

# 1 Performance improvement of a direct carbon solid oxide fuel cell through 2 integrating an Otto heat engine

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11

12 **Abstract:** A novel system consisting of an external heat source, a direct carbon solid oxide fuel  
13 cell (DC-SOFC), a regenerator and an air standard Otto cycle engine is proposed to improve  
14 the performance of the DC-SOFC. Considering the electrochemical/chemical reactions,  
15 ionic/electronic charge transport, mass/momentum transport and heat transfer, a 2D tubular  
16 DC-SOFC model shows that the overall heat released in the cell can be smaller than, equal to  
17 or larger than the heat required by the internal Boudouard reaction. Three different operating  
18 modes of the proposed system are identified, and accordingly, analytical expressions for the  
19 equivalent power output and efficiency of the proposed system are derived under different  
20 operating conditions. The modeling results show that the Otto heat engine can effectively  
21 recover the waste heat from the DC-SOFC for additional power production especially at large  
22 operating current density. Comprehensive parametric studies are conducted to investigate the  
23 effects of the different operating conditions of DC-SOFC on its performance and heat  
24 generation. The effects of compression ratio, internal irreversibility factor and power  
25 dissipation of the Otto heat engine on the system performance improvement are also studied.

26

27 **Keywords:** Solid oxide fuel cell; Carbon gasification; Air standard Otto heat engine;

28 Performance improvement; Parametric study

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## 32 1. Introduction

33 The increasing global attention on energy crisis drives worldwide research interest in clean  
34 and high efficiency energy conversion devices, such as solid oxide fuel cells (SOFCs). SOFCs  
35 are all solid-state devices working at a high temperature (e.g. 800°C). A typical SOFC has a  
36 sandwiched structure with a dense electrolyte between a porous anode and a porous cathode  
37 [1-3]. Fuels (e.g. H<sub>2</sub>) and oxidants (e.g. O<sub>2</sub>) are supplied to the anode and cathode, respectively.  
38 Through electrochemical reactions, chemical energy in fuels and oxidants can be converted  
39 into electrical power directly with a high efficiency. As fuels and oxidants are separated by the  
40 dense electrolyte, the post-process of emission gases is relatively easy.

41 Apart from gas fuels like H<sub>2</sub> and CO, the utilization of solid carbons in SOFCs has received  
42 rising attention as these widely spreaded solid fuels have high volumetric energy density, which  
43 can easily be obtained at a low cost. There are two main methods for direct solid carbon  
44 utilization in the SOFCs. One is electrochemical oxidation of solid carbon that is in direct  
45 contact with the electrode catalyst (usually called as direct carbon fuel cell, DCFC) [1, 2],  
46 aiming for a high thermodynamic efficiency. However, this method yields a low power density  
47 due to difficult transport of solid carbon and poor contact between the carbon particles and the  
48 electrochemical reaction sites (triple phase boundaries: TPBs). The other method is solid  
49 carbon indirect utilization through an agent (usually called as direct-carbon solid oxide fuel  
50 cell, DC-SOFC), which converts solid carbon into gas fuel such as CO for the electrochemical  
51 reaction at the TPBs [3, 4]. Compared with the first method, the second method provides a  
52 much higher power density due to easy gas transport and good contact between gas fuel and  
53 the TPBs. With verifications of its mechanism [5, 6], catalysts are developed to further improve  
54 the performance of DC-SOFCs [7-10]. Besides, the concept of CO and electrical power co-  
55 generation is proposed and analyzed. The results suggest that a much higher exergy efficiency  
56 can be achieved by the DC-SOFC than DCFC [11]. Different agents have also been compared  
57 to explore the application of DC-SOFC[12]. It is found that DC-SOFC with H<sub>2</sub>O as

58 gasification agent for H<sub>2</sub> and CO production could achieve higher performance than that with  
59 CO<sub>2</sub> agent due to fast gasification kinetics using H<sub>2</sub>O agent and low activation loss associated  
60 with H<sub>2</sub> electrochemical oxidation. To further understand the detailed chemical/physical  
61 process in the DC-SOFCs, mathematical models are developed [13-16]. Our recent  
62 mathematical model analyses [17] prove the existence of heat balance in DC-SOFC when it  
63 operates at a relative low current density. When the DC-SOFC operates at a high current density  
64 to provide a large power density, the heat generated from the irreversible electrochemical losses  
65 and enthalpy change exceeds the heat demand by Boudouard reaction. Therefore, the efficiency  
66 of DC-SOFCs can be further improved at a wide range of operating current density by utilizing  
67 the waste heat [18].

68 Various thermodynamic cycles including Carnot cycle[19], Stirling cycle[20], Ericsson  
69 cycle[21], Brayton cycle[22], Rankine cycle[23], Braysson cycle[24] and Kalina cycle[25]  
70 have been used for the conversion of heat into power. Compared with these cycles, Otto cycle  
71 has interesting perspectives as the rapid combustion process takes place at a constant volume,  
72 which indicates an excellent potential to integrate with other systems. By applying the air-  
73 standard analysis on Otto cycle, a number of modeling works have been conducted on air-  
74 standard Otto cycle heat engines [26-29] to illustrate the thermodynamic aspects of engine  
75 performance. Gumus et al.[30] compared the performance of a reversible Otto cycle based on  
76 its maximum power, maximum power density and maximum efficient power, where they  
77 conclude that the design parameters at maximum efficient power conditions lead to more  
78 efficient engines than that at the maximum power condition. Besides, the maximum efficient  
79 power criterion may have a significant power advantage compared with maximum power  
80 density criterion. By considering multiple irreversible losses, Zhao et al. [31, 32] evaluated the  
81 performance of an irreversible Otto heat engine and determined the optimum criteria. Chen et  
82 al. [33] further evaluated the performance of the air-standard Otto cycle with different specific  
83 heats of working fluid [34, 35] by using different objective functions and heat transfer laws.  
84 Apart from aforementioned works focusing on Otto heat engine itself, there is another work  
85 done by Eldighidy [36], where an air-standard Otto cycle is proposed to harvest solar energy

86 for power generation. Obviously, it is a feasible method for the air-standard Otto cycle heat  
87 engine to harvest the waste heat from DC-SOFC for performance improvement. An up-to-date  
88 literature survey shows that there is no work reported on this subject.

89 In this work, a numerical model is developed to analyze the performance improvement of  
90 DC-SOFC by combining it with an air-standard Otto cycle heat engine. Based on the numerical  
91 analysis, three system operation modes are specified under different operating conditions.  
92 Besides, the performance of the proposed system is evaluated based on the output power and  
93 efficiency expressions. The advantages of the system are also demonstrated through numerical  
94 calculations. Finally, the effects of several design parameters and operating conditions on the  
95 performance of the system are discussed.

## 96 **2. System description**

97 As shown in Fig. 1 (a), the proposed system mainly consists of a DC-SOFC, an external  
98 heat source, an air standard Otto cycle heat engine and a regenerator. The DC-SOFC generates  
99 electrical power  $P_{\text{SOFC}}$  (W) by consuming solid carbon. To ensure the normal operation of the  
100 DC-SOFC, certain amount of heat  $Q$  ( $\text{J S}^{-1}$ ) should be provided to DC-SOFC at low operating  
101 current density (DC-SOFC in the endothermic mode), and the corresponding heat and mass  
102 transfer are shown in Fig. 1 (b). Otherwise, the air standard Otto cycle heat engine should be  
103 connected to utilize the waste heat from the DC-SOFC for additional power ( $P_{\text{Otto}}$ ) production,  
104 and the corresponding heat and mass transfer are shown in Fig. 1 (c). It should be noted that  
105 the CO reformation process is inside the anode of the DC-SOFC, and the excess heat generated  
106 in the SOFC component is carried out by the outlet products to power the Otto engine for  
107 additional power generation. In calculation, partial differential equations for CO reformation  
108 and SOFC component are coupled in COMSOL MULTIPHYSICS<sup>®</sup>. The generated heat (an  
109 output variable from DC-SOFC) is then an input variable in the calculation of Otto engine. The  
110 regenerator in the system preheats the inlet solid carbon and gas by outlet high-temperature  
111 gases.

