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1 Analysis of the Effect of Syngas Substitution of Diesel on the Heat Release Rate and  
2 Combustion Behaviour of Diesel-Syngas Dual Fuel Engine

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10

11 **Abstract**

12 The Heat Release Rate (HRR) model of ICEs is known to be most sensitive to the ratio of  
13 specific heats,  $\gamma$ , which is known to be depended on temperature and the excess air ratio,  $\lambda$ .  
14 The HRR of ICEs cannot be measured directly. As such, accurate HRR models, as well as  
15 accurate expressions of  $\gamma$  and  $\lambda$  are required to model the HRR behaviour of ICEs  
16 mathematically. In this work, an improved HRR model based on  $\gamma(T, \lambda)$  was used to  
17 investigate the effect of syngas substitution of diesel at constant energy on the Heat Release  
18 Rate (HRR) behaviour and the combustion phasing in a 5.7 kW engine out and 4.3 kW  
19 generator output, single cylinder, dual fuel, Reactivity Controlled Compression Ignition (RCCI)  
20 mode CI engine. An improved global excess air ratio,  $\lambda_g$  was used in the HRR analysis of the  
21 dual fuel engine. The engine was run on 10, 25, and 45% syngas substitution (by energy) and  
22 at 1, 2, 3, and 4 kW loads (generator output) for each syngas substitution. The improved dual  
23 fuel engine HRR model was validated by comparing the measured fuel consumption by energy  
24 (input energy) per (thermodynamic) cycle to the predicted fuel consumption by energy per  
25 cycle for the tested conditions. The values of the fuel consumption predicted by the Leeds  
26 HRR model were also compared to the predictions of the HRR models that were based on

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27  $\gamma(T)$ . The overall average error in the predictions of the fuel input energy by the Leeds HRR  
28 model was 2.41% with a standard deviation of 1.65. The overall average errors in the other  
29 models ranged from 6.26 to 8.29%. The SoC, MFB50, PP, and PHRR occurred later for the  
30 diesel-syngas dual fuels compared to baseline diesel due to increased ignition delay as the  
31 fraction of syngas was increased. The current work showed that the use of diesel-syngas dual  
32 fuel in diesel engines in Nigeria (a developing country) can potentially reduce CO<sub>2</sub> emissions  
33 by up to ~0.26 million tonnes.

34 Key words: Dual-fuel engine, combustion, syngas, RCCI, global lambda, modelling

### 35 **Nomenclature**

36 Symbols:

37	$A_s$	Surface area
38	$b$	Coefficients of ratio of specific heats function for burned mixtures
39	$c_m$	Mean piston speed
40	$c_p$	Specific heat capacity at constant pressure
41	$c_v$	Specific heat capacity at constant volume
42	$h$	Heat transfer coefficient
43	$h_{bb}$	Enthalpy of blow-by gases
44	$K_1$	Constant
45	$m$	Amount of gas in cylinder
46	$\dot{m}$	Mass flow rate
47	$m_{bb}$	Mass of blow-by gases
48	$m_f$	Mass of injected fuel
49	$p$	Pressure
50	$p', p''$	Differentials of pressure
51	$Q$	Heat released from injected fuel
52	$Q_b$	Heat loss through blow-by gases

53	$Q_w$	Heat loss through cylinder walls
54	$q_e$	Heat of evaporation of fuel
55	$R$	Universal gas constant
56	$R'$	Ratio of length of connecting rod to crank radius
57	$r$	Compression ratio
58	$T$	Temperature
59	$V$	Volume
60	$W$	Pressure–volume work

61

62 Greek symbols:

63	$\gamma$	Specific heats ratio
64	$\delta$	Blow-by gap
65	$k_1, k_2$	Constants
66	$\lambda$	Excess air ratio
67	$\phi$	Equivalence ratio
68	$\pi$	Constant
69	$\rho$	Density
70	$\theta$	Crank Angle Degree

71 Subscripts:

72	$bb$	Blow–by
73	$d$	Displaced
74	$e$	Evaporation
75	$eff$	Effective
76	$g$	Global
77	$m$	Mean
78	$mod$	Modified
79	$ref$	Reference

80	<i>s</i>	Surface
81	<i>stoich</i>	Stoichiometric
82	<i>w</i>	Wall
83	Abbreviations:	
84	AFR	Air Fuel Ratio
85	aTDC	After Top Dead Centre
86	bTDC	Before Top Dead Centre
87	CAD	Crank Angle Degree
88	CHR	Cumulative Heat Release
89	CI	Compression Ignition
90	CN	Cetane Number
91	Cv	Calorific value
92	DI	Direct Injection
93	DoC	Duration of Combustion
94	EGR	Exhaust Gas Recirculation
95	EoC	End of Combustion
96	EVC	Exhaust Valve Closing
97	GTL	Gas-to-Liquid
98	HRR	Heat Release Rate
99	HVO	Hydrotreated Vegetable Oil
100	ICE	Internal Combustion Engine
101	ID	Ignition Delay
102	IMEP	Indicated Mean Effective Pressure
103	IVC	Intake Valve Closing
104	LTC	Low Temperature Combustion
105	MFB	Mass Fraction Burned
106	MFIS	Multiple Fuel Injection Strategy
107	PHRR	Peak Heat Release Rate

108	PP	Peak Pressure
109	PT	Peak Temperature
110	RCCI	Reactivity Controlled Compression Ignition
111	rpm	Revolutions per minute
112	SG	Diesel-syngas dual fuel
113	SoC	Start of Combustion
114	ULSD	Ultra Low Sulphur Diesel

115

## 116 **1. Introduction**

117 The utilization of syngas in diesel generators will widen the fuel choices and availability in  
 118 those developing countries with abundant biomass to produce syngas [1]. Fossil fuels require  
 119 large-scale refining and transport infrastructure, and are also subject to geopolitical events  
 120 that can affect social stability, price and availability [2,3]. Diesel supply is limited in many rural  
 121 and remote areas creating a constraint to sustainable development. Diesel-syngas dual fuel  
 122 is beneficial and desirable in developing countries because it provides alternative fuel sources  
 123 and enhances the use of renewable fuels for electricity generation. The use of diesel-syngas  
 124 dual fuel for electricity generation can be achieved through Reactivity Controlled Compression  
 125 Ignition (RCCI) technology.

126 RCCI technology is a combustion technology that involves the utilization of at least two fuels  
 127 of different reactivities to optimize the phasing of the combustion in Compression Ignition (CI)  
 128 engines. The use of two fuels of different reactivities or Cetane Number (CN) in CI engines  
 129 has the potential to reduce the Peak Pressure Rise Rate (PPRR), the Peak Heat Release  
 130 Rate (PHRR), the Peak Pressure (PP), and the Peak Temperature (PT). Therefore, RCCI is  
 131 a Low Temperature Combustion (LTC) technology that can potentially reduce engine-out NOx  
 132 emissions. The determination and optimization of the combustion phasing of diesel-syngas  
 133 dual-fuel RCCI engines require accurate Heat Release Rate (HRR) models. The HRR models  
 134 of ICEs are based on the First Law of thermodynamics [4]. The accuracy of the HRR models

135 of Internal Combustion Engines (ICEs) is strongly depended on the specific heats ratio ( $\gamma$ ).  
136 The specific heats ratio,  $\gamma$  on the other hand has been shown to be strongly depended on the  
137 temperature ( $T$ ) of the gases in the cylinder as well as the excess air ratio ( $\lambda$ ) [5]. Therefore,  
138 accurate models (expressions) of  $\lambda$  are also required in HRR analysis. The Leeds HRR model  
139 has been validated for liquid fuels: pure diesel as well as alternative diesels: Gas-to-Liquid  
140 (GTL) diesel and Hydrotreated Vegetable Oil (HVO) diesel [5,6]. The improved accuracy of  
141 the Leeds HRR model is mainly due to the expression of  $\gamma$  as a function of  $T$  and  $\lambda$ . The aim  
142 of the current work was to validate and apply the Leeds HRR model to diesel-syngas dual-fuel  
143 combustion in an RCCI engine. The current work was carried out on a 5.7 kW, single cylinder,  
144 RCCI mode engine with a modern combustion chamber design (re-entrant bowl piston).  
145 Notwithstanding, the model results here presented are generally applicable to RCCI mode  
146 diesel-syngas dual-fuel engines.

#### 147 1.1 Previous works on diesel-syngas dual fuel HRR analysis

148 The effect of simulated syngas substitution of diesel on the combustion characteristics and  
149 engine performance was investigated by Garnier et al. [7] using a Litter-Petter diesel engine.  
150 The authors validated their HRR model (derived from Wiebe's Law) by comparing it graphically  
151 to the model that was derived from the measured pressure-crank angle degree (P-CAD) data.  
152 According to the authors, the PHRR decreased in the first stage of the combustion when the  
153 pilot fuel (diesel) was <45-50%. The authors reported that the Ignition Delay (ID) decreased  
154 as the syngas substitution increased. Le Anh and Hoang [8] studied the effect of diesel-syngas  
155 dual fuel on a 3-cylinder, 8.75 kW diesel engine. The authors utilized real syngas in their work  
156 and reported that the HRR of the engine increased as the flow of syngas was increased. The  
157 authors attributed this to the high flame speed of the hydrogen and the carbon monoxide  
158 components of the tested syngas. According to the authors, the engine-out CO increased as  
159 the ratio of syngas increased in the dual fuel. The maximum substitution of diesel that was  
160 reported was 60% at the investigated engine condition (1,500 rpm and an Indicated Mean  
161 Effective Pressure (IMEP) of 6.54 bar).

