



## 25 **1. Introduction**

26 Application of venting is one of the cheapest and simplest ways to mitigate gas explosion  
27 despite the complexity of the vent process (Mercx et al., 1992). In order to study the venting  
28 process and mechanisms, there have been numerous experimental, numerical and analytical  
29 studies (Bradley and Mitcheson, 1978; Ferrara et al., 2006; Russo and Di Benedetto, 2007;  
30 Kasmani et al., 2013) on vented gas explosions. Based on a large amount of experimental data  
31 and analytical predictions, some correlations (Swift, 1989; Rota et al., 1991; Molkov et al.,  
32 2000) have been proposed and adopted in the vented gas explosion design codes (Rodgers and  
33 Zalosh, 2013), such as the National Fire Protection Association-68 (NFPA-68).

34 However, the majority of existing vented gas explosion studies are conducted by using small  
35 to medium enclosures. For example, (Ferrara et al., 2008) gained experimental data from a  
36 pilot scale ( $0.2 \text{ m}^3$ ) cylindrical vessel for the analysis of interaction between internal and  
37 external vented gas explosions. The study on the flame propagation and gas explosion in  
38 propane/air mixtures done by Liu et al. (Liu et al., 2015) were performed in a  $1.16 \text{ m}^3$  explosion  
39 chamber. Similarly, in the investigation of temperature and initial enclosure pressure effects on  
40 gas explosion by Cammarota et al. (Cammarota et al., 2010), the explosion tests were  
41 performed in the cylindrical tank reactor with a diameter of 0.135m and a height of 0.4m.

42 Although there are some large-scale vented gas explosion experimental studies (Solberg et al.,  
43 1981; Harrison and Eyre, 1987; Tomlin et al., 2015), most of the explosion chambers used for  
44 experiments were cuboid-shaped chambers. Very limited literatures of vented gas explosion  
45 were conducted in large-scale cylindrical tanks. It is pointed out by (Catlin, 1991) that the  
46 scale effect on vented gas explosion is not negligible since the turbulence strain rate and  
47 chemical time scale ratio in larger scale explosions are different.

48 Therefore, in order to study large-scale vented gas explosions in cylindrical tanks, it is essential  
49 to investigate them in actual scale models. Even though the authors have performed a series of  
50 experiments by using 1.5m diameter and 1m height tanks (Li et al., 2017; Li and Hao, 2018;  
51 Li et al., 2018), large explosion pressures over 15 kPa were rarely obtained. Especially the  
52 external pressures, i.e., pressure recorded outside the explosion tank, from these tests were  
53 generally below 2 kPa. For a more meaningful structure safety or structure response study,  
54 large pressures from large-scale experiments are expected. However, large-scale experiments  
55 are impractical for most labs owing to the cost and safety concerns. Consequently,  
56 Computational Fluid Dynamics (CFD) simulations are conducted in this study to investigate  
57 larger scale vented gas explosions, existing experimental data are used for numerical data  
58 calibration.

59 In addition to the focus on large-scale vented gas explosion study, effectiveness of separation  
60 gap between adjacent tanks on gas explosion pressure and impulse mitigation is another main  
61 investigation objective in this study. Firstly, a series of small-medium scale methane-air  
62 explosion experiments conducted by the authors with different gas concentrations, vent area  
63 sizes and tank combinations are briefly introduced. Secondly, CFD simulations corresponding  
64 to all experiments are carried out. The CFD simulation accuracy is validated by comparing the  
65 numerical data with experimental data. Sensitivity study of CFD models consisting of a large  
66 explosion tank and a large adjacent tank with scaled-up grids is conducted. The empirical  
67 relations derived by the authors are applied in this study along with new adjustments for  
68 prediction of explosion pressures. Lastly, parametric studies are carried out to investigate the  
69 effectiveness of separation distance between adjacent tanks on mitigation of pressures and  
70 impulses from large-scale vented explosions in a cylindrical tank.

## 71 **2. Vented gas explosion experiments and CFD simulation calibration**

### 72 **2.1 Experimental details and CFD simulation setups**

73 A series of vented gas explosions with different methane-air gas concentrations (the  
74 concentrations presented in this article are in volume basis), vent opening designs and tank  
75 layouts were conducted. The experimental data analyzed in this study and details of equipment  
76 parameters can be found in data presented in the authors' previous work (Li et al., 2017; Li and  
77 Hao, 2018; Li et al., 2018). Table 1 summarizes the experimental details.

78 **Table 1 Experimental details of different vented gas explosion cases**

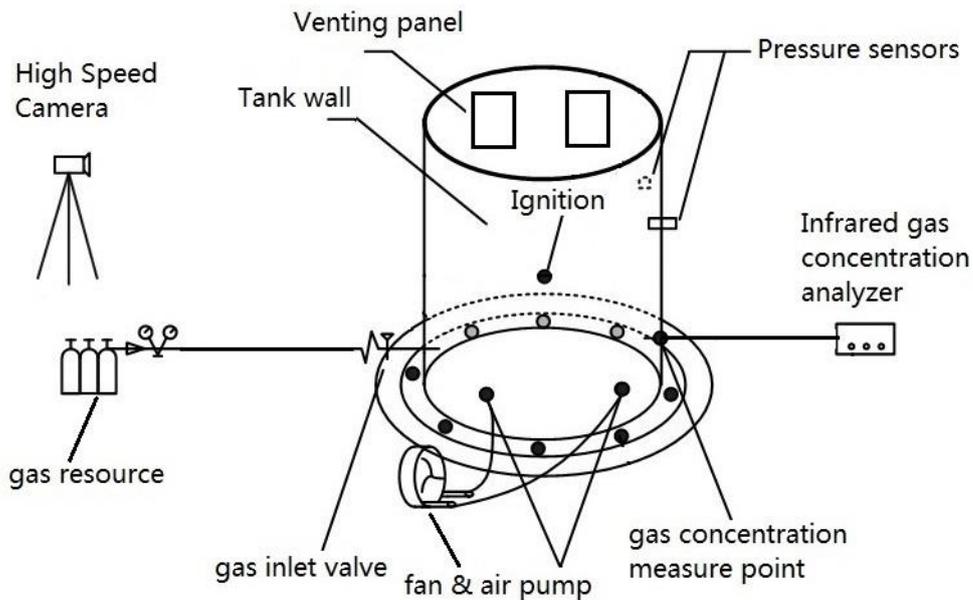
Case No.	Gas concentration (vol %)	Tank dimension (m)	Sensor location	Vent opening
1	6.5	1.5m diameter, 1m height	On tank wall at 0.75m height	One 130×280 mm <sup>2</sup> panel on roof edge
2	6.5	1.5m diameter, 1m height	On tank wall at 0.75m height	One 305×610 mm <sup>2</sup> panel on roof
3	6.5	1.5m diameter, 1m height	On tank wall at 0.75m height	Two symmetric 305×610 mm <sup>2</sup> panel on roof
4	9.5	1.5m diameter, 1m height	On tank wall at 0.75m height	One 305×610 mm <sup>2</sup> panel on roof
5	9.5	1.5m diameter, 1m height	On tank wall at 0.75m height	Two symmetric 305×610 mm <sup>2</sup> panel on roof
6	12.5	1.5m diameter, 1m height	On tank wall at 0.75m height	One 305×610 mm <sup>2</sup> panel on roof
7	9.5	8 of 1.5 diameter and 1m height tanks in group	On tank wall at 0.75m height	Two symmetric 305×610 mm <sup>2</sup> panel on roof

79  
80 For explosion cases No. 1 to 6, cylindrical tanks of 1.0m height and 1.5m diameter were  
81 designed according to the American Petroleum Institute Standard (API-650, 2007). Tank walls  
82 are made of Q345B steel with tensile strength of 0.47 GPa and yield strength of 0.35 GPa (Li  
83 and Hao, 2018). The total vent area sizes vary from 0.036 m<sup>2</sup> to 0.37 m<sup>2</sup> in these 6 cases. The  
84 methane-air concentrations of 6.5 vol %, 9.5 vol % and 12.5 vol% were tested. One larger-  
85 scale vented gas explosion test, namely case No. 7, was also carried out. This gas explosion  
86 test consisted of 8 tanks of the same size used in case No. 1 to 6 to study the pressures on the  
87 adjacent tanks from vented explosions in the tank located at the center of the tank group.

88 All tanks' bottom plates are anchored to a reinforced concrete foundation to ensure the tanks  
89 stay stationary during the vented explosion testing. High Speed Video Camera (HSVC), Gas

90 Flow Control System (GFCS) and Piezo-resistive sensors are used. The sensors are installed to  
91 record internal pressures in all the cases. A recirculation pump to fill methane into the tank and  
92 an infrared methane analyzer to control methane-air concentration are used in the GFCS. The  
93 fan and air pump as seen in Fig. 1 are used to continuously fill and mix the flammable  
94 atmosphere in the tank. In order to ensure the homogeneity of the gas concentration inside the  
95 tank, about 10 to 20 minutes is required to mix the gas mixture. A probe connected to the air  
96 pump is inserted into the tank from the gas concentration measuring point as seen in Fig. 1,  
97 while the other side of the air pump connected to the infrared gas concentration analyzer  
98 provided up-to-date gas concentration data. When the gas concentration inside the tank reached  
99 a steady data of 9.5 vol % for 10 minutes as indicated by the infrared methane analyzer, the  
100 homogenization of gas mixture for the whole region was deemed achieved.

