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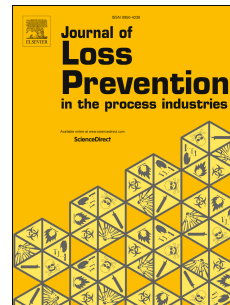
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# Evaluation of explosion characteristics of 2-methylfuran/air mixture

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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	$\phi$	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  $\phi$  in order to warrant 90-95% certitude.

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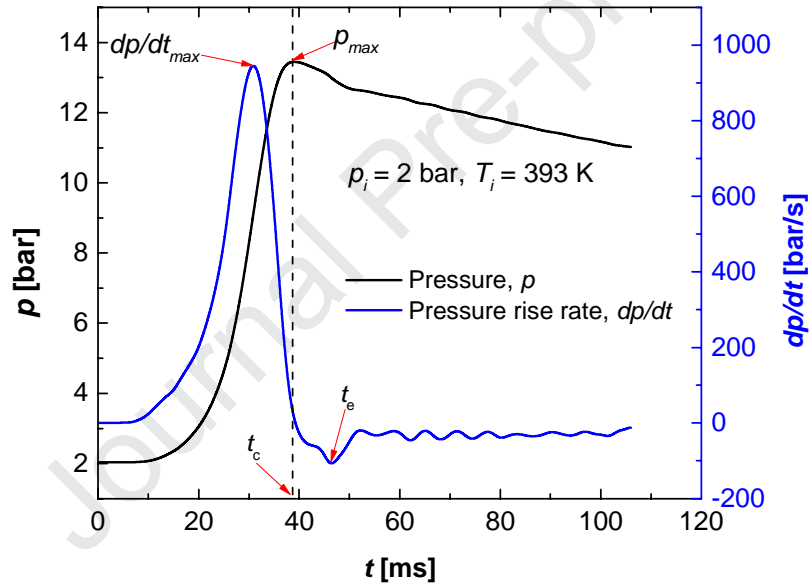
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169

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.

183



184

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  $\phi = 1.0$ .

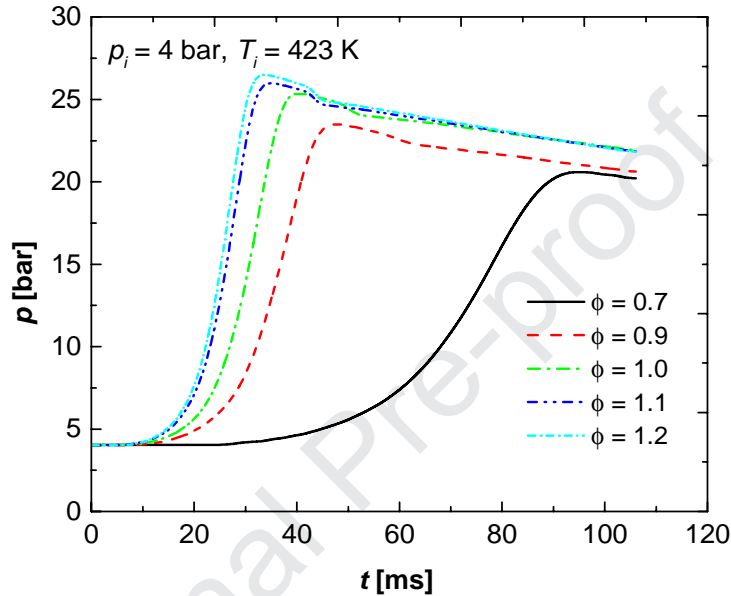
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188 **3.1. Explosion pressure and peak explosion pressure**

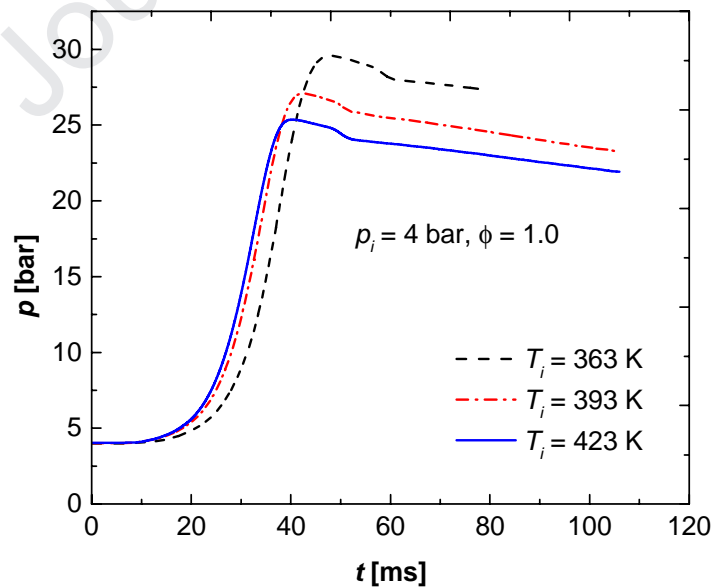
189 Fig. 2 shows  $p$  contours at  $p_i = 4$  bar and  $T_i = 423$  K for different  $\phi$ . Similar contours were obtained  
 190 for the different  $p_i$ ,  $T_i$  and  $\phi$  values investigated in this document. With reference to Fig. 2, it can be  
 191 noticed that the value of  $p$  is sensitive to  $\phi$ , therefore, the magnitude of  $p$  increases with increasing  
 192  $\phi$ . 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  $\phi$  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



