanger (a crystallizer such as a condenser, or a vessel) also plays a 227 role of a cold energy storage vessel. As depicted by Xie et al. [10], in CBHS-VCRS, 228 the CO<sub>2</sub> gases discharged from the compressor are injected into a crystallizer, and then 229 the cold energy is stored via the clathrates forming during the off-peak period. Later the 230 hydrate slurries are expanded via a slurry pump and directly delivered to the users (heat 231 exchangers such as evaporators) during the on-peak period. In addition, those typical 232 energy storage strategies widely used in conventional CTESs [12], such as full storage, 233 load-levelling storage and partial storage, still can be applied to the novel hydrate-based 234 refrigeration systems. Xie et al. [10] investigated a CHB-VCRS with CTES under two 235 operation strategies, i.e., full storage and load-levelling storage for an office room and 236 a storeroom. The former one was adopted by using the hourly energy storage, and the 237 latter one chose the monthly cold storage. The peak load of the storeroom in the hottest 238 month was cut by 22% but facing a huge initial investment on the storage tank. Zhou et 239 al. [13] modeled and experimented a fluidized bed based CTES system with a variable 240 cooling load in the summer of the Netherlands. The CO<sub>2</sub> hydrates were used as PCMs. 241 The energy efficiency of this CTES system with nighttime production was improved 242 by 23%-43% compared with the conventional system. At the meantime, the investment 243 costs of the hydrate slurry tank were notably reduced. In addition to common indicators, 244 such as cooling load, power consumption and life cycle cost (summation of initial 245 capital cost and operation cost) [14], environmental considerations need also be 246 included in evaluation of a CHB-VCRS incorporating CTES technologies. For instance, 247 Dai et al introduced a life cycle climate performance to indicate the  $CO_2$  emissions of 248 the CO<sub>2</sub> system over the whole lifetime [15], an indicator including pollution emissions 249 to express the environmental performance for different strategies [16].

In summary, the CO<sub>2</sub> hydrate-based refrigeration systems existed in literature have two characteristics: 1) the formation and dissociation are arranged at the high-pressure 252 (condensation) and low-pressure (evaporation) stages; 2) the formation and dissociation 253 pressure should be relatively low at the temperature of the application scenarios. The 254first one brings the high initial investment, complex configuration and low system 255 reliability, due to the multi-phase compressor (or vapor compressor plus water pump) 256 and the slurry pump. The second one increases the difficulty and cost of preparation of 257 mixed CO<sub>2</sub> hydrate. Therefore, in this work, a two-stage CHB-VCRS using pure CO<sub>2</sub> 258 hydrate was proposed. The equilibrium pressures of formation and dissociation have 259 the same level. Thus both of them can be arranged at the low-pressure stage, which only 260 need simplified reform at the evaporation side for the conventional VCRS This created 261 the feasibility for the improvement of the proposed CHB-VCRS system performance 262 by applies existed advanced technologies of conventional VCRS, such as the two-stage 263 compression. In addition, the exothermic reaction of CO<sub>2</sub> hydrate generated in a reactor 264 of the proposed system was cooled by the two-phase CO<sub>2</sub> injected itself, rather than 265 extra external cooling. The present work develop the numerical model of the proposed 266 system and applies it to conduct the thermodynamic and economic analyses. A 267 comparison of CHB-VCRS and conventional single-stage CO<sub>2</sub> vapor-compression 268 (SC-VCRS, the baseline) considering different CTES operation strategies and different 269 time-of-use electricity tariffs is implemented. In the end, this paper summarized the 270 results of all these efforts and discussed the potential feasibility of new CHB-VCRSs 271to replace the conventional SC-VCRS.

272

# 273 2. Description of carbon dioxide hydrate-based vapor-compression refrigeration 274 system

As depicted in Fig. 1(a), a two-stage cycle is adopted for the present CHB-VCRS, aiming to reduce the compressor discharge temperature. The thermodynamic processes 277 of the cycle are given in Fig. 1(b). The whole system is divided into three substages: 278 the high-pressure stage, the saturated-vapor  $CO_2$  (State 6) is inhaled to a high-pressure 279 stage compressor and becomes supercritical state (State 7). Then it is cooled and reaches 280 the pseudo-critical temperature at the exit of the gas-cooler (State 1). Finally, a portion 281 of CO<sub>2</sub> out of the gas-cooler experiences a subcooling during a coil submerging inside a flash tank (State 2) and goes into the tank reactor; the intermediate-pressure stage, the 282 283 remaining portion CO<sub>2</sub> from the gas-cooler becomes two-phase (State 8) undergoing an 284 expansion process and then is delivered into the flash tank directly. The liquid CO<sub>2</sub> 285 cools the coil and vaporizes to be saturated vapor state (State 6). In addition, a portion 286 of superheated vapor CO<sub>2</sub> discharged from a low-stage compressor is cooled by the 287 liquid CO<sub>2</sub> to be saturated vapor state (State 6) in the flash tank as well. All the saturated 288 vapor CO<sub>2</sub> at State 6 is provided to the high-stage compressor; and lastly, the low-289 pressure stage, where the CO<sub>2</sub> hydrates are formatted in a tank reactor. Different from 290 the conventional hydrate-based refrigeration system, there is no external cooling 291 mediate supplied to the formation tank, such as a bubble column reactor. The two-phase 292  $CO_2$  (State 3) with low temperature and low pressure injected into the aqueous solution 293 via a nozzle, not only provides gas source for CO<sub>2</sub> hydrate formation, but also absorbs 294 the heat from the exothermic hydration reaction. The redundant saturated-vapor CO<sub>2</sub> is 295 discharged from the port at the top of the tank and delivered to the low-stage compressor. 296 The  $CO_2$  hydrate slurry is pumped to a heat exchanger to melt and then the mixture of 297 water and vapor CO<sub>2</sub> go through a liquid-vapor separator. Water is circulated back to 298 the tank reactor for reusing and the saturated-vapor  $CO_2$  (State 4) is compressed by the 299 low-stage compressor together with saturated-vapor CO<sub>2</sub> from the reactor. Moreover, 300 the cooling tower supplies the enough cooling water to reduce the operating temperature 301 in the gas cooler.



(...)





Figure 1 Schematic and P-h diagram of CHB-VCRS

The two-stage CHB-VCRS is characterized as follows. The pressure losses in all components and pipelines are negligible. Equations (1a) and (1b) expresses the balance of mass flow rates and their ratio at high-stage and low-stage, which significantly affect the system performance.

$$m_{\rm CO_2,H} = m_{\rm CO_2,I} + m_{\rm CO_2,L}, \quad m_{\rm CO_2,H} \ge m_{\rm CO_2,L}$$
(1a)

$$r = \frac{m_{\rm CO_2,H}}{m_{\rm CO_2,L}} \tag{1b}$$

A subcooling parameter, *a*, is defined by Torrella et al. [17] to indicate the subcooler effectiveness in the flash tank, as expressed by Eq. (2). It is noted that  $h_L$  is the enthalpy of saturated liquid CO<sub>2</sub> (State L) at intermediate pressure.

$$a = \frac{h_1 - h_2}{h_1 - h_L} \quad (0 \le a \le 1) \tag{2}$$

In addition, the energy balance of the inter-pressure stage can be expressed by Eq. 317 (3). Taking into account Eqs. (1-2), the mass flow ratio, *r*, can be derived based on the 318 subcooling parameter, *a*, by Eq. (4):

$$m_{\rm CO_2,L}h_1 + m_{\rm CO_2,L}h_1 + m_{\rm CO_2,L}h_5 = m_{\rm CO_2,H}h_{6(V)} + m_{\rm CO_2,L}h_2$$
(3)

$$r = \frac{h_5 - h_1 + a(h_1 - h_L)}{h_{6(V)} - h_1}$$
(4)

