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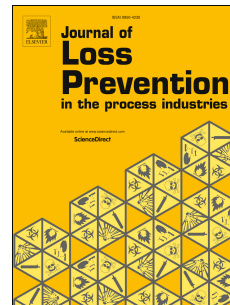
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Evaluation of explosion characteristics of 2-methylfuran/air mixture

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Abstract

Herein, the explosion characteristics such as the peak explosion pressure, maximum pressure rise rate and deflagration index of 2-methylfuran (MF) /air mixture have been investigated at high pressures and temperatures. Knowledge of these parameters can be used in the safety assessment of MF explosions. The explosion experiments were performed at the initial pressure of 1, 2, 3, and 4 bar, the initial temperature of 333, 363, 393, and 423 K and the equivalence ratio of 0.7-1.4 using a constant volume combustion bomb. The pressure data obtained from the experiment were carefully processed to examine MF peak explosion pressure, maximum pressure rise rate, explosion time as well as the deflagration index. Explosion characteristics of MF were sensitive to the initial pressure and temperature conditions and the mixture concentration. An increment in the initial pressure triggered a dramatic growth in the peak explosion pressure, maximum rate of pressure rise and the deflagration index. Alternatively, an increment in the initial temperature decreased the peak explosion pressure, maximum pressure rise rate and the deflagration index. By and large, MF explosion parameters obtained in this investigation can offer firsthand information on MF explosion hazard assessment at high pressures and temperatures.

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Keywords: 2-methylfuran (MF); Explosion characteristics; Explosion pressure; Pressure rise rate; Deflagration index; Explosion time

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Nomenclature		<i>Subscript</i>	
V	Combustion vessel volume, m^3	max	Maximum
T	Temperature, K	i	Initial
p	Explosion pressure, bar	L	Laminar
p_{max}	Peak explosion pressure, bar	c	Combustion
dp/d_{max}	Maximum pressure rise rate, bar/s	e	End
	Time after ignition, ms		
	Explosion time, ms	<i>Greek Symbol</i>	
t_e	End of explosion time, ms	ϕ	Equivalence ratio
dp/d	Pressure rise rate, bar/s		
T_i	Initial temperature, K		
p_i	Initial pressure, bar		
S_L	Laminar burning velocity, m/s		
K_G	Deflagration index, bar*m/s		

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82 1. Introduction

83 Annually, chemical or gas explosion accident kill and injure hundreds of people globally (Beck,
84 2016; OECD, 2013; World Health Organization, 2009; Wu et al., 2019). As a matter of fact, an
85 explosion can occur in industries, household, confined and unconfined space, process equipment as
86 well as in offshore/marine structures when a flammable gas or highly evaporative liquid is
87 accidentally discharged into the atmosphere and meet a strong ignition source. In compliance with
88 this, the explosion characteristics of distinct flammable or highly evaporative fuels have to be
89 thoroughly studied. To this end, having knowledge of the explosion characteristics such as the peak
90 explosion pressure, maximum pressure rise rate, explosion time and deflagration index is useful to
91 improve safety. In essence, the deflagration index is used as the foundation for the design of
92 pressure tanks and safety relief valves for chemical storage as well as vents, high pressure and
93 temperature combustors/furnace. The magnitude of the deflagration index characteristically
94 determines the severity of the explosion. Therefore, higher deflagration indices/values indicate the
95 possibility of extremely dangerous explosion. Considerable investigations have been performed in
96 the literature to study the explosive behavior of gaseous and liquid fuels in recent years. Just to
97 mention a few, quite a bit of these investigations used hydrogen (Li et al., 2015; Li et al., 2018a,
98 2018b; Sun and Li, 2017), methane/methanol (Cui et al., 2018; Kundu et al., 2018; Mitu and
99 Brandes, 2015; Tang et al., 2014), ethanol (Mitu et al., 2018; Mitu and Brandes, 2017) and syngas
100 (Tran et al., 2017) fuels. The authors sought to investigate the impact of initial pressure, initial
101 temperature and equivalence ratio on the peak explosion pressure, maximum rate of pressure rise,
102 explosion time and deflagration index of these fuels. For instance, Hu et al. (2017) have
103 investigated the explosion characteristics of butanol/isooctane blends and corroborated that at rich
104 mixtures and elevated pressures the peak pressure exhibited oscillatory behaviour which reduced
105 the explosion time and increased the maximum pressure rise rate. In another study, Shen et al.
106 (2017b) showed that methane has a higher upper flammability limit than ethane. What's more, Li et
107 al. (2015) have evaluated the explosion characteristics of alcohol (ethanol, 1-butanol, 1-pentanol)
108 /air mixtures. Their results showed that 1-pentanol had the largest peak explosion pressure and
109 maximum pressure rise rate on the rich regime of the mixture when compared with ethanol and 1-
110 butanol. They asserted that this occurrence was due to the difference in heat loss of the various
111 alcohols. On one hand, the maximum pressure rise rate was insensitive to the initial temperature
112 variation. More recently, Sun (2018) also studied the explosion properties of syngas and reported
113 that within his investigated conditions the deflagration index was below 30 MPa*m/s.

114 Laminar burning velocity (LBV) is another significant parameter which quantifies the
115 physicochemical properties of premixed flames/combustion. Essentially, it is used to validate the
116 chemical mechanism of a specific fuel and gives essential information about the burning process
117 and flame dynamics (Bao et al., 2017). The burning velocity of a premixture is somehow related to
118 the explosion pressure development, meanwhile, it is very influential in predicting explosion
119 hazards (Huzayyin et al., 2008). Several studies have been performed to study the burning speeds of
120 different fuels in the literature (Askari et al., 2017; Mannaa et al., 2015; Mitu et al., 2015; Reyes et
121 al., 2018). Moreover, some of these studies evaluated the correlation between the burning velocity
122 and explosion parameters (Dahoe, 2005; Dahoe and de Goey, 2003; Saeed, 2017; Zhang et al.,
123 2019b). Recently, Ma et al., (2013a, 2013b) studied the burning characteristics of 2-methylfuran
124 (MF) / air mixtures and reported that MF had unstable flames and higher burning velocities

125 compared to isooctane and 2,5-dimethylfuran. In another study, the following researchers (Somers
126 et al., 2013; Xu et al., 2018; Zhongyang et al., 2018) also studied the LBV of 2-methylfuran at
127 elevated pressures and temperatures and evaluated the correlation between the burning velocities
128 and the initial pressure and temperature.