162 Le Anh and Hoang [8] utilized the flow rates of diesel, syngas, and air to evaluate the global  
163 excess air ratio, as shown in Equation 1.

$$164 \quad \lambda = \frac{\dot{m}_{air}}{[(\dot{m}_{diesel} \times AFR_{stoich\_diesel}) + (\dot{m}_{syngas} \times AFR_{stoich\_syngas})]} \quad 1$$

165  $\dot{m}_{air}$ ,  $\dot{m}_{diesel}$ , and  $\dot{m}_{syngas}$  are the mass flow rates of air, diesel, and syngas respectively,  
166  $AFR_{stoich}$  is the stoichiometric air-fuel ratio (AFR). The use of the flow rates in Equation 1 can  
167 lead to errors in the estimated values of the global  $\lambda$  because the combustion of fuel in ICEs  
168 is a periodic phenomenon.

169 Guo et al. [9] investigated the effect of syngas fraction and composition on the energy  
170 efficiency, cylinder pressure, exhaust temperature, and combustion stability in a 2.44 L, 74.6  
171 kW, single cylinder, diesel engine. Two real syngases and one simulated syngas were used  
172 by the authors. The authors reported that the ID and PP increased as the syngas fraction in  
173 the dual fuel was increased (contrary to what was reported by Garnier et al. [7]). This  
174 underscores the need to further investigate the effect of syngas substitution of diesel on the  
175 ID of diesel-syngas dual fuel engines.

176 Mahgoub et al. [10] investigated the effect of CO<sub>2</sub> removal from a simulated syngas on the  
177 performance of syngas dual-fuel engine at 1,850 rpm. A simulated, typical syngas and a  
178 simulated high hydrogen syngas were used in the investigation. Biodiesel blend (B50) was  
179 used as the direct-injection (pilot) fuel. The authors reported a maximum pilot fuel substitution  
180 of 47% with simulated syngas. The authors did not investigate the effect of the dual fuel on  
181 the ID of the engine.

182 Kousheshi et al. [11] investigated the effect of various types of syngas mixtures on the  
183 combustion process and the emission characteristics in diesel-syngas RCCI engine using a  
184 2.44 L, single cylinder diesel engine. The HRR of the dual-fuel engine was modelled using a  
185 commercial software (CONVERGE). The authors reported that, as the ratio of hydrogen in the



186 syngas increased, the ID decreased, the crank angle at which 50% of the injected fuel was  
187 burned (MFB50) was advanced, while the HRR became steeper.

188 Rith et al. [12] studied the effect of increasing the flow rate of real syngas on the PHRR. The  
189 authors utilized a 5.7 kW, single cylinder, naturally aspirated diesel engine in their  
190 investigation. The engine was run at 3,000 rpm and 35, 53, and 70% loads. The authors  
191 reported that the PHRR decreased and occurred later as the flow rate of the syngas was  
192 increased.

193 The foregoing discussion shows that contradicting results have been reported in literature in  
194 terms of the effect of syngas substitution of diesel on the ID of CI engines. Therefore, there is  
195 a need to further investigate the effect of syngas substitution of diesel on the phasing of the  
196 combustion as well as the ID of CI engines. In the current work, the modified  $\gamma$  function of  
197 Ceviz and Kaymaz [13],  $\gamma_{mod}(T, \lambda)$  (Equation 2) and the Leeds HRR model developed by  
198 Olanrewaju et al. [5] were validated for a 5.7 kW diesel-syngas dual-fuel engine.

$$199 \gamma_{mod} = b_1 + b_2T + b_3/\lambda + b_4T^2 + b_5/\lambda^2 + b_6T/\lambda + b_7T^3 + b_8/\lambda^3 + b_9T/\lambda^2 + b_{10}T^2/\lambda \quad 2$$

200  $T$  in Equation 2 represents the temperature of the gases in the combustion chamber. The  
201 values of the constants  $b_1$  to  $b_{10}$  in Equation 2 are given in the Appendix as reported by Ceviz  
202 and Kaymaz [13].

## 203 **2. Methodology**

### 204 **2.1 Diesel-syngas dual-fuel engine HRR model development**

205 The Leeds HRR model shown in Equation 3 [5] was adopted in the current work to model the  
206 HRR of the diesel-syngas dual-fuel engine.

$$207 \frac{dQ}{d\theta} = \frac{\gamma}{\gamma-1} p \frac{dV}{d\theta} + \frac{1}{\gamma-1} V \frac{dp}{d\theta} + \frac{dQ_w}{d\theta} + h_{bb} \frac{dm_{bb}}{d\theta} + q_e \frac{dm_f}{d\theta} \quad 3$$

208 The terms in Equation 3 were explained in the previous works [5,6]. The last term in Equation  
209 3 (heat loss due to the evaporation of the injected fuel mass) was determined in the current

210 work after the HRR and CHR profiles were generated from the basic input data (P-CAD data).  
211 The heat absorbed from the combustion chamber to vaporize the injected fuel was estimated  
212 by multiplying the product of the total input energy and the fraction of diesel by the ratio of the  
213 heat of evaporation and Cv of diesel.

214 The instantaneous volume of the cylinder,  $V$  was calculated from Equation 4 [14].

$$215 \quad V = (V_d/(r - 1)) + (V_d/2)[R' + 1 - \cos \theta - \sqrt{R'^2 - \sin^2 \theta}] \quad 4$$

216  $V_d$  is the displaced volume,  $r$  is the compression ratio, and  $R'$  is the ratio of the length of the  
217 connecting rod to the crank radius.

218 The global excess air ratio ( $\lambda_g$ ) that was used in Equation 2 was improved by using the trapped  
219 masses of air, syngas, and diesel rather than the flow rates as shown in Equation 5.

$$220 \quad \lambda_g = \frac{m_{air}}{[(m_{diesel} \times AFR_{stoich\_diesel}) + (m_{syngas} \times AFR_{stoich\_syngas})]} \quad 5$$

221  $m_{air}$ ,  $m_{diesel}$ , and  $m_{syngas}$  in Equation 5 represent the trapped masses of air, diesel, and  
222 syngas respectively. The volumetric efficiency of the engine for air intake during the intake  
223 stroke was determined by experiment as 85%. The ratio of specific heats,  $\gamma$  was estimated by  
224 substituting the modified expression for  $\lambda_g$  (Equation 5) into Equation 2.

225 The Leeds HRR model was validated for the dual-fuel RCCI engine by comparing the  
226 predicted fuel input energy per thermodynamic cycle to the input energy per cycle estimated  
227 from the injected fuel masses. The predictions of the Leeds HRR model were also compared  
228 to those obtained by using the  $\gamma$  functions of Gatowsky et al. [15], Brunt and Emtage [16],  
229 Egnell [17], and Blair [18] in the HRR model.

## 230 2.2 Model assumptions

231 The following assumptions were made to apply the improved Leeds HRR model to diesel-  
232 syngas dual-fuel RCCI engine:

- 233 1. Single zone combustion (combustion parameters were uniform in the cylinder).

- 234 2. A zero-dimensional (transient) HRR model.
- 235 3. Ideal gas behaviour.
- 236 4. The concentration of oxygen in the residual gas in the clearance volume after the
- 237 exhaust stroke is close to that of air due to lean combustion in diesel engines.

238 2.3 Engine description and instrumentation

239 The details of the engine, instrumentation and test conditions that were used are summarized

240 in Tables 1, 2 and 3. Each of the tested fuels (SG0 (baseline diesel), SG10, SG25, and SG45)

241 was tested at the power conditions given in the third column of Table 3. The basic model input

242 data (the P-CAD data) were measured by a pressure sensor and AVL FlexIFEM Indi 601 (2-

243 channel). The pressure data were averaged over 50 cycles and logged by LabView software.

244 The HRR model was solved and analyzed in Microsoft Office Excel software.

245 Table 1 Engine specifications

Parameter	Specification
Type	4-stroke, single cylinder
Make	Yanmar, 2019 model year, EU Stage V emission compliant,
Rated power	5.7 kW
Speed	3,000 rpm
Bore x Stroke	86 mm x 75 mm
Compression ratio	20.9:1
Displacement	435.66 cm <sup>3</sup>
Total cylinder volume	457.55 cm <sup>3</sup>
Injection pressure	~20 MPa
Injection timing	13° bTDC

246

247

248 Table 2 Instrumentation

<b>Parameter</b>	<b>Equipment specification</b>
Cylinder pressure	AVL FlexIFEM Indi 601 (2-channel), AVL GH14D transducer
Fuel consumption (Diesel)	Scale (ADAM CPW plus-35)
Syngas flow	Omega FMA-1622
Temperature	K-type thermocouples

249

250 Table 3 Test conditions

<b>Test</b>	<b>Dual fuel</b>	<b>Power, kW</b>	<b>Syngas substitution of diesel, % by energy</b>	<b>Equivalent syngas flow, kg/h</b>	<b>Diesel flow, kg/h</b>
1	SG0	1	0	0	0.745
2		2	0	0	0.925
3		3	0	0	1.12
4		4	0	0	1.451
5	SG10	1	10	0.651	0.673
6		2	10	0.806	0.832
7		3	10	0.976	1.008
8		4	10	1.267	1.307
9	SG25	1	25	1.627	0.558
10		2	25	2.016	0.695
11		3	25	2.437	0.839
12		4	25	3.164	1.091
13	SG45	3	45	4.388	0.616
14		4	45	5.695	0.799

251

252

253 2.4 Fuel properties

254 The properties of the diesel and syngas fuels are given in Tables 4 and 5 respectively. The  
255 selected properties of the ULSD fuel (red diesel) used in the test complied with BS2869 (2010)  
256 Class A2. A simulated syngas produced by BOC was used with a heating value of 5.047  
257 MJ/kg.