112 For simplification, the following assumptions are adopted [15]

- 113 • Electrochemical reactions spatially take place at triple phase boundaries (TPBs),  
114 which are assumed to be uniformly distributed in the porous electrodes. Electronic  
115 and ionic conduction phases in the porous electrodes are continuous and  
116 homogeneous;
- 117 • Ionic and electronic charge transport processes take place in the PEN (Positive  
118 Electrode-Electrolyte-Negative electrode assembly), and the charge transfer  
119 reaction can take place at TPB sites throughout the porous electrode;
- 120 • All gases (CO, CO<sub>2</sub>, O<sub>2</sub> and N<sub>2</sub>) involved in the DC-SOFC are ideal gases and the  
121 gas flow is incompressible;
- 122 • Internal relaxation times in the adiabatic processes are negligible;
- 123 • Heat transfer irreversibility between the DC-SOFC and the Otto heat engine is  
124 neglected;
- 125 • Irreversibility in the two adiabatic processes is neglected;
- 126 • Working substance air of Otto heat engine is assumed to behave as an ideal gas.

127

## 128 **2.1 DC-SOFC**

129 In DC-SOFCs, solid carbon in anode chamber is gasified by CO<sub>2</sub> to generate CO molecules,  
130 which then diffuse into the porous anode and react with O<sup>2-</sup> ions at the TPB sites. The produced  
131 CO<sub>2</sub> molecules in electrochemical reactions subsequently diffuse back to the anode chamber  
132 and continue the Boudouard reaction for CO generation. These processes repeat between the  
133 anode chamber and the porous anode for power generation as long as there is enough solid  
134 carbon in the anode chamber.

135 A previously developed 2D numerical model is adopted to describe the electrochemical  
136 /chemical reactions, ionic/electronic charge transport, mass/momentum transport and heat  
137 transfer in the tubular DC-SOFC.

### 138 **2.1.1 Chemical reaction model**

139 In anode chamber, the Boudouard reaction converts solid carbon into CO by consuming

140 CO<sub>2</sub>, i.e.,  
 141 C + CO<sub>2</sub> = 2CO. (1)

142 Its reaction rate can be calculated as [37]

$$143 R_{rb} = k_{rb} \exp(-E_{rb}/RT) c_{CO_2}. \quad (2)$$

### 144 2.1.2 Electrochemical reaction model

145 At anode TPB sites, CO molecules electrochemically react with O<sup>2-</sup> ions and release  
 146 electrons, i.e.,



148 The above mentioned O<sup>2-</sup> ions are transported from cathode TPB sites, where O<sub>2</sub> molecules  
 149 are reduced into O<sup>2-</sup>, i.e.,



151 The equilibrium potential ( $E_{CO}$ ) for above reactions can be determined by [38]

$$152 E_{CO} = E_{CO}^0 + \frac{RT}{2F} \ln \left[ \frac{P_{CO}^L (P_{O_2}^L)^{1/2}}{P_{CO_2}^L} \right], \quad (5)$$

153 where  $R$  is the universal gas constant and  $F$  is Faraday constant.  $T$  is operating temperature and  
 154  $P^L$  is local gas partial pressure.  $E_{CO}^0$  is the standard potential (V), which can be calculated by

$$155 E_{CO}^0 = 1.46713 - 0.0004527T. \quad (6)$$

156 For the calculation of the operating potential ( $E$ ), both activation overpotential ( $\eta_{act}$ ) and  
 157 ohmic overpotential ( $\eta_{ohmic}$ ) should be considered, i.e.,

$$158 E = E_{CO}^0 - \eta_{act} - \eta_{ohmic}. \quad (7)$$

159 The relationship between current density and above two overpotential losses are described  
 160 by Butler-Volmer equation (Eq. (8)) and ohm law (Eq. (9)), respectively[39], i.e.,

$$161 i = i_0 \left\{ \exp\left(\frac{\alpha n F \eta_{act}}{RT}\right) - \exp\left(-\frac{(1-\alpha) n F \eta_{act}}{RT}\right) \right\}, \quad (8)$$

162 and

163  $i = -\sigma^{\text{eff}}\nabla(\phi),$  (9)

164 where  $i$  is operating current density,  $i_0$  is exchange current density,  $\alpha$  is the electron transfer  
 165 coefficient and  $n$  is the number of transferred electrons per electrochemical reaction.  $\sigma^{\text{eff}}$  and  
 166  $\phi$  are effective conductivity ( $\text{S m}^{-1}$ ) and electric potential (V), respectively.

167 **2.1.3 Mass and momentum transport model**

168 Mass and momentum transport are, respectively, calculated by the extended Fick's model (Eq.  
 169 (10)) and Navier-Stokes equation (Eq. (11)) [15], i.e.,

170 
$$N_m = -\frac{1}{RT} \left( \frac{B_0 y_m P}{\mu} \frac{\partial P}{\partial z} - D_m^{\text{eff}} \frac{\partial (y_m P)}{\partial z} \right) \quad (m = 1, 2, \dots, l),$$
 (10)

171 and

172 
$$\rho \frac{\partial u}{\partial t} + \rho u \nabla u = -\nabla p + \nabla \left[ \mu \left( \nabla u + (\nabla u)^T \right) - \frac{2}{3} \mu \nabla u \right] - \frac{\varepsilon \mu u}{k},$$
 (11)

173 where  $B_0$  is the permeability ( $\text{m}^2$ ) of the porous electrodes,  $y_m$  is the mole fraction of  
 174 component  $m$ ,  $\mu$  is the gas viscosity ( $\text{N m}^{-1} \text{s}^{-1}$ ),  $D_m^{\text{eff}}$  is the overall effective diffusion  
 175 coefficient ( $\text{m}^2 \text{s}^{-1}$ ) of component  $m$ ,  $\rho$  ( $\text{kg m}^{-3}$ ) is the gas density and  $u$  ( $\text{m s}^{-1}$ ) is the velocity  
 176 vector.

177 **2.1.4 Heat transfer model**

178 The heat transfer process is described by the general heat balance equation [17]

179 
$$\rho C_p u \cdot \nabla T + \nabla \cdot (-\lambda_{\text{eff}} \nabla T) = Q,$$
 (12)

180 where  $C_p$  is the heat capacity,  $u$  is the fluid velocity field,  $\lambda_{\text{eff}}$  is the effective heat  
 181 conductivity and  $Q$  is the heat source term.

182 The above model is validated by fitting simulation results ( $I$ - $V$  characteristics) with  
 183 experimental data and good agreement has been found in Ref. [17]. The DC-SOFC model is



184 described by partial differential equations, which are handled by nonlinear finite elements  
 185 method using commercial software COMSOL MULTIPHYSICS®.

186 The power output of the DC-SOFC is determined by

$$187 \quad P_{\text{SOFC}} = V \times I, \quad (13)$$

188 where  $V$  (V) and  $I$  (A) are output voltage and current, respectively.

189 Considering the irreversible polarization losses and enthalpy changes in DC-SOFC, its  
 190 electrical efficiency

$$191 \quad \eta_{\text{SOFC}} = \frac{P_{\text{SOFC}}}{P_{\text{SOFC}} + Q} \quad (14)$$

192 can be defined, where  $Q$  ( $\text{J s}^{-1}$ ) is the overall heat released from the DC-SOFC, which is  
 193 defined as positive in this paper. The heat  $Q$  can be further expressed as

$$194 \quad Q = Q_e - Q_c, \quad (15)$$

195 where  $Q_c$  ( $\text{J s}^{-1}$ ) is the absorbed heat by the Boudouard reaction and  $Q_e$  ( $\text{J s}^{-1}$ ) includes heat  
 196 released from the electrochemical reaction and overpotential losses. Thus,  $Q_e$  can be  
 197 calculated as

$$198 \quad Q_e = -T\Delta S \times \frac{I}{2F} + (E - V)I. \quad (16)$$

199 When  $Q_e = Q_c$ , i.e.,  $Q = 0$ , the thermal neutral current

$$200 \quad I_{\text{tn}} = \frac{Q_c}{-T\Delta S/2F + E - V_{\text{tn}}} \quad (17)$$

201 can be obtained, where  $V_{\text{tn}}$  (V) is the thermal neutral voltage corresponding to  $I_{\text{tn}}$ .