129 In the meantime, in the long haul, 2-methylfuran has the potential as an alternative fuel. In
130 addition, it also used in the pharmaceutical industry and the manufacturing of pesticides. MF is
131 highly flammable, has a lower flash point and easy to vaporize, therefore, any leakage of MF poses
132 a potential threat to human life and properties. If MF is inappropriately handled during production,
133 transportation and storage it can cause a fire outbreak as well as an explosion if any leaked MF
134 meets a strong ignition source. Therefore, firsthand information about its explosion characteristics is
135 relevant for accident and safety evaluations. In spite of the progress made in the investigation of
136 explosion characteristics of many fuels in previous publications, to the best knowledge of the
137 authors, there is no information on MF explosion characteristics such as the peak explosion
138 pressure, maximum pressure rise rate, explosion time and deflagration index in the literature. In
139 addition, the explosion characteristics of liquid fuels, most especially liquid biofuels are rarely
140 studied in the literature. Therefore, this work intends to examine the explosion features of 2-
141 methylfuran at elevated pressures and temperatures. The main purpose of this work is to investigate
142 the influence of initial pressure, initial temperature and the equivalence ratio on MF explosion. 2-
143 methylfuran explosion characteristics were experimentally determined using a constant volume
144 combustion chamber (CVCC) at the initial temperature (333, 363, 393 and 423 K), initial pressure
145 (1, 2, 3, and 4 bar) and equivalence ratio (0.7-1.4). The experimental explosion pressure data were
146 well examined to determine MF peak explosion pressure, maximum pressure rise rate and explosion
147 time. Last but not most definitely not least, 2-methylfuran LBV data were mapped against the
148 equivalence ratio.

149

150 2. Analysis of experimental device and method

151 The experimental instrumentation has been shown elsewhere (Zhongyang et al., 2018). The
152 experiment was done in a CVCC which has an inner length to diameter ratio of ($L/D = 1.0$). The
153 CVCC has an inner volume of 2.067 L. In addition, experimental data of the testing rig have been
154 validated in this paper (Zhongyang et al., 2018). The CVCC also comprises of a high-speed imaging
155 (Schlieren) system and a data recording system. It also has quartz windows which permits viewing
156 and recording of flame images. The CVCC has six heating units on its sides used to control the
157 initial temperature. Moreover, the initial mixture temperature was measured with a K-Type
158 thermocouple (WRNK-231) which is accurate to $\pm 0.75\%$. Altogether the combustion pressure was
159 recorded by a piezoelectric pressure sensor (Kistler 6115A) and a charge amplifier (Kistler 5018A).
160 Meanwhile, the initial pressure was determined with a high precision pressure gauge (Keller
161 LEX1). The resolution of the pressure sensor is 0.0001 MPa. Therefore, 0.1-3% of inaccuracy was
162 generated by the initial pressure. The sampling frequency of the pressure recording unit is 75MHz.
163 The mixture was ignited with two electrodes of diameter 0.4mm opposite with each other and the
164 ignition unit. The ignition or spark energy of the experiment is 10mJ (Xu et al., 2014). The mean of
165 three testing data was used for each ϕ in order to warrant 90-95% certitude.

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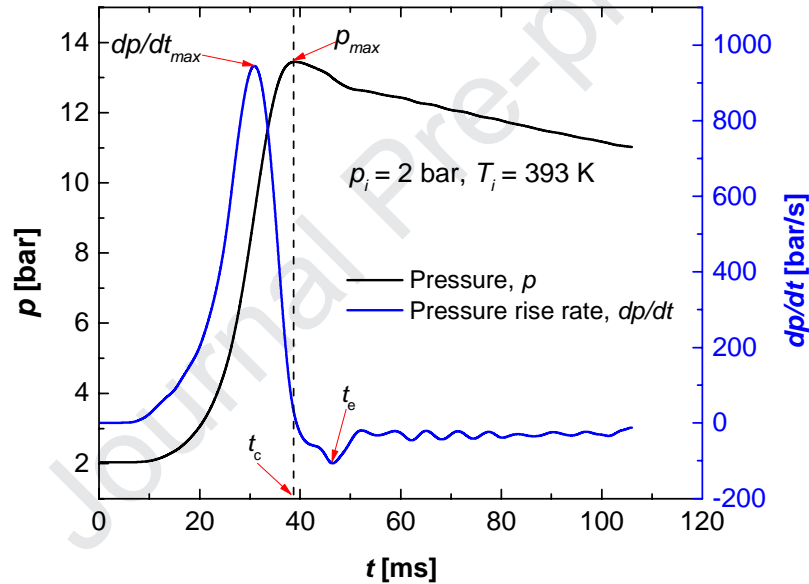
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170 **3. Results and discussion**

171 The experimentally recorded pressure data have some level of noise in the data; therefore, it is
 172 difficult and inaccurate to determine the explosion parameters from the raw pressure data. In this
 173 regard, the raw pressure history was filtered or smoothed using a low-pass band filter in Python.
 174 Fig. 1 shows a typical example of smooth explosion pressure (p) and pressure rise rate (dp/dt)
 175 cartography at the initial pressure (p_i) of 2 bar, the initial temperature (T_i) of 393 K and
 176 stoichiometric fuel/air ratio of $\phi = 1.0$. As shown in Fig. 1, the pressure steadily increases after
 177 ignition and reaches the peak at p_{max} . However, after obtaining p_{max} the pressure starts to drop due
 178 to heat loss to the CVCC wall when the flame front reaches the wall. The combustion/explosion
 179 time was attained at the time (t_c). The maximum pressure rise rate was recorded at the point
 180 (dp/dt_{max}). At last, the combustion process was completed at the time (t_e). It is worth to mention
 181 that p_{max} , t_c , and dp/dt_{max} are the important parameters typically used in the safety assessment of
 182 a specific fuel/chemical, hence, herein they are the only parameters discussed.

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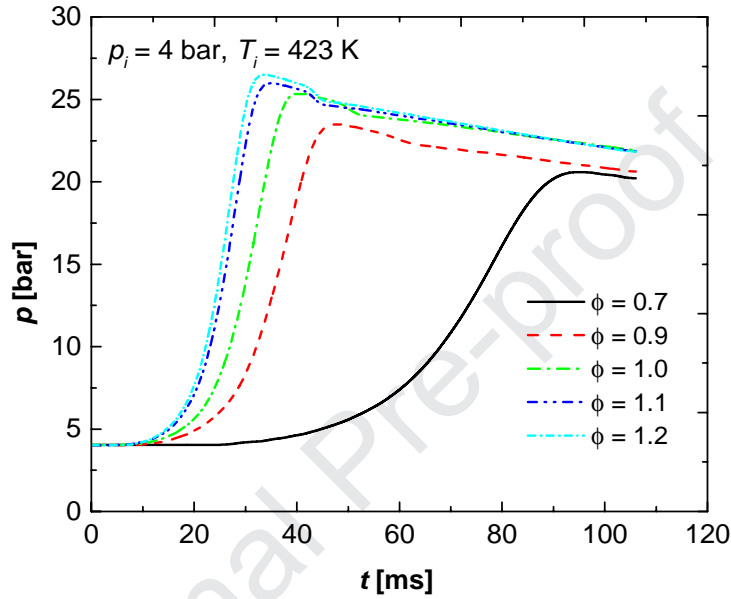
185 **Fig. 1.** Illustration of in-chamber explosion pressure evolution and pressure rise rate contours at $T_i =$
 186 393 K and $p_i = 2$ bar and $\phi = 1.0$.