258 Table 4 Properties of diesel

<b>Property</b>	<b>Diesel</b>
Kinematic viscosity @ 40 °C, mm <sup>2</sup> /s	~2.7
Density @ 15 °C, kg/m <sup>3</sup>	840
Cetane Number (CN)	~48
LHV, MJ/kg	~44
Sulphur content, wt%	<10

259

260 Table 5 Composition of simulated syngas

<b>Component</b>	<b>Mol %</b>	<b>Molar weight, kg/kgmol</b>	<b>LHV, MJ/kg</b>
Hydrogen	15	2.016	121
CO	20	28.01	10.8
CH <sub>4</sub>	4	16.04	50
O <sub>2</sub>	0.98	32	-
CO <sub>2</sub>	12	44.01	-
N <sub>2</sub>	48.02	28.01	-

261

262 2.5 Determination of the Start of Combustion (SoC) and the End of Combustion (EoC)

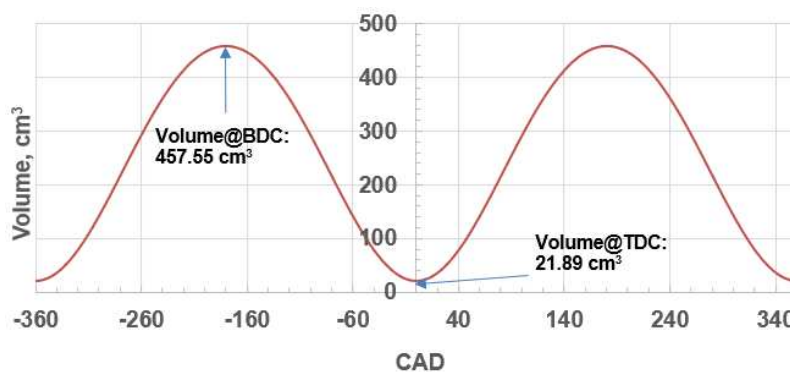
263 The Cumulative Heat Release (CHR) profiles were determined from the modelled HRR  
264 profiles for the tested conditions. Thereafter, the fuel burn profiles were determined from the

265 HRR and the CHR profiles. The Start of Combustion (SoC) was determined for each of the  
266 tested modes by direct inspection of the HRR profile, the first and the second derivatives of  
267 the measured P-CAD data,  $p'$  and  $p''$  respectively. The SoC was taken as the points on the  
268 derivatives where the curves were minimum and then followed by a sudden, consistent rise in  
269 value. The End of Combustion (EoC), on the other hand, was the crank angle at which the  
270 fuel burn profile began to level off after the MFB50.

### 271 3. Results and discussion

#### 272 3.1 Estimated instantaneous volume of the cylinder

273 Figure 1 presents the estimated instantaneous volume of the cylinder of the engine. The  
274 volumes of the cylinder of the engine at the BDC (total volume) and at the TDC (clearance  
275 volume) were  $\sim 458 \text{ cm}^3$  and  $\sim 22 \text{ cm}^3$  respectively.



276

277 Fig. 1 Instantaneous volume of the cylinder of the Gen-set engine

#### 278 3.2 Estimated properties of the simulated syngas

279 The data in Table 5 were used to estimate the stoichiometric AFR ( $AFR_{stoich\_syngas}$ ), the  
280 density, and the Lower Heating Value (LHV) of the syngas. One (1) mole of syngas was taken  
281 as the basis for the estimates. The estimated average molar weight of the simulated syngas  
282 was 25.593 kg/kmol while the estimated stoichiometric AFR, density, and LHV were 1.316 by  
283 mass,  $1.067 \text{ kg/m}^3$ , and 5.047 respectively. The details of the estimates are given in the  
284 Appendix (Tables A.2 and A.3).

285 3.3 Pressure-crank angle data

286 The pressure-crank angle data of the tested conditions were the basic model input data for  
287 the diesel-syngas dual-fuel engine HRR analysis that was carried out. Figure 2 presents the  
288 basic input data. Figure 2 graphically depicts the potential of diesel-syngas dual fuels to reduce  
289 the Peak Pressure (PP) in dual-fuel RCCI engines. As shown in the figure, the PP values for  
290 the tested dual fuels (SG10, SG25, and SG45) decreased below the baseline (SG0) as the  
291 fraction of syngas increased in the dual fuels. Also, the crank angle timing of the PP increased  
292 above the baseline as the flow rate of the syngas increased at constant energy. This was due  
293 to the relatively low CN of syngas compared to pure diesel. Generally, the peak pressures  
294 increased for each of the tested fuels as the power of the engine was increased. Furthermore,  
295 contrary to what was reported by Guo et al. [9], Figure 2 shows that the PP decreased below  
296 the baseline as the fraction of syngas increased.

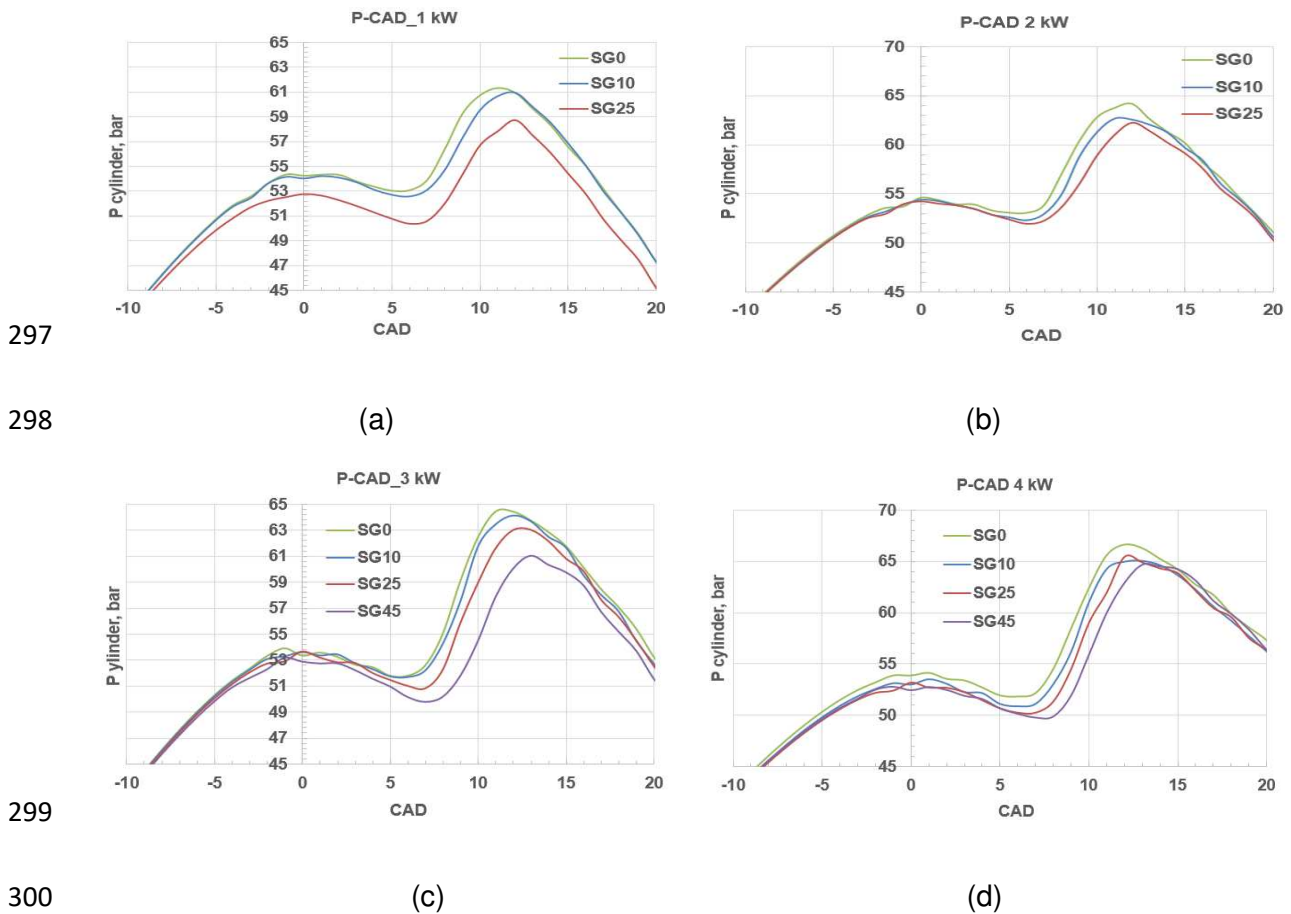
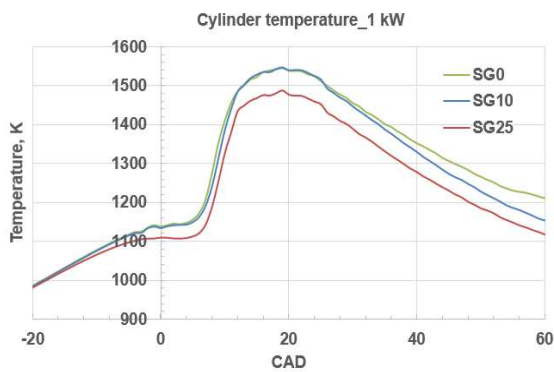


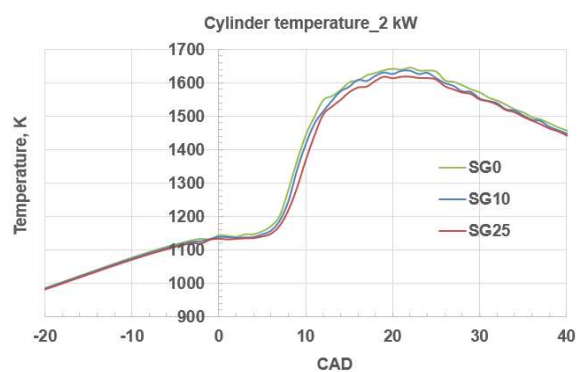
Fig. 2 Pressure traces for the dual fuels at the tested conditions

302 3.4 Calculated instantaneous cylinder temperatures

303 The calculated in-cylinder temperatures are presented in Figure 3. Figure 3 shows that, at  
304 each of the tested loads, the temperature of the flame decreased below baseline diesel as the  
305 fraction of the syngas in the dual fuel was increased. As was the case for the PP, the Peak  
306 Temperature (PT) also increased for each of the tested fuels as the load on the engine was  
307 increased.