101 The ignition sources are electric spark plugs. Centre ignitions are conducted for all tests.  
102 Ambient temperature is between 15 degree and 28 degree at the experiment site. To facilitate  
103 comparison with the numerical simulation data, all starting times of the raw experimental data  
104 are adjusted to zero.



105  
106 **Fig. 1 Gas flow control system scheme (Li and Hao, 2018).**

107 For numerical simulation, a commercial CFD software FLACS v10.7 (Gexcon, 2017), which  
 108 relies on the Reynolds-Averaged Navier-Stokes (RANS)  $k-\epsilon$  model equations, burning velocity  
 109 data, correlations, energy balance and turbulence equations (Hjertager, 1984, 1993; Arntzen,  
 110 1998; Ferrara et al., 2006), is utilized in this study for vented gas explosion simulation. The  
 111 finite volume method is used in FLACS to solve the compressible Navier-Stokes equations,  
 112 and the SIMPLE pressure algorithm (Patankar, 1980) is employed for the highly confined  
 113 explosion simulation. In FLACS, the laminar burning velocity and flame turbulent burning  
 114 velocity are based on the pre-defined tables and Bray's expression (Bray, 1990). During the  
 115 vented gas explosion simulation, diffusion is increased by a factor of beta and reaction rate is  
 116 reduced by a factor of  $1/\beta$ , which eventually thickens the flame zone in combustion  
 117 modelling. The flame thickness is between 3 and 5 grid cells under the selected beta value in  
 118 FLACS (Vyazmina and Jallais, 2016).

119 For all simulations, the atmosphere pressure of 1 barg is used as the initial condition, tank roof  
 120 and wall are modelled as rigid in FLACS. Grid cells are modelled as cubical in the combustion  
 121 region. The combustion region's volume is specified to be at least 9 times larger than the tank

122 size. Based on the authors' previous sensitivity studies (Li et al., 2017; Li and Hao, 2018; Li et  
123 al., 2018), a grid size of 0.05m within the combustion region is used for small-scale simulation  
124 (1.5m diameter and 1m height tank) in this study, while 0.5-1m grid cell is more commonly  
125 used for large-scale oil and gas explosion simulation, such as explosion in a fixed offshore  
126 platform. Starting from the venting direction, the grid cells are stretched with an increment  
127 ratio between 4-10%.

## 128 **2.2 Different vent opening designs of 6.5 vol % gas concentration case**

129 As seen in Fig. 2 (a) to (c), three different vent openings are designed for the 6.5 vol % methane-  
130 air concentration explosion tests. From case No.1 to case No. 3, the vent areas are 0.036 m<sup>2</sup>,  
131 0.19 m<sup>2</sup> and 0.37 m<sup>2</sup>, respectively. A hinged light-weight steel panel sealed with latex foam, a  
132 polyethylene film and two REMBE vent panels with activation pressure of 15 kPa (REMBE,  
133 2015) are used for the aforementioned three cases. The ignition point is located at the center of  
134 each tank.

135 Fig. 3 shows the FLACS 3D geometries of the corresponding experimental cases. 10% meshing  
136 increment is used for the grid stretching. 15 grid cells are specified at the smallest vent panel.  
137 Eulerian boundary condition is used for these three CFD simulations as in the authors' previous  
138 study (Li et al., 2017) that focused on the internal pressure simulation, and since the reflection  
139 effect of pressure wave to internal pressure is minimum as the z-direction domain is sufficiently  
140 large. Whereas the PLANE\_WAVE boundary conditions are generally used in the following  
141 large-scale simulations to eliminate pressure wave reflection effect (Hansen et al., 2010;  
142 Hansen and Johnson, 2015; Cen et al., 2017). Monitor points are located close to tank's vent  
143 panel and on tank's wall at different heights, as seen in Fig. 4. The monitor points at height of  
144 0.75m on tank wall are used to record the internal pressures of vented gas explosions in FLACS.  
145 Hinged panels with weight of 1 kN/m<sup>2</sup> are used for model case No. 1 and case No. 3, while the  
146 POPOUT relief panel in FLACS is used to model the polyethylene film panel for case No. 2.

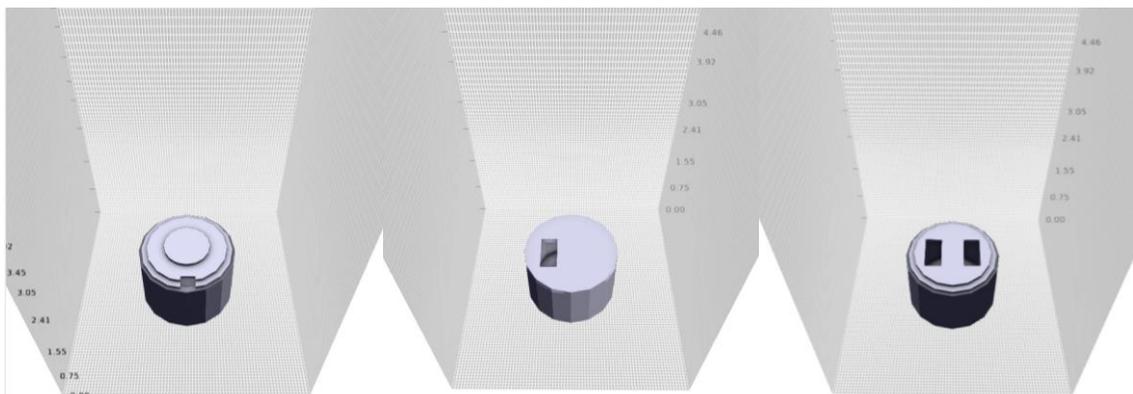
147 The activation pressure for the venting design case No.1 and No. 2 are 6.6 kPa and 1.4 kPa,  
 148 which are corresponding to the initial vent opening pressure in the experiment Case No. 3 by  
 149 Li et al., (2017) and the opening pressure in the 6.5 vol % gas concentration experiment by Li  
 150 and Hao (2018), respectively.



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 152 (a) Venting design case No. 1 (b) Venting design case No. 2 (c) Venting design case No. 3

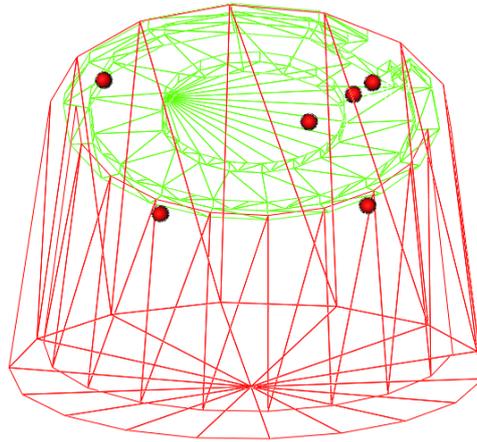


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 154 (d) Case No. 1 during explosion (e) Case No. 2 during explosion (f) Case No. 3 during explosion  
 155 Fig. 2 6.5 vol % gas concentration experiments for case No.1, No.2 and No. 3



156  
 157 (a) Venting design case No. 1 (b) Venting design case No. 2 (c) Venting design case No. 3  
 158 Fig. 3 6.5 vol % gas concentration CFD models for case No.1, No.2 and No. 3

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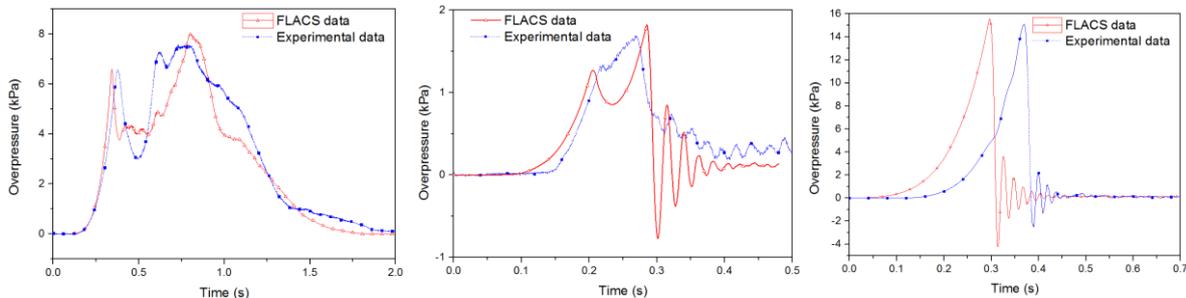


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**Fig. 4 Locations of monitor points**

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**(a) Venting design case No. 1 (b) Venting design case No. 2 (c) Venting design case No. 3**

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**Fig. 5 Comparison of experimental data and FLACS data for 6.5 vol % gas concentration case No.1, No.2 and No. 3**