In the present work, the CHB-VCRS provides the hydrate slurries which generate and melt at the equilibrium temperature of 7 °C. Assume that there is no pressure drop during hydrate formation and dissociation, the low-stage pressure equals to the corresponding equilibrium pressure, 2.78 MPa. Figure 2 (a) illustrates the variation of the mass flow ratio, r, as function of the subcooling parameter, a, at different inter-stage pressures,  $P_{\rm I}$ , when the high-stage pressure,  $P_{\rm H}$ , is fixed at 9 MPa. The intermediate-

stage pressure is also an significant parameter for a two-stage compression system. It can be observed that the mass flow ratio, r, increases together with increasing of the subcooling parameter, a, and the intermediate pressure,  $P_{\rm I}$ . Moreover, there is a little sharper increase of the mass flow ratio when the intermediate-stage pressure decreases. A COP expression, as seen in Eq. (5), can be established using the subcooling parameter, a. The power consumption of the water pump here at low-stage (between the liquid-vapor separator and the tank reactor) is negligible.

$$COP = \frac{h_{4} - h_{3}}{\frac{h_{5s} - h_{4}}{\eta_{\text{isen,L}}} + r \times \frac{h_{7s} - h_{6(V)}}{\eta_{\text{isen,H}}}}{\frac{h_{4} - h_{3}}{\frac{h_{5s} - h_{4}}{\eta_{\text{isen,L}}} + \left[\frac{h_{5} - h_{1} + a(h_{1} - h_{L})}{h_{6(V)} - h_{1}}\right] \times \frac{h_{7s} - h_{6(V)}}{\eta_{\text{isen,H}}}}$$
(5)

332 where  $\eta_{\text{isen,L}}$  and  $\eta_{\text{isen,H}}$  represent the isentropic efficiency at low-stage and high-stage 333 pressures, respectively.

Actually, the inter-stage pressure,  $P_{\rm I}$ , plays an important role in the optimization of the two-stage system. As depicted in Fig. 2(b), the COP increases with increasing of the subcooling parameter, a, at a fixed inter-stage pressure. As shown in Fig. 1(b), a bigger subcooling means a larger difference in specific enthalpy between the states 3 and 4, and then results in more CO<sub>2</sub> hydrate generated. Moreover, with the increasing of the subcooling parameter, the optimum inter-stage pressure on the basis of maximum COP is moving to the higher value of the inter-stage pressure.











Figure 2 Schematic and P-h diagram of CO<sub>2</sub> hydrate-based VCR system

#### 348 **3.Mathematical model**

349 The first law of thermodynamic is implemented to each component of the system.

350 There are some assumptions as following:

- 351 1) The system is under steady state conditions.
- 352 2) The expansion of  $CO_2$  in the nozzle of the reactor is assumed as isenthalpic.
- 353 3) The pressure losses in all pipelines and components are negligible.

354 4) The heat losses in all pipelines and components are negligible.

- 355 5) The power consumption of the water pump between the liquid-vapor separator356 and the tank reactor at low-stage is negligible.
- 357

#### 358 **3.1 Gas cooler**

Tube-in-tube heat exchanger is selected as the gas cooler. The water flows in the annulus while the  $CO_2$  flows counter-currently along the inner tube. Due to the thermophysical properties of  $CO_2$  dramatically vary with temperature and pressure in the supercritical region, the gas cooler is discretized into a number of small elements. The energy conservation equations are applied in both sides of water and  $CO_2$  in each element. The heat balance can be expressed by the following equations:

$$Q(i) = \dot{m}_{\rm CO_2}(h_{\rm CO_2}(i) - h_{\rm CO_2}(i+1)) = \dot{m}_{\rm w}Cp_{\rm w}(i)(T_{\rm w}(i) - T_{\rm w}(i+1))$$
(6a)

$$Q(i) = UA(i) \times LMTD(i) \tag{6b}$$

365 where *i* refers to the element index along the calculation direction.

366 The overall heat transfer coefficient is obtained by:

$$\frac{1}{UA(i)} = \frac{1}{h_{\rm w}(i)A_{\rm o}} + \frac{\ln(d_{\rm o}/d_{\rm i})}{2\pi k_{\rm wall}l} + \frac{1}{h_{\rm CO_2}(i)A_{\rm i}}$$
(7)

367 where l is the length of the element.

Type and source	Equations
CO <sub>2</sub> in gas cooler	(f/8)(Re-1000)Pr
(Dang and Hihara [18])	$Nu = \frac{107 + 12.7 (f/8)^{1/2} (Pr^{2/3} - 1)}{107 + 12.7 (f/8)^{1/2} (Pr^{2/3} - 1)}$
	$f = [1.82\log(Re) - 1.64]^{-2}$
	$\left(\frac{Cp_{\rm b}\mu_{\rm b}}{k_{\rm b}} \text{ for } Cp_{\rm b} > Cp\right)$
	$Pr = \begin{cases} Cp\mu_{\rm b}/k_{\rm b} & \text{for } Cp_{\rm b} < Cp \ , \mu_{\rm b}/k_{\rm b} \ge \mu_{\rm f}/k_{\rm f} \end{cases}$
	$(Cp\mu_f/k_f \text{ for } Cp_b < Cp \text{ , } \mu_b/k_b < \mu_f/k_f$
	$\bar{C}p = \frac{n_{\rm b} - n_{\rm wall}}{T - T}$
	$I_{\rm b} - I_{\rm wall}$ (f/8)(Re - 1000)Pr
Water in gas cooler	Nu = (0,7,6)(10,-100,6)(1,7,7,7,7,7,7,7,7,7,7,7,7,7,7,7,7,7,7,7
(Gnielinsk [19])	$f = [1.82] \log(Re) - 1.64]^{-2}$
Cooling tower	$AU = 746 m_{\rm w}^{0.43} m_{\rm a}^{1.03}$
(Lebrun and Silva [20])	ii u
CO <sub>2</sub> evaporation	$\alpha_{\rm ob} = 0.023 \frac{k_1}{k_1} R e_1^{0.8} P r_1^{0.4}$
(Hwang et al. [21])	$D_h$
	$\Gamma$ ( 1 for $\frac{1}{x_{tt}} > 0.1$
	$F = \left\{ 2.35 \left( \frac{1}{x_{\rm H}} + 0.213 \right)^{0.150} \text{ for } \frac{1}{1} < 0.1 \right\}$
	$1  (0)^{0.5} (\mu)^{0.1} (\gamma)^{0.9}$
	$\frac{1}{X_{\mu}} = \left(\frac{\mu_{1}}{\rho}\right)  \left(\frac{\mu_{V}}{\mu_{1}}\right)  \left(\frac{\lambda}{1-\gamma}\right)$
	$k_1^{0.79} C p_1^{0.49} $
	$\alpha_{\rm nb} = 0.00122 \frac{n_1}{\sigma^{0.45} u^{0.29} u^{0.24} \Lambda h_{\rm r}} \Delta T_{\rm sat}^{0.24} \Delta P_{\rm sat}^{0.75}$
	$\Delta P_{\text{sat}} = P_{\text{sat}}(T_{\text{wall}}) - P_{\text{sat}}(T_{\text{sat}}) \text{ and}$
	$\Delta T_{\rm sat} = T_{\rm wall} - T_{\rm sat}$
	$S = \frac{1 - \exp(-\beta)}{\rho}$ with $\beta = \frac{F\alpha_{\rm cb}X_0}{\mu}$ and
	$\sigma^{\mu} = [\sigma^{-1}]^{0.5}$
	$X_0 = 0.05 \left[ \frac{1}{g(\rho_l - \rho_v)} \right]$
Single-phase CO <sub>2</sub> in	$Nu = 0.023 Re^{0.8} Pr^{0.4}$
evaporator	
(Mac Adams [22])	$N_{ev} = i D_{a} D_{ev} \frac{1}{3}$
(Wang et al. 23])	$Nu = JRePr^{-7}$
(() ang et an 20])	$j = 0.086Re^{P_1}N^{P_2}\left(\frac{T_{\rm P}}{D_{\rm c}}\right)  \left(\frac{T_{\rm P}}{D_{\rm h}}\right)  \left(\frac{T_{\rm P}}{P_{\rm t}}\right)$
	$P1 = 0.261 = \frac{0.042N}{0.042N} + 0.159\log\left(N\left(\frac{F_{\rm P}}{P}\right)^{0.41}\right)$
	$FI = -0.501 - \frac{1}{\log_e(Re)} + 0.150\log_e\left(N\left(\frac{1}{D_c}\right)\right)$
	$0.042 \left(\frac{P_1}{P_1}\right)^{1.42}$
	$P2 = -1.224 - \frac{(D_{\rm h})}{\log (P_{\rm c})}$
	0.058N
	$P3 = -0.083 + \frac{1}{\log_e(Re)}$
	$RA = [725 + 1, 21]_{co}$ ( <i>Re</i> )
	$P4 = -5.735 + 1.2100 e(\overline{N})$