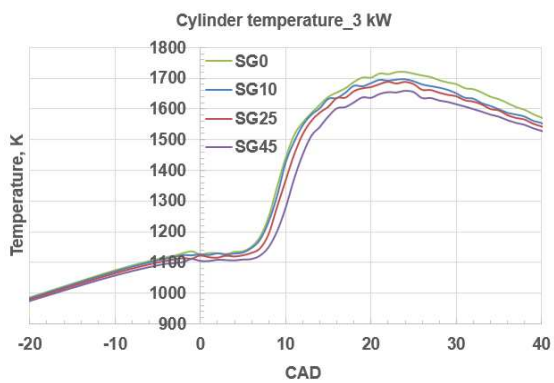
308



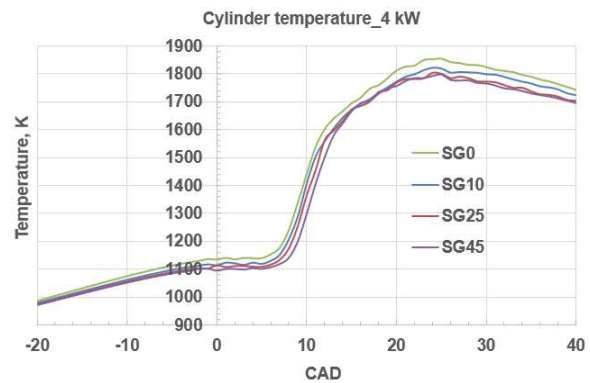
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(a)

(b)



310



311

(c)

(d)

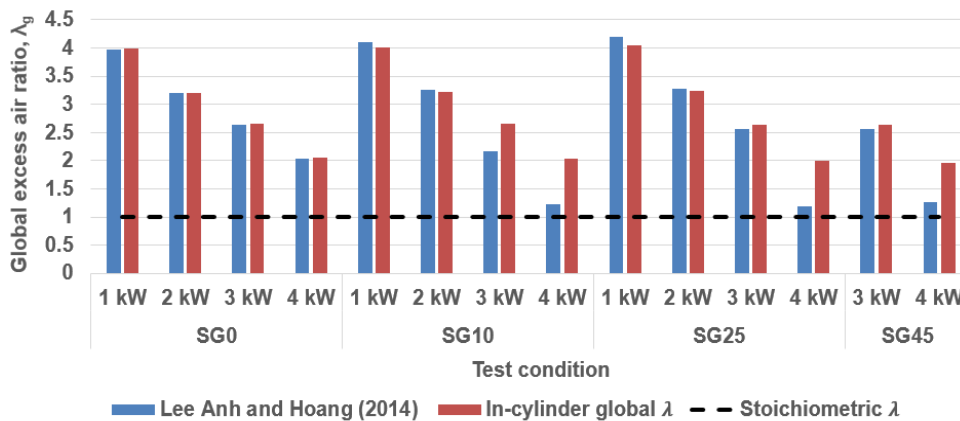
312 Fig. 3 Modelled in-cylinder temperatures

313 3.5 Estimated global excess air ratio,  $\lambda_g$

314 The values of the global excess air ratio,  $\lambda_g$  for the diesel-syngas dual-fuel RCCI engine were  
315 estimated from Equations 1 and 5 and compared graphically as shown in Figure 4. It shows



316 that, for dual fuel operations at the relatively high loads, the values estimated for the  $\lambda_g$  by  
 317 Equation 1 deviated drastically from the values estimated by Equation 5 (the improved  
 318 equation for  $\lambda_g$ ). Furthermore, the estimated values of  $\lambda_g$  for the engine from Equation 1 were  
 319 near-stoichiometric at 4 kW for the tested diesel-syngas dual fuels (SG10, SG25, and SG45).  
 320 Diesel engines are known to operate in lean combustion mode. Therefore, the improved  
 321 equation for  $\lambda_g$  which is based on the trapped masses of the gases and diesel fuel (Equation  
 322 5) is more accurate than the equation that is based on the flow rates of the fuels and air  
 323 (Equation 1).



324

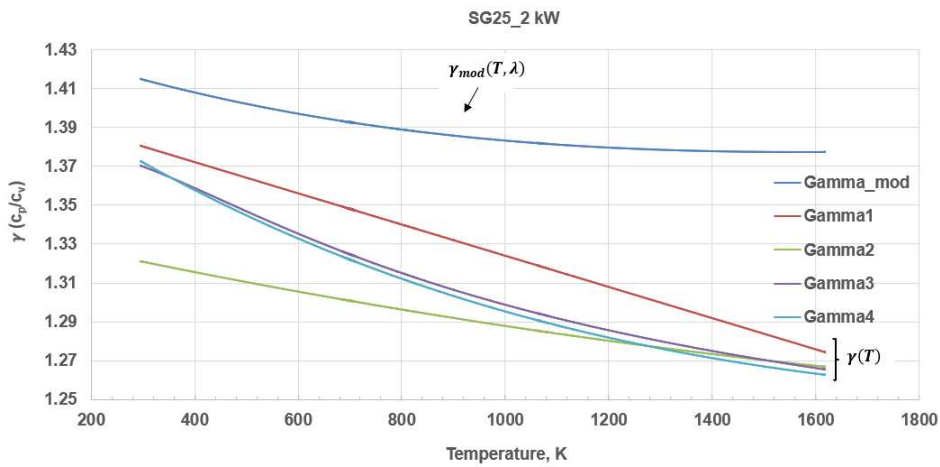
325 Fig. 4 Comparison of the estimated values of the global excess air ratio,  $\lambda_g$

326 Figure 4 shows that as the load on the engine increased for each of the tested fuels,  $\lambda_g$   
 327 decreased (the combustion became richer). This was due to the increase in the masses of the  
 328 diesel-syngas dual fuel as the load on the engine was increased. The increase in the flow rate  
 329 and the trapped mass of the syngas led to a decrease in the trapped mass of air.  
 330 Consequently,  $\lambda_g$  decreased as the power of the engine increased.

331 3.6 Comparison of the modified  $\gamma$  function and the  $\gamma$  functions from literature for diesel-  
 332 syngas dual fuels

333 The modified  $\gamma$  function ( $\gamma_{mod}$ ) and the  $\gamma$  functions from literature were compared graphically  
 334 as shown in Figure 5 (for 25% and 45% syngas substitution at 2 kW and 4 kW respectively).

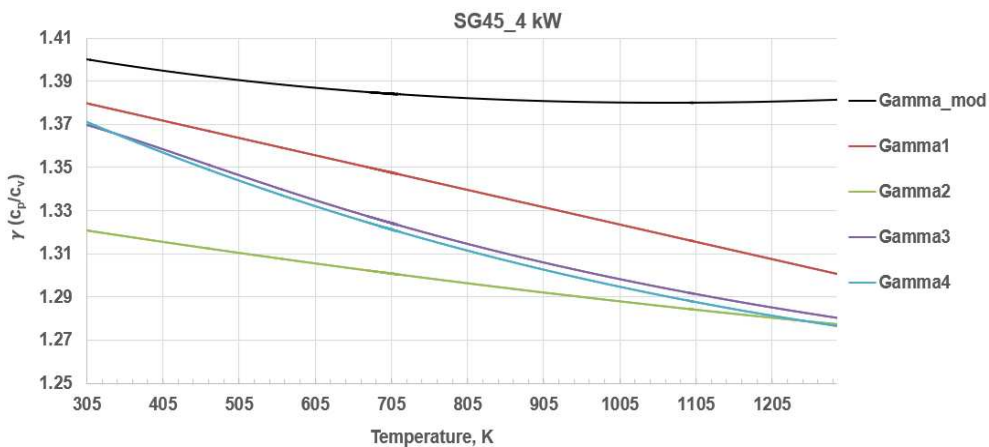
335 Gamma1 to Gamma4 in Figure 5 represent the  $\gamma$  models of Gatowsky et al. [15], Brunt and  
 336 Emtage [16], Egnell [17], and Blair [18] respectively while Gamma\_mod represents the  
 337 modified  $\gamma$  function. Figure 5 shows that the values of  $\gamma$  estimated from  $\gamma_{mod}$  for the diesel-  
 338 syngas dual-fuel RCCI engine were higher than the  $\gamma$  values estimated from the models from  
 339 literature that expressed  $\gamma(T)$ . This implies that  $\gamma$  also has a strong dependence on  $\lambda$  for diesel-  
 340 syngas dual-fuel RCCI engines. The same trend shown in Figure 5 was observed for all the  
 341 tested modes.