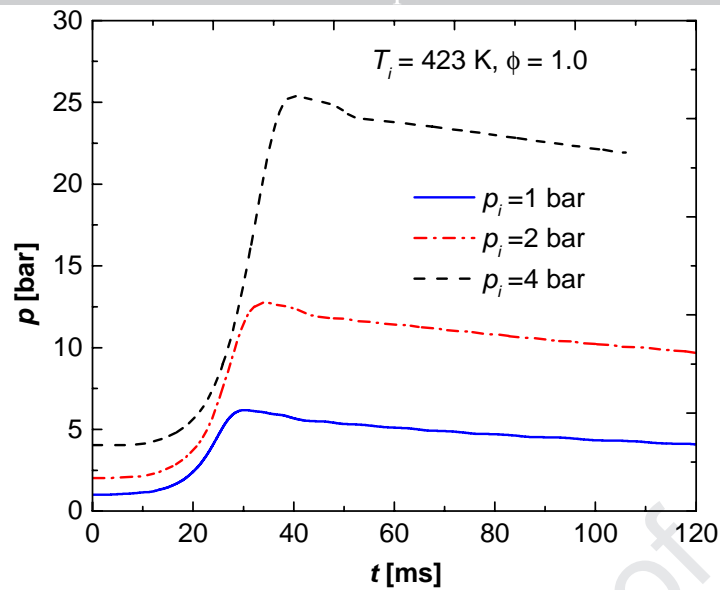
197 of  $p$  is lower at a higher  $T_i$  owing to a higher mass burning rate and flame speed at a higher  $T_i$ .  
 198 Accordingly, the combustible mixture takes a shorter time to reach the peak of  $p$ . In addition to this,  
 199 the mass of MF/air unburnt mixture in the CVCC was decreased (less 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  $\phi = 1.0$ .

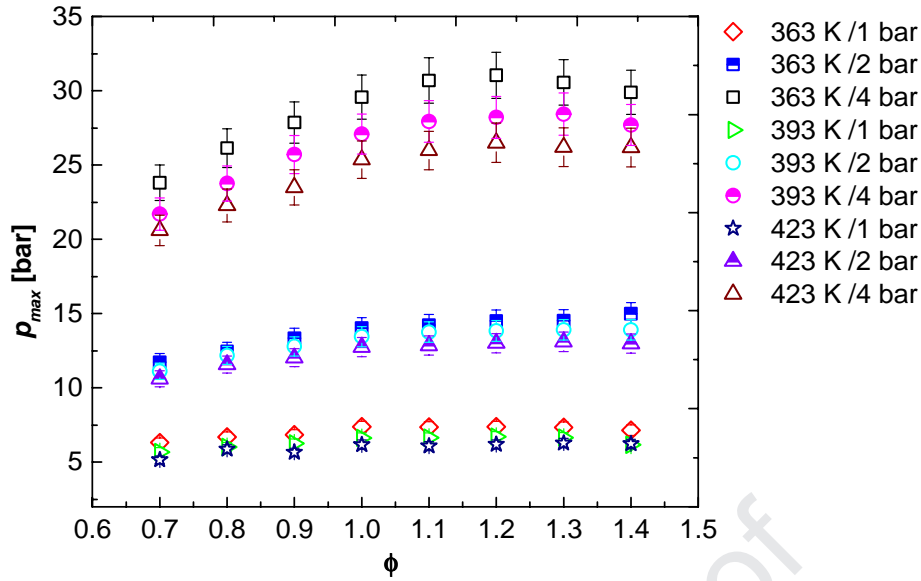
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216 The peak explosion pressure ( $p_{max}$ ) quantify the energy distribution of combustion propagating  
 217 waves (Shen et al., 2017b). Therefore,  $p_{max}$  can be used to determine the heat energy from the  
 218 explosion. Fig. 5 depicts the values of  $p_{max}$  as a function of  $\phi$  at  $p_i = 1-4$  bar and  $T_i = 363-423$  K. In  
 219 general, the values of  $p_{max}$  increases with increasing  $\phi$ . 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  $\phi$  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.