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The experimental internal pressure-time histories are compared with FLACS simulation data

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as shown in Fig. 5. The internal pressures extracted from the monitors in FLACS are at the

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same locations of the sensors installed in the tests. It can be seen that the internal pressure data

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predicted by FLACS agree well with the experimental data. The differences in overpressure

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peaks obtained from FLACS and experiments are less than 10%, although the first peaks

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appear earlier in numerical simulations than the peaks in the experiments, which is consistent

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with the observation in other researchers' studies (Pedersen and Middha, 2012; Vyazmina and

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Jallais, 2016). For small vent area cases No. 1 and No. 2, there are two obvious overpressure

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peaks while there is only one overpressure peak for case No. 3 with larger vent area. The main

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reason is that the small vent panel in case No. 1 and case No. 2 results in longer duration of

177 venting process and more unburned gas is consumed inside the tank. Further flame expansion  
178 and pressure growth are developed in these two cases due to the external explosion outside the  
179 chamber. When the flame area reaches its highest value during external explosion, the second  
180 overpressure peak is generated. Whereas for case No. 3, a larger amount of unburned and  
181 burned gases are vented due to the large vent area (2 panels activate at early stage). As more  
182 unburned gas is jetted out in case No. 3, less unburned gas is consumed during the combustion.  
183 Therefore, the instant reduction of internal pressure is expected when the panels open. Owing  
184 to the large vent area, there is no external explosion that contributes to the generation of second  
185 overpressure peak in case No. 3.

### 186 **2.3 Different vent opening designs of 9.5 vol % gas concentration case**

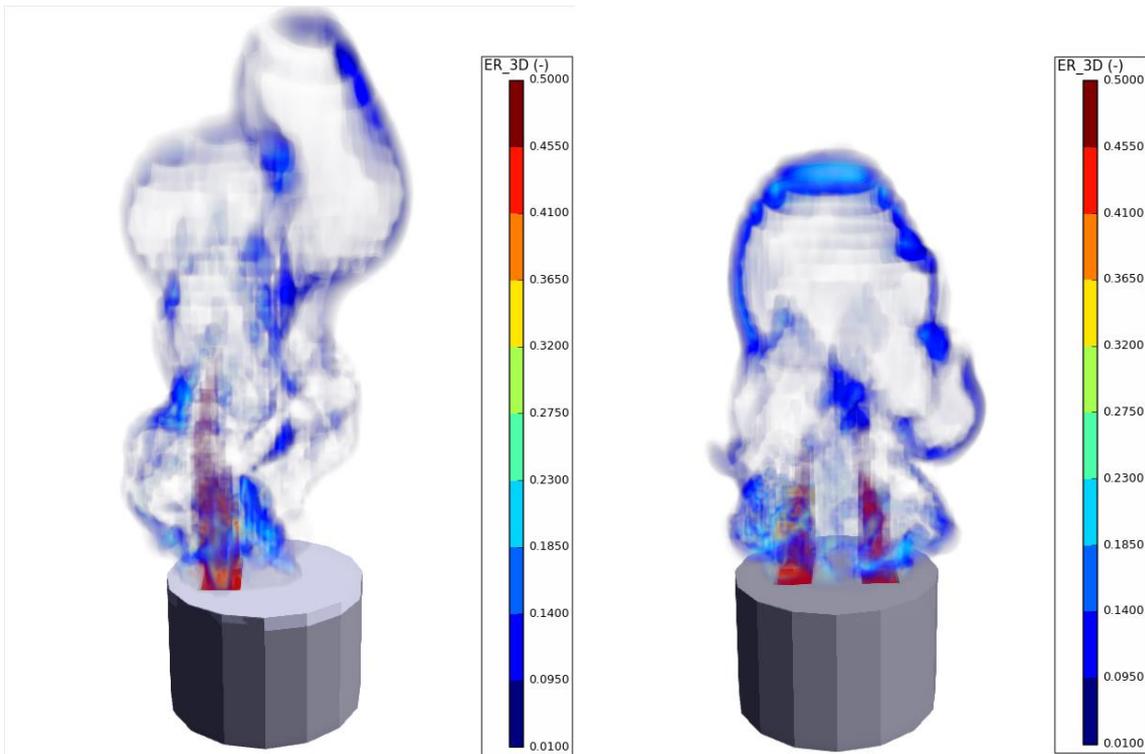
187 The same tank used for 6.5 vol % gas concentration explosion is also used for the 9.5 vol %  
188 gas concentration in case No. 4 and case No. 5. Only one vent panel on the left hand side is  
189 activated for case No. 4, while the panel on the other side is sealed by welding with a yield  
190 strength of 0.45 GPa and tensile strength of 0.53 GPa, as seen in Fig. 6(a). For case No. 5, two  
191 vent panels are designed. Plastic films are used as the vent panels. The sensor installations,  
192 methane-air gas mixing and gas concentration control system are the same as in the 6.5 vol %  
193 vented gas explosion cases.

194 The tanks in experiments are modelled in 1:1 ratio in FLACS, as seen in Fig. 7. Rigid roof and  
195 wall are assumed. Centre ignitions are applied for the both cases. POPOUT activation panels  
196 with activation pressure of 0.01 barg in FLACS are used to model the plastic film vent panels  
197 installed on the roof. The cuboid boundary region has the x-direction and y-direction  
198 dimensions more than 4 times larger than the tank radius. The z-direction is the venting  
199 direction, therefore, the z-direction dimension is modelled to be 10 times longer than the tank  
200 height. Cubical mesh grids are uniformly distributed inside the combustion region, while other  
201 grids are stretched with an increment ratio of 7% towards the venting direction.



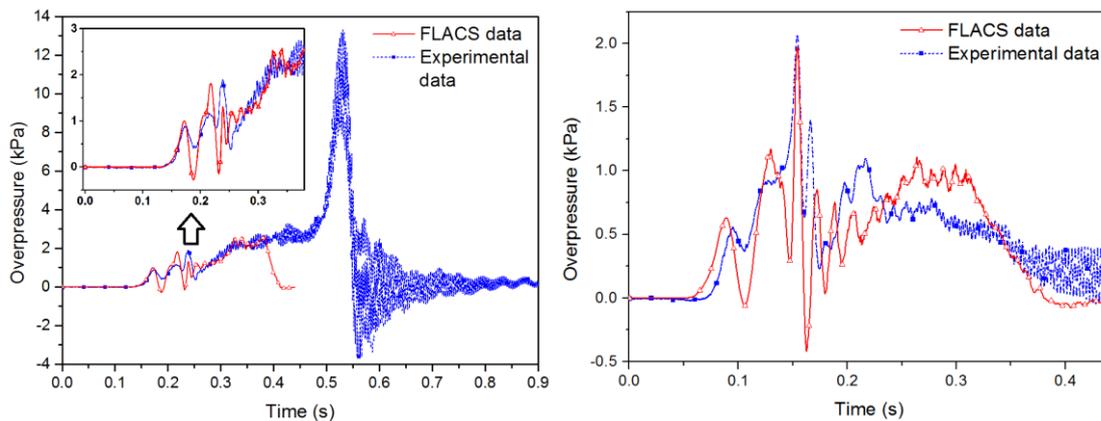
(a) Design case No. 4 with one vent panel      (b) Design case No. 5 with two vent panels  
**Fig. 6 9.5 vol % gas concentration experiments for case No.4, No.5**

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(a) Design case No. 4 with one vent panel      (b) Design case No. 5 with two vent panels  
**Fig. 7 9.5 vol % gas concentration CFD models for case No.4, No.5**

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 210 (a) Design case No. 4 with one vent panel (b) Design case No. 5 with two vent panels  
 211 Fig. 8 Comparison of experimental data and FLACS data for 9.5 vol % gas concentration case  
 212 No.4, No.5

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214 As seen in Fig. 7, flame developments from vented gas explosion in the both cases are well  
 215 projected in FLACS 3D view. The comparison of internal pressures from experiments and  
 216 numerical data in Fig. 8 further verifies the accuracy of FLACS simulation. For the  
 217 stoichiometric methane concentration of 9.5 vol % case with one vent panel in Fig. 8(a),  
 218 internal overpressure peaks owing to vent opening and external explosion outside the vent are  
 219 well predicted by FLACS. In the zoomed-in figure, pressure-time histories due to geometry-  
 220 induced flame instabilities and turbulence production before 0.4 s are well modelled in FLACS  
 221 as well. However, due to the fact that the explosion-generated structural vibrations/inductions  
 222 are not taken into account in FLACS, the overpressure peak (i.e. 13 kPa at 0.52s in Fig. 8(a))  
 223 due to flame-acoustic interactions (Bauwens et al., 2010) cannot be reproduced by FLACS  
 224 (Hisken, 2018). As a matter of fact, so far there is no reliable CFD tool being able to accurately  
 225 calculate the acoustically driven pressures (Tolias et al., 2018; Vyazmina et al., 2018).  
 226 Moreover, feedback between acoustics generated by the structure of the chamber and the  
 227 combustion process is more dominate in front ignition cases of vented gas explosion (Bauwens  
 228 et al., 2012; Vyazmina and Jallais, 2016). The front ignition explosion study is not within the  
 229 scope of this article, all experiments and CFD simulations are based on center ignition  
 230 explosions in this study.