342

(a)

343



344

(b)

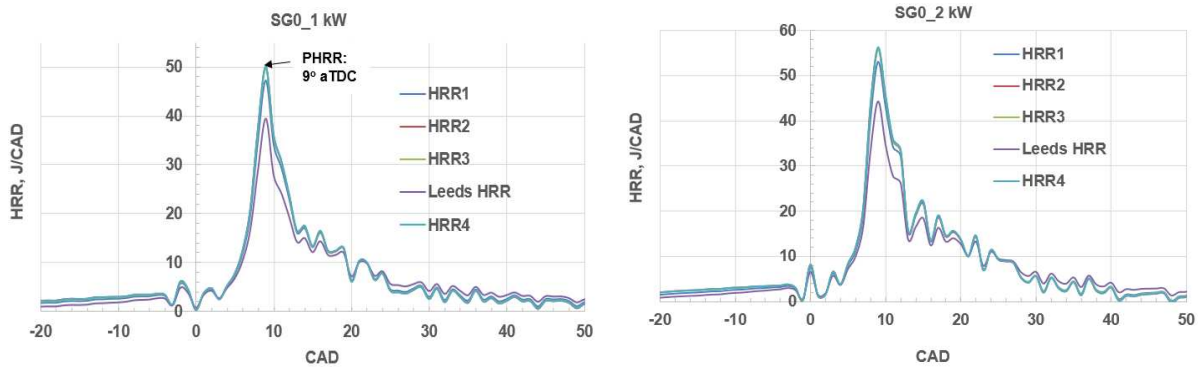
345

346 Fig. 5 Comparison of the modified  $\gamma$  function ( $\gamma_{mod}$ ) to the  $\gamma$  functions from literature (a)

347 SG25\_2 kW mode (b) SG45\_4 kW mode

348 3.7 Sensitivity of diesel-syngas dual-fuel RCCI engine HRR model to  $\gamma$  functions

349 The HRR profiles which were derived from the investigated  $\gamma$  and HRR models are shown in  
350 Figures 6 to 9. Figures 6 depicts the modelled HRR profiles for pure diesel (SG0) while the  
351 HRR profiles for SG10, SG25, and SG45 are depicted in Figures 7, 8, and 9 respectively.  
352 HRR1, HRR2, HRR3, and HRR4 were respectively based on the four  $\gamma$  functions from  
353 literature (Gamma1 to Gamma4).

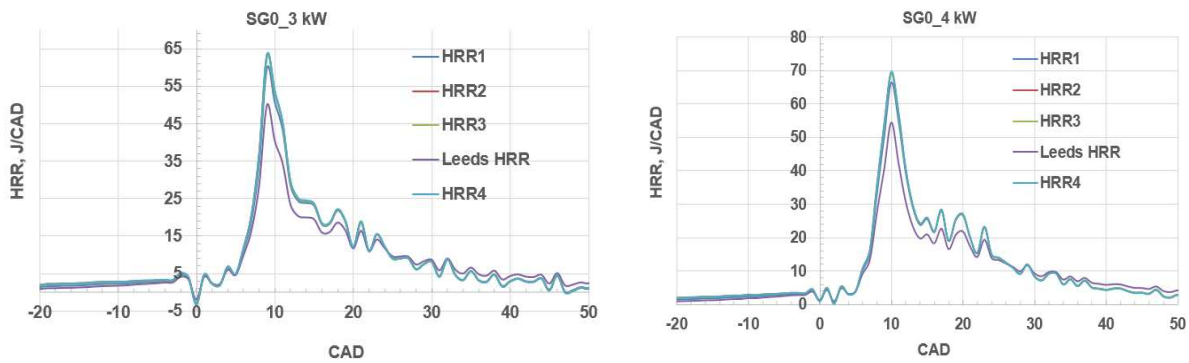


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(a)

(b)



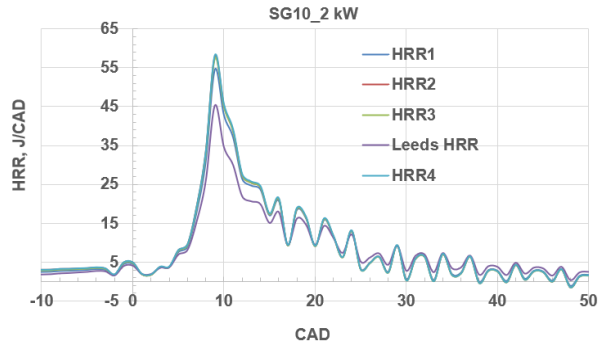
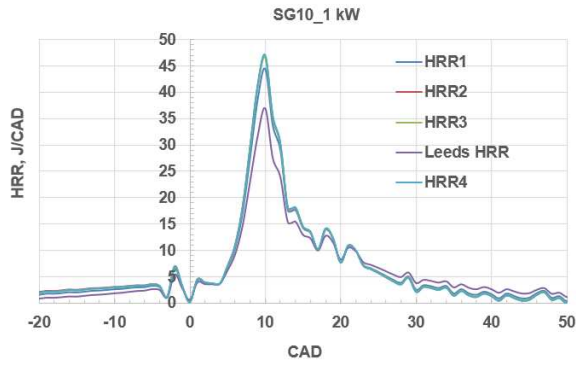
356

357

(c)

(d)

358 Fig. 6 Modelled HRR profiles for pure diesel (SG0)

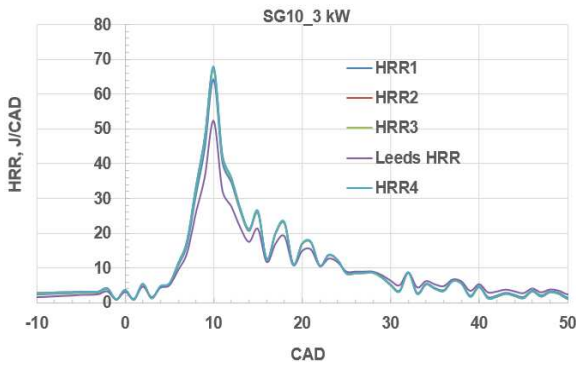


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(a)

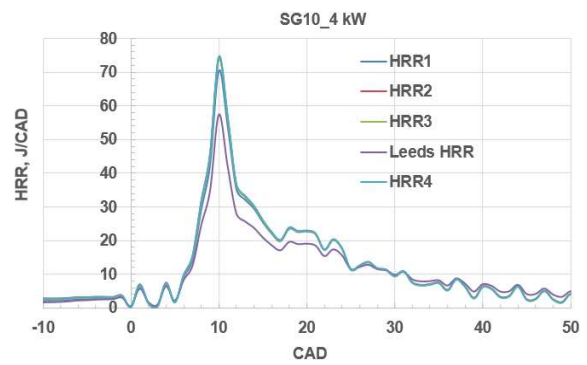
(b)



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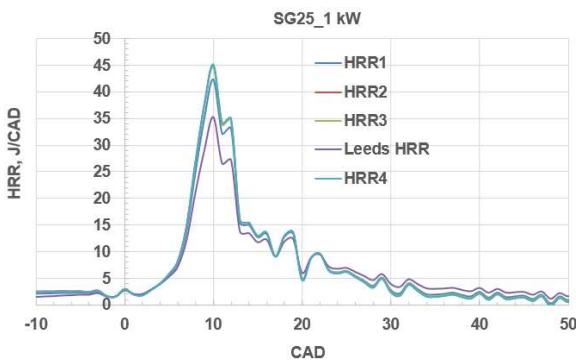
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(c)



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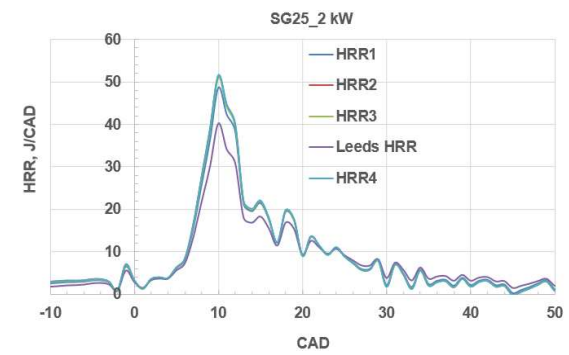
363 Fig. 7 Modelled HRR profiles for SG10



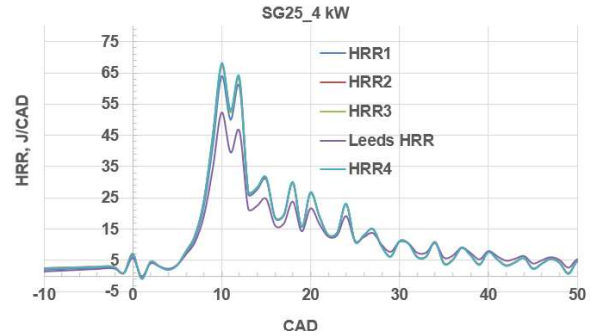
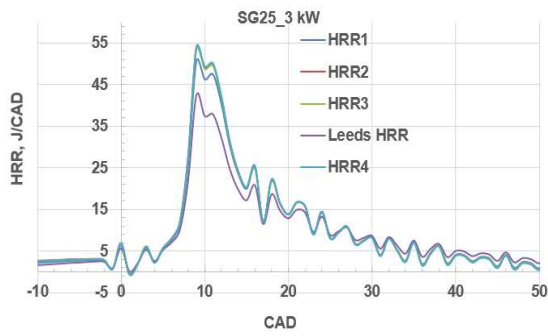
364

365

(a)



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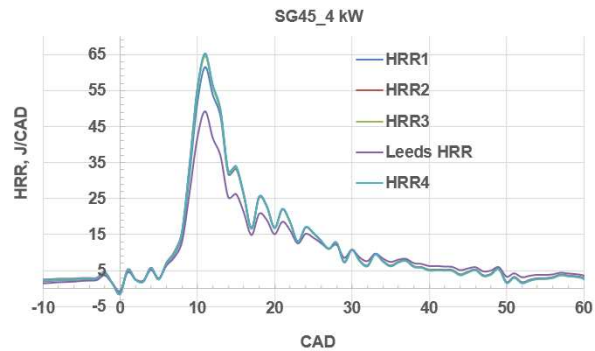
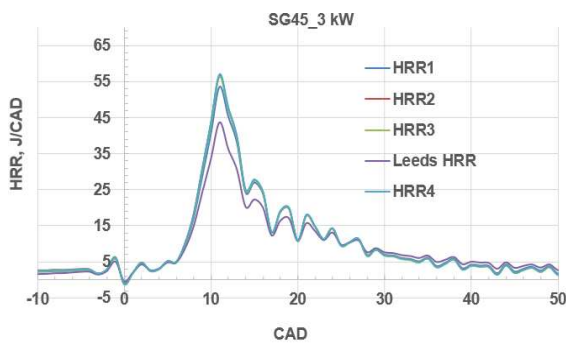
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(c)