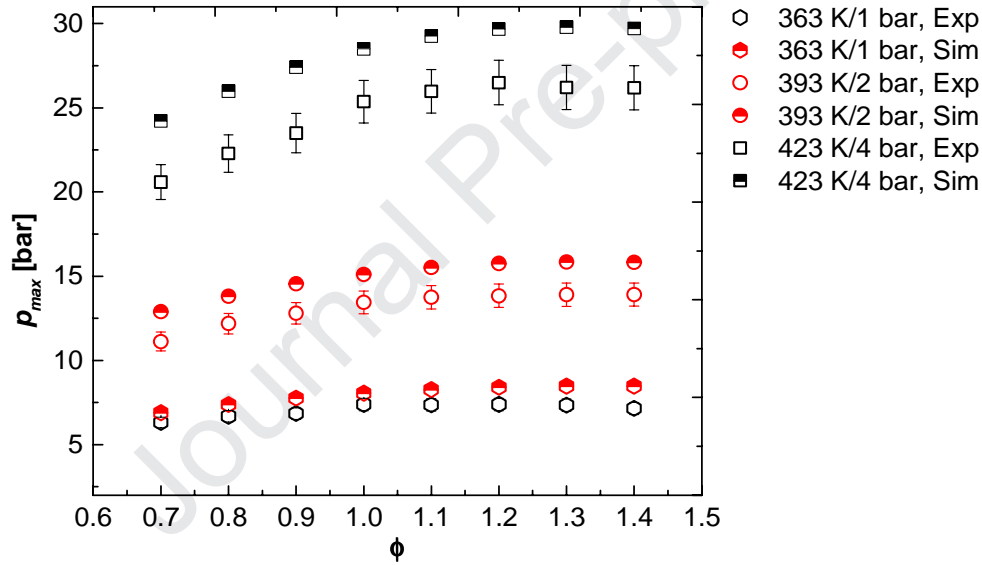
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243

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

245



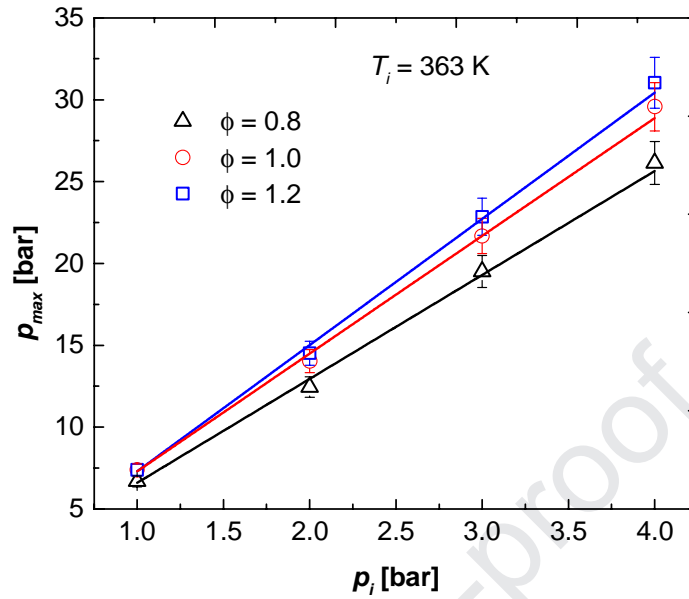
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247 **Fig. 6.** Experimental and simulated  $p_{max}$  at  $T_i = 363, 393,$  and  $423$  K,  $p_i = 1, 2,$  and  $4$  bar and  $\phi =$   
248  $0.7\text{-}1.4$ . Legend:  $p_i$  is led by  $T_i$ . Exp and Sim refer to the experimental and simulated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

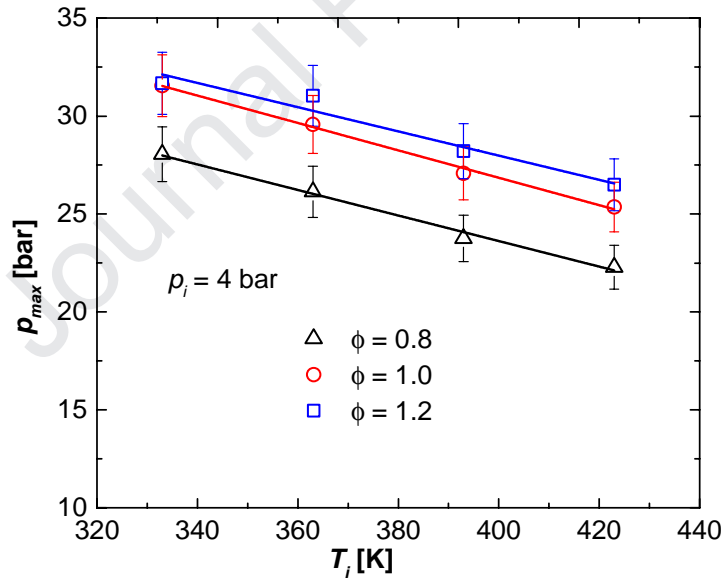
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250 Fig. 7 describes the effect of  $p_i$  on  $p_{max}$  at  $\phi = 0.8, 1.0,$  and  $1.2$  and  $T_i$  of  $363$  K. In conformity  
251 with Fig. 7, it can be realized that in some way  $p_i$  increases linearly with  $p_{max}$  values. The explosion  
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  $6.689\text{-}26.139$  bar ( $\phi = 0.8$ ),  $7.388\text{-}29.577$  bar ( $\phi = 1.0$ ) and  $7.388\text{-}$   
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