231 In terms of the two-panel vented gas explosion in Fig. 8(b), the first two peaks due to vent  
232 panel opening are accurately predicted by FLACS, although the predicted flame arrival time is  
233 slightly earlier. Meanwhile, FLACS simulation data after 0.15s closely resemble overpressure  
234 peaks resulted from external explosion and the oscillations due to Rayleigh-Taylor instabilities  
235 (Solberg et al., 1981; Tsuruda and Hirano, 1987) in experiments. By comparing the 9.5 vol %  
236 cases No. 4 and No.5, it is worth noting that increasing the vent area from one-panel size to  
237 two-panel size results in the elimination of acoustically driven overpressure peak.

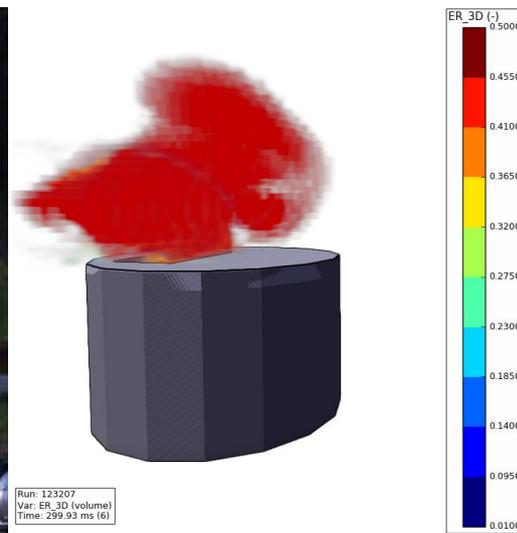
#### 238 **2.4 One vent opening of 12.5 vol % gas concentration case**

239 Following the above studies on lean combustion of 6.5 vol % concentration case and  
240 stoichiometric gas explosion case (i.e. 9.5 vol % methane-air mixture), the vented gas explosion  
241 with rich methane-air mixture of 12.5 vol % is also investigated. The same tank and  
242 corresponding experimental setups from case NO. 1 to case NO. 5 are used in this section,  
243 except the gas concentration is controlled at 12.5 vol %.

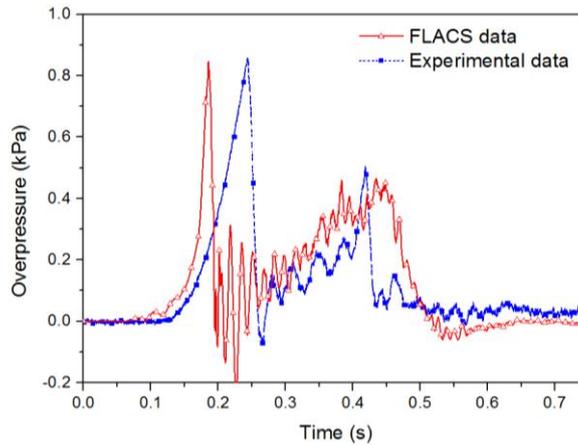
244 Similarly, the FLACS model has 1:1 ratio of the experimental geometry. The panel type,  
245 boundary, meshing grid size, aspect ratio of the grid increment, etc. are kept the same as in the  
246 previous cases.



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248 (a) Experiment for case No. 6



(b) FLACS model for case No. 6



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 250 **(c) Comparison of experimental data and FLACS data**  
 251 **Fig. 9 Experimental and FLACS data for 12.5 vol % gas concentration case No.6**

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 253 Compared to the stoichiometric gas explosion in Fig. 6 and Fig. 7, it is interesting to note the  
 254 combustion of fuel-rich mixture at 12.5 vol % generates more visible red flame as shown in  
 255 Fig. 9(a) and (b). Despite the fact that the same polyethylene sheets are utilized as the vent  
 256 panels, it is notable that the first internal overpressure peak (0.85 kPa in Fig. 9(c)) which is  
 257 related to the vent activation pressure in the 12.5 vol % case is smaller than the first peak (1  
 258 kPa) in the one-panel 9.5 vol % case in Fig. 8. Additionally, the rate of pressure rise (pressure  
 259 increases in the first peak with duration of approximately 0.3s) in 9.5 vol % case is faster than  
 260 the rate (pressure increases with duration of approximately 0.7s) in the richer fuel mixture case  
 261 (12.5 vol %). The explanation is that laminar burning velocity at stoichiometric methane  
 262 concentration of 9.5 vol % is the greatest (i.e. 0.38 m/s) so that the combustion rate reaches the  
 263 highest (Nishimura et al., 2013). When methane-air mixture concentration increases from 9.5  
 264 vol % to 12.5 vol %, the laminar burning velocity decreases from 0.38 m/s to 0.19 m/s. Slower  
 265 laminar flame velocity implies lower combustion rate, which eventually results in smaller  
 266 overpressure peak and lower rate of pressure rise (Bao et al., 2016).  
 267 For the 12.5 vol % fuel-rich mixture, FLACS predicted data also agree well with experimental  
 268 data as shown in Fig. 9(c) in terms of the magnitudes of overpressure peak and combustion  
 269 duration. However, the first peak calculated by FLACS has a narrower shape and more

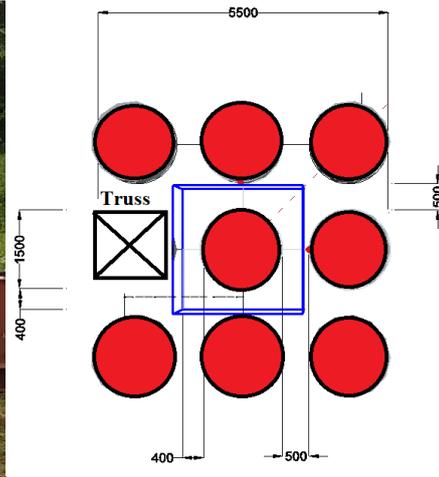
270 oscillations are seen between the first peak and the second peak. Overall, the FLACS predicted  
271 internal pressure-time data are reasonable.

## 272 **2.5 Vented gas explosion in a tank group**

273 From case No. 1 to No. 6, experiments and numerical simulations are conducted based on a  
274 single tank with volume of  $1.77 \text{ m}^3$ . In this section, the experimental and numerical scale  
275 increases from a single tank to 8 tanks in a group. As seen in Fig. 10, the tank in the center of  
276 the group is confined by an enclosed polyethylene film region with dimensions of  
277  $2300 \times 2300 \times 1500 \text{ mm}^3$ . 7 enclosed tanks are used to encircle the middle tank and 1 upright  
278 truss equipped with water cooling system is placed on one side of the tank group. The  
279 separation distance between each two tanks varies from 500 mm to 1000 mm, as shown in Fig.  
280 11. Same experimental facilities and equipment used in case No. 1 to case No. 6 are employed  
281 in the tank group testing. Four vales for air inlet, gas inlet, air outlet and gas outlet are equipped  
282 for the middle tank. Two fire-resistant fans, a recirculation pump and an infrared methane  
283 analyzer are used for gas mixing and gas concentration control.

284 The center ignition is located inside the middle tank. 9.5 vol % methane-air concentration  
285 inside the middle tank and the enclosed film region is used for all tests. The middle tank has  
286 no vent covers, which means the vent activation pressure is dependent on the film failure from  
287 the cuboid region. Beside the three different separation distances arranged for experiments, all  
288 experimental setups are kept the same during explosion tests.

289 Similarly, the FLACS simulations for three tank group explosions with three different  
290 separation distances have the same numerical simulation setups used in the aforementioned  
291 cases from No.1 to No. 6. Except the simulation boundaries are extended to cover the whole  
292 tank group. The simulation domain has the dimensions of  $18000 \times 18000 \times 18000 \text{ mm}^3$ .