202 Based on the above governing equations and parameters in Table 1, the relationship  
 203 between  $Q$  and operating current density  $i$  ( $i = I/A$ ,  $\text{A m}^{-2}$ ) are obtained as shown in Fig. 2.  
 204 It is seen that  $Q$  increases from negative to positive values with increasing current density.  
 205 When  $i < i_{\text{tn}}$ , i.e.,  $Q < 0$ , the heat produced due to the polarization losses and enthalpy  
 206 change of the electrochemical reaction is less than the heat required for the Boudouard reaction.  
 207 Certain amount of heat  $|Q|$  should be supplied from the external heat source to the DC-SOFC  
 208 to maintain its operating temperature. In this case, the external heat source in Fig. 1(a) should  
 209 be switched on while the air standard Otto heat engine is off. When  $i = i_{\text{tn}}$ , i.e.,  $Q = 0$ , the  
 210 heat generation equals the heat consumption by Boudouard reaction in the DC-SOFC, which

211 means the DC-SOFC can work in a thermally self-sustained manner. When  $i > i_{tn}$ , i.e.,  $Q >$   
 212 0, the heat generated exceeds the required heat for the Boudouard reaction. The air standard  
 213 Otto heat engine should be switched on to utilize the waste heat from DC-SOFC for extra  
 214 electrical power ( $P_{\text{Otto}}$ ) generation. As also shown in Fig. 2, a larger  $i_{tn}$  is needed at a higher  
 215 operating temperature to generate more heat for the endothermic Boudouard reaction. Less  
 216 netheat is generated for a given current density at a higher operating temperature, as the faster  
 217 Boudouard reaction at a higher temperature consumes more heat from DC-SOFC.

218

## 219 **2.2 Air standard Otto cycle heat engine**

220 The air standard Otto cycle is composed of two adiabatic processes (1→2 and 3→4) and  
 221 two isochoric processes (2→3 and 4→1), as shown in Fig. 3.  $T_1$ ,  $T_2$ ,  $T_3$  and  $T_4$  are  
 222 temperatures of the working substance at the state points 1, 2, 3 and 4. The heat flow from the  
 223 DC-SOFC,  $Q$ , is provided to the Otto cycle heat engine at the volume  $V_2$ . After producing  
 224 power  $P_{\text{Otto}}$ , the remaining heat  $Q_r$  is released at the volume  $V_2$ . Considering instantaneous  
 225 adiabats, the period of the Otto cycle [40]

$$226 \quad \tau_t = t_{1V} + t_{2V} = K_1(T_3 - T_2) + K_2(T_4 - T_1) \quad (18)$$

227 can be calculated, where  $t_{1V}$  and  $t_{2V}$  are, respectively, the heating and cooling times;  $K_1$   
 228 and  $K_2$  are temperature-independent constants ( $\text{s K}^{-1}$ ).

229 From the first law of thermodynamics, the reversible work

$$230 \quad W_{\text{Otto},r} = C_{V_1}(T_3 - T_2) - C_{V_2}(T_4 - T_1) \quad (19)$$

231 done by the Otto cycle heat engine can be calculated, where  $C_{V_1}$  and  $C_{V_2}$  are the heat  
 232 capacities of gases in the compression and power strokes, respectively.

233 Thus, the reversible power is shown as

$$234 \quad P_{\text{Otto},r} = \frac{W_{\text{Otto},r}}{\tau_t} = \frac{C_{V_1}(T_3 - T_2) - C_{V_2}(T_4 - T_1)}{K_1(T_3 - T_2) + K_2(T_4 - T_1)}. \quad (20)$$

235 If the reversible work with adiabats given by  $TV^{(\gamma-1)} = \text{constant}$ , then Eq. (20) can be

236 further rewritten as [40, 41]

$$237 \quad P_{\text{Otto},r} = \frac{C_{V_1} - C_{V_2} r^{(1-\gamma)}}{K_1 + K_2 r^{(1-\gamma)}}, \quad (21)$$

238 where  $\gamma = C_P / C_V$ ,  $C_P$  and  $C_V$  are, respectively, constant-pressure heat capacity ( $\text{J K}^{-1}$ ) and  
239 constant-volume heat capacity ( $\text{J K}^{-1}$ ), and  $r = V_1/V_2$  is the compression ratio.

240 Considering a dissipation term represented by a friction force proportional to the velocity,  
241 the friction force

$$242 \quad F_f = -\omega v = -\omega \frac{dx}{dt} \quad (22)$$

243 can be obtained, where  $\omega$  is the friction coefficient which takes into account the global losses,  
244  $v$  is the piston velocity, and  $x$  is the piston displacement. Then, the friction-related power  
245 loss

$$246 \quad P_f = -\omega \frac{dx}{dt} \frac{dx}{dt} = -\omega v^2 \quad (23)$$

247 can be calculated [41].

248 The piston mean velocity can be expressed as

$$249 \quad \bar{v} = \frac{x_1 - x_2}{\Delta t_{12}} = \frac{x_2 (r - 1)}{\Delta t_{12}}, \quad (24)$$

250 where  $x_2$  is the piston position at minimum volume and  $\Delta t_{12}$  is the time spent in the power  
251 stroke. Counted the piston friction-like losses, the power output is reduced from  $P_{\text{Otto},r}$  to

$$252 \quad P_{\text{Otto},P} = P_{\text{Otto},r} - P_f = \frac{C_{V_1} - C_{V_2} r^{(1-\gamma)}}{K_1 + K_2 r^{(1-\gamma)}} - b (r - 1)^2, \quad (25)$$

$$253 \quad \text{where } b = \frac{\omega x_2^2}{(\Delta t_{12})^2}.$$

254 In addition to the piston friction-like losses, irreversible losses from mass transfer, friction,  
255 eddy and other irreversible effects inside the cyclic working fluid should be considered. The  
256 total irreversible effects within the working fluid can be characterized by the internal  
257 irreversibility factor [40]

$$I_R = \frac{\Delta S_{W1}}{|\Delta S_{W2}|} = \frac{C_{V1} \ln(T_3/T_2)}{C_{V2} \ln(T_4/T_1)} = \frac{C_{V1}}{C_{V2}}, \quad (26)$$

where  $\Delta S_{W1}$  and  $\Delta S_{W2}$  are entropy changes ( $J K^{-1}$ ) along the hot isothermal branch and the cold isothermal compression branch. The internal irreversibility factor is in the range of  $0 < I_R \leq 1$ .

Considering the finite-time evolution of the cycle's compression and power strokes, piston friction-like losses and internal irreversibility of working fluid, the efficiency and power output of the air standard Otto heat engine are, respectively, given by [40-42]

$$\eta_{Oto} = 1 - r^{1-\gamma} - \frac{b(r-1)^2}{C_{V2}} (K_1 + K_2 r^{1-\gamma}), \quad (27)$$

and

$$P_{Oto} = Q \left[ 1 - r^{1-\gamma} - \frac{b(r-1)^2}{C_{V2}} (K_1 + K_2 r^{1-\gamma}) \right], \quad (28)$$

where the relevant parameters for the air standard Otto cycle are summarized in Table 2.

### 2.3 The regenerator

The regenerator works as a heat exchanger continuously preheating the inlet solid carbon and air by the high-temperature outlet gases. The products are cooled down to the environmental temperature with the solid carbon and oxygen being heated to the operating temperature of the DC-SOFC. According to the thermodynamic parameters given in Ref. [18], one can prove that

$$\Delta Q_{CO} - (\Delta Q_C + \Delta Q_{O_2}) > 0, \quad (29)$$

and

$$\Delta Q_{CO_2} - (\Delta Q_C + \Delta Q_{O_2}) > 0, \quad (30)$$

where  $\Delta Q_{CO} = \dot{m} \int_{T_0}^T C_{CO} d\tau$ ,  $\Delta Q_C = \dot{m} \int_{T_0}^T C_C d\tau$ ,  $\Delta Q_{O_2} = 0.5 \dot{m} \int_{T_0}^T C_{O_2} d\tau$ ,  $\Delta Q_{CO_2} = \dot{m} \int_{T_0}^T C_{CO_2} d\tau$ ,

$\Delta Q_{CO_2} = \dot{m} \int_{T_0}^T C_{CO_2} d\tau$ ,  $\dot{m}$  is the molar consumption rate of solid carbon,  $T_0$  is the ambient

281 temperature (K),  $C_j$  is the isobaric molar heat capacities ( $\text{J mol}^{-1} \text{K}^{-1}$ ) for species  $j$  ( $j = \text{solid}$   
 282 carbon, CO, O<sub>2</sub> or CO<sub>2</sub>). As only CO and CO<sub>2</sub> are present in the anode outlet gas, we can  
 283 conclude that the heat contained in the products is always enough to preheat the reactants to  
 284 attain the operating temperature of the DC-SOFC regardless of its molar fraction of CO and  
 285 CO<sub>2</sub> (the inlet N<sub>2</sub> in air is supposed to be preheated by the outlet N<sub>2</sub>). Since some high-  
 286 effectiveness regenerators have already been reported [43], it is appropriate to assume that the  
 287 regenerator in Fig. 1 (a) performs perfect regeneration.