187

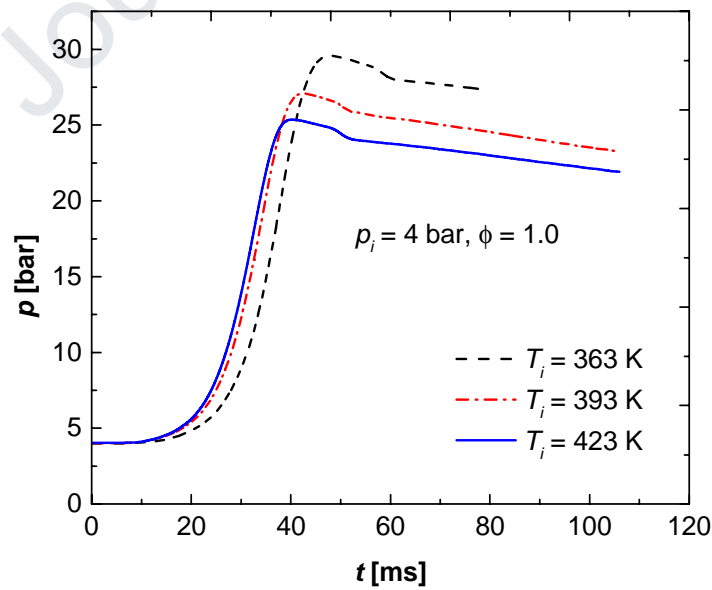
188 **3.1. Explosion pressure and peak explosion pressure**

189 Fig. 2 shows p contours at $p_i = 4$ bar and $T_i = 423$ K for different ϕ . Similar contours were obtained
 190 for the different p_i , T_i and ϕ values investigated in this document. With reference to Fig. 2, it can be
 191 noticed that the value of p is sensitive to ϕ , therefore, the magnitude of p increases with increasing
 192 ϕ . Parallel trends have been observed in previous studies (Li et al., 2015, Cui et al., 2018; Mitu and
 193 Brandes, 2015; Tang et al., 2014). The reduced amount of fuel at $\phi = 0.7$ and 0.9 led to less heat
 194 energy released from the combustion phenomena and lower p values. The opposite is true for $\phi =$
 195 1.0, 1.1 and 1.2. The peak value of p increased from 20.593 bar to 26.495 bar when ϕ increased
 196 from 0.7 to 1.2. Fig. 3 displays p values at $p_i = 4$ bar, $T_i = 363$ -423 K and $\phi = 1.0$. The magnitude

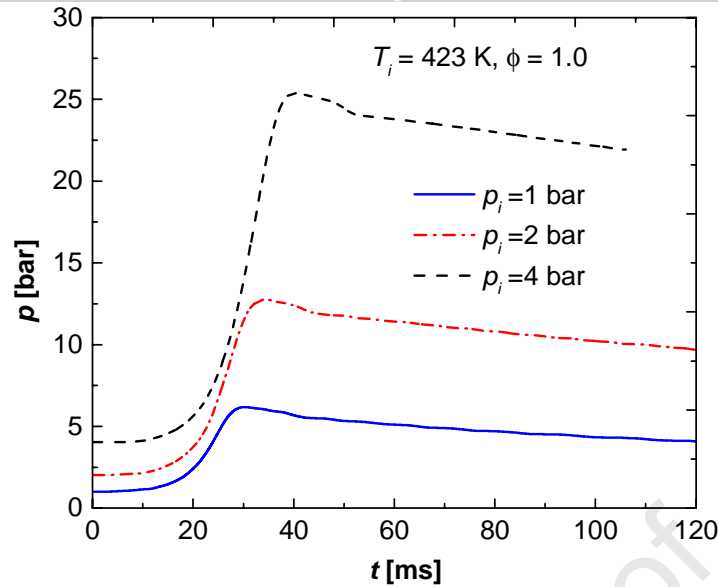
197 of p is lower at a higher T_i owing to a higher mass burning rate and flame speed at a higher T_i .
 198 Accordingly, the combustible mixture takes a shorter time to reach the peak of p . In addition to this,
 199 the mass of MF/air unburnt mixture in the CVCC was decreased (less heat energy from
 200 combustion) at a higher T_i , thence, leading to the decreased peak value of p . The peak values of p
 201 obtained at 363 K, 393 K and 423 K are 29.577 bar, 27.084 bar, and 25.364 bar. Furthermore, it can
 202 be noticed in Fig. 4 that an increment in the value of p_i increased the magnitude of p due to the
 203 robustness of the combustion process which generated a higher amount of heat energy. The highest
 204 values of p increased from 6.077 bar to 25.364 bar when the value of p_i increased from 1 bar to 4
 205 bar.
 206



207
 208 **Fig. 2.** In-chamber p evolution versus t at $\phi = 0.7-1.2$, $T_i = 423$ K and $p_i = 4$ bar.
 209



210
 211 **Fig. 3.** A plot of p versus t at $T_i = 363-423$ K, $p_i = 4$ bar and $\phi = 1.0$.
 212



213

214 **Fig. 4.** A plot of p against t at $T_i = 423$ K, $p_i = 1-4$ bar and $\phi = 1.0$.

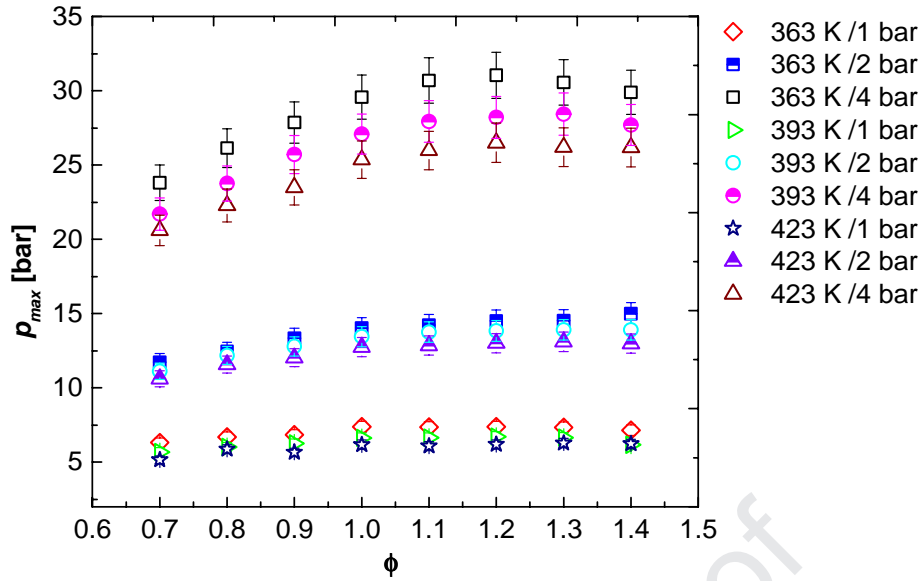
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216 The peak explosion pressure (p_{max}) quantify the energy distribution of combustion propagating
 217 waves (Shen et al., 2017b). Therefore, p_{max} can be used to determine the heat energy from the
 218 explosion. Fig. 5 depicts the values of p_{max} as a function of ϕ at $p_i = 1-4$ bar and $T_i = 363-423$ K. In
 219 general, the values of p_{max} increases with increasing ϕ . In lean mixtures, the amount of MF fuel in
 220 the CVCC is less leading to less release of heat energy and lower p_{max} . On the other hand,
 221 combustion becomes more robust as ϕ increases, consequently, the value of p_{max} also increases. As
 222 shown in Fig. 5, somewhat p_{max} decreases at some of the rich mixtures due to an insufficient
 223 amount of oxygen in the CVCC leading to incomplete combustion and a reduced amount of heat
 224 released.