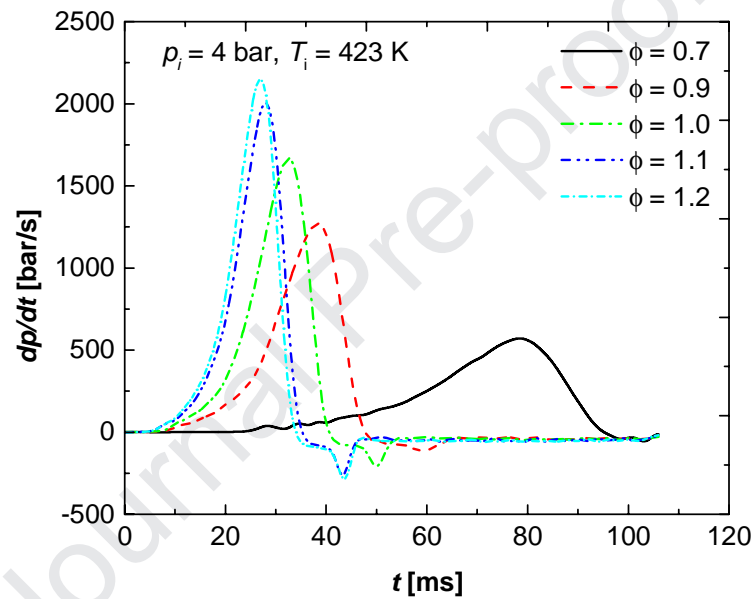
### 270 3.2. Pressure rise rate, maximum pressure rise rate and deflagration index

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  $\phi$ , underlining the sensitivity of  $dp/d$  to  $\phi$ . The peak of  $dp/d$  value increased  
 277 from 571.3 bar/s to 2147.3 bar/s when  $\phi$  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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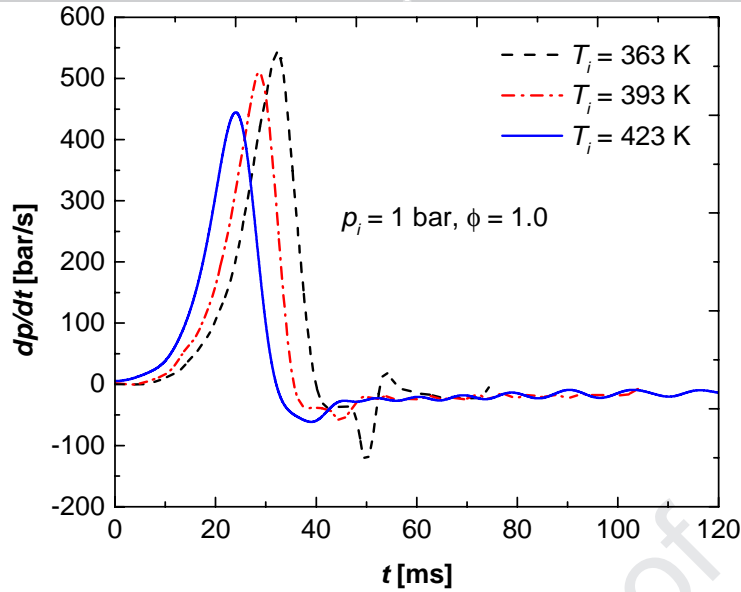
290 **Fig. 9.** A graph of pressure rise rate contours at  $T_i = 423$  K,  $p_i = 4$  bar and  $\phi = 0.7-1.2$ .

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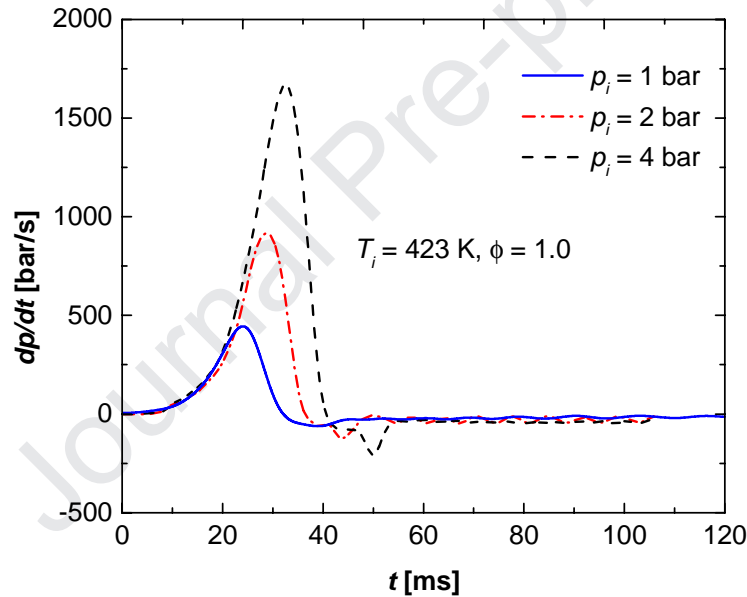
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296 **Fig. 10.** Pressure rise rate maps at  $p_i = 1$  bar,  $T_i = 363$ - $423$  K and  $\phi = 1.0$ .  
297