(d)

367

368 Fig. 8 Modelled HRR profiles for SG25



369

(a)

(b)

370

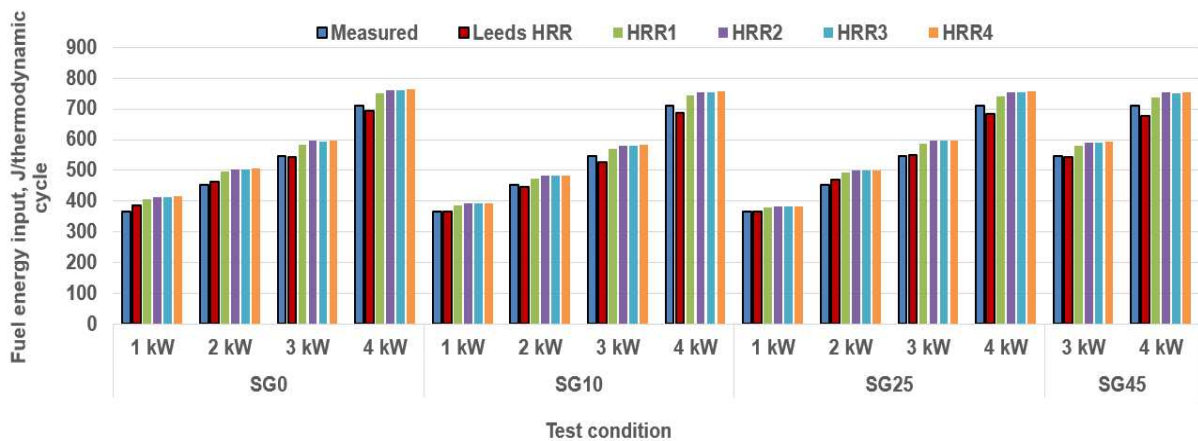
371 Fig. 9 Modelled HRR profiles for SG45

372 The sensitivity of the HRR model of the dual-fuel RCCI engine to  $\gamma$  functions is clearly depicted  
 373 in the figures as different PHRR values were predicted by the five HRR models for the same  
 374 engine mode. The Leeds HRR model predicted the lowest PHRR for all the tested dual fuels  
 375 and power conditions. Figure 5 shows that  $\gamma(T, \lambda)$  gives estimates of  $\gamma$  that are higher than  
 376 the estimates from the functions that expressed  $\gamma(T)$ . However, Figures 6 to 9 show that, for  
 377 both baseline diesel and the diesel-syngas dual fuels, the HRR model that utilized  $\gamma(T, \lambda)$   
 378 predicted lower PHRR values for the dual-fuel RCCI engine than the HRR models that utilized  
 379  $\gamma(T)$ . Though the five HRR models showed the same trend, they predicted different PHRR for  
 380 the tested dual fuels and engine loads, just as in the cases of single-fuel ULSD and the  
 381 alternative diesel operations [5,6]. The observed differences in the PHRR predictions of the

382 investigated HRR models necessitated the validation of the Leeds HRR model for the diesel-  
 383 syngas dual-fuel RCCI engine.

### 384 3.7.1 Validation of the Leeds HRR model

385 The Cumulative Heat Release (CHR) profiles for the tested dual fuels and power conditions  
 386 were derived from the HRR profiles (strictly for the heat that was released as a result of the  
 387 combustion of the injected fuel masses). Figure A.1 presents the CHR profiles for the tested  
 388 dual fuels and power conditions. The HRR and CHR profiles for the tested conditions were  
 389 used to predict the fuel input energy of the dual-fuel RCCI engine per thermodynamic cycle.  
 390 The fuel energy input (in J/thermodynamic cycle) predicted by the Leeds HRR model and the  
 391 HRR models that were based on  $\gamma(T)$  were compared to the measured fuel energy input to  
 392 validate the models. Figure 10 presents the result of the validation of the HRR models. The  
 393 analysis which was carried out to compare the predicted fuel energy input to the measured  
 394 fuel energy input is summarized in Table A.4.



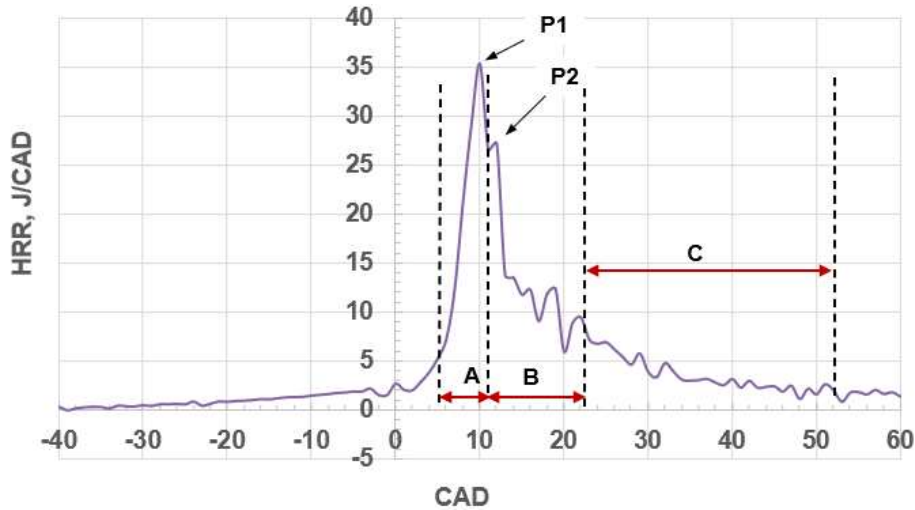
395  
 396 Fig. 10 Comparison of the measured and the predicted fuel energy inputs for the investigated  
 397 diesel-syngas dual fuels

398 The red bars with dark borderline in Figure 10 represent the values of the fuel energy input  
 399 predicted by the Leeds HRR model. The Leeds HRR model predicted the fuel input energy of  
 400 the dual-fuel RCCI engine for baseline diesel (SG0), SG10, SG25, and SG45 at the tested  
 401 conditions of power with an overall average (absolute) error of 2.41% compared to the

402 measured fuel energy input (blue bars with black borderline). The percentage errors of the  
403 fuel energy input predicted by the Leeds HRR model ranged from -4.59 to +5.41, with a  
404 standard deviation of 1.65. The overall average errors which were obtained for off-road diesel  
405 and the alternative diesel fuels (GTL and HVO diesels) for a 96 kW Multiple Fuel Injection  
406 Strategy (MFIS) IVECO diesel engine were 1.41% and 4.86% respectively [5,6]. The overall  
407 average errors in the predicted fuel energy input by the other HRR models that were based  
408 on  $\gamma(T)$  ranged from 6.26 to 8.29%. The HRR models that were based on  $\gamma(T)$  overpredicted  
409 the fuel consumption of the diesel-syngas dual-fuel engine because the significant effect of  $\lambda$   
410 on  $\gamma$  was not considered in the models. Figure 10 clearly shows that the accuracy of the HRR  
411 model of diesel engines for predicting the combustion behaviour of diesel-syngas dual fuels  
412 in the dual-fuel RCCI diesel engine was enhanced by using  $\gamma(T, \lambda)$ .

### 413 3.7.2 Effect of syngas substitution of diesel at constant energy on the combustion behaviour 414 of RCCI diesel engines

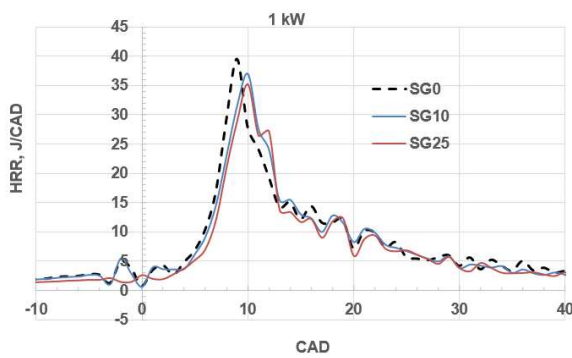
415 The effect of syngas substitution of diesel on the combustion behaviour of diesel engines was  
416 investigated by plotting the HRR profiles for the tested dual fuels on the same graph for each  
417 of the tested engine loads. The three phases of the combustion of the injected diesel-syngas  
418 fuel masses in the cylinder of the dual-fuel engine [7] are depicted in Figure 11 for 25% syngas  
419 substitution of diesel at 1 kW. The rate of release of heat during the rapid/premixed combustion  
420 phase (phase A) was the highest. The heat that was released in stage A was due to the  
421 premixed combustion of the DI diesel and some of the injected syngas. The first HRR peak  
422 (P1) in Figure 11 resulted from the premixed combustion of the pilot injection fuel (diesel).  
423 Stage B resulted from the premixed combustion of the port injected fuel (syngas) as well as  
424 the remaining diesel. The second HRR peak (P2) in Figure 11 resulted from the premixed  
425 combustion of syngas. The HRR reduced drastically during the mixing-controlled combustion  
426 phase (phase C) as the combustion became less spontaneous than it was in the previous  
427 stages.