225 Furthermore, the values of p_{max} are somehow higher at a lower T_i and increases dramatically as
 226 p_i increases. The reason for a higher p_{max} at a lower T_i is due to the increased mass of the unburnt
 227 MF mixture in the CVCC (higher heat energy from MF explosion) which subsequently increased
 228 the value of p_{max} . Again, a total reduction in the burning mass of MF mixture and heat loss could
 229 also possibly cause a decrease in the explosion peak pressure when T_i was increased. On one hand,
 230 at a higher p_i MF explosion becomes more and more energetic leading to a higher release of
 231 thermal energy, and a higher p_{max} as depicted in Fig. 5.

232 The experimental p_{max} data are compared to simulated p_{max} data in Fig. 6. The numerical data
 233 were obtained using constant-volume combustion in CANTERA (Goodwin et al., 2017) and MF
 234 comprehensive chemical mechanism (Cheng et al., 2017). Comparatively, the experimental p_{max}
 235 values are lower than the simulated results. The disparity between the experiment and the simulated
 236 p_{max} is attributable to heat loss (conduction and radiation) in the CVCC during the experiment
 237 which reduces the pressure rise whereas the numerical analysis assumes adiabatic condition. In
 238 addition, somehow some of the fuel could be stuck in the vessel due to adsorption and couldn't burn
 239 during combustion, which could lead to reduced peak pressures (Zhang et al., 2019a). Moreover,
 240 likewise, the observations made in Fig. 5, an increment in the initial pressure promotes strenuous
 241 combustion and the release of higher thermal energy and peak explosion pressures.

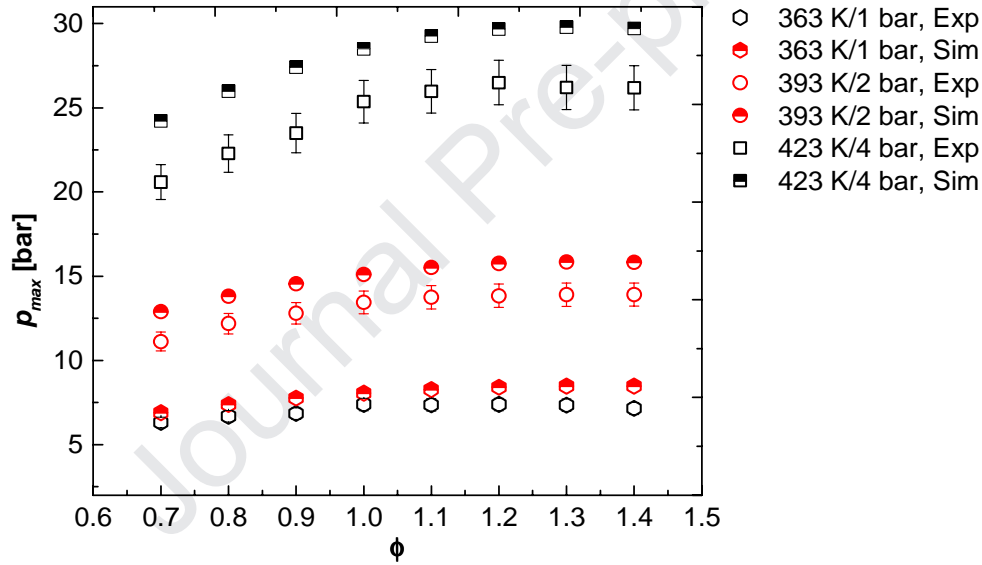
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244 **Fig. 5.** A chart of p_{max} against ϕ at $T_i = 363$ - 423 K and $p_i = 1$ - 4 bar. Legend: p_i is led by T_i .

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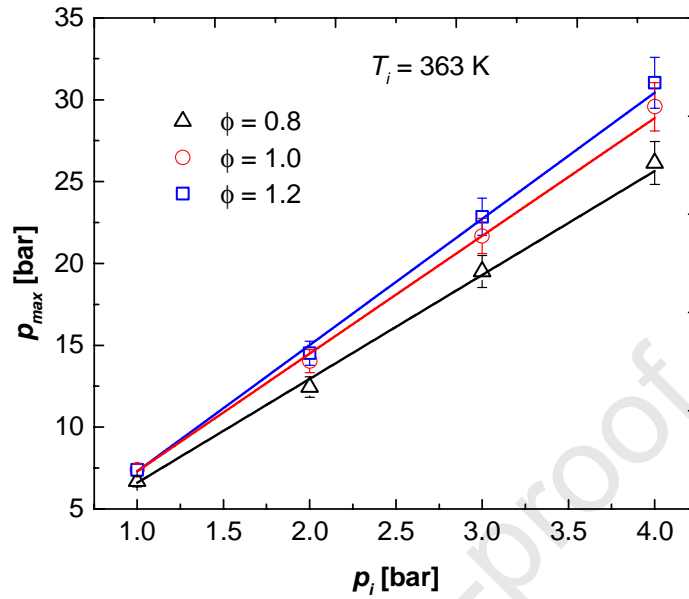
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247 **Fig. 6.** Experimental and simulated p_{max} at $T_i = 363$, 393 , and 423 K, $p_i = 1$, 2 , and 4 bar and $\phi =$
248 0.7 - 1.4 . Legend: p_i is led by T_i . Exp and Sim refer to the experimental and simulated results.