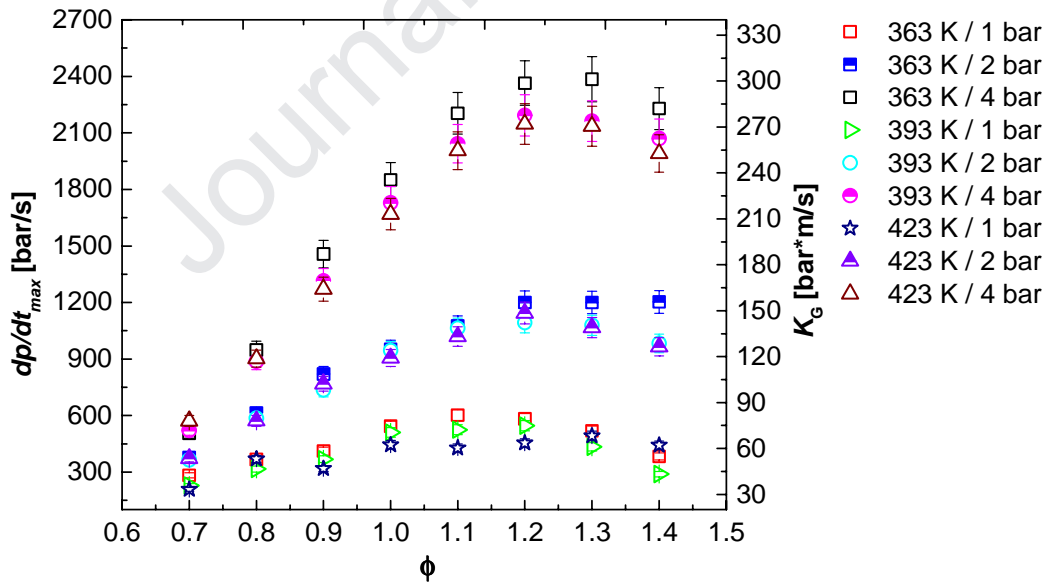


298  
299 **Fig. 11.** Effects of  $p_i$  on  $dp/dt$  at  $T_i = 423$  K and  $\phi = 1.0$ .  
300

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  $V^{1/3}$ .

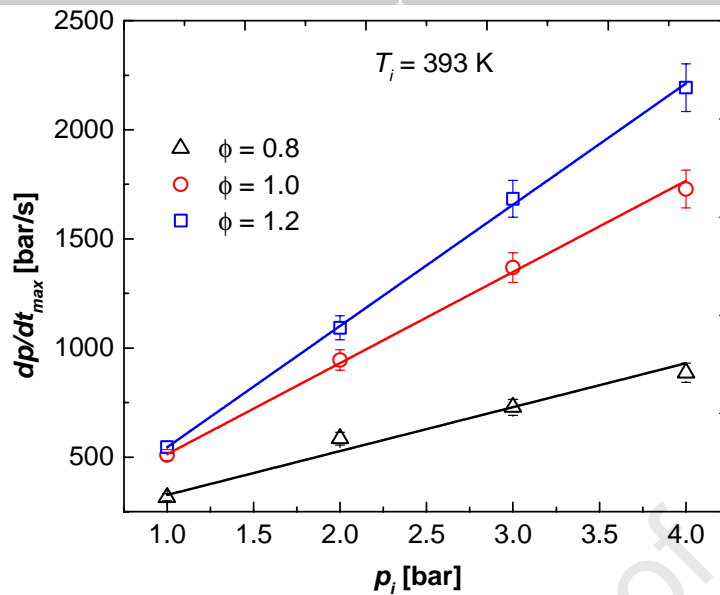
321 Again, Fig. 12 shows  $K_G$  values graphed against  $\phi$  at  $T_i = 363$ -423 K and  $p_i = 1$ -4 bar. The  
 322 values of  $K_G$  have a similar tendency as  $dp/d_{max}$  due to its linear dependence on  $dp/d_{max}$ . The  
 323 magnitude of  $K_G$  values rise with increased  $\phi$ . Besides, 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  $\phi$  at  $p_i = 1$ -4 bar and  $T_i = 363$ -423 K. Legend:  $p_i$  is led by  $T_i$ .

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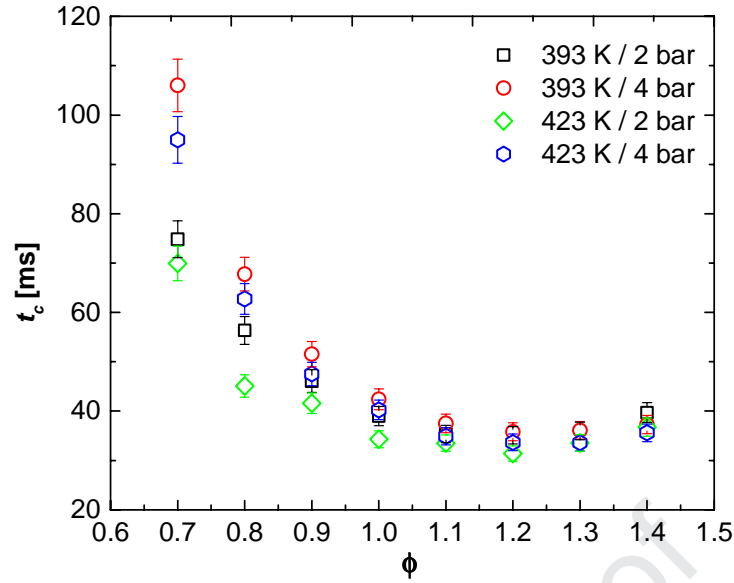
337 **Fig. 13.** A chart of  $dp/dt_{max}$  against  $p_i$  at  $T_i = 393$  K and  $\phi = 0.8, 1.0,$  and  $1.2$ . The solid lines are  
 338 linear fit.