## 369 Table 1 Summary of correlations for heat transfer

The correlation of the heat transfer coefficient of the supercritical CO<sub>2</sub> in tubes is from Dang and Hihara [18]. The heat transfer coefficient for the water side is obtained via the Gnielinsk correlation [19]. The details can be found in Table 1. In addition, the flowchart of the heat transfer calculation in a segment can be found in Fig. B1.

375

#### 376 **3.2 Cooling tower**

A simplified model of direct contact cooling tower was developed by Lebrun et al. In the model assumed the humid air was replaced by a fictitious perfect gas and the temperature of which is the wet-bulb temperature. Therefore, as depicted in Fig. A1, the wet-bulb temperature of the moist air can be iteratively calculated by Eq. (8).

$$T_{\rm wb} = T - \frac{p_{\rm sat}(T_{\rm wb}) - (\phi_{\rm a} / 100) p_{\rm sat}(T)}{k p_{\rm atm}}$$
(8)

381 where k is a constant,  $p_{\text{atm}}$  is the atmospheric pressure,  $\phi_{a}$  is the relative humidity and

 $p_{sat}(T_{wb})$  and  $p_{sat}(T)$  are the air saturation vapor pressures at T and  $T_{wb}$ , respectively.

383 The energy balance on the air side can be given:

$$Q = \dot{C}_{a, fic} (T_{wb, ex} - T_{wb, su}) = \dot{m}_{a} C p_{a, fic} (T_{wb, ex} - T_{wb, su})$$
(9)

384 where  $Cp_{air,fic}$  defines as a fictitious specific heat by Eq. (10).

$$Cp_{a,\text{fic}} = \frac{(h_{a,\text{ex}} - h_{a,\text{su}})}{(T_{\text{wb,ex}} - T_{\text{wb,su}})}$$
(10)

The water flows in counter current arrangement with the air flow in cooling tower, thus the energy balance on the water side can be given by:

$$Q = \dot{C}_{w}(T_{w,su} - T_{w,ex}) = \dot{m}_{w}Cp_{w}(T_{w,su} - T_{w,ex})$$
(11)

In accordance with the definition of an equivalent heat exchanger for the simulation of the direct contact cooling tower, the heat flow rate can be calculated by Eq. (12). The effectiveness of a counter flow cooling tower is given by Eq. (13).

$$Q = \varepsilon_{\rm fic} \dot{C}_{\rm min} \left( T_{\rm w,su} - T_{\rm a,wb,su} \right) \tag{12}$$

$$\mathcal{E}_{\rm fic} = \frac{1 - \exp(-NTU_{\rm fic}(1 - \omega))}{1 - \omega \exp(-NTU_{\rm fic}(1 - \omega))}$$
(13)

390 The fictitious,  $NTU_{\text{fic}}$ , is defined in Eq. (14). The fictitious cooling tower heat 391 transfer coefficient,  $AU_{\text{fic}}$ , is related to the real water-air overall heat transfer coefficient, 392 AU, and the moist air specific heat,  $Cp_{\text{a}}$ , in Eq. (15).

$$NTU_{\rm fic} = \frac{AU_{\rm fic}}{\dot{C}_{\rm min}} \tag{14}$$

$$AU_{\rm fic} = AU \frac{Cp_{\rm a,fic}}{Cp_{\rm a}}$$
(15)

393  $Cp_a$  here is assumed constant and equal to 1025 J kg<sup>-1</sup> K<sup>-1</sup> in good approximation 394 (ASHRAE1997 [26]). The real water-air overall heat transfer coefficient for the cooling 395 tower, *AU*, can be obtained by the correlation (Table 1) of Lebrun and Silva [20]. In 396 addition, the flowchart of the modeling of direct contact cooling tower can be found in 397 Fig. A2.

398

#### 399 3.3 Variable-speed Compressor

400 A model of variable-speed compressor is applied to determinate the mass flow rate, 401 the power consumption and the discharge  $CO_2$  state of the compressor. Equations (16) 402 and (17) are the curve fits by Nguyen and Eslami-Nejad [27] for an open-type  $CO_2$ 403 compressor and used to calculate the isentropic efficiency and volumetric efficiency at 404 nominal frequency, respectively.

$$\eta_{\rm isen,nom} = 1.006 - 0.121 \frac{P_1}{P_2} \tag{16}$$

$$\eta_{\rm vol,nom} = 1.079 - 0.1053 \frac{P_1}{P_2} \tag{17}$$

405 where  $P_1$  and  $P_2$  are the discharge and suction pressures.

Equation 18 derived from the manufacturer data of a carbon dioxide compressor is implemented to calculate both the isentropic and volumetric efficiencies at any arbitrary frequency, *f*, between the range of 0 to 65 Hz.

$$\frac{\eta}{\eta_{\rm nom}} = 0.91 + 0.18f_{\rm r} - 0.09f_{\rm r}^{\,2} \tag{18}$$

409 where  $f_r$  refers to the frequency ratio of  $f/f_{nom}$ .

The enthalpy of the  $CO_2$  at the discharge (States 5 and 7),  $h_1$ , of the compressor is obtained using Eq. (19), and the power consumption is calculated by Eq. (20). The mass flow rate in the loop is calculated by Eq. (21).

$$h_1 = h_2 + \frac{h_{1s} - h_2}{\eta_{isen}}$$
(19)

$$W_{\rm com} = \dot{m}_{\rm CO_2} (h_1 - h_2) \tag{20}$$

$$\dot{m}_{\rm CO_2} = \eta_{\rm vol} \rho_{\rm CO_2} V_{\rm rev} f \tag{21}$$

413 Where  $h_{1s}$  is the isentropic enthalpy,  $h_2$  is the suction enthalpy,  $\rho_{CO2}$  is the density at the 414 suction of the compressor and  $V_{rev}$  is the displacement volume of the compressor.