288

## 289 **2.4 The performance of the proposed system**

290 As the waste heat from DC-SOFC is used to preheat the activated carbon and air at the inlet  
 291 of the cell, the heat loss from the DC-SOFC system to the environment is negligible against  
 292 the electrical power ( $P_{\text{SOFC}}$ ). Adding the contribution of the air standard Otto cycle heat engine,  
 293 the equivalent power output ( $P$ ) and equivalent efficiency ( $\eta$ ) of the proposed system can be,  
 294 respectively, expressed as

$$295 \quad P = \begin{cases} = P_{\text{SOFC}} & (i < i_{\text{tn}}) \\ = P_{\text{SOFC}} + P_{\text{Otto}} & (i \geq i_{\text{tn}}) \end{cases}, \quad (31)$$

296 and

$$297 \quad \eta = \begin{cases} = \frac{P_{\text{SOFC}}}{P_{\text{SOFC}} + |Q|} & (i < i_{\text{tn}}) \\ = \frac{P_{\text{SOFC}} + P_{\text{Otto}}}{P_{\text{SOFC}} + Q} & (i \geq i_{\text{tn}}) \end{cases}. \quad (32)$$

## 298 **3. Results and discussion**

299 Based on the mathematical models above which have been well validated by the previous  
 300 studies[15] and relevant parameters given in Table 1 and Table 2, the performance  
 301 characteristics of the proposed system can be analyzed. The parameters are taken as default  
 302 ones unless they are specifically mentioned.

### 3.1 Performance characteristics of air standard Otto heat engine

The basic performance characteristics of the air standard Otto heat engine are shown in Fig. 4. As can be found in Fig. 4 (a), the efficiency ( $\eta_{\text{Otto}}$ ) increases with increasing compression ratio ( $r$ ) at different power dissipation ( $b$ ) values at the beginning. After reaching the peak efficiency values,  $\eta_{\text{Otto}}$  decreases with a further increase in compression value. Besides, a higher efficiency and larger effective interval compression ratio can be achieved at smaller power dissipation value. When power dissipation is decreased to zero, the friction losses in the Otto heat engine can be negligible. In this situation, Eqs. (27) and (28) can be, respectively, reduced into

$$\eta_{\text{Otto}} = 1 - r^{1-\gamma} / I_R, \quad (33)$$

and

$$P_{\text{Otto}} = Q(1 - r^{1-\gamma} / I_R). \quad (34)$$

As can be found in Fig. 4(b), the equivalent power density of the air standard Otto heat engine  $P_{\text{Otto}}^*$  increases with the increasing operating current density of the DC-SOFC  $i$  and the increasing internal irreversibility factor  $I_R$ . The effect of the internal irreversibility factor on its power output becomes more significant at larger operating current density as more heat is generated from DC-SOFC. With the internal irreversibility factor reaching 1, the Otto heat engine achieves its upper limit power density. In this situation, Eqs. (27) and (28) can be, respectively, reduced into

$$\eta_{\text{Otto}} = 1 - r^{1-\gamma} - \frac{b(r-1)^2}{C_{V_2}} (K_1 + K_2 r^{1-\gamma}), \quad (35)$$

and

$$P_{\text{Otto}} = Q \left[ 1 - r^{1-\gamma} - \frac{b(r-1)^2}{C_{V_2}} (K_1 + K_2 r^{1-\gamma}) \right]. \quad (36)$$

### 3.2 Power density improvement of the proposed system

The equivalent power densities of the DC-SOFC, Otto heat engine and proposed system

328 are compared at different operating temperatures as shown in Fig. 5, where  $P_{\text{SOFC}}^* = P_{\text{SOFC}}/A$   
329 and  $P^* = P/A$  are the power densities for the DC-SOFC and the proposed system,  
330 respectively. When  $i \leq i_{\text{tn}}$ , the curves of  $P^* \sim i$  and  $P_{\text{SOFC}}^* \sim i$  are overlapped as no waste  
331 heat is transferred to Otto heat engine for extra power production. In the range of  $i > i_{\text{tn}}$ ,  $P_{\text{Otto}}^*$   
332 keeps growing with larger operating current density as more heat is provided from the DC-  
333 SOFC. While for the DC-SOFC, its power density  $P_{\text{SOFC}}^*$  first increases and then decreases  
334 with the increasing  $i$ . As a result, the power density is significantly improved in the proposed  
335 system and  $P^*$  increases to attain a maximum value with increasing  $i$ .

336 The elevated operating temperature improves the performance of the DC-SOFC by  
337 promoting its chemical/electrochemical reactivity and ionic conductivity. However, the power  
338 density of the Otto heat engine at the same operating current density decreases with increasing  
339 operating temperature due to less waste heat supply, as shown by Fig. 2. As  $P_{\text{SOFC}}^*$  is more  
340 sensitive to the operating temperature than  $P_{\text{Otto}}^*$ , a higher operating temperature is preferred  
341 for the proposed system to obtain a higher output power density. For example, when the DC-  
342 SOFC works at a current density of  $30000 \text{ A m}^{-2}$ , the equivalent power density of the proposed  
343 system approximately increases from  $5550 \text{ W m}^{-2}$  at  $1073 \text{ K}$  to  $7950 \text{ W m}^{-2}$  at  $1173 \text{ K}$ , which  
344 are about 79.6% and 33.3% larger than that of the stand-alone DC-SOFC, respectively.

345

### 346 **3.3 Efficiency characteristics of proposed system**

347 Apart from power density, the equivalent efficiencies of the DC-SOFC, Otto heat engine  
348 and proposed system under different operating temperature are also compared as shown in Fig.  
349 6. Similarly, the  $\eta \sim i$  and  $\eta_{\text{SOFC}} \sim i$  curves are overlapped in the region of  $i \leq i_{\text{tn}}$  and the  
350 proposed system has the largest efficiency  $\eta$  when  $i > i_{\text{tn}}$ . The efficiency of the DC-SOFC is  
351 quite high at small operating current density, where it reaches a peak efficiency of 100% at  $i_{\text{tn}}$   
352 as DC-SOFC is thermally self-sustained. With a further increase in operating current density,

353  $\eta_{\text{SOFC}}$  decreases to less than  $\eta_{\text{Otto}}$  (which does not vary with the operating temperature). When  
354 the DC-SOFC works at a current density of  $30000 \text{ A m}^{-2}$ , the equivalent efficiency of the  
355 proposed system increases from 46.8% at 1073 K to 60.8% at 1173 K mainly due to the  
356 significant efficiency improvement of the DC-SOFC, whose efficiency increases from 26.4%  
357 at 1073 K to 45.4% at 1173 K. A higher operating temperature is thus more favored to obtain  
358 a higher efficiency of the proposed system.

359

### 360 **3.4 Effect of distance between carbon layer and anode electrode**

361 In DC-SOFCs, the distance between carbon layer and anode ( $D_{ce}$ ) will increase over time  
362 due to the consumption of solid carbon, resulting in the change of  $z$  in Eq. (10). As a result, the  
363 gas transportation between carbon layer and anode significantly affects the power output and  
364 heat generation in the proposed system. As shown in Fig. 7, as the distance between carbon  
365 layer and anode is decreased from  $559 \mu\text{m}$  to  $59 \mu\text{m}$ , a significant output power density  
366 improvement of the proposed system is found. The peak power density of the proposed system  
367 increases from  $5030 \text{ W m}^{-2}$  at  $559 \mu\text{m}$  to  $6990 \text{ W m}^{-2}$  at  $59 \mu\text{m}$ . As analyzed in our previous  
368 papers [15, 17], a small distance between carbon layer and anode helps to maintain a high fuel  
369 concentration in anode, which brings in a high output power density. Meanwhile, more heat  
370 can be provided from the DC-SOFC at higher operating current density, allowing more power  
371 to be generated through Otto heat engine. As a result, higher power density and efficiency of  
372 the proposed system can be obtained at a smaller distance, and this effect becomes more  
373 pronounced at a larger current density.

374

### 375 **3.5 Effect of compression ratio**

376 The effect of compression ratio ( $r$ ) on the performance of the proposed system appears  
377 only in the region of  $i > i_{\text{in}}$ , as shown in Fig. 8. For a given current density, it is observed that  
378 there exists peak values for the power density and efficiency of the proposed system with the  
379 change of compression ratio, indicating the existence of an optimum compression ratio. Based



380 on the parameters given in Table 1 and Table 2, the optimum value for the compression ratio is  
 381 found to be 9.26. Moreover, the optimum value for the compression ratio is closely related to  
 382 the friction-like coefficient. The optimum value of compression ratio ( $r_{opt}$ ) under different  
 383 dissipation power ( $b$ ) are listed in Table 3 by using the extremum condition  $\partial\eta_{Otto}/\partial r = 0$ ,  
 384 from which a smaller  $r_{opt}$  can be found at a larger  $b$ . It can be also found from Fig. 8 that the  
 385 effect of compression ratio on the performance of the proposed system becomes more  
 386 significant as the operating current density increases.