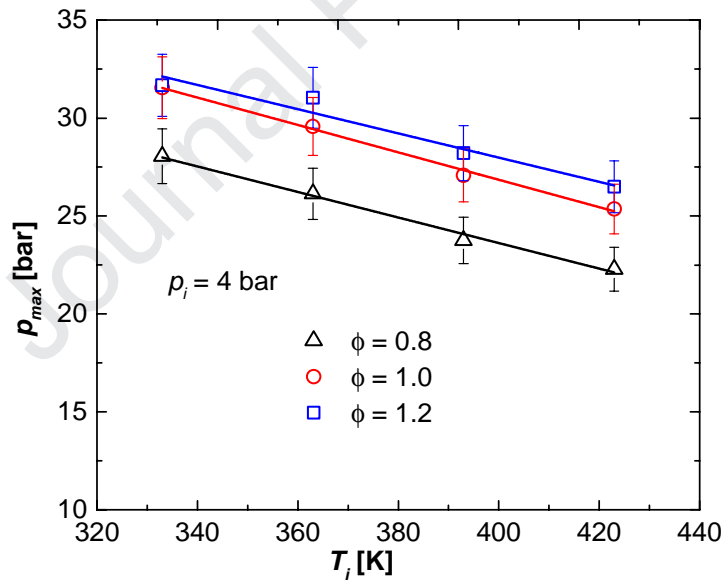
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250 Fig. 7 describes the effect of p_i on p_{max} at $\phi = 0.8$, 1.0 , and 1.2 and T_i of 363 K. In conformity
251 with Fig. 7, it can be realized that in some way p_i increases linearly with p_{max} values. The explosion
252 becomes brisk when p_i is increased which will lead to a higher discharge of heat from the
253 combustion and high pressure rise. Here, as the values of p_i increased from 1 bar to 4 bar, p_{max}
254 values also increased from 6.689 - 26.139 bar ($\phi = 0.8$), 7.388 - 29.577 bar ($\phi = 1.0$) and 7.388 -
255 31.041 bar at $\phi = 1.2$. Fig. 8 also illustrates the impact of T_i on p_{max} at p_i of 4 bar and $\phi = 0.8$, 1.0 ,
256 and 1.2 . Similar correlations have been noticed in past studies (Mitu et al., 2012; Saeed, 2017) for
257 distinct fuels. As can be observed in Fig. 8, p_{max} values somehow decrease linearly with increasing
258 T_i . When T_i was increased the density of MF mixture in the CVCC decreased which resulted in
259 rapid burning speed and decreased p_{max} values. When T_i increased from 333 K to 423 K, p_{max}

260 decreased from 28.057 bar to 22.285 bar at ($\phi = 0.8$). At the same time, p_{max} decreased from
 261 31.553 bar to 25.364 bar at ($\phi = 1.0$) as well as 31.677 bar to 26.495 bar at ($\phi = 1.2$) when T_i
 262 increased from 333 K to 423 K.
 263



264
 265 **Fig. 7.** Effect of p_i on p_{max} at $\phi = 0.8, 1.0,$ and 1.2 and $T_i = 363$ K. The solid lines are linear fit.
 266



267
 268 **Fig. 8.** Effect of T_i on p_{max} at $\phi = 0.8, 1.0,$ and 1.2 and $p_i = 4$ bar. The solid lines are linear fit.
 269

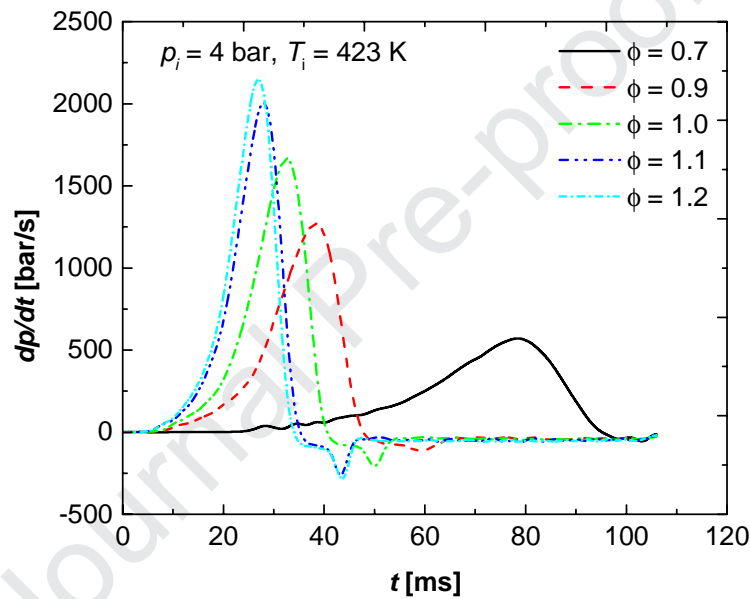
270 3.2. Pressure rise rate, maximum pressure rise rate and deflagration index

271 Fig. 9 displays the plot of pressure rise rate (dp/d) versus t at $\phi = 0.7-1.2$, $p_i = 4$ bar and $T_i =$
 272 423 K. As can be observed in Fig. 9, for each of the dp/d map ($\phi = 0.7-1.2$), dp/d initially
 273 increases and reaches the maximum value and decrease afterwards. Moreover, due to excessive heat
 274 transfer to the CVCC wall the explosion pressure p decreases and the values of dp/d become

275 negative as illustrated in Fig.9. In accordance with Fig. 9, the values of dp/d somehow increases
 276 with increasing ϕ , underlining the sensitivity of dp/d to ϕ . The peak of dp/d value increased
 277 from 571.3 bar/s to 2147.3 bar/s when ϕ increased from $\phi = 0.7$ to 1.2, obtaining the highest value
 278 at $\phi = 1.2$. Fig. 10 also shows the comparison of dp/d at $T_i = 363, 393$ and 423 K, $p_i = 1$ bar and
 279 $\phi = 1.0$.

280 According to Fig. 10, the peak of dp/d increases with a lower T_i . Thus, increased MF burning
 281 velocity or speed as well as decreased explosion pressure and maximum pressure rise rate depends
 282 on increased T_i . The highest values of dp/d are 542.905 bar/s (363 K), 509.712 bar/s (393 K) and
 283 444.523 bar/s for 423 K. Fig. 11 represents the variation of dp/d with p_i at $T_i = 423$ K and $\phi =$
 284 1.0. As shown in Fig. 11, the values of dp/d almost increased twofold with increased p_i . In
 285 addition, when p_i increased from 1 bar to 4 bar the value of dp/d increased from 444.523 bar/s to
 286 1668.99 bar/s. As aforementioned in Section 3.1, this could be due to more and more energetic MF
 287 explosion at increased p_i .