415

#### 416 **3.4 Flash tank**

In the present model, seeing in Fig. 1, the two-phase CO<sub>2</sub> (State 8) and superheated

- 418 vapor CO<sub>2</sub> (State 5) enter the flash tank, and exit as saturated vapor CO<sub>2</sub> (State 6) from
- 419 the top port of the flash tank. The following simplifications are adopted.
- 420 1) Two Phases separate perfectly inside the flash tank.
- 421 2) There is no pressure drop inside the flash tank.

422 3) The vapor and liquid in the flash tank are in thermodynamic equilibrium.

423

$$\dot{m}_{\rm CO_2,H}(h_1 - h_2) = \dot{m}_{\rm CO_2,I}(h_6 - h_8) + \dot{m}_{\rm CO_2,L}(h_5 - h_6)$$
(22)

424

#### 425 **3.5 Expansion valve**

The expansion processes from State 1 to State 8 and from State 2 to State 3 are assumed that the enthalpy value before an expansion value is equal to that after the expansion value, i.e.,  $h_1=h_8$  and  $h_2=h_3$ .

429

#### 430 **3.6 Carbon dioxide hydrate decomposer and carbon dioxide evaporator**

The CO<sub>2</sub> hydrates format in the tank reactor at temperature of 7 °C and circulates the hydrate slurry to melt at 7 °C as well. Thus, the low-stage pressure equals to the equilibrium pressure, 2.78 MPa, corresponding to the equilibrium temperature of 7 °C. The LMTD method is calculate the heat transfer area of the CO<sub>2</sub> hydrate decomposer and the CO<sub>2</sub> evaporator (finned-tube heat exchangers here as adopted). The overall heat transfer coefficient and the heat transfer area are calculated by Eqs. (23) and (24).

$$\frac{1}{U} = \frac{A_{\rm i}}{h_{\rm a}(i)A_{\rm o}} + \frac{A_{\rm i}\ln(d_{\rm o}/d_{\rm i})}{2\pi k_{\rm wall}l} + \frac{1}{h_{\rm hyd/CO_2}}$$
(23)

$$A = \frac{Q}{U \times LMTD}$$
(24)

The evaporator of the SC-VCRS is divided into two parts, namely two-phase and single-phase. The air inlet and outlet temperatures are assumed as 23 °C and 18 °C with temperature difference of 5 °C. The orders of magnitude of the heat transfer coefficients for CO<sub>2</sub> evaporation and single-phase in tubes are obtained by of Hwang et al. [21] and Mac Adams [22] correlations. They are round 40000 W/m<sup>2</sup> k and 2000 W/m<sup>2</sup> k in the tubes with diameter of 10 mm. Those values are also recommended by Diaby et al. [36]. The value for air is of the order of magnitude of 100 W/m<sup>2</sup> k, which is obtained by the correlation of Wang et al. [23]. For the convective heat transfer coefficient of the  $CO_2$ hydrate slurry in tubes, the research by Oignet et al. [28] suggested that the value can reach 3500 W/m<sup>2</sup> k for solid fraction of 14 vol.% with a Reynolds number around 2300.

447

#### 448 **3.7 Performance evaluation**

449 As defined in Eq. (25), the COP of the system is the ratio of cooling capacity and 450 total power consumption. The total power consumption comes from the compressors in 451 the primary  $CO_2$  loop, which is referred in Eq. (20), as well as the water pump and the 452 air fan in the cooling tower loop. Relevant correlations can be found in Table 2.

$$COP = \frac{Q_{\text{cooling}}}{W_{\text{comp,H}} + W_{\text{comp,L}} + W_{\text{pump,ct}} + W_{\text{fan,ct}}}$$
(25)

453

454 Table2 Details of power consumption correlations for cooling tower

Component	Correlation
Pump power [29]	$W_{\rm pump} = 3.57 m_{\rm w} H \rho_{\rm w} / \eta_{\rm pump,ct}$
Fan power [30]	$W_{\rm fan} = (1+u) \times 3600 m_{\rm a} / (10728 \rho_{\rm mix})$
Water make-up flow rate [29]	$m_{\rm w,m\_up} = EC/(C-1)$
Water blow-down flow rate [29]	$m_{\rm w,b\_down} = E/(C-1)$

455 *u*: water vapor to dry air ratio,  $\rho_{mix}$ : humidity air density, *C*: cycle of concentration

456

#### 457 **3.8 Economical model**

Equation (26) is used to determine the total operating cost of design day. It mainly consists of two parts, namely the cost of the electricity consumption and the cost of the water make-up and blow-down. The latter part is produced from the water supplied to the cooling tower due to the reduction of evaporation loss and the daily maintain

$$C_{\rm op} = C_{\rm op,E} + C_{\rm w,m\_up} = \int_0^{t_{\rm op}} e_{\rm tariff} W dt + \int_0^{t_{\rm op}} w_{\rm tariff} V_{\rm w} dt$$
(26)

462 where  $e_{\text{tariffs}}$  and  $w_{\text{tarffs}}$  refer to the localized electricity (£ kWh<sup>-1</sup>) and water (£ m<sup>-3</sup>) tariff 463 rates, respectively.  $V_{\text{w}}$  is the water volume cost.  $w_{\text{tarffs}}$  is estimated to 2 £/m<sup>3</sup>.

Table 1 gives the water flow rates of make-up and blow-down for the cooling tower.
Blow-down and make-up are as functions of evaporation loss, which can be calculated
by Eq. (27).

$$E = 0.00546m_{\rm w,ct}R\tag{27}$$

467 Where *R* refers to the range of cooling tower, *Rang:*  $R = T_{w,su} - T_{w,ex}$ .

The correlations listed in Table 3 are used to estimate the capital costs of the main components in the vapor-compression refrigeration systems.

470

#### 471 Table 3 Details of capital cost correlations for main components

Component	Correlation	
Compressor [31]	$C_{\rm comp} = 10167.5 m_{\rm CO_2}^{0.46}$	
Gas cooler [31]	$C_{\rm gc} = 2382.9 A_{\rm gc}^{0.68}$	
CO <sub>2</sub> hydrate decomposer and CO <sub>2</sub> evaporator [32]	$C_{\rm dec/evap} = 1397.9 A_{\rm dec/evap}^{0.89}$	
Cooling tower [29]	$C_{\rm ct} = 148.05(13.11m_{\rm w})^{0.79}(0.12R)^{0.57}(0.18A)^{-0.9924} + (0.022T_{\rm wb} + 0.)^{2.441}$	
Expansion valve [31]	$C_{\text{eval}} = 114.5m_{\text{CO}_2}$	
Flash tank [33]	$C_{\rm flash-tank} = 280.3 m_{\rm CO_2}^{0.67}$	
Hydrate tank [34]	$C_{\rm hyd-tank} = 8.67 \times 10^{2.9211 \exp{(0.1416 \log V_{\rm tank})}}$	
$P_{anal} P_{-} T = T = A_{nnnogalit} A_{-} T = T_{n-1}$		

472 *Rang:*  $R = T_{w,su} - T_{w,ex}$ , *Approach:*  $A = T_{w,ex} - T_{air,wb,su}$ 

473

In addition, Equation (28) is used to calculate the total annual cost, including three parts: the annual repayment of initial capital investment, the total annual operation cost and the annual salvage value.

$$C_{\text{tot}} = CRF \times C_{\text{cap}} + C_{\text{op}} - SV\left(\frac{i}{(1+i)^n - 1}\right)$$
(28)

477 The capital recovery factor (CRF) in Eq. (29) is defined as the ratio of a constant 478 annuity to the present value of receiving that annuity for a given length of lifetime [35].