387

### 388 **3.6 Effect of internal irreversibility factor and dissipation power**

389 The effects of internal irreversibility factor ( $I_R$ ) and dissipation power ( $b$ ) on the  
 390 performance of the proposed system are shown in Fig. 9, where the involved values of  
 391 compression ratio are assigned from Table 3 to maximize the efficiency of the Otto heat engine.  
 392 In the region of  $i > i_{in}$ , significant effects of irreversibility factor and dissipation power can be  
 393 found at large operating current density as more heat is provided from the DC-SOFC to the  
 394 Otto heat engine. The power density and efficiency of the proposed system both increase with  
 395 increasing  $I_R$  or decreasing  $b$ . When both the internal irreversible losses and the friction-like  
 396 losses are negligible, the power density and efficiency of the proposed system can be drawn as  
 397 the black square lines in Fig. 9. In this situation, Eqs. (27) and (28) can be reduced into

$$398 \quad \eta_{Otto} = 1 - r^{1-\gamma}, \quad (37)$$

399 and

$$400 \quad P_{Otto} = Q(1 - r^{1-\gamma}). \quad (38)$$

401

## 402 **4. Conclusions**

403 The previously developed 2D tubular DC-SOFC model shows that the overall heat

404 generated in the cell could be smaller than, equal to or higher than the heat demand by the  
405 internal Boudouard reaction. A novel hybrid system consists of a DC-SOFC, an external heat  
406 source, a regenerator and an Otto heat engine is proposed to improve the performance of the  
407 DC-SOFC. Based on the thermal characteristics of the DC-SOFC, three operation modes are  
408 presented. The analytical expressions for the proposed system under different operating  
409 conditions are derived to evaluate its performance. The results show that the proposed system  
410 is technically feasible and effective, and the equivalent power density of the proposed system  
411 could be increased by up to 80% compared to the stand-alone DC-SOFC. Comprehensive  
412 parametric studies show that there exists an optimum value for the compression ratio to  
413 maximize the efficiency of the Otto heat engine, and increasing the operating temperature,  
414 operating current density and internal irreversibility factor will increase the overall power  
415 density and efficiency of the proposed system. Furthermore, decreasing dissipation power and  
416 the distance between carbon layer and anode electrode are also benefit to improve the  
417 equivalent power density and efficiency of the DC-SOFC based hybrid system.

418

#### 419 **Acknowledgement**

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425

426 **Nomenclature**

427 **Abbreviation**

CHP	Combined heat and power
DC-SOFC	Direct-carbon solid oxide fuel cell
LSM	Strontium-doped lanthanum manganite
Otto	Otto heat engine
SCCM	Standard cubic centime per minute
SOFC	Solid oxide fuel cell
TPB	Triple phase boundary
YSZ	Yttrium stabilized zirconium

428

429 **Roman**

$b$	Power dissipation due to friction, W
$B_0$	Permeability coefficient, $m^2$
$c_{CO_2}$	Molar concentration of carbon dioxide, $mol \cdot m^{-3}$
$C_p$	$C_p$ is constant-pressure heat capacity, $J \cdot K^{-1}$
$C_v$	$C_v$ is constant-volume heat capacity, $J \cdot K^{-1}$
$C_{V_1}$	Heat capacity of the gases in the compression stroke, $J \cdot K^{-1}$
$C_{V_2}$	Heat capacity of the gases in the power strokes, $J \cdot K^{-1}$
$D_{ce}$	Distance between carbon layer and anode, $\mu m$
$D_m^{eff}$	Effective diffusivity of species $m$ , $m^2 \cdot s^{-1}$
$E_{act}$	Activation energy, $J \cdot mol^{-1}$
$E_{CO}$	Equilibrium potential for carbon monoxide oxidization, V
$E_{CO}^0$	Standard equilibrium potential for carbon monoxide oxidization, V

$E_{eq}$	Equilibrium Nernst potential, V
$F$	Faraday constant, $96485 \text{ C}\cdot\text{mol}^{-1}$
$F_f$	Friction force, N
$i_o$	Exchange current density, $\text{A}\cdot\text{m}^{-2}$
$I$	Electrical current, A
$I_R$	Internal irreversibility factor
$K_1 ; K_2$	Constant temperature rate in Eq. (18), ( $\text{s K}^{-1}$ )
$n$	Number of electrons transferred per electrochemical reaction
$N_i$	Flux of mass transport, $\text{kg}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$
$p$	(partial) Pressure, Pa
$P$	Power output, W
$P_f$	Friction-related power loss, W
$P_{Otto,r}$	Reversible power of the Otto heat engine, W
$r$	Compression ratio
$R$	Gas constant, $8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
$R_{ce}$	Reaction rate of Boudouard reaction, $\text{mol}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$
$\Delta S_{W1}$	Entropy change along the hot isothermal branch, $\text{J}\cdot\text{K}^{-1}$
$\Delta S_{W2}$	Entropy change along the cold isothermal compression branch, $\text{J}\cdot\text{K}^{-1}$
$\Delta t_{12}$	Time spent in the power stroke, s
$T$	Temperature, K
$T_{1-4}$	Temperatures of the working substance at the state points 1, 2, 3 and 4
$u$	Velocity field, $\text{m}^3\cdot\text{s}^{-1}$
$V$	Volume fraction
$V_1$	Working substance volume along the constant-volume cooling branch, $\text{m}^3$

$V_2$	Working substance volumes along the constant-volume heating branch, $\text{m}^3$
$W_{\text{Otto},r}$	Reversible work of the Otto heat engine, W
$x_2$	Piston position at minimum volume, m
$y_k$	Molar fraction of component k

#### Greek letters

$\alpha$	Charge transfer coefficient
$\beta_{\text{H}_2}$	Electrochemical kinetics parameter for $\text{H}_2$
$\gamma$	Ratio of specific heats
$\varepsilon$	Porosity
$\eta$	Efficiency
$\eta_{\text{act}}$	Activation polarization, V
$\eta_{\text{ohmic}}$	Ohmic polarization, V
$\kappa$	Permeability, $\text{m}^2$
$\lambda$	Thermal conductivity, $\text{W}\cdot\text{m}^{-1}\text{K}^{-1}$
$\mu$	Dynamic viscosity of fluid, $\text{Pa}\cdot\text{s}$
$\theta$	Friction coefficient, $\text{J}\cdot\text{s}\cdot\text{m}^{-2}$
$\rho$	Fluid density, $\text{kg}\cdot\text{m}^{-3}$
$\sigma$	Conductivity, S/m
$\tau$	Tortuosity
$\tau_t$	Period of the Otto cycle, s
$\emptyset$	Potential, V

#### Subscripts

an	Anode
ca	Cathode

CO	Carbon monoxide
CO <sub>2</sub>	Carbon dioxide
H <sub>2</sub>	Hydrogen
l	Ionic phase
O <sub>2</sub>	Oxygen
r	Reversible
s	Electronic phase

#### Superscripts

0	Parameter at equilibrium conditions
eff	Effective
L	Local

430

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557

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560 Table 2. Parameters used in Otto heat engine.

561 Table 3. Optimum value of compression ratio  $r_{opt}$  under different power dissipation  $b$ , the

562 other parameters are as the same in Table 1 and Table 2.