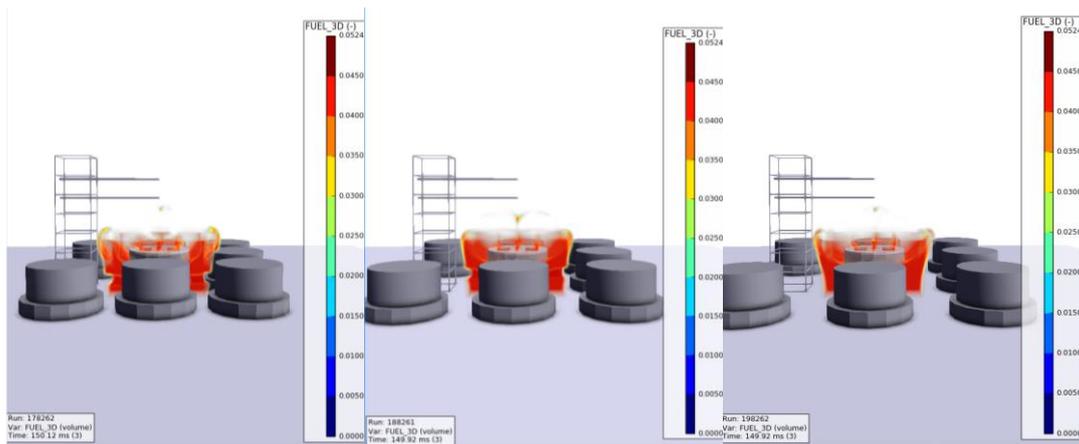
(a) Realistic tank group setup in field (b) Plane graph of the 500m gap example  
**Fig. 10 Tank group testing setup in experiment**

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(a) 500mm separation distance (b) 750mm separation distance (c) 1000mm separation distance  
**Fig. 11 Snapshots of different separation distance cases in experiments**

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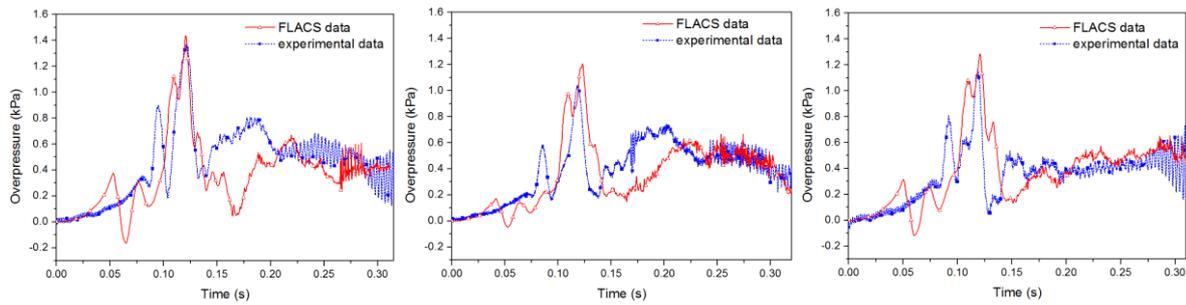


(a) 500mm separation distance (b) 750mm separation distance (c) 1000mm separation distance

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**Fig. 12 3D models of different separation distance cases in FLACS**



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**(a) 500mm separation distance (b) 750mm separation distance (c) 1000mm separation distance**  
**Fig. 13 Internal pressure comparison between experimental data and FLACS simulation results**

309 The fuel combustion inside the confined region is well simulated in FLACS as seen in Fig. 12.  
310 However, the 0.015mm polyethylene films modelled as light-weight PLASTIC relieve panels  
311 in FLACS are invisible. In FLACS, the internal pressure time histories from the 500mm,  
312 750mm and 1000mm separation distance explosion cases are extracted from the monitors  
313 inside the center tank. All pressure data are then compared with internal pressures recorded in  
314 experiments. The comparison is shown in Fig. 13. In general, the first overpressure peaks and  
315 the maximum pressures for all the cases in FLACS agree well with experimental data, although  
316 the first peaks from experiments start later than those in FLACS. In all experiments, the  
317 Rayleigh-Taylor instability induced pressures after 0.15s as seen in Fig. 13 are well recorded.  
318 The correspondingly estimated pressure-time histories in FLACS also satisfactorily  
319 demonstrate such instability oscillations. To sum up, for the vented gas explosions with  
320 multiple tanks, FLACS provides accurate internal pressure calculation and the predicted  
321 pressure development tendencies inside the tank also agree with the experimental data.

### 322 **3. Large-scale vented gas explosion simulation for large storage tanks**

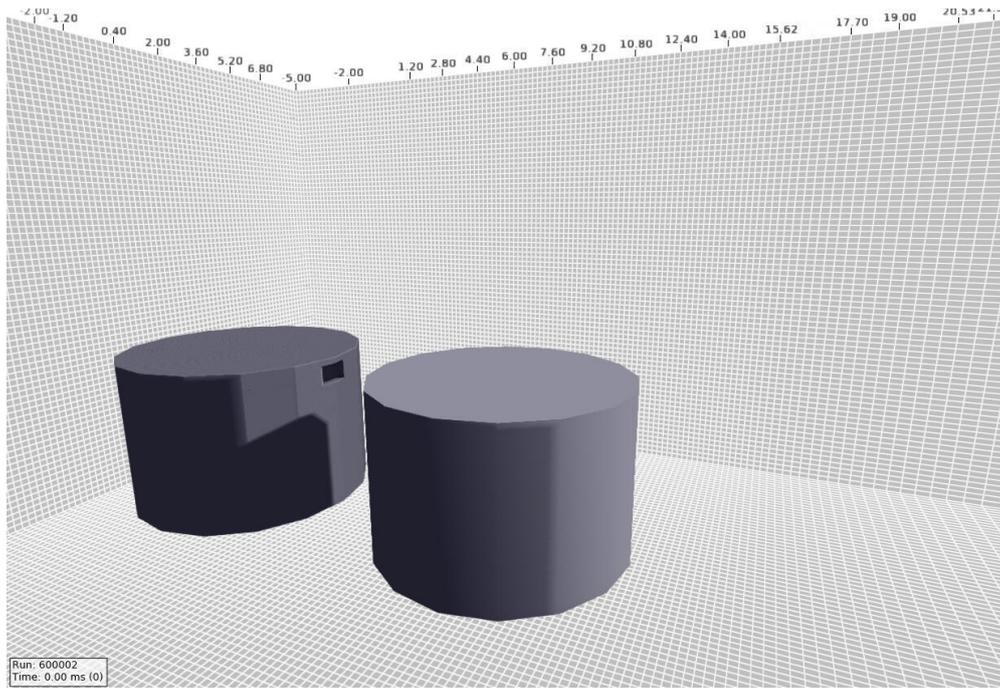
#### 323 **3.1 Grid sensitivity study of large-scale CFD simulation**

324 The aforementioned vented gas explosions from case No. 1 to No. 6 are based on the 1.5m  
325 diameter and 1m height tanks (volume = 1.77 m<sup>3</sup>). Even though 8 tanks are used in the tank  
326 group study with 9 times larger simulation domain size, the grid size still has to be kept as

327 small as possible so that at least 6-8 grid cells are guaranteed for the vent opening resolution in  
328 each tank in FLACS (Gexcon, 2017). Moreover, the maximum overpressure peak calculated  
329 by FLACS for cases from No. 1 to No. 6 is 15 kPa.

330 In this study of large scale vented gas explosions, the tank volumes considered are in the range  
331 of 95 m<sup>3</sup> to 308 m<sup>3</sup>. Much higher overpressures (higher than 1bar or 100kPa) from such large  
332 scale gas explosions are expected. To find the compromise between the simulation accuracy  
333 and efficiency for such large-scale vented gas explosion, a new grid sensitivity analysis is  
334 conducted to select the suitable grid size. In this study, a cylindrical tank with diameter of 7m  
335 and height of 4m (volume of 154 m<sup>3</sup>, which is in the middle of the tank volume range) is chosen  
336 for the sensitivity study, as seen in Fig. 14.

337 Both the internal pressures and external pressures between two tanks are calculated in this  
338 section. Monitors inside the pressure donor tank on the left hand side and monitors on the wall  
339 of pressure acceptor tank on the right hand side as seen in Fig. 14 are set to record the pressures.  
340 The pressure donor tank is filled with 9.5 vol % stoichiometric methane-air mixture. Ignition  
341 is at the center of the donor tank. Vent opening (600x1000 mm<sup>2</sup>) is on the top of the donor  
342 tank's side wall facing the pressure acceptor tank. Vent activation pressure is assumed as zero.  
343 The acceptor tank has the same dimensions of the donor tank, the separation distance between  
344 the two tanks is kept as 1m in the sensitivity study. CFLC = 5 and CFLV = 0.5 for simulations  
345 within the explosion region are used. Since the external pressures outside the donor tank are of  
346 interest, the time step condition STEP "KEEP\_LOW" is applied to reduce smearing of the  
347 pressure waves (Hansen and Johnson, 2015). The simulation domain has dimensions of  
348 45000×18000×15400 mm<sup>3</sup>.



**Fig. 14 3D model of 7m diameter and 4m height tanks in FLACS simulation**

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350  
351

352 According to FLACS user guide, the grid resolution should be chosen to obtain an adequately  
353 accurate simulation result within an acceptable time frame, which is about a few hours or at  
354 least overnight for an explosion simulation. It is not suggested to start a CFD simulation on a  
355 grid that will be running for days (Gexcon, 2017). For the 7m diameter and 4m height tank, the  
356 grid size of 0.1m results in explosion calculation running for more than 2 days. Therefore, the  
357 grid size starting from 0.15m is chosen for the sensitivity study. As seen in Table 2, 5 different  
358 grid sizes in the range of 0.15 mm to 0.25 mm are selected for CFD simulation.