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1}$$
(29)

Where *i* refers to the annual interest and *n* is the years of the system lifetime. Salvage value, *SV*, the estimated value that an asset will realize upon its sale at the end of its useful life (is given in Table 4 as a percentage of the initial capital cost).

482

#### 483 Table 4 Parameters of economic analysis

Parameter	Value
Annual interest rate (%)	14
Salvage value rate (%)	10

484

#### 485 **3.9 Modelling procedure**

The flowchart of modeling of the CHB-VCRS is showed in Fig. 3. The procedures of detailly iterating the frequencies of the compressors at low-pressure stage,  $f_{\rm L}$ , and high-pressure stage,  $f_{\rm H}$ , are presented in Fig. 4, respectively. The residual values of  $\varepsilon$ (in Figs. 3, A2, B1 and B2) are adopted very carefully to ensure an appropriate computation cost and a deviation between  $Q_{\rm target}$  and  $Q_{\rm calculate}$  within ±0.5%. The codes are written in FORTRAN. The thermodynamic and transport properties of the working fluids are calculated by REFPROP 9.0.



Figure 3 Flowchart of modelling of CHB-VCRS



The ambient dry-bulb temperature and relative humidity records for Birmingham and London in the United Kingdom on the design day of 31 July are as shown in Fig. 5, which is used as the typical ambient conditions for the simulation. It illustrates that London had higher dry-bulb temperature, lower humidity as well as more remarkable

- their diurnal change due to the urban hot island effect [36], though both cities have a
  marine west coast climate. The weather data in the figure is sourced from Typical
  Meteorological Year 2 (TMY2) files in TRNSYS 17 libraries [37].
- 513



514

515

Figure 6 Time-variant pricing of design day

517 Time-of-use pricing of the electricity in Fig. 6 is used for the estimation of the 518 operating cost. The electricity utilities often construct their tariffs around on-peak and 519 off-peak schedules, which have strong incentives for the customer to shift the cooling 520 load from on-peak to off-peak. Economy 7 and Economy 10 are two energy price plans 521 suggested by the UKPower [38] to the customers who prefer a 'time of use' tariff. These 522 two plans mean charge a cheaper rate for seven and ten nighttime hours than during the rest of the day. The off-peak hours are most likely being consecutive period between 523 524 22:30 and 8:30. For the simplification, two periods, i.e., 12 on-peak hours (10:00 to 525 22:00) and 12 off-peak hours (22:00 to 10:00), are created in this work. The average price of electricity during on- and off-peak are 20.03 and 9.76 pence per kilowatt-hour
(with ratio of 2.1) for the standard rate (between April 2019-April 2020), respectively.
These data is sourced from the English Housing Survey [39]. In addition, the economic
parameters affected by the electricity prices ratio of on- and off-peak (range from 1.0
to 8.0) will be discussed in the following sections.

531



532

533 Figure 7 Capacities of SC-VCRS, CHB-VCRS with LS and CHB-VCRS with FS

534

The cooling load profile (solid-square) in Fig. 7 is calculated by TRNSYS 17. It is modeled under Birmingham weather conditions during 24 hours of a typical summer day in a typical meteorological year. The reference building of SFH 45 recommended by the IEA standard [40] is selected. It is assumed to be occupied from 9:00 to 20:00 in a 12-hour cooling of design days. The design room temperature is 20 °C and other input data can be found in Table 5. This building has a peak load of 39.54 kW at 15:00 with a total cooling requirement of 376.3 kWh. Moreover, a total of 150 days during the

- 542 whole summer (5 days  $\times$  4 weeks  $\times$  6 months + 30 days) is selected, considering the
- heating season in Birmingham from 1st October to 30th April. Extra 30 days are design
- 544 margin.
- 545
- 546 Table 5 Input data of building cooling load calculation

Component	Description/value	
Design room temperature (°C)	20.00	
Building type	SFH 45 [40]	
Building gross area (m <sup>2</sup> )	1440	
Working hours	9:00 to 20:00	
Average occupant number per hour (person)	8	
Average electrical gain per hour (W)	580	
Annual working days (day)	150	
Derating factor	0.70	

548 The load profile in the figure defines the real-time cooling capacity for the nonstorage single-stage CO<sub>2</sub> vapor-compression refrigeration system (SC-VCRS), which 549 550 is descripted in Fig. 8. Therefore, the design capacity of the SC-VCRS equals the peak 551load. It means that the compressor is only running at the nominal frequency when full 552 capacity of 39.54 kW cooling is required. The compressor runs in variant-speed to meet 553 the cooling load during the rest time. Notice that, different from the two-stage system 554 in Fig. 1, there is no split of the CO<sub>2</sub> flow at the exit of the gas-cooler for the SC-VCRS. 555 The supercritical  $CO_2$  with high pressure and high temperature (State 5 in Fig. 8) 556 discharged from the compressor would be cooled to reach State 2 directly. There is no 557 flash tank, and the subcooling (from State 1 to State 2) is operated in the gas-cooler. 558 Then experiencing an expansion process, the two-phase CO<sub>2</sub> with low pressure and low 559 temperature (State 3) is delivered into the evaporator. Finally, the superheated vapor

560 CO<sub>2</sub> (State 4) flows back to the compressor. The flowchart of modeling of the variant-

561 speed SC-VCRS can be found in Fig. (C1)

562



563

564

Figure 8 P-h diagram of SC-VCRS (baseline)

565

566 The procedure for the SC-VCRS is not the case when designing the size of a VCRS 567 with CTES, the design capacity of which must be able to meet the total cooling load 568 over the working-hour period. Therefore, it is significant to accurately calculate the 569 total integrated load. A derating factor is introduced to estimate the efficiency losses in 570 CTES charge-discharge cycles at nigh time. Generally, this factor is related to the 571standards of the ice-storage tank from the manufacturer. In this work, the value of the 572 derating factor is estimated at 0.70, which is recommended by Silvertti [41] in design 573 of an ice slurry based CTES. This factor typically varies between 0.65 and 0.70. Based 574 on the discussion above, the design capacity of a VCRS with CTES can be calculated 575 using the following equation:

Canacity kW =	total kWh	(30)
	day hours + derating factor × nighty hours	(30)

576 Load-leveling storage and full storage strategies are implemented for the CHB-577 VCRS, and compared with the non-storage SC-VCRS (as baseline). As presented in 578 Fig. 7, the CHB-VCRS with LS evenly transfers the entire on-peak cooling load to the 579 whole design day, which means the system works at constant capacity throughout 24 580 hours. During the on-peak period, when the cooling load is less than the design capacity, 581 the excess coolth energy is stored. Conversely, when the load exceeds the capacity, the 582 additional demand is discharged from the storage. For the CHB-VCRS with FS, the 583 system operates on its full capacity from 22:00 to 10:00 (12 hours), which transfers the 584 entire on-peak cooling load to the off-peak period. The design capacities of CHB-VCRS 585 under LS and FS strategies calculated by Eq. (30), are 17.84 kW and 43.33 kW, 586 respectively. The FS system does not run during on-peak time, therefore it requires 587 relatively large refrigeration and storage capacities. As listed in Table 6, the capacity of 588 the CHB-VCRS with LS is just 45% of the SC-VCRS while the capacity of the FS 589 system is 10% higher than the baseline.