339

### 340 3.3. Explosion time

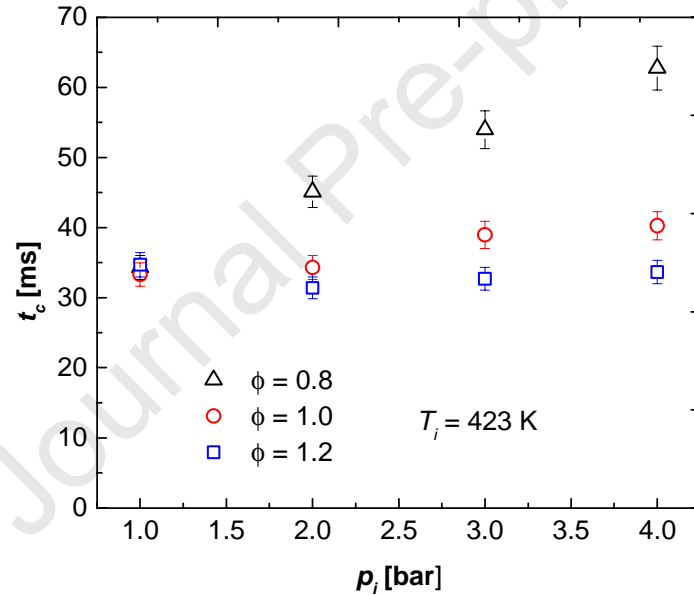
341 Herein, the explosion time ( $\tau$ ) describes the time at which  $p_{max}$  was obtained. The explosion time  
 342 is very crucial in safety assessment and design of combustion devices. Fig. 14 shows  $\tau$  values at  
 343 the investigated conditions,  $p_i = 2$  and  $4$  bar and  $T_i = 393$  and  $423$  K at different  $\phi$ . The values of  
 344  $\tau$  decreases with increasing  $\phi$  until it attains the minimum value and starts to increase again with  $\phi$ .  
 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  $\phi$ . Here  $\tau$  values  
 347 presented in Fig. 14 are in somewhat sensitive to  $p_i$  and  $T_i$ . By and large, the values of  $\tau$  somehow  
 348 increased with increased  $p_i$  and decreased with increased  $T_i$ . An increment in  $T_i$  caused a decrease  
 349 in  $\tau$  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  $\tau$  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  $\tau$  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).  
 358





359  
360  
361

**Fig. 14.** A plot of  $\tau_c$  with  $\phi$  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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365

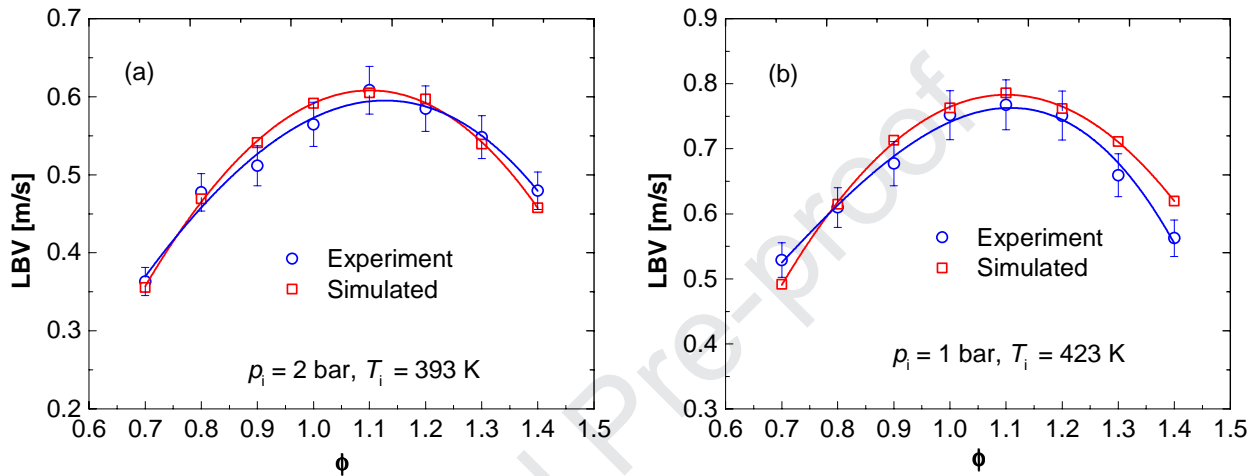
**Fig. 15.** A graph of  $\tau_c$  against  $p_i$  at  $\phi = 0.8, 1.0$ , and 1.2 and  $T_i = 423$  K.