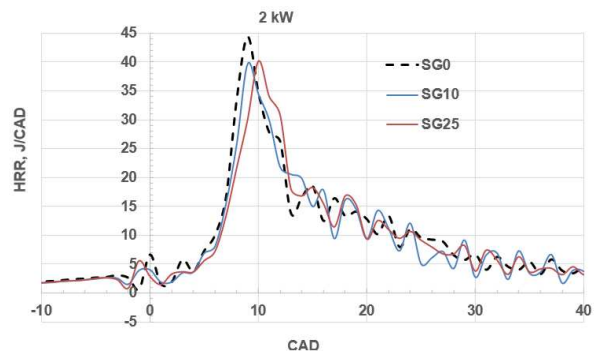
428

429 Fig. 11 Stages of the combustion of the diesel-syngas dual-fuel in the RCCI engine

430 Figure 12 depicts the effect of increasing the fraction of syngas in the dual fuel and the load  
 431 on the engine on the combustion behaviour of the RCCI engine. Generally, it was observed in  
 432 Figure 12 that, as the fraction of syngas increased for each of the tested conditions of power,  
 433 the HRR profiles of the dual fuels (SG10, SG25, and SG45) shifted to the right of the profile  
 434 for baseline diesel (SG0). This was because the tendency of the dual fuel to auto-ignite (the  
 435 effective CN of the dual fuel) decreased as the fraction of syngas was increased. The relatively  
 436 low CN of syngas increased the ID of the dual fuels as the syngas fraction increased. As a  
 437 result of the observed increase in the ID for the diesel-syngas dual fuels above the baseline,  
 438 the PHRR (and the PP; Figure 2) for the dual fuels (SG10, SG25, and SG45) occurred later  
 439 than pure diesel (SG0). Rith et al. [12] also reported that the PHRR occurred later than  
 440 baseline diesel as the flow rate of syngas was increased.



441

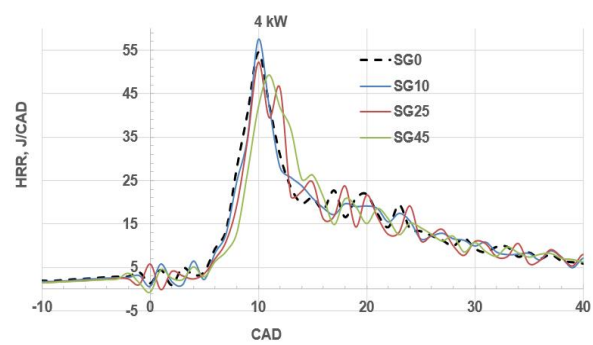
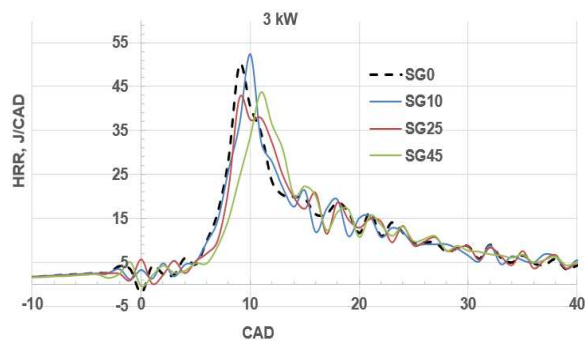


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(a)

(b)





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(c)

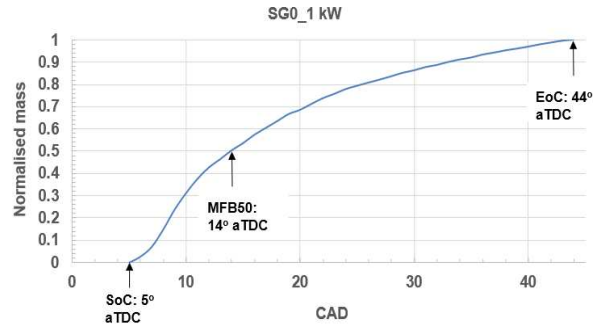
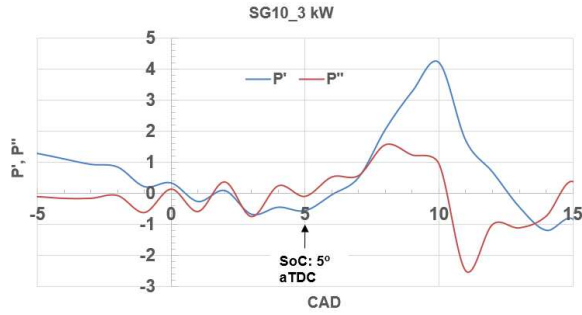
(d)

445 Fig. 12 Effect of syngas concentration on the combustion behaviour of the diesel-syngas dual-  
 446 fuel RCCI engine

447 Furthermore, Rith et al. [12] reported that the PHRR decreased below the baseline as the  
 448 fraction of syngas increased. Contrary to what was reported by the authors, Figure 12 shows  
 449 that at the relatively high load conditions (3 and 4 kW), the values of the PHRR for the lowest  
 450 syngas fraction (SG10) were higher than those for pure diesel (SG0). The observed high  
 451 PHRR for SG10 above the baseline could be because the premixed combustion of diesel  
 452 (represented by P1 in Figure 11) and the premixed combustion of the port injected syngas (P2  
 453 in Figure 11) occurred at the same crank angle at the lowest syngas fraction (SG10).

### 454 3.7.3 Combustion phasing for the diesel-syngas dual fuel RCCI engine

455 The Start of Combustion (SoC), the End of Combustion (EoC), and the MFB50 were  
 456 determined from the HRR profiles, the derivatives of the P-CAD data, and the derived fuel  
 457 burn profiles for the tested conditions as shown in Figures 13 and 14. The crank angle timings  
 458 for the PP, PT and PHRR were determined from the pressure, temperature, and HRR profiles,  
 459 respectively. Table 6 presents the combustion phasing for the tested conditions. The Duration  
 460 of Combustion (DoC) was estimated as the difference between the EoC and the SoC.



461

462 Fig. 13 Determination of SoC: SG10\_3 kW

462 Fig. 14 SoC, MFB50, EoC for SG0 at 1 kW

463 Table 6 Combustion phasing for the tested conditions

		CAD						
Dual fuel	Power, kW	SoC	MFB50	EoC	DoC	PP	PT	PHRR
SG0	1	5	14	44	39	11	19	9
	2	5	14.5	48	43	12	22	9
	3	5	16	52	47	11	24	9
	4	4	18	67	63	12	26	10
SG10	1	6	14	43	37	12	19	10
	2	6	15	48	42	11	22	9
	3	5	16	50	45	12	24	10
	4	5	19	67	62	13	24	10
SG25	1	6	14.5	53	47	12	19	10
	2	6	16	58	52	12	22	10
	3	5	17	60	55	13	24	9
	4	5	19	67	62	12	24	10
SG45	3	6	17.5	60	54	13	24	11
	4	6	19	65	59	13	25	11

464

465 Table 6 shows that the SoC, MFB50, PP, and PHRR occurred later for the diesel-syngas dual

466 fuels compared to pure diesel. Table 6 also shows that the DoC increased above the baseline

467 for the relatively high syngas flow rates (SG25 and SG45). This could be attributed to the  
 468 delayed and slow combustion of the CO in the syngas.

469 The values of the Peak Pressure (PP), the Peak Temperature (PT), and the PHRR for the  
 470 tested conditions are presented in Table A.5. The table shows that the values for the PP, and  
 471 the PT decreased below the baseline for the tested diesel-syngas dual fuels. This was due to  
 472 the relatively low Cv of syngas.

473 3.7.4 Effect of syngas substitution of diesel on the Ignition Delay (ID) of the dual-fuel RCCI  
 474 engine

475 The values of the Ignition Delay (ID) for the tested conditions were estimated by adding the  
 476 corresponding SoC crank angles to the Start of Injection (Sol) crank angle of the engine (13°  
 477 bTDC). Table 7 presents the estimated values of the ID.

478

479 Table 7 Ignition Delay (ID) values for the investigated fuel blends and engine loads

<b>Fuel blend</b>	<b>Power, kW</b>	<b>ID, CAD</b>	<b>ID, milliseconds</b>
SG0	1	18	1
	2	18	1
	3	18	1
	4	17	0.94
SG10	1	19	1.06
	2	19	1.06
	3	18	1
	4	18	1
SG25	1	19	1.06
	2	19	1.06
	3	18	1
	4	18	1

SG45	3	19	1.06
	4	19	1.06

480

481 The values of the ID for the tested conditions (Table 7) showed that diesel-syngas dual fuels  
 482 increase the ID in dual-fuel RCCI engines. The results for the ID in the current work contradict  
 483 what was reported by Garnier et al. [7].

484 **3.8 Estimation of possible CO<sub>2</sub> savings from the utilization of diesel-syngas dual fuel**  
 485 **in diesel engines**

486 Table 8 shows that the use of 45% (by energy) syngas substitution of diesel in a typical  
 487 developing country (Nigeria) can reduce CO<sub>2</sub> emissions by ~0.26 million tonnes per year. The  
 488 estimate in Table 8 is based on the consumption of diesel in Nigeria for the year 2019 [19] and  
 489 the maximum syngas substitution that was used in the current work.

490 Table 8 Possible reduction in CO<sub>2</sub> emissions from the substitution of diesel with syngas

S/n	Item	Calculation	Value
1	Syngas substitution of diesel by energy, %		45
2	Consumption of diesel in Nigeria in 2019 [19], million tonnes	-	0.19
3	CO <sub>2</sub> emission per kg of diesel combusted [20], kg CO <sub>2</sub> /kg diesel	-	3.1
4	CO <sub>2</sub> emissions from the combustion of diesel in Nigeria, million tonnes	0.19 x 3.1	0.58
5	Reduction in CO <sub>2</sub> emissions for 45% substitution of diesel by energy, million tonnes	45 x 0.58/100	~0.26

491

492

493

#### 494 **4. Conclusion**

495 In this work, the improved Leeds HRR model was validated and applied to a diesel-syngas  
496 dual-fuel RCCI Gen-set engine to investigate the effect of syngas substitution of diesel on the  
497 engine. The current work showed that the accuracy of the HRR model of the diesel-syngas  
498 dual-fuel RCCI engine was also strongly depended on the specific heats ratio ( $\gamma$ ). The effect  
499 of the excess air ratio ( $\lambda$ ) on  $\gamma$  was also investigated in this work for dual-fuel RCCI diesel  
500 engines.  $\lambda$  was found to have a significant effect on  $\gamma$ . In the current work, the accuracy of the  
501 Leeds HRR model for the analysis of the combustion behaviour of the dual-fuel RCCI engine  
502 was further enhanced by the use of in-cylinder global lambda function ( $\lambda_g$ ). The Leeds HRR  
503 model based on  $\gamma_{mod}(T, \lambda)$  predicted the fuel input energy of the engine with an average  
504 (absolute) error of 2.41%. The errors in the fuel input energy predicted by the Leeds HRR  
505 model ranged from -4.59 to +5.41%, with a standard deviation of 1.65. The average error in  
506 the fuel input energy predictions of the other models which were based on  $\gamma(T)$  ranged from  
507 6.26 to 8.29%. The error in the predictions of the other models was because  $\lambda$  was neglected  
508 in the models. Therefore, in this work, it was shown that the accuracy of the HRR model of  
509 diesel-syngas dual-fuel RCCI engines is enhanced by using  $\gamma(T, \lambda)$ . It was found that the SoC,  
510 MFB50, PP, and PHRR occurred later for the diesel-syngas dual fuels compared to baseline  
511 diesel due to the observed increase in the Ignition Delay as the fraction of syngas was  
512 increased. It was observed in the current work that diesel-syngas dual fuels led to a decrease  
513 in the Peak Pressure (PP) and the Peak Temperature (PT) below the baseline. The current  
514 work also showed that 45% by energy substitution of diesel with syngas in Nigeria (a  
515 developing country) can potentially reduce CO<sub>2</sub> emissions by ~0.26 million tonnes.