590

#### 591 Table 6 Summary of capacity calculation

Description	Capacity (kW)	Comparison
SC-VCRS	39.54	100%
CHB-VCRS with LS	17.84	45%
CHB-VCRS with FS	43.33	110%

<sup>592</sup> 

593 A series of trial-runs are implemented to figure out the configurations of the main 594 components, including the gas cooler, the compressor and the cooling tower. The basic 595 configurations are firstly determined, when the system operates in full design capacity 596 (compressors run at nominal frequency). The maximum pressure at high stage of design 597 day is obtained. For a normal VCRS, higher high-stage pressure results in a loss of COP. 598 In order to maintain the CO<sub>2</sub> systems always running in the trans-critical region and a 599 relatively high overall COP of whole design day, further refining and finalizing of the 600 configurations is implemented. The iterative steps are to ensure the high-stage pressure 601 be located as close as possible to the critical pressure (7.38 MPa), when the system 602 operates under the conditions of the lowest dry-bulb temperature and lowest relative 603 humidity. At this point, it reaches the minimum pressure at high stage of system of 604 design day. Table 7 lists the final configurations and the other important system 605 parameters.

Table 7 Specification of system component design parameters and controls

Component	Parameter	Value
CHB-VCRS		
CO <sub>2</sub> hydration and dissociation	Equilibrium temperature (°C)	7.0
Gas cooler (LS)	Heat transfer area (m <sup>2</sup> )	0.43
Gas cooler (FS)	Heat transfer area (m <sup>2</sup> )	1.39
Mass flow rate ratio	$m_{ m CO_2,H}/m_{ m CO_2,L}$	3
Compressor (LS)	Displacement volume -H (cm <sup>3</sup> rev <sup>-1</sup> )	27
	Displacement volume -L (cm <sup>3</sup> rev <sup>-1</sup> )	38
Compressor (FS)	Displacement volume -H (cm <sup>3</sup> rev <sup>-1</sup> )	66
	Displacement volume -L (cm <sup>3</sup> rev <sup>-1</sup> )	93
Cooling tower (LS)	Air supply mass flow rate (kg s <sup>-1</sup> )	2.80
	Water supply mass flow rate (kg s <sup>-1</sup> )	0.47
Cooling tower (FS)	Air supply mass flow rate (kg s <sup>-1</sup> )	3.24
	Water supply mass flow rate (kg s <sup>-1</sup> )	1.15
SC-VCRS		
Evaporator	Evaporating temperature (°C)	7.0
Gas cooler	Heat transfer area (m <sup>2</sup> )	0.14
Compressor	Displacement volume (cm <sup>3</sup> rev <sup>-1</sup> )	42

Cooling tower	Air supply mass flow rate (kg s <sup>-1</sup> )	3.25
	Water supply mass flow rate (kg s <sup>-1</sup> )	1.45
Common design		
Gas cooler	Inner diameter of inner tube (m)	0.012
	Outer diameter of inner tube (m)	0.018
	Inner diameter of outer tube (m)	0.027
	Fictitious subcooling degree (-)	0.5
Dissociation reactor/evaporator	Outer diameter (m)	0.00952
	Inner diameter (m)	0.0082
	Tube pitch (m)	0.0254
	Fin pitch (m)	0.002
Compressor	Superheating (°C)	15.0
Cooling tower	Range/ $T_{w,su}$ - $T_{w,ex}$ (°C)	10.0
	Cycle of concentration	4
	Water pump efficiency	0.6

609 5. Comparison of coefficient of performance, power consumption and operating

610 **cost** 

611 Figures 9 demonstrate the hourly variations of the COP. In general, the COP of the 612 SC-VCRS is higher than those of both the HBC-VCRSs. There are three reasons. One 613 is the higher low-stage pressure of the SC-VCRS, 4.18 MPa, corresponding to 7 °C 614 evaporation temperature. Whereas the low-stage pressure of the CHB-VCRSs is only 615 2.78 MPa, corresponding to 7 °C equilibrium temperature. The other is the variable-616 speed compressor for the SC-VCRS. It can maintain the high-stage pressure of the SC-617 VCRS operating at a relative low-level, especially at worst weather conditions and 618 when the hourly cooling load has great fluctuation. The last and most important is the 619 different characteristics between single-stage and two-stage thermodynamic cycles. 620 Compared to the single-stage system for the COP formula for the two-stage system 621 (seeing Eq. (5)), the enthalpy difference of the second term on the denominator needs

to be multiplied by the mass flow ratio of high- and low-stages, *r* (with the value of 3.0
in present simulation), which significantly decrease the COP.

624



## 625

626

627

Figure 9 Time-variant COP of design day

628 In addition, the COP of the CHB-VCRS with LS has non-obvious improvement at 629 nighttime, only 8-17% and 5-12% for Birmingham and London, respectively, as it is 630 only slightly affected by ambient temperature and humidity. The system is operating 631 with constant capacity in all working hours, thus the COP mainly depends on the 632 compressor power consumption. Therefore, the compression ratio and the mass flow 633 rate are considerable factors. The temperature of the cooling water supplied to the gas 634 cooler strongly affects the high-stage pressure. In the present case, the dry-bulb 635 temperature at nighttime is lower than that at daytime, which improves the performance 636 of the cooling tower, however, the relative humidity increases at nighttime which 637 depresses the cooling tower. Based on this, the cooling water temperature is relative 638 stable, as a result that the high-stage pressure changes very slightly. Coupled with the 639 almost unchanged mass flow rates ratio of the high- and low-stages, the compression 640 ratio and the mass flow rate hence fluctuate moderately. The hourly variations of the 641 frequencies of the high- and low-stage compressors for the CHB-VCRS can be found 642 in Fig. 10. They are slightly changed from 58 Hz to 61 Hz. All of these led to the COP 643 fluctuation of CHB-VCRS smoothly and slightly. The overall COP of the FS system is 644 a litter higher than that of the LS system, because of the diminution part, i.e., daytime 645 COP, influencing the overall performance for the latter system. On the contrary, the 646 COP of the SC-VCRS changes dramatically. The mass flow rate of CO<sub>2</sub> in the gas 647 cooler has strong influence. The SC-VCRS raises or reduces the compressor frequency 648 to adjust the mass flow rate to meet the higher or lower cooling requirements all day. 649 As depicted in Fig. 10, the frequency of the SC-VCRS obviously varies from 33 Hz to 650 60 Hz. When the notably reduced mass flow rate of supercritical CO<sub>2</sub> passes through 651 the gas cooler, the high-stage pressure has to decrease to balance the heat transfer 652 between the  $CO_2$  and the water sides. Consequently, the COP rises significantly. 653 Conversely, the COP drops sharply.



Figure 10 Time-variant compressor frequency of design day





Figure 11 Time-variant total power consumption of design day

661 Figures 11 present the hourly variations of the total power consumption. It has the 662 similar tendency with the frequencies in Fig. 10. As seen in Fig. 11, the total power 663 consumption mainly comes from the compressors, which depends on the compression 664 ratio and the mass flow rate. Because of the largest cooling capacity, the CHB-VCRS 665 with FS has the highest hourly power consumption. The detailed distributions of the 666 power consumption are presented in Fig. 12. As depicted, the CHB-VCRS with FS has 667 the maximum total power consumption of design day, but the lowest ratio of the part 668 from cooling tower occupied. The non-storage system has the smallest total power 669 consumption, but the largest percentage consumed by the cooling tower. More details 670 can be found in Table 8. Additionally, the FS system consumes the lowest power of 671 cooling tower and the LS system expends the highest.