563

564 Table 1. Model parameters used in DC-SOFC [15, 44, 45].

Parameters	Value or expression	Unit
Ionic conductivity		
$\sigma_{\text{GDC}}$	$\frac{100}{T} \times 10^{(6.66071 - \frac{5322.92}{T})}$	$\text{S m}^{-1}$
$\sigma_{\text{YSZ}}$	$3.34 \times 10^4 e^{-\frac{10300}{T}}$	$\text{S m}^{-1}$
Electronic conductivity		
$\sigma_{\text{silver}}$	$\frac{1.59 \times 10^8}{(0.0038T - 0.1134)}$	$\text{S m}^{-1}$
Porosity		
$\varepsilon_{\text{an}}$	0.46	
$\varepsilon_{\text{ca}}$	0.46	
Electrode volume fraction		
$V_{\text{GDC}}$	0.21	
$V_{\text{silver}}$	0.79	
TPB length of electrode		
Anode	$2.14 \times 10^5$	$\text{m}^2 \text{m}^{-3}$
Cathode	$2.14 \times 10^5$	$\text{m}^2 \text{m}^{-3}$
Tortuosity		
$\tau_{\text{an}}$	3	
$\tau_{\text{ca}}$	3	
Exchange current density		
$i_0^{\text{CO}}$	450	$\text{A m}^{-2}$
$i_0^{\text{O}_2}$	400	$\text{A m}^{-2}$

Charge transfer coefficient		
$\alpha_{\text{CO}}$	0.5	
$\alpha_{\text{O}_2}$	0.5	
Equilibrium constant of Boudouard reaction	$k_{\text{rb}} = 6 \times 10^{13}$	1/s
Activation energy of Boudouard reaction	$E_{\text{rb}} = 248$	$\text{kJ mol}^{-1}$

565

566



567 Table 2. Parameters used in Otto heat engine [46, 47].

Parameter	Value
Constant-volume heat capacity during the compression stroke, $C_{V_1}$ (J K <sup>-1</sup> )	0.2988
Constant-volume heat capacity during the power stroke, $C_{V_2}$ (J K <sup>-1</sup> )	0.4372
Constant temperature rate, $K_1$ (s K <sup>-1</sup> )	$8.128 \times 10^{-6}$
Constant temperature rate, $K_2$ (s K <sup>-1</sup> )	$1.867 \times 10^{-5}$
Compression ratio, $r$	9.26
Specific heat ratio, $\gamma$	1.4
Dissipation power due to friction $b$ (W)	32.5

568

569

570 Table 3. Optimum value of compression ratio  $r_{opt}$  under different power dissipation  $b$ , the

571 other parameters are as the same in Table 1 and Table 2.

$b$ (W)	0	16.25	32.5	48.75
$r_{opt}$	-	12.48	9.26	7.80

572

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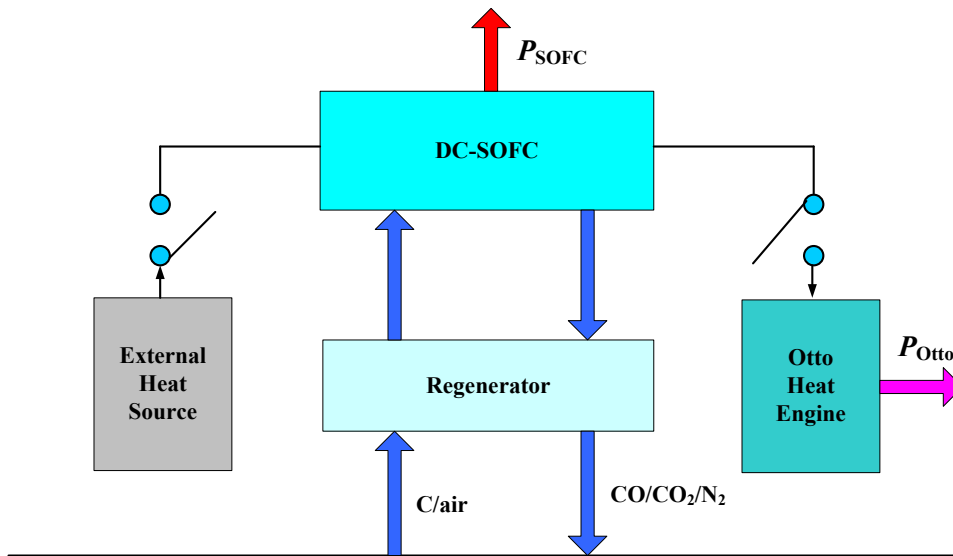
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592 performance of the proposed system at 1123 K.

593

594 Fig. 1.

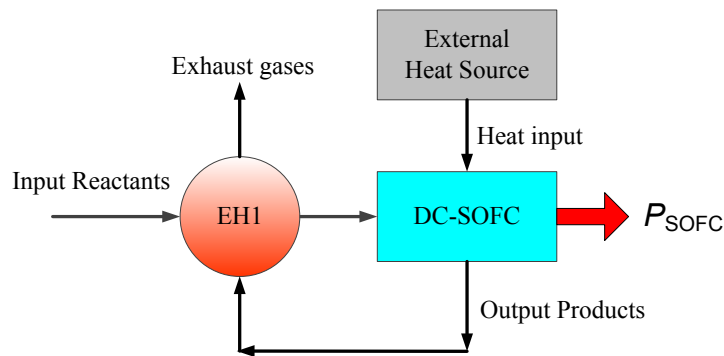


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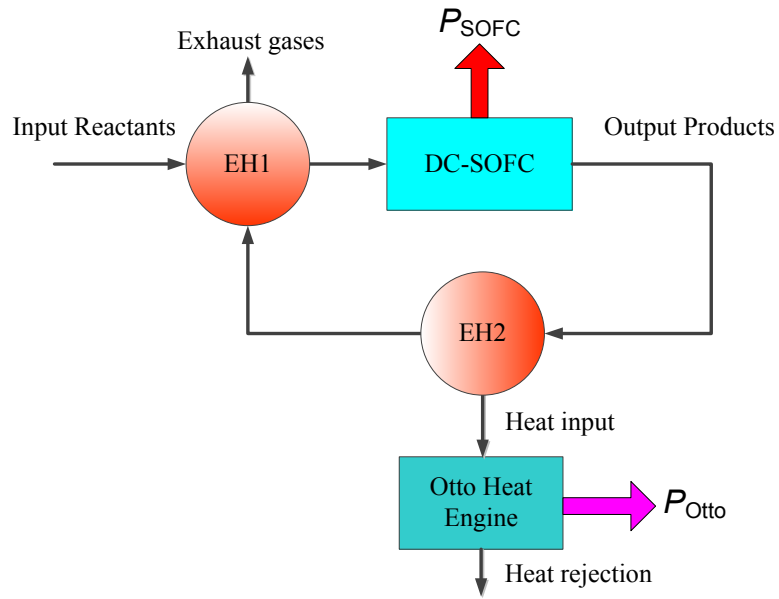
Fig. 1. (a) Schematic diagram of a DC-SOFC based system.

597



598

599 Fig. 1. (b) Schematic diagram of the heat and mass transfer process at small operating current  
600 density.



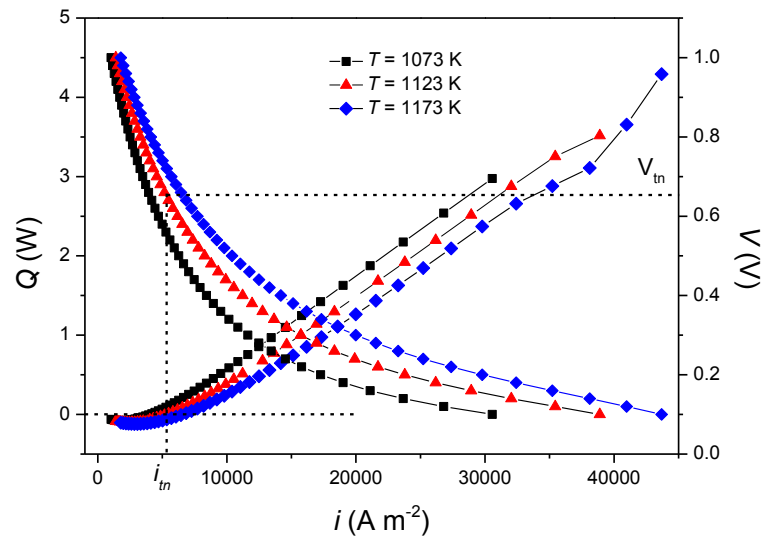
601

602 Fig. 1. (c) Schematic diagram of the heat and mass transfer process at large operating current

603 density.