### 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  $\gamma$  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.  
 400  
 401  
 402

403 **Acknowledgements**

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407 **References:**

- 409 Askari, M.H., Ashjaee, M., Karaminejad, S., 2017. Experimental and numerical investigation of the  
410 laminar burning velocity and combustion characteristics of biogas at high pressures. *Energy*  
411 and Fuels 31, 14169–14179.
- 412 Bao, X., Jiang, Y., Xu, H., Wang, C., Lattimore, T., Tang, L., 2017. Laminar flame characteristics  
413 of cyclopentanone at elevated temperatures. *Appl. Energy* 195, 671–680.
- 414 Beck, M., 2016. The risk implications of globalisation: An exploratory analysis of 105 major  
415 industrial incidents (1971-2010). *Int. J. Environ. Res. Public Health* 13, 1–21.
- 416 Cheng, Z., Niu, Q., Wang, Z., Jin, H., Chen, G., Yao, M., Wei, L., 2017. Experimental and kinetic  
417 modeling studies of low-pressure premixed laminar 2-methylfuran flames. *Proc. Combust.*  
418 *Inst.* 1295–1302.
- 419 Cui, G., Wang, S., Liu, J., Bi, Z., Li, Z., 2018. Explosion characteristics of a methane/air mixture at  
420 low initial temperatures. *Fuel* 234, 886–893.
- 421 Dahoe, A.E., 2005. Laminar burning velocities of hydrogen-air mixtures from closed vessel gas  
422 explosions. *J. Loss Prev. Process Ind.* 18, 152–166.
- 423 Dahoe, A.E., de Goey, L.P.H., 2003. On the determination of the laminar burning velocity from  
424 closed vessel gas explosions. *J. Loss Prev. Process Ind.* 16, 457–478.
- 425 Di Sarli, V., Benedetto, A. Di, 2012. Sensitivity to the presence of the combustion submodel for  
426 large eddy simulation of transient premixed flame-vortex interactions. *Ind. Eng. Chem. Res.*  
427 51, 7704–7712.
- 428 Faghih, M., Gou, X., Chen, Z., 2016. The explosion characteristics of methane, hydrogen and their  
429 mixtures: A computational study. *J. Loss Prev. Process Ind.* 40, 131–138.
- 430 Goodwin, D.G., Moffat, H.K., Speth, R.L., 2017. *Cantera: An Object-oriented Software Toolkit for*  
431 *Chemical Kinetics, Thermodynamics, and Transport Processes.*
- 432 Hu, E., Tian, H., Zhang, X., Li, X., Huang, Z., 2017. Explosion characteristics of n-butanol/iso-  
433 octane-air mixtures. *Fuel* 188, 90–97.
- 434 Huzayyin, A.S., Moneib, H.A., Shehatta, M.S., Attia, A.M.A., 2008. Laminar burning velocity and  
435 explosion index of LPG-air and propane-air mixtures. *Fuel* 87, 39–57.
- 436 Kundu, S.K., Zanganeh, J., Eschebach, D., Badat, Y., Moghtaderi, B., 2018. Confined explosion of  
437 methane-air mixtures under turbulence. *Fuel* 220, 471–480.
- 438 Li, D., Zhang, Q., Ma, Q., Shen, S., 2015. Comparison of explosion characteristics between  
439 hydrogen/air and methane/air at the stoichiometric concentrations. *Int. J. Hydrogen Energy* 40,  
440 8761–8768.
- 441 Li, Q., Cheng, Y., Huang, Z., 2015. Comparative assessment of the explosion characteristics of  
442 alcohol-air mixtures. *J. Loss Prev. Process Ind.* 37, 91–100.
- 443 Li, Y., Bi, M., Huang, L., Liu, Q., Li, B., Ma, D., Gao, W., 2018a. Hydrogen cloud explosion  
444 evaluation under inert gas atmosphere. *Fuel Process. Technol.* 180, 96–104.
- 445 Li, Y., Bi, M., Li, B., Zhou, Y., Gao, W., 2018b. Effects of hydrogen and initial pressure on flame