672



673

Figure 12 Details of total power consumption of design day

675



	COP <sub>overall</sub>	W <sub>comp</sub> (kWh)	W <sub>ct</sub> (kWh)	$C_{\mathrm{op,E}}$ (£)	$C_{ m w,m\_up}$ (£)	$C_{ m op}$ (£)
Birmingham						
SC-VCRS	2.67	140.83	12.78	30.13	1.67	31.80
CHB-VCRS with LS	1.78	251.85	19.69	40.74	0.58	41.32
CHB-VCRS with FS	1.85	290.30	11.81	29.50	1.40	30.90
London						
SC-VCRS	2.66	141.47	12.78	30.31	1.67	31.98
CHB-VCRS with LS	1.80	246.12	19.69	40.14	0.58	40.72
CHB-VCRS with FS	1.92	280.96	11.81	28.59	1.40	29.99





### Figure 13 Details of total operating cost of design day





Figure 14 Total operating cost variation with the electricity prices ratio

Figure 13 presents the detailed distribution of the daily operation cost. In general, the CBH-VCRS with FS has the lowest total operating cost, which is 26.4% and 6.3% lower than those of the LS system and the SC-VCRS, respectively. Major operating cost comes from the compressors, almost 90% of total. The operating cost of the cooling tower includes the electricity and water consumption. The former is higher and occupies no more than 7.7%. The SC-VCRS consumes the maximum amount of the water every day, and the LS system has the most saving on it. More details are listed in Table 8.



695 the price ratios of 1.3 and 1.8, respectively. The third one means that the  $C_{op}$  of the SV-

696 VCRS exceeds that of the LS system at the price ratios of 6.5.

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#### 698 **6. Comparison of initial capital cost and total annual cost**

The initial capital cost and its influence on the total annual cost and the payback
period of additional expense under different electricity tariffs structures are carried out
in this section.

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Figure 15 Details of initial capital cost for three systems

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Figure 15 gives the detailed distribution of the main components cost. Because of the largest design capacity, the CHB-VCRS with FS pays the highest initial capital cost, 708 which is 44.4% and 75.5% higher than those of the CHB-VCRS with LS and the SC-709 VCRS. The compressor is absolutely the major cost. This part accounts for 80.8%, 710 72.3% and 72.0% of the total costs for the conventional, LS and FS systems, 711 respectively. For the CHB-VCRS, the hydration tank is the second major cost, which 712 comprises 14.2% and 14.5% for the LS and FS systems, respectively. For the non-713 storage SC-VCRS, the second costly equipment is evaporator, which is around 10.8% 714 of total. The hydrate decomposer of the LS and FS systems only make a spend of about 715 8.0% and 5.6%. The gas cooler and cooling tower for the three systems occupy the costs 716 of the total in the range of 1.6-6.3%. The rest components, such as the expansion valve 717 and flash tank, expends less than 1% of the total. Based on these, it can be found that 718 the cost of the CO<sub>2</sub> compressor shows the greatest impact on the total initial capital cost, which thus has the greatest potential to cut down the investment. 719

As well known, initial capital cost control is a basic design principle in engineering. This method has great potential particularly with the development of new materials and the globalization of industry. Therefore, the economic feasibility of the CHB-VCRS proposed in this work will be discussed in comparison of the annual costs that replacing the conventional SC-VCRS considering the improvement of the initial capital cost considering the variation of initial capital cost.

726









733 Figures 16(a) and 16(b) illustrate the indication range of the initial capital cost for 734 the CHB-VCRS with LS that is worthy of replacing the SC-VCRS when the lifetime is 735 set within 15 years. Generally, the total annual cost decreases with the increasing of the 736 system lifetime. The electricity price ratio of on- and off-peak is adopted as 2.1 in Fig 737 16(a). The light-shadow area in the figure is called  $C_{cap,LS}$  perfect range, which indicates the LS system can absolutely replace the base line when its initial capital cost is less 738 739 than 88% of  $C_{cap,SC}$ . The white area that the  $C_{cap,LS}$  larger than 98% of  $C_{cap,SC}$  means 740 there is totally no worthy replacement. For the dark-shadow area between 88% and 98% 741 of  $C_{cap,SC}$ , the lifetime of the CHB-VCRS with LS need be calculated carefully for 742 replacing the baseline. Taking the case in the enlarged area (enclosed by dotted line), 743 the red line of 90% is the limitation for the LS system with the 10-year system lifetime. 744 In fact, the control range of the initial capital cost for the LS system is quite narrow and 745 the ceiling cannot beyond 100% when the electricity prices ratio set as 2.1, due to no 746 advantage on the operation cost (as depicted in Fig. 14).

747 Fig 16(b) investigate the economic feasibility of the CHB-VCRS with LS affected 748 by the increasing of the electricity prices ratio. The ceiling and floor line of the control 749 area intersect at the point of (6.5, 100%). Comparing Fig. 14, the operation costs of the 750 CHB-VCRS with LS and the SC-VCRS reach identical at the price ratio of 6.5. The 751 corresponding vertical  $C_{op}$  criticality line (brown solid) divides the map into two zones. 752 On the left hand side, it is the  $C_{op,LS}$  advantage zone. Whereas on the right hand side, it 753 is the  $C_{op,LS}$  disadvantage zone. The control range become more and more narrow when 754 the price ratio approaches to  $C_{op}$  criticality line. 1-year boundary and 15-year boundary 755 switch their characteristics if crossing the zones. Generally, in the  $C_{op,LS}$  disadvantage 756 zone, the LS system should reduce their initial capital cost lower than 100% of baseline, 757 that the CHB-VCRS would have the feasibility of replacing the SC-VCRS. However,

in the  $C_{op,LS}$  advantage zone, the CHB-VCRS start to have the flexibility on the initial capital cost. In this case, because of no advantage on the operating cost, the LS system nearly have no any flexibility, only 104.5% of  $C_{cap,SC}$  even when the electricity ratio is 8.0. At last, noticed that the red dash line in Fig 16(b) points out the positions of those key boundary lines which exist in Fig. 16(a).

763 Figures 17(a) and 17(b) has the identical function as Figs. 16(a) and 16(b). These 764 two maps are then used to assess the economic feasibility for the CHB-VCRS with FS. 765 The electricity prices ratio in Fig17(a) is 4.0. The control range of 109-160% for the FS 766 system is wider than that for the LS system. Different from the LS system, seeing Fig. 767 14, the FS system has superior advantage over the SC-VCRS on the operation cost. 768 Thus the  $C_{op,FS}$  advantage zone is huge and overwhelms the  $C_{op,FS}$  disadvantage zone in 769 Fig. 17(b). As viewed, the FS system has more flexibility, even the  $C_{cap,FS}$  is over 250% of  $C_{cap,SC}$  when the electricity prices ratio set as 8.0, A specific system lifetime (within 770 771 15 years) can be found, which means the FS system is worthy of replacing the SC-772 VCRS.