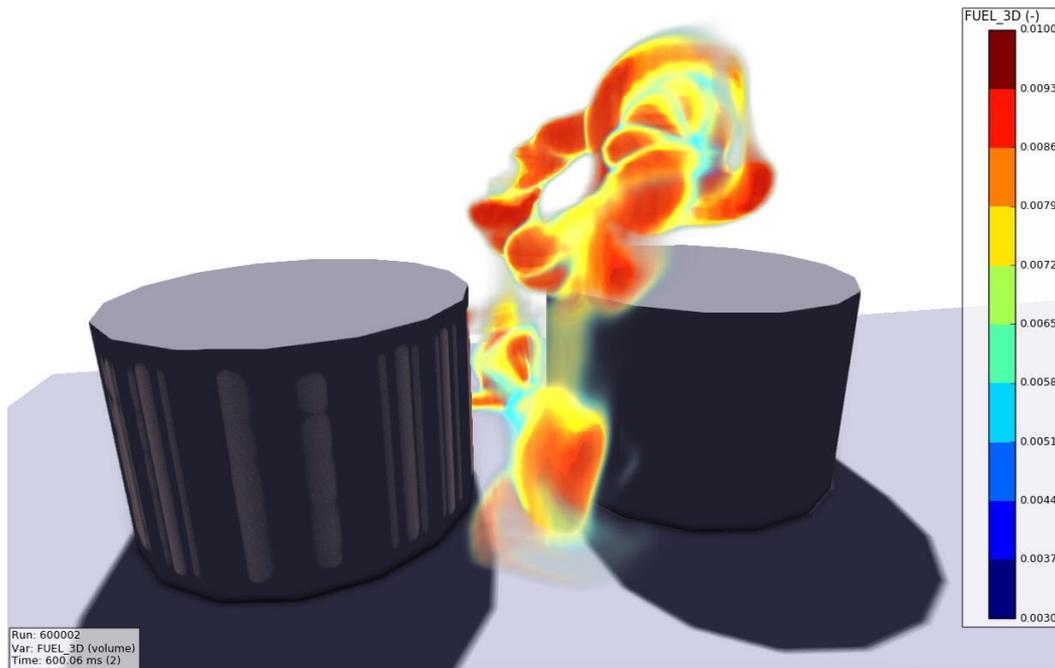
359 **Table 2 Sensitivity study details of selected grid size, predicted internal pressure and**  
360 **comparison of pressures between two different grid size cases**

<b>Grid size (m)</b>	0.15	0.18	0.2	0.22	0.25
<b>Peak internal pressure (kPa)</b>	237.9	243.4	250.5	255.7	260.5
<b>Difference between neighboring data (%)</b>	-	2.26%	2.83%	2.03%	1.84%
<b>Computational time for 8-core computer</b>	28 hrs	16 hrs	12 hrs	8.5 hrs	6 hrs

361  
362

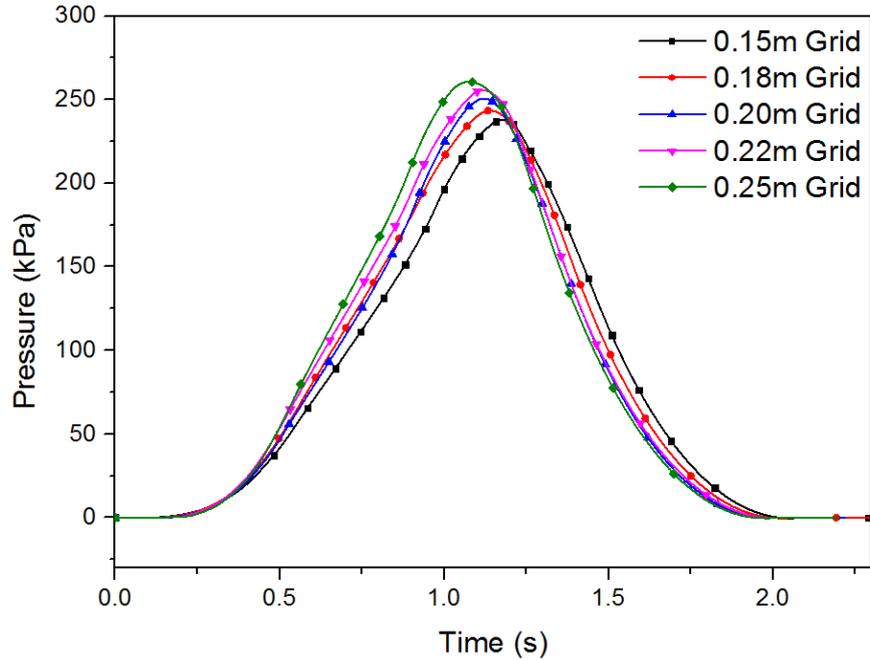
363 Fig. 15 shows the 3D model of flame development during the vented gas explosion. For  
364 demonstration purpose, the fuel mass fraction is set between 0.003 and 0.01 in the figure. The  
365 time is set at 600ms (i.e. at the early stage of simulation). The cylindrical gas cloud inside the  
donor tank is ignited at the center of the tank, the unburned and burned gases are jetted out of

366 the tank from the 600x1000 mm<sup>2</sup> vent opening. The internal overpressure-time history data are  
367 extracted from all simulations and shown in Fig. 16. Internal pressures are obtained from the  
368 same monitors located on the wall at the same height of 1m inside the pressure donor tank.  
369 Since the overpressures inside the tank are homogeneously distributed, only the monitor point  
370 located at the height of 1m is used to record the maximum explosion overpressures.



371 **Fig. 15 Flame development of the vented gas explosion from the donor tank in FLACS**

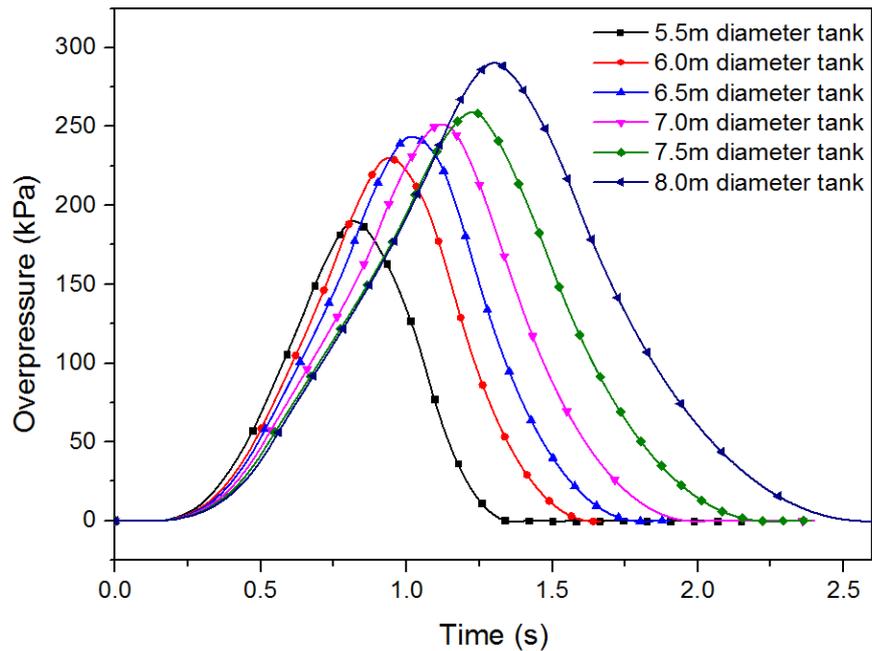
372  
373  
374 In the comparison of Fig. 16, the highest overpressure peak is 260.5 kPa by using 0.25 m grid,  
375 the lowest overpressure peak is 237.9 kPa by using 0.15 m grid. From 0.15 m grid to 0.25 m  
376 grid, the overpressure peak increases marginally. The pressure difference between each two  
377 neighboring cases is below 3%. The maximum difference between the most far-end cases (i.e.  
378 the 0.15 m grid case and the 0.25m grid case) is 8.7%, which is deemed acceptable. Therefore  
379 it can be concluded that the grid sensitivity in the range of 0.15 m to 0.25 m is convergent.  
380 However, the CFD calculation time can increase up to 300 % when the grid size decreases from  
381 0.25 m to 0.15 m. In order to improve the computational efficiency and to ensure minimum  
382 15 grid cells available at vent opening, grid size of 0.2 m is chosen for all large-scale vented  
383 gas explosion simulations in this study.



384  
385 **Fig. 16 Comparison of internal pressures from different grid size simulations**  
386

387 **3.2 Analysis of internal pressures from vented explosion with different tank**  
388 **volumes by using VMEOC correlations**

389 Having decided the grid cell size of 0.2m, the internal pressures of tanks with volume sizes in  
390 the range of 95 m<sup>3</sup> to 308 m<sup>3</sup> are calculated. Specifically, the variable in tank volume is the  
391 diameter, which increases from 5.5m to 8.0m in the CFD simulation. While the tank height is  
392 kept at 4m and the vent opening size of 600x1000 mm<sup>2</sup> is also unchanged. Vent activation  
393 pressure is zero.