#### 516 **Acknowledgements**

517 This work was supported by the Engineering and Physical Sciences Research Council  
518 (EPSRC) for a GCRF grant: Creating resilient sustainable micro-grids through hybrid  
519 renewable energy systems (CRESUM-HYRES), grant number EP/R030243/1 and by the

520 Petroleum Technology Development Fund (PTDF), Nigeria; and the National Agency for  
 521 Science and Engineering Infrastructure (NASENI), Nigeria.

522 **Appendix**

523 Table A.1 Values of the coefficients in Equation 2 [13]

Coefficients ( $\gamma_b$ )	Values
$b_1$	1.498119965
$b_2$	-0.00011303
$b_3$	-0.26688898
$b_4$	4.03642e-08
$b_5$	0.273428364
$b_6$	5.7462e-05
$b_7$	-7.2026e-12
$b_8$	-0.08218813
$b_9$	-1.3029e-05
$b_{10}$	2.35732e-08

524

525 Table A.2 Stoichiometric AFR of the simulated syngas

Species	Composition in syngas, mol %	Molar mass, kg/kgmol	Mass, kg	Stoichiometric O <sub>2</sub> requirement, kmol	N <sub>2</sub> , kmol	Air mass, kg
H <sub>2</sub>	0.15	2.016	0.302	0.075	0.282	10.3
CO	0.2	28.01	5.602	0.100	0.376	13.733
CH <sub>4</sub>	0.04	16.04	0.642	0.080	0.301	10.987
O <sub>2</sub>	0.0098	32	0.314	-0.0098	-0.037	-1,346
CO <sub>2</sub>	0.12	44.01	5.281	-	-	-
N <sub>2</sub>	0.4802	28.014	13.452	-	-	-
Total	1		25.593			33.674

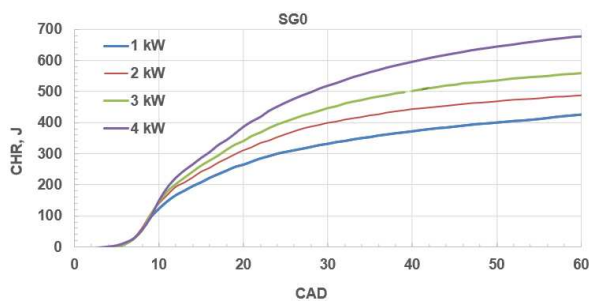
$$AFR_{\text{stoich\_syngas}}: 33.674/25.593 = 1.316 \text{ kg/kg}$$

526

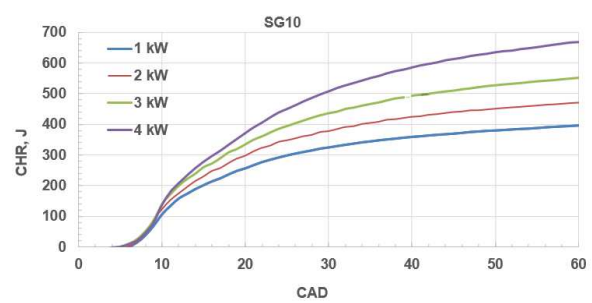
527 Table A.3 Density and the Lower Heating Value (LHV) of the simulated syngas

Species	Composition, mol %	Molar mass, kg/kgmol	Mass, kg	Mass fraction	Density, kg/m <sup>3</sup>	LHV, MJ/kg
H <sub>2</sub>	0.15	2.016	0.302	0.012	0.0899	121
CO	0.2	28.01	5.602	0.219	1.165	10.8
CH <sub>4</sub>	0.04	16.04	0.642	0.025	0.668	50
O <sub>2</sub>	0.0098	32	0.314	0.012	1.331	0
CO <sub>2</sub>	0.12	44.01	5.281	0.206	1.842	0
N <sub>2</sub>	0.4802	28.014	13.452	0.526	1.165	0
Total	1		25.593	1		
Simulated syngas					1.067	5.047

528



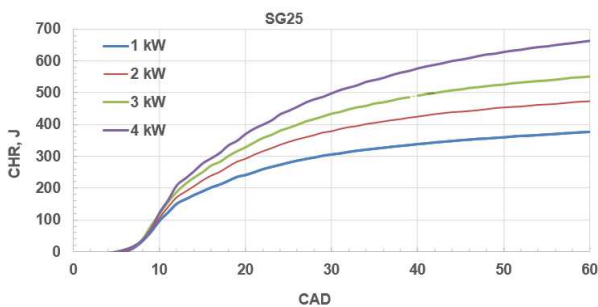
529



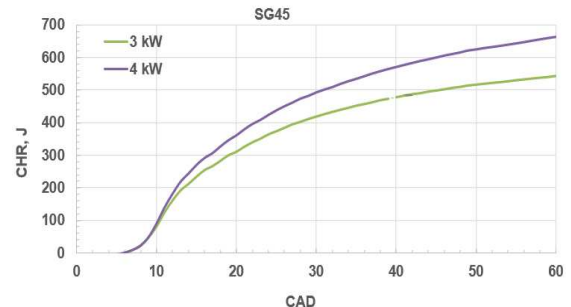
530

(a)

(b)



531



532

(c)

(d)

533 Fig. A.1 CHR profiles for the tested fuels

Table A.4 Validation of the Leeds HRR model for diesel-syngas dual fuel RCCI engine

Dual fuel	Power, kW	Global lambda, $\lambda_g$	Energy input, J/thermodynamic cycle					% Deviation from measured input energy					
			Measured	Leeds HRR	HRR1	HRR2	HRR3	HRR4	Leeds HRR	HRR1	HRR2	HRR3	HRR4
SG0	1	3.99	364.71	384.45	406.5	414	412.9	414.5	5.41	11.46	13.51	13.21	13.65
	2	3.21	463.5	495.5	488.64	504.4	503.66	505.55	2.49	9.57	11.54	11.37	11.79
	3	2.66	542.42	584.16	595.57	594.6	597	587.25	-0.85	6.78	8.87	8.69	9.13
	4	2.05	709.87	694.76	751.2	762.46	762	764.7	-2.13	5.82	7.41	7.34	7.72
SG10	1	4.01	364.71	365.85	386.9	393.5	392.8	394.1	0.31	6.08	7.89	7.7	8.06
	2	3.22	452.22	445.54	474.17	482.63	481.83	483.56	-1.48	4.85	6.72	6.55	6.93
	3	2.65	547.07	526.37	568.58	580.37	579.32	581.8	-3.78	3.93	6.09	5.9	6.35
	4	2.03	709.87	685.9	742.54	754.84	754	756.9	-3.38	4.60	6.33	6.22	6.63
SG25	1	4.04	364.71	365.68	378	382	381.6	382.46	0.27	3.64	4.74	4.63	4.87
	2	3.23	452.22	469.6	493.03	499.53	498.96	500	3.84	9.02	10.46	10.34	10.57
	3	2.64	547.07	551.3	587.2	597.17	596.3	598.3	0.77	7.34	9.16	9	9.36
	4	2.00	709.87	683.8	741.13	754.1	753.25	756.13	-3.67	4.4	6.23	6.11	6.52
SG45	3	2.63	547.07	543.18	579.94	590.86	589.66	591.87	-0.71	6	8	7.79	8.19
	4	1.96	709.87	677.3	738.7	754.78	751.54	754.6	-4.59	4.06	6.33	5.87	6.3
Average of absolute error, %:									2.41	6.26	8.09	7.91	8.29



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Standard deviation:	1.65	2.28	2.33	2.32	2.32
% error range:	-4.59 - +5.41	3.64 - 11.46	4.74 - 13.51	4.63 - 13.21	4.87 - 13.65

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Table A.5 Model results for the Peak Pressure (PP), Peak Temperature (PT), and Peak Heat Release Rate (PHRR) for the tested dual fuels

Dual fuel	Power, kW	PP, bar	PT, K	PHRR, J/CAD
SG0	1	61.31	1548.07	39.5
	2	64.14	1646.54	44.3
	3	64.45	1719.39	49.95
	4	66.66	1840.84	54.42
SG10	1	60.96	1544.57	36.95
	2	62.66	1636.71	45.36
	3	64.17	1696	52.37
	4	65.01	1822.95	57.5
SG25	1	58.7	1488.23	35.27
	2	62.24	1617.32	40.15
	3	63.03	1687.08	42.4
	4	65.48	1802.12	52.2
SG45	3	61.07	1658.01	43.7
	4	64.71	1796.52	49.25

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