Figure 17 Initial capital cost control for CHB-VCRS with FS

The payback years of additional expenses when a system with larger operation cost but lower initial capital cost is replaced by a specific system with lower operation cost, but larger initial capital cost can be calculated iteratively by the following equation:

$$C_{\text{op,diff}}\left(\frac{i(1+i)^n - 1}{i(1+i)^n}\right) + SV\left(\frac{1}{(1+i)^n}\right) = C_{\text{cap,diff}}$$
(31)

In Eq. (31), *n* refers to the payback years.  $C_{op,diff}$  is defined as the value of savings in the annual operating cost (e.g., based on Fig. 18, the difference in annual operating costs of the SC-VCRS and the CHB-VCRS with FS), and  $C_{cap,diff}$  is considered as the difference between the initial capital costs of the two systems. *SV* in Eq. (31) is assumed as 10% of  $C_{cap,diff}$ .

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Figure 18 Payback period for extra capital cost in case of replacing SC-VCRS with

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CHB-VCRS with FS in a system lifetime of 15 years

793 As aforementioned, the burden on the operation cost of the SC-VCRS over that of 794 the CHB-VCRS with FS is enlarged significantly with the increasing of the electricity 795 prices ratio. This will strongly influence on the payback years of the additional expenses 796 on the initial capital investment. As depicted in Fig. 18, the system lifetime of 15 years 797 is pre-set, lower the burden results in the slop of the curve become steeper, which means 798 the growth of the flexibility on the initial capital cost for the FS system would be smaller 799 when the payback years is planned from 1 to the maximum value of 15. For instance, 800 the growth of the flexibility would decrease from 51.0% of  $C_{cap,SC}$  (109-159%) to 4.3% 801 of  $C_{cap,SC}$  (101-105%), if the electricity prices ratio increases from 4.0 to 2.0. In 802 addition, Figure 18 can be used as an indication map to estimate the profit years in case of the SC-VCRS replaced by the CHB-VCRS with LS in the lifetime of 15 years. 803 804 Taking the electricity prices ratio of 4.0 as the example: If  $C_{\text{cap,FC}}$  is larger than 159% 805 of  $C_{cap,SC}$ , replacing with the FS system that the system cannot complete the payback 806 for the extra expanses on the initial capital cost within 15 years; If  $C_{cap,FC}$  is smaller 807 than 105% of  $C_{cap,SC}$ , the FS system can accomplish the payback and make the profits 808 since the first operation year; If  $C_{\text{cap,FC}}$  is 130.0% of  $C_{\text{cap,SC}}$ , a value between 105-159%, 809 it can be figured out (red-dash lines) in Fig. 18 that the FS system can pay off the extra 810 expenses and start to earn the profits in the fifth year.

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#### 812 **7. Conclusions**

This paper proposed a new two-stage CHB-VCRS, which arranged formation and dissociation at the low-pressure stage and used pure CO<sub>2</sub> hydrates as the primary refrigerant. Detailed mathematic models were developed. The numerical simulations of the proposed CHB-VCRS applying two CETS operation strategies, i.e., load-levelling storage and full storage, were conducted under continuous 24 hours of design day in the summer of Birmingham and London. In addition, a conventional non-storage SCVCRS was modelled as the baseline, which was used to make performance comparison
based on thermo-economic analyses. The following conclusions are achieved:

- 821 (1) For two-stage CHB-VCRS, when the high- and low-stage pressures were fixed,
  822 there existed an optimum inter-stage pressure on the basis of maximum COP.
  823 This value increased with the increasing of the subcooling parameter.
- (2) The design cooling capacity of the CHB-VCRS with LS was around 40% lower
  than that of the non-storage SC-VCRS. The design capacity of the CHB-VCRS
  with FS have the largest one, 10% larger than that of the baseline.
- 827 (3) In general, the CHB-VCRS with FS had the lowest annual operation cost, and
  828 with the incentivization of electricity-price ratio (from 2 to 8), this savings was
  829 significantly enlarged.
- (4) The CHB-VCRS with LS saved most on the water consumption, whereas the
   non-storage SC-VCRS consumed most.
- (5) The initial capital cost of the CHB-VCRS with FS was 71.1% and 44.4% higher
  than those of the SC-VCRS and the CHB-VCRS with LS, respectively. The
  compressor was the major cost for all the three systems.
- (6) Compared to the FS operation, the CHB-VCRS using LS strategy had wider
  economic feasibility in replacing of the conventional SC-VCRS, because of the
  advantage on the annual operation cost. With higher electricity-price ratio, the
  LS system had more flexibility on the initial capital cost.
- (7) A payback-year map for the CHB-VCRS with FS was developed to estimate
   the profit years when it replaces the non-storage SC-VCRS based on a 15-year
- 841 lifetime under different electricity-price ratios.
- 842

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846

#### 847 Appendix A

848 This part provides the procedure of calculation of moist air properties and the flow 849 chart of simplified modeling of cooling tower.

The relative humidity is the ratio of the actual water vapor partial pressure in moist air and the water vapor partial pressure in moist air at saturation, can be expressed by Eq. (A1) [42]:

$$\phi = \frac{p_{\rm w}}{p_{\rm ws}} \times 100 \tag{A1}$$

where  $p_w$  refer to the actual air vapor pressure, kPa.  $p_{ws}$  is the air saturation vapor pressure, kPa, are calculated by Eq. (A2)

$$p_{\rm ws} = (at^3 + bt^2 + ct + d) \times 0.1 \tag{A2}$$

where *a*, *b*, *c* and *d* are constants with values of [43]:

$$a = 6.6 \times 10^{-4}; b = 4.6 \times 10^{-3}; c = 4.58 \times 10^{-1}; d = 6.63$$

856 The saturation humidity ratio,  $W_s$ , can be calculated by Eq. (A3).

$$W_{\rm s} = 0.621945 \frac{p_{\rm ws}}{p_{\rm atm} - p_{\rm ws}}$$
 (A3)

857

7 Similarly, the humidity ratio *W*, can be calculated by Eq. (A4).

$$W = 0.621945 \frac{p_{\rm w}}{p_{\rm atm} - p_{\rm w}}$$
(A4)

858 The moist air specific enthalpy in kJ/kg then becomes:

$$h = 1.006t_{\rm db} + W(2501 + 1.86t_{\rm db}) \tag{A5}$$

The wet-bulb temperature can be determined by Eq. (A6).

$$t_{\rm wb} = t_{\rm db} - \frac{p_{\rm ws}(t_{\rm wb}) - (\phi/100) p_{\rm ws}(t_{\rm db})}{k p_{\rm atm}}$$
(A6)

where *k* is a constant,  $p_{\text{atm}}$  is the atmospheric pressure and  $p_{\text{ws}}(t_{\text{wb}})$  and  $p_{\text{ws}}(t_{\text{db}})$  are the air saturation vapor pressure at  $t_{\text{wb}}$  and  $t_{\text{db}}$  respectively.

$$k = 6.53 \times 10^{-4}$$

Figure A1 presents the flow chart of the iterative method to determine the wet-bulb temperature by Eqs. (A2) and (A6).

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868 Figure A2 presents the flowchart of modeling of the direct contact cooling tower869 as follow.

Figure A1 Flowchart of wet-bulb temperature iteration





Figure A2 Flowchart of modeling of direct contact cooling tower

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#### 874 Appendix B

This part presents the flowchart of heat transfer calculation in a segment of gas cooler. Figure B1 is a simplified procedure and focus on presenting the main iterations during the process.





Figure B1 Flowchart of heat transfer calculation in a segment

#### 882 Appendix C

883 This part gives the flowchart of modeling of single-stage CO<sub>2</sub> vapor-compression

refrigeration system with variable-speed compressor.



Figure C1 Flowchart of modelling of SC-VCRS (baseline)

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