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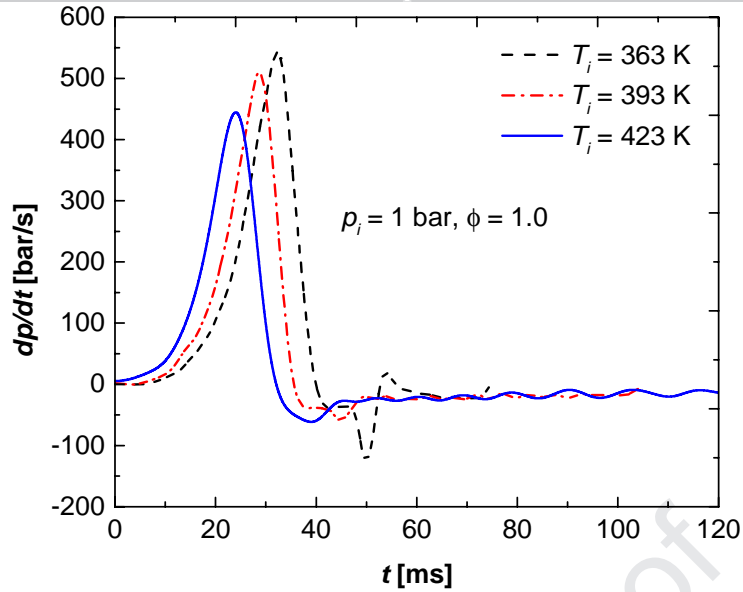
290 **Fig. 9.** A graph of pressure rise rate contours at $T_i = 423$ K, $p_i = 4$ bar and $\phi = 0.7-1.2$.

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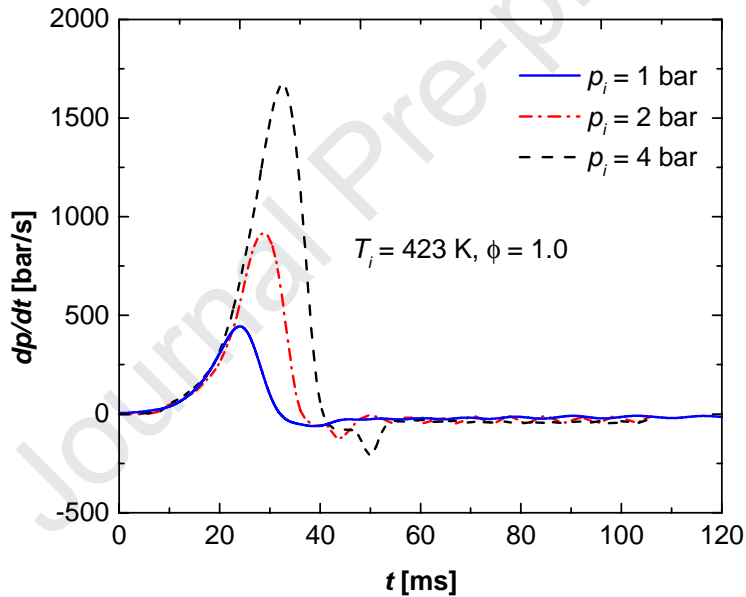
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296 **Fig. 10.** Pressure rise rate maps at $p_i = 1$ bar, $T_i = 363$ - 423 K and $\phi = 1.0$.
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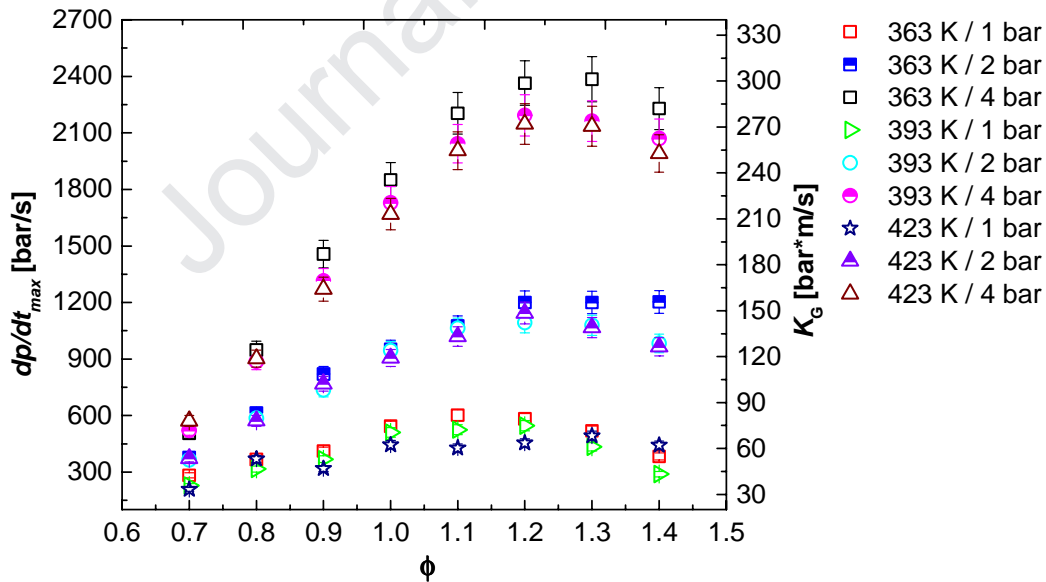


298
299 **Fig. 11.** Effects of p_i on dp/dt at $T_i = 423$ K and $\phi = 1.0$.
300

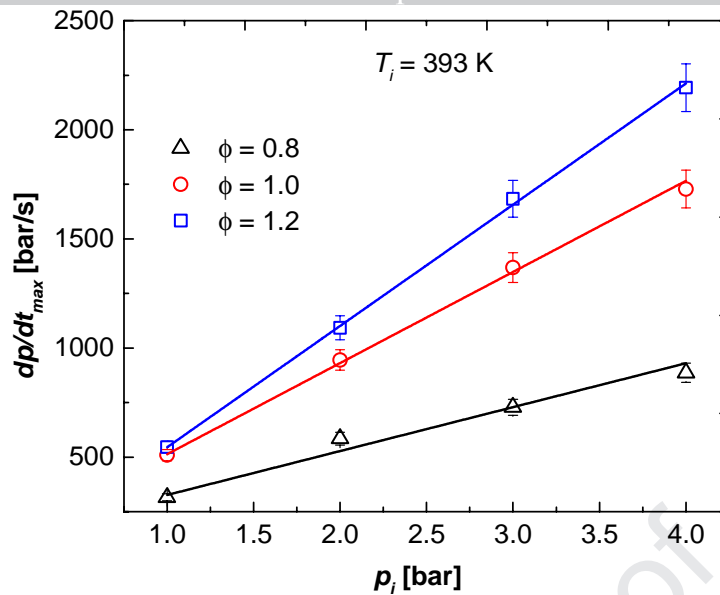
301 The maximum pressure rise rate dp/dt_{max} is a significant parameter used to describe the
302 explosion build-up pressure. It is a very influential parameter in the estimation of the deflagration
303 index (K_G). Fig. 12 compares dp/dt_{max} at $T_i = 363$ - 423 K, $p_i = 1$ - 4 bar and $\phi = 0.7$ - 1.4 . As
304 depicted in Fig. 12, dp/dt_{max} values are fairly higher at a lower T_i when compared to dp/dt_{max}
305 values at a higher T_i . Truly, increased T_i dictates higher burning velocity and reduced p_{max} .
306 However, the combined effect of the burning velocity and p_{max} determines the magnitude of the
307 maximum pressure rise rate. In addition, the values of dp/dt_{max} increases drastically when p_i
308 increases. As shown in Fig. 12, dp/dt_{max} values are somehow insensitive to p_i at some of the
309 equivalence ratios.