604

605 Fig. 2.



606

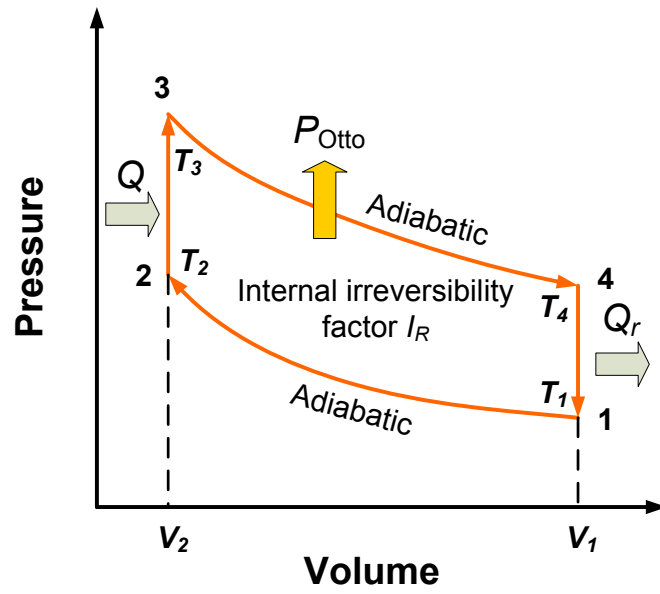
607 Fig. 2. The curves of  $Q$  and  $V$  versus current density under different operating temperature,

608 where  $i_{tn} = I_{tn}/A$ ,  $A$  is the polar plate area of the DC-SOFC,  $V_{tn}$  is the voltage

609 corresponding to  $i_{tn}$ .

610

611 Fig. 3.



612

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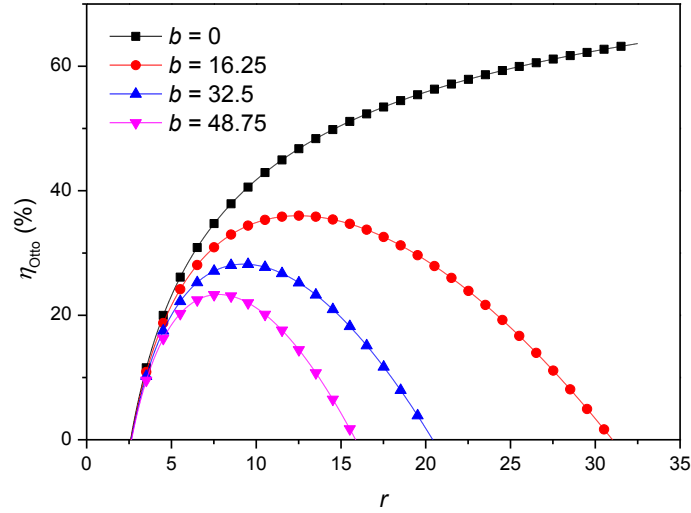
Fig. 3. The pressure-volume diagram of the internal irreversible Otto cycle.

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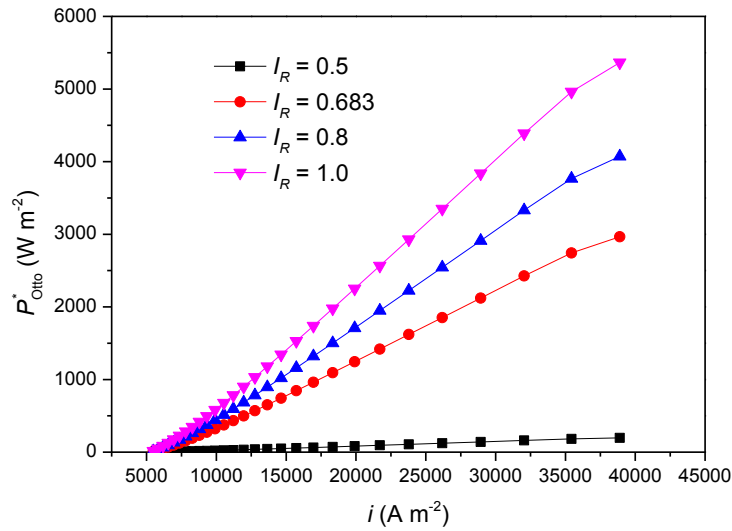
616 Fig. 4.

(a)



617

(b)



618

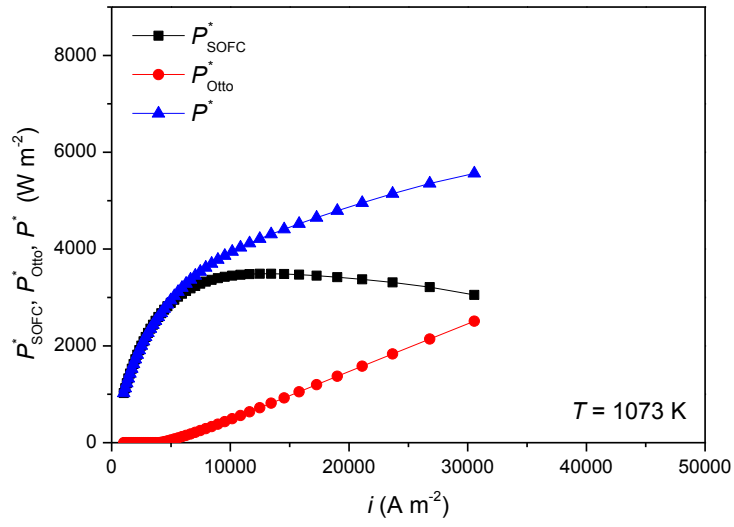
619 Fig. 4. The (a) efficiency, and (b) equivalent power density of the Otto heat engine under

620 different operating conditions, where  $P_{\text{Otto}}^* = P_{\text{Otto}} / A$  is the equivalent power density of the

621 Otto heat engine.

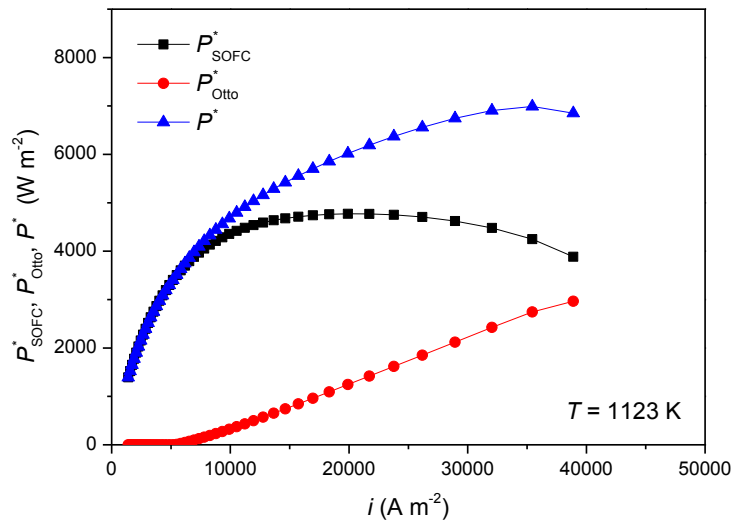
622

(a)



624

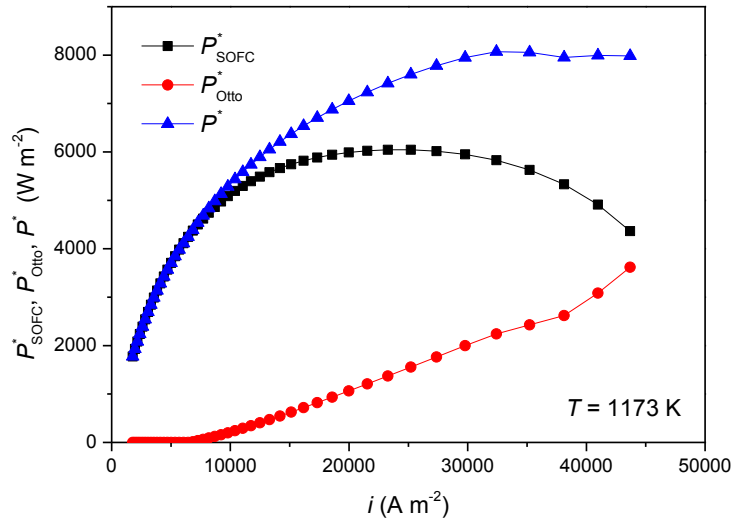
(b)



625



(c)



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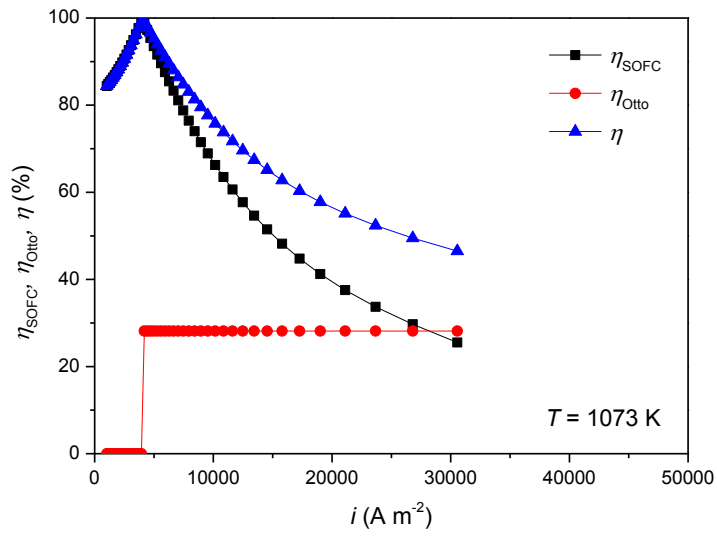
627 Fig. 5. Equivalent power densities of the DC-SOFC, Otto heat engine and proposed system at

628 (a) 1073 K, (b) 1123 K and (c) 1173 K.