**Fig. 17 Internal pressures recorded inside the donor tanks for different tank diameter cases**

As seen in Fig. 17, the internal overpressure peak increases proportionally with the tank diameter, as well as the duration of the explosion pressure time history. Therefore, the impulse, which is the integral of the overpressure over time, increases even more significantly than the overpressure peak. This is because the larger tank diameter has larger gas cloud inside the tank. Since the tank volume/diameter is the only variable, the larger gas cloud will generate more combustion energy once the cloud is ignited, thereby increasing both the pressure and impulse inside the tank.

In the authors' previous study (Li et al., 2017), a series of simplified correlations named Vented Methane-air Explosion Overpressure Calculation (VMEOC) correlations were proposed to predict the internal pressure from vented gas explosion under tank size of  $50\text{m}^3$ . In this section, the VMEOC correlations are used to predict the internal pressures from the above 5 larger-scale vented gas explosions. Additionally, another two explosion cases with different vent areas are included as seen in Table 3.

412 **Table 3 Parameter details of different tanks used in the internal pressure analysis by using**  
 413 **VMEOC correlations**

Explosion No.	Tank diameter (m)	Vent area (m <sup>2</sup> )	Tank roof area (m <sup>2</sup> )	Ratio <sup>#</sup> of $A_{vo} \times D / (A_{rf} \times H)$
1	5.5	0.6	23.8	0.034
2	6	0.6	28.3	0.032
3	6.5	0.6	33.2	0.029
4	7	0.6	38.5	0.027
5	7.5	0.6	44.2	0.025
6	8	0.6	50.3	0.024
7	7	0.8	38.5	0.036
8	7	1.0	38.5	0.045

414 <sup>#</sup> The parameters of  $A_{vo}$ ,  $D$ ,  $A_{rf}$ ,  $H$  represent the vent area, diameter of tank, roof area and tank  
 415 height/depth for the ratio used in the vent activation effect calculation.

416  
 417 Table 3 summarizes the parameter details for these 8 explosion cases. In VMEOC correlations,  
 418 depending on the ratio related to the vent area, tank roof area and tank volume, the internal  
 419 overpressure peak is calculated as (pressure activation is equal to zero in FLACS simulation):

420 **i. Enclosure with small vent area ratio ( $(A_{vo} / A_{rf}) \cdot V^{1/3} \leq 0.08$ )**

421 
$$P_{\max} = 1.613 \cdot \ln \left[ \left( \phi_{\text{gas}}^* |1 - \ln \phi_{\text{gas}}^*| - 2.1 |1 - \phi_{\text{gas}}^*| \right) P_{\text{act}}^* A_{\text{vo}}^* + 4 \right] - 1.93 \quad (1)$$

422 **ii. Enclosure with large vent area ratio ( $(A_{vo} / A_{rf}) \cdot V^{1/3} > 0.08$ )**

423 
$$P_{\max} = 1.613 \cdot \ln \left[ \left( \phi_{\text{gas}}^* |1 - \ln \phi_{\text{gas}}^*| - 2.1 |1 - \phi_{\text{gas}}^*| \right) \cdot \left( 3 \cdot P_{\text{act}}^{*0.3} - 1.7 P_{\text{atm}} \right) A_{\text{vo}}^* + 4 \right] - 1.93 \quad (2)$$

424 where  $P_{\max}$  is the internal overpressure peak,  $\phi_{\text{gas}}^*$  is the effective gas equivalence ratio,  $P_{\text{act}}^*$  is  
 425 the effective vent activation pressure,  $A_{\text{vo}}^*$  is the effective vent area ratio, and  $P_{\text{atm}}$  is the  
 426 atmosphere pressure.

427 In order to decide which equation to use, the ratio of  $\gamma_{\text{vent}}$  is calculated as:

428 
$$\gamma_{\text{vent}} = \frac{A_{\text{vo}}}{A_{\text{rf}}} \cdot V^{1/3} \quad (3)$$

429 where  $\gamma_{vent}$  is the vent area to tank roof area and tank volume ratio,  $A_{vo}$  is the vent area,  $A_{rf}$  is  
 430 the roof area,  $V$  is the tank volume.

431 In Table 3, the ratios of  $\gamma_{vent}$  are all over 0.08 except explosion No. 5 and No. 6. Therefore,  
 432 equation (1) is used for explosion No. 5 and No. 6, while equation (2) is used for other  
 433 explosion cases.

434 In equation (1) and equation (2), the effective gas equivalence ratio of  $\phi_{gas}^*$  is calculated as:

$$435 \quad \phi_{gas}^* = 3.5 \ln \left( -4 \left| \ln(\phi_{gas} - 0.1) \right| \left( \frac{1}{\phi_{gas} + 0.1} \right)^{0.7} - \left| -1 + \phi_{gas} \right| + 6 \right) + \frac{16.80 \left( \frac{P_{act}}{P_o} \right)^{0.75}}{V} \quad (4)$$

- 4.1

436 where  $\phi_{gas}$  is the equivalence ratio of gas,  $P_{act}$  is the vent activation pressure, and  $P_o$  is the  
 437 initial pressure (e.g. atmosphere pressure) inside the enclosure prior to ignition.

438 The effective vent area ratio of  $A_{vo}^*$  is calculated as:

$$439 \quad A_{vo}^* = 4.5 \left( 0.03530 + 0.01765 \left( \frac{1}{1.2} \frac{H}{D} - 1 \right)^2 \right) D^{1.82} A_{vo}^{\left( -\frac{2D}{H} \right)} - 0.65 \quad (5)$$

440

441 The effective vent activation pressure of  $P_{act}^*$  is determined by:

442 If  $\frac{A_{vo} D}{A_{rf} H} > 0.04$ ,

$$443 \quad P_{act}^* = 2.52 \ln \left( 1 + P_{act}^{1.4} \sqrt{\frac{A_{vo} D}{A_{rf} H}} \right) + 1.26 P_o \ln \left( \frac{0.02 V}{A_{vo}} \right) + 2 \quad (6)$$

444

445

446 If  $\frac{A_{vo} D}{A_{rf} H} \leq 0.04$ ,

447 
$$P_{act}^* = 0.45 P_{act} + 1.26 P_o \ln \left( \frac{0.02 V}{A_{vo}} \right) + 2 \quad (7)$$

448 In Table 3, only explosion case No. 8 has the ratio of  $A_{vo} \times D / (A_{rf} \times H)$  larger than 0.04, while  
 449 others are lower than 0.04. The equations (6) and (7) are used accordingly.

450 By substituting all parameters calculated from equation (3) to equation (7) into equation (1)  
 451 and equation (2), internal overpressure peaks of Pmax are calculated and compared with  
 452 FLACS estimated results as shown in Table 4.

453 **Table 4 VMEOC correlations calculated overpressure peaks and FLACS predicted**  
 454 **overpressure peaks for explosion cases in Table 3**

Explosion No.	VMEOC correlations calculated pressure (kPa)	FLACS predicted pressure (kPa)	Difference between VMEOC and FLACS data
1	509.4	190.5	268.10%
2	562.9	230.4	244.75%
3	613.7	244.3	251.52%
4	662.1	251.6	263.80%
5	767.3	260.4	295.13%
6	815.2	290.1	281.11%
7	493.6	169.3	292.07%
8	363.9	112.4	324.96%

455  
 456 It is seen in Table 4 that VMEOC correlations estimated overpressure peaks are about 3 times  
 457 the overpressure peaks of FLACS. The 3 times difference between two sets of data is mainly  
 458 due to the simulation scale difference. It is worth pointing out that the current CFD models are  
 459 in large-scale, while the correlations derived earlier were based on small-medium scale tanks.  
 460 The secondary reason is the grid cell size difference between the numerical models used in  
 461 VMEOC correlation development and the numerical models in the current simulation. In  
 462 authors' previous study on VMEOC correlations, all CFD simulations (over 350 cases) were  
 463 conducted based on 0.05 m grid size, while the grid size in current cases are 0.2m. As seen in  
 464 section 3.1, from grid size 0.18 m to 0.2 m, the overpressure peak difference is 2.83%. The  
 465 pressure difference can be even larger if the grid size increases from 0.05 m to 0.2 m. The  
 466 previously derived VMEOC can be used to predict overpressure for a tank with volume up to

467 50m<sup>3</sup>. However, for case No.6 with 154m<sup>3</sup> tank in Table 4, the pressure predicted by the original  
468 VMEOC is 815.2 kPa, which is even larger than the highest pressure (i.e. 750 kPa) from an  
469 idealized vented explosion (i.e. explosion from a nearly fully-closed vessel) with 9.5 vol %  
470 methane-air mixture (NFPA-68, 2007). In other words, the previously derived VMEOC  
471 overestimates pressure for vented gas explosion from a tank with size over 50m<sup>3</sup>. Therefore, in  
472 this study, a factor of  $\alpha$  is required to adjust the VMEOC correlations for large-scale vented  
473 gas explosion. However, owing to the cost and safety concerns for large-scale experiments,  
474 only CFD simulations are conducted in current study. The sensitivity study in section 3.1  
475 assures large-scale simulation results' convergence and accuracy.  $\alpha$  equals to 0.35 is  
476 determined in this study based on all large-scale CFD simulation data. As a guidance in this  
477 study, the factor of  $\alpha$  is only used as a reference factor, which may vary depending on the  
478 simulation scale and grid size selection.