310 The deflagration index (K_G) measures the intensity of the combustion or explosion process.
 311 Therefore, the higher the value of the deflagration index the more intense the explosion risk. The
 312 deflagration index forms the basis for the design of explosion devices and safety assessment.
 313 Fundamentally, the deflagration index is quantified as, $K_G = dp/d_{max} \cdot V^{1/3}$ (Dahoe and de Goey,
 314 2003; Saeed, 2017). V denotes the CVCC inner volume. Invariably, explosion advancement is
 315 influenced by the volume of a vessel. Accordingly, an increment in the volume (radius) of a vessel
 316 results in an increment in the flame propagation time. Therefore, the pressure rise during the
 317 explosion is volume-variant. However, according to the definition of cube-root law or K_G ,
 318 multiplying dp/d_{max} by $V^{1/3}$ renders K_G volume-independent irrespective of the vessel size
 319 (Dahoe, 2005; Dahoe and de Goey, 2003; Faghieh et al., 2016; Xie et al., 2016). Thus, dp/d_{max} is
 320 normalized by $V^{1/3}$.

321 Again, Fig. 12 shows K_G values graphed against ϕ at $T_i = 363$ -423 K and $p_i = 1$ -4 bar. The
 322 values of K_G have a similar tendency as dp/d_{max} due to its linear dependence on dp/d_{max} . The
 323 magnitude of K_G values rise with increased ϕ . Besides, an increment in p_i dramatically increases
 324 K_G values due to more vigorous combustion. Thus, at a higher p_i , the propagating flame front
 325 becomes more vigorous and instable, hence, generating a higher p_{max} and dp/d_{max} as well as K_G .
 326 Herein, K_G values of MF range from 200-300 bar*m/s at $p_i = 4$ bar, $T_i = 363$ K, 393 K and 423 K,
 327 and $\phi = 1.0$ -1.4. Fig. 13 also depicts the variation of dp/d_{max} with p_i at $T_i = 393$ K and $\phi = 0.8$,
 328 1.0, and 1.2. Fig. 13 discloses that MF dp/d_{max} values are greater at a higher p_i and to a certain
 329 degree varies linearly with p_i values. Herein, dp/d_{max} increased from 315.645-886.725 bar/s ($\phi =$
 330 0.8), 509.712-1728.69 bar/s ($\phi = 1.0$), and 545.877-2192.92 bar/s ($\phi = 1.2$) when p_i increased from
 331 1 bar to 4 bar.
 332



333
 334 **Fig. 12.** dp/d_{max} and K_G plots with ϕ at $p_i = 1$ -4 bar and $T_i = 363$ -423 K. Legend: p_i is led by T_i .
 335



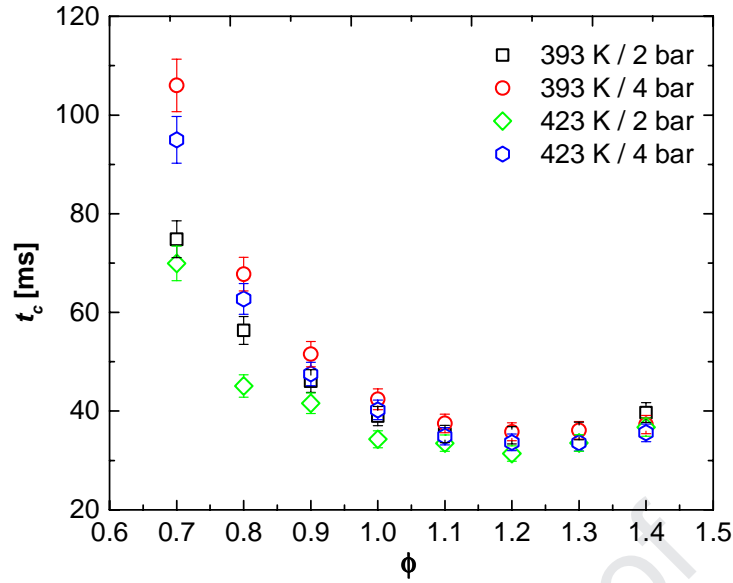
336

337 **Fig. 13.** A chart of dp/dt_{max} against p_i at $T_i = 393$ K and $\phi = 0.8, 1.0,$ and 1.2 . The solid lines are
 338 linear fit.