629

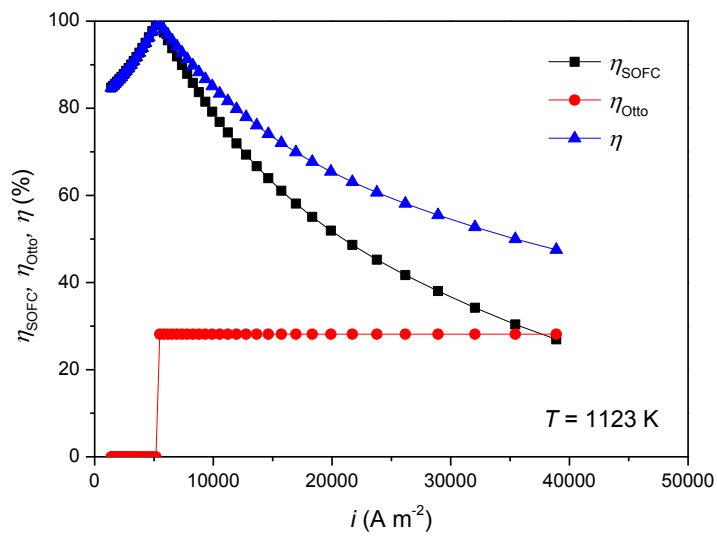
630 Fig. 6.

(a)

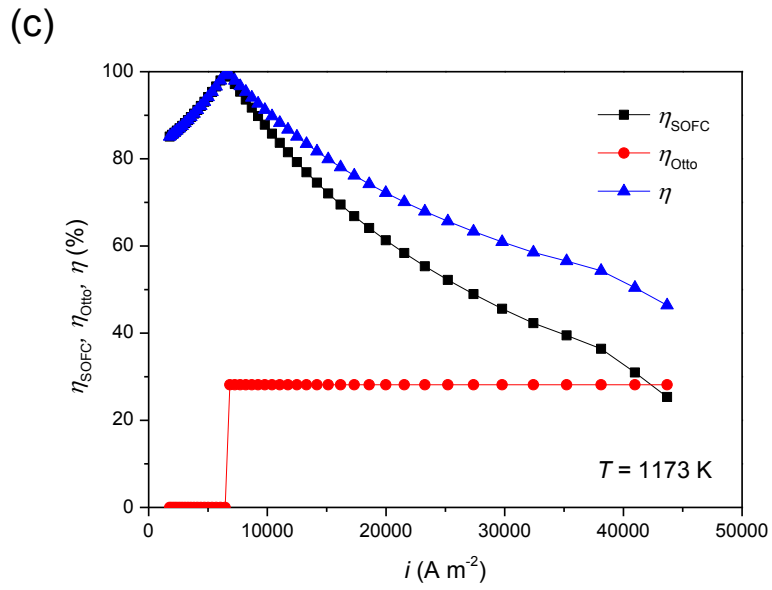


631

(b)



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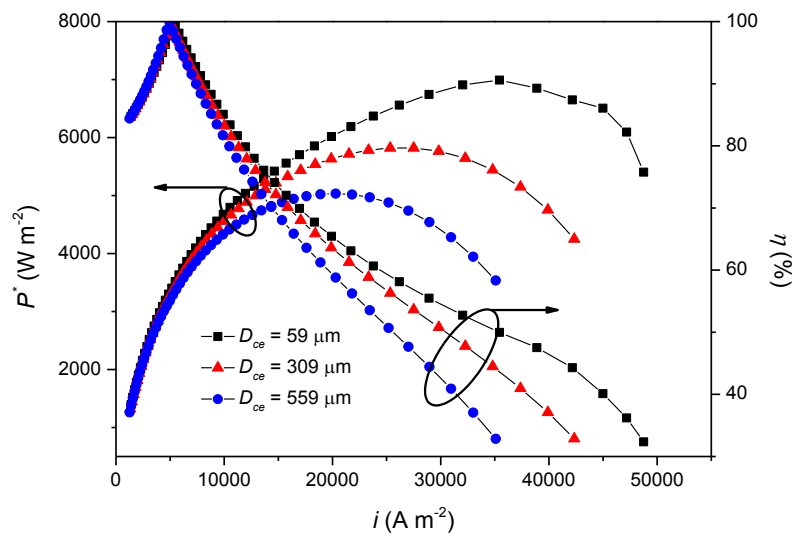
633

634 Fig. 6. Equivalent efficiencies of the DC-SOFC, Otto heat engine and proposed system at (a)

635 1073 K, (b) 1123 K and (c) 1173 K.

636

637 Fig. 7.



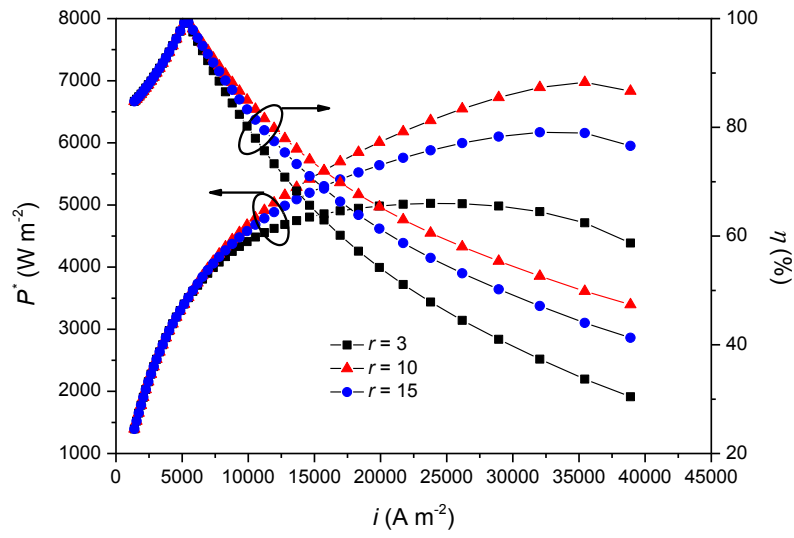
638

639 Fig. 7. Effects of distance between carbon layer and anode electrode on the performance of the

640 proposed system at 1123 K.

641

642 Fig. 8.

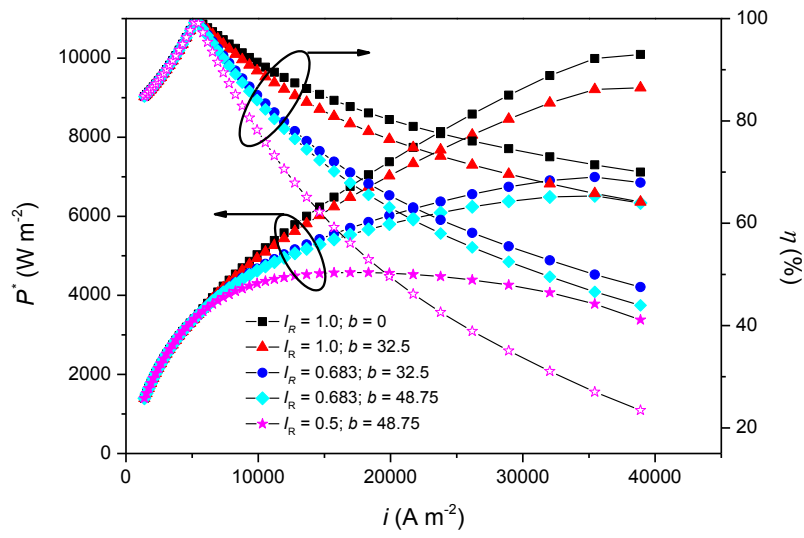


643

644 Fig. 8. Effects of compression ratio on the performance of the proposed system at 1123 K.

645

646 Fig. 9.



647

648 Fig. 9. Effects of compression ratio and power dissipation of the Otto heat engine on the  
649 performance of the proposed system at 1123 K.

650