- 446 characteristics and explosion pressure of methane/hydrogen fuels. *Fuel* 233, 269–282.
- 447 Ma, X., Jiang, C., Xu, H., Ding, H., Shuai, S., 2013a. Laminar burning characteristics of 2-  
448 methylfuran and isooctane blend fuels. *Fuel* 116, 281–291.
- 449 Ma, X., Jiang, C., Xu, H., Shuai, S., Ding, H., 2013b. Laminar burning characteristics of 2-  
450 methylfuran compared with 2,5-dimethylfuran and isooctane. *Energy and Fuels* 27, 6212–  
451 6221.
- 452 Mannaa, O., Mansour, M.S., Roberts, W.L., Chung, S.H., 2015. Laminar burning velocities at  
453 elevated pressures for gasoline and gasoline surrogates associated with RON. *Combust. Flame*  
454 162, 2311–2321.
- 455 Mitu, M., Brandes, E., 2017. Influence of pressure, temperature and vessel volume on explosion  
456 characteristics of ethanol/air mixtures in closed spherical vessels. *Fuel* 203, 460–468.
- 457 Mitu, M., Brandes, E., 2015. Explosion parameters of methanol-air mixtures. *Fuel* 158, 217–223.
- 458 Mitu, M., Brandes, E., Hirsch, W., 2018. Mitigation effects on the explosion safety characteristic  
459 data of ethanol/air mixtures in closed vessel. *Process Saf. Environ. Prot.* 117, 190–199.
- 460 Mitu, M., Giurcan, V., Razus, D., Oancea, D., 2012. Temperature and pressure influence on ethane-  
461 air deflagration parameters in a spherical closed vessel. *Energy and Fuels* 26, 4840–4848.
- 462 Mitu, M., Razus, D., Giurcan, V., Oancea, D., 2015. Normal burning velocity and propagation  
463 speed of ethane-air: Pressure and temperature dependence. *Fuel* 147, 27–34.
- 464 OECD, 2013. 25 years of chemical accident prevention at OECD.
- 465 Omari, A., Tartakovsky, L., 2016. Measurement of the laminar burning velocity using the confined  
466 and unconfined spherical flame methods - A comparative analysis. *Combust. Flame* 168, 127–  
467 137.
- 468 Reyes, M., Tinaut, F. V., Horrillo, A., Lafuente, A., 2018. Experimental characterization of burning  
469 velocities of premixed methane-air and hydrogen-air mixtures in a constant volume  
470 combustion bomb at moderate pressure and temperature. *Appl. Therm. Eng.* 130, 684–697.
- 471 Saeed, K., 2017. Determination of the explosion characteristics of methanol – Air mixture in a  
472 constant volume vessel. *Fuel* 210, 729–737. <https://doi.org/10.1016/j.fuel.2017.09.004>
- 473 Shen, X., Xiu, G., Wu, S., 2017a. Experimental study on the explosion characteristics of  
474 methane/air mixtures with hydrogen addition. *Appl. Therm. Eng.* 120, 741–747.
- 475 Shen, X., Zhang, B., Zhang, X., Xiu, G., 2017b. Explosion characteristics of methane-ethane  
476 mixtures in air. *J. Loss Prev. Process Ind.* 45, 102–107.
- 477 Somers, K.P., Simmie, J.M., Gillespie, F., Burke, U., Connolly, J., Metcalfe, W.K., Battin-Leclerc,  
478 F., Dirrenberger, P., Herbinet, O., Glaude, P.A., Curran, H.J., 2013. A high temperature and  
479 atmospheric pressure experimental and detailed chemical kinetic modelling study of 2-methyl  
480 furan oxidation. *Proc. Combust. Inst.* 34, 225–232.
- 481 Sun, Z.Y., 2018. Laminar Explosion Properties of Syngas. *Combust. Sci. Technol.* 1–16.
- 482 Sun, Z.Y., Li, G.X., 2017. Turbulence influence on explosion characteristics of stoichiometric and  
483 rich hydrogen/air mixtures in a spherical closed vessel. *Energy Convers. Manag.* 149, 526–  
484 535.
- 485 Tang, C., Zhang, S., Si, Z., Huang, Z., Zhang, K., Jin, Z., 2014. High methane natural gas/air  
486 explosion characteristics in confined vessel. *J. Hazard. Mater.* 278, 520–528.
- 487 Tran, M.V., Scribano, G., Chong, C.T., Ho, T.X., 2017. Influence of hydrocarbon additions and  
488 dilutions on explosion behavior of syngas/air mixtures. *Int. J. Hydrogen Energy* 42, 27416–  
489 27427.

- 490 World Health Organization, 2009. Manual for the public health management of chemical incidents,  
491 World Health Organization.
- 492 Wu, Y.-C., Laiwang, B., Shu, C.-M., 2019. Investigation of an explosion at a styrene plant with  
493 alkylation reactor feed furnace. *Appl. Sci.* 9, 503.
- 494 Xie, Y., Wang, J., Cai, X., Huang, Z., 2016. Pressure history in the explosion of moist syngas/air  
495 mixtures. *Fuel* 185, 18–25.
- 496 Xu, C., Fang, D., Luo, Q., Ma, J., Xie, Y., 2014. A comparative study of laser ignition and spark  
497 ignition with gasoline-air mixtures. *Opt. Laser Technol.* 64, 343–351.
- 498 Xu, C., Wang, H., Li, X., Zhou, W., Wang, C., Wang, S., 2019. Explosion characteristics of a  
499 pyrolysis biofuel derived from rice husk. *J. Hazard. Mater.* 369, 324–333.
- 500 Xu, C., Zhong, A., Wang, H., Jiang, C., Sahu, A., Zhou, W., Wang, C., 2018. Laminar burning  
501 velocity of 2-methylfuran-air mixtures at elevated pressures and temperatures: Experimental  
502 and modeling studies. *Fuel* 231, 215–223.
- 503 Zhang, L., Ma, H., Pan, J., Shen, Z., Wang, L., Liu, R., Zhao, K., 2019a. Effects of hydrogen  
504 addition on the explosion characteristics of n-hexane/air mixtures. *Int. J. Hydrogen Energy* 44,  
505 2029–2038.
- 506 Zhang, L., Ma, H., Shen, Z., Wang, L., Liu, R., Pan, J., 2019b. Influence of pressure and  
507 temperature on explosion characteristics of n-hexane/air mixtures. *Exp. Therm. Fluid Sci.* 102,  
508 52–60.
- 509 Zhongyang, L., Oppong, F., Wang, H., Li, X., Xu, C., Wang, C., 2018. Investigating the laminar  
510 burning velocity of 2-methylfuran. *Fuel* 234, 1469–1480.
- 511

## 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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