339

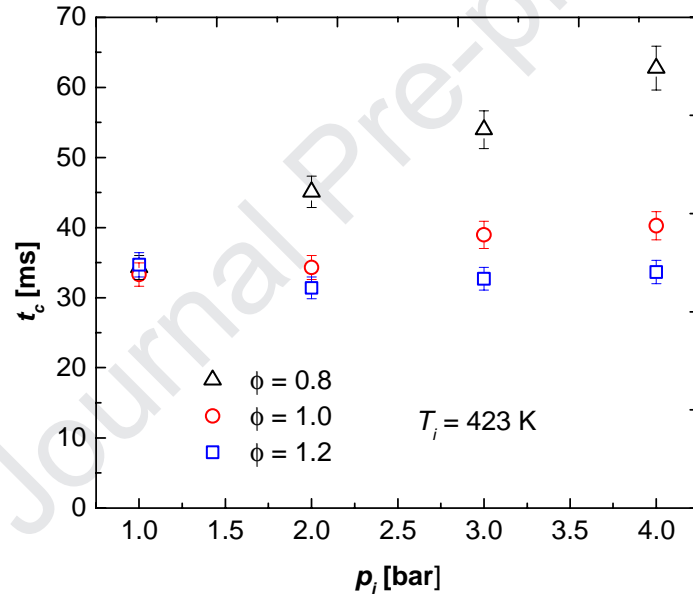
340 3.3. Explosion time

341 Herein, the explosion time (τ) describes the time at which p_{max} was obtained. The explosion time
 342 is very crucial in safety assessment and design of combustion devices. Fig. 14 shows τ values at
 343 the investigated conditions, $p_i = 2$ and 4 bar and $T_i = 393$ and 423 K at different ϕ . The values of
 344 τ decreases with increasing ϕ until it attains the minimum value and starts to increase again with ϕ .
 345 Due to less quantity of fuel in lean fuel mixtures, the explosion was not brisk, therefore, the
 346 combustion time was prolonged. Moreover, reverse reflection is true for increased ϕ . Here τ values
 347 presented in Fig. 14 are in somewhat sensitive to p_i and T_i . By and large, the values of τ somehow
 348 increased with increased p_i and decreased with increased T_i . An increment in T_i caused a decrease
 349 in τ owing to a faster flame speed. However, at rich mixtures the influence of T_i on the explosion
 350 time is somewhat insignificant. This could be as a consequence of equivalence ratio effects on the
 351 explosion pressure rise in rich mixtures. Fig. 15 also shows the relationship between p_i and τ at
 352 $\phi = 0.8, 1.0,$ and 1.2 and $T_i = 423$ K. According to Fig. 15, somewhat p_i exhibits a close linear
 353 correlation with τ at the different equivalence ratios. Explosion time is closely associated with the
 354 flame speed, so, the fastness of the flame speed determines the explosion time. In this study, the
 355 explosion time was relatively longer when p_i increased. Thus, when p_i was increased the mass or
 356 density of MF mixture also increased which extended the explosion time due to low flame speed. A
 357 parallel remark was made in these treatises (Cui et al., 2018; Hu et al., 2017; Xu et al., 2019).
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Fig. 14. A plot of τ_c with ϕ at $p_i = 2$ and 4 bar and $T_i = 393$ and 423 K. Legend: p_i is led by T_i .



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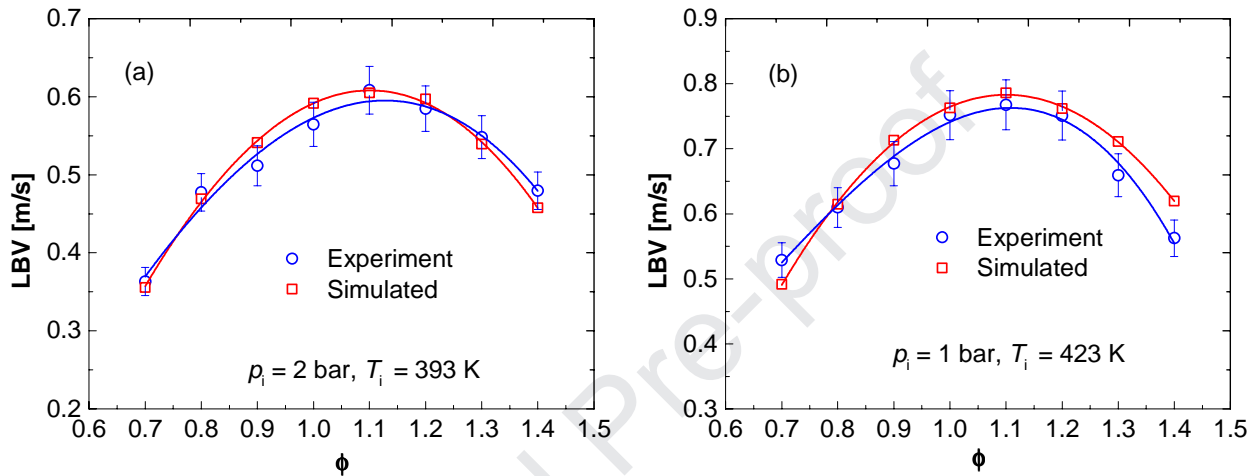
Fig. 15. A graph of τ_c against p_i at $\phi = 0.8, 1.0$, and 1.2 and $T_i = 423$ K.

3.4. 2-methylfuran LBV

366 Using the well-established burning velocity relation in equation (1), the pressure history data were
367 used to determine the experimental burning velocities of MF at the investigated conditions. The
368 LBVs at the initial conditions were evaluated from the $S_L(p)$ curve employing extrapolation (Dahoe
369 and de Goey, 2003; Omari and Tartakovsky, 2016; Shen et al., 2017a).
370

$$S_L = \frac{1}{(p_{\max} - p_i)} \frac{1}{3} \left(\frac{4\pi}{3V} \right)^{-1/3} \left(\frac{p_i}{p} \right)^{1/\gamma} \left[1 - \left(\frac{p_i}{p} \right)^{1/\gamma} \left(\frac{p_{\max} - p}{p_{\max} - p_i} \right) \right]^{-2/3} \frac{dp}{dt} \quad (1)$$

371 p_{max} and p denote the peak explosion pressure and explosion pressure whereas p_i and γ refer to the
 372 initial pressure and the specific heat of the unburnt mixture. V and dp/dt refer to the CVCC inner
 373 volume and the explosion pressure rise rate. Fig. 16(a)-(b) compares the experimental and simulated
 374 burning velocities of MF at $p_i = 1$ bar and 2 bar as well as $T_i = 393$ K and 423 K. The simulated
 375 LBVs were computed with CANTERA thermochemical code (Goodwin et al., 2017) using Cheng
 376 et al. (2017) MF mechanism. It is worth noting that the LBV data of this work at $T_i = 363$ K have
 377 been compared to literature data (Ma et al., 2013a) in (Zhongyang et al., 2018) to validate the
 378 accuracy of this investigation. In conformity with Fig. 16(a)-(b), the experimental and the simulated
 379 LBVs have a parallel tendency. However, the experimental burning velocities are somehow
 380 underpredicted compared to the calculated results.
 381



382
 383 Fig. 16. Comparison of MF experimental and simulated burning velocities. The solid lines represent
 384 a polynomial fit.
 385

386 4. Conclusions

387 The explosion characteristics of 2-methylfuran have been evaluated at high pressure (1, 2, 3, and
 388 4 bar) and temperature (333-423 K) conditions and equivalence ratio ($\phi = 0.7$ -1.4) in a constant
 389 volume combustion chamber. The important explosion parameters were determined from well-
 390 processed pressure data obtained from the experiment. The experimental peak explosion pressure
 391 data were compared to simulated data. It was found that the simulated results were higher than the
 392 experimental data due to heat loss to the chamber walls during the combustion process in the
 393 experiment. The explosion parameters were sensitive to the initial pressure, initial temperature and
 394 equivalence ratio. 2-methylfuran peak explosion pressure, maximum pressure rise rate and the
 395 deflagration index decreased with increased initial temperature, however, they increased with
 396 increased initial pressure. In addition, the magnitude of the explosion parameters increased as the
 397 equivalence ratio increased. The deflagration index of 2-methylfuran was found to be quite higher
 398 at higher pressures, reactive, and rich mixtures. In conclusion, the explosion time somehow
 399 decreased with increased initial temperature and increased with a higher initial pressure.
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 401
 402

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Highlights

- Explosion characteristics of 2-methylfuran were studied at elevated pressures and temperatures.
- The influence of initial pressure, initial temperature and equivalence ratio on 2-methylfuran explosion characteristics were assessed.
- The connexion between 2-methylfuran laminar burning velocity and the explosion indices such as the peak explosion pressure, maximum pressure rise rate and the severity factor were examined.

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