479 For vented gas explosion with zero vent activation pressure in different simulation domain  
480 scale, the adjusted VMEOC correlations are expressed as:

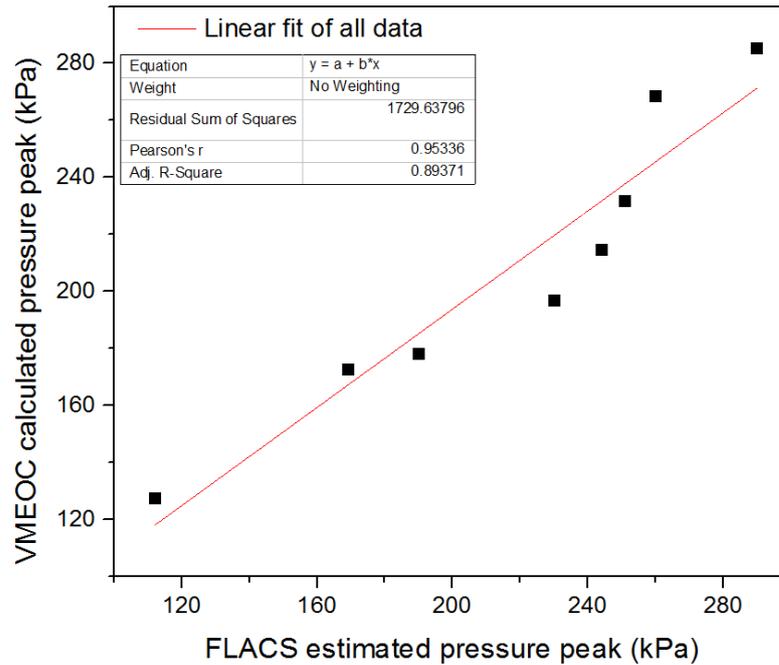
481 **iii. Enclosure with small vent area ratio** ( $(A_{vo} / A_{rf}) \cdot V^{1/3} \leq 0.08$ )

482 
$$P_{\max} = \alpha \left\{ 1.613 \cdot \ln \left[ \left( \varphi_{\text{gas}}^* |1 - \ln \varphi_{\text{gas}}| - 2.1 |1 - \varphi_{\text{gas}}| \right) P_{\text{act}}^* A_{vo}^* + 4 \right] - 1.93 \right\} \quad (8)$$

483 **iv. Enclosure with large vent area ratio** ( $(A_{vo} / A_{rf}) \cdot V^{1/3} > 0.08$ )

484 
$$P_{\max} = \alpha \left\{ 1.613 \cdot \ln \left[ \left( \varphi_{\text{gas}}^* |1 - \ln \varphi_{\text{gas}}| - 2.1 |1 - \varphi_{\text{gas}}| \right) \cdot (3 \cdot P_{\text{act}}^{*0.3} - 1.7 P_{\text{atm}}) A_{vo}^* + 4 \right] - 1.93 \right\} \quad (9)$$

485 By using the correction factor of  $\alpha = 0.35$ , the adjusted VMEOC correlations predicted  
486 overpressure peaks are updated and compared with FLACS calculated results, as shown in Fig.  
487 18. It is noted that the R-square value between two sets of data is 0.89, which means the newly  
488 adjusted VMEOC correlations can predict internal pressures with 89% accuracy for these large-  
489 scale vented gas explosions.



490  
 491 **Fig. 18 Comparison of FLACS estimated internal overpressure peak and VMEOC calculated**  
 492 **data**  
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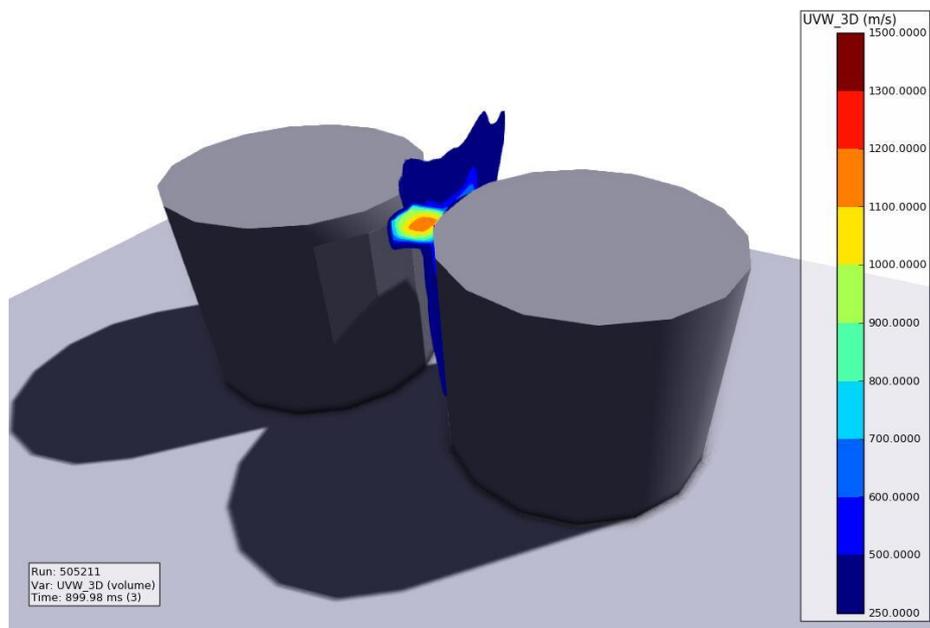
494 **3.3 Analysis of external pressures from vented explosion with different tank**  
 495 **volumes by using dimensionless correlations**

496 In the comparison of internal pressures from different donor tanks in the above section, the  
 497 explosion pressure from the vented gas explosion can be over 2 barg (i.e. 200 kPa), which may  
 498 generate supersonic flow velocity if detonation occurs. It is defined that gas explosion includes  
 499 two scenarios, i.e., deflagration and detonation. For deflagration, the flame propagates with  
 500 subsonic velocity in the range of 1-1000 m/s. While the detonation wave has flame velocity  
 501 over 1500 m/s (Bjerketvedt et al., 1997; Pasman, 2015).

502 For vented gas explosion in the aforementioned cases in Table 3 and Table 4 , the flame velocity  
 503 in external explosion is highly likely to reach sonic speed (i.e. 343 m/s). Therefore, the correct  
 504 selection of flame development criterion in FLACS is important, especially when the external  
 505 pressures are the study focus in this section. Taking the tank of explosion No. 1 and No. 5 in  
 506 Table 3 as examples, the tank in case No. 1 has the smallest diameter of 5.5m among all the  
 507 considered cases, the tank in case No. 5 has a relatively large diameter of 7.5m. The flame

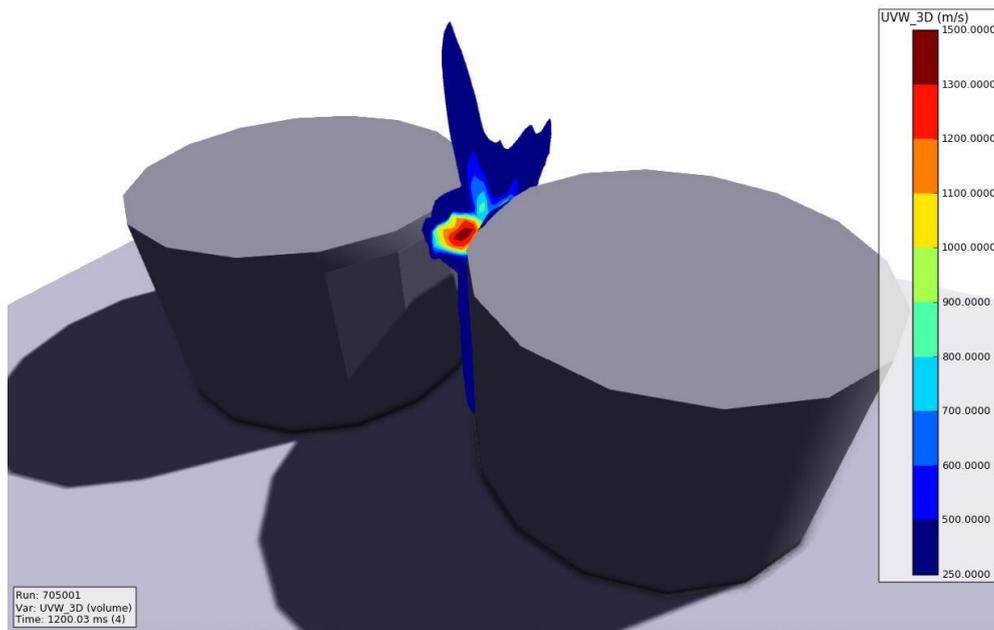
508 velocities at 0.9s and 1.2s generated from the donor tank (tank filled with gas cloud) for two  
509 cases are shown in Fig. 19. It is clearly seen that the flame speed from the vent in case No. 1  
510 can propagate at a speed over 1000 m/s, which is beyond the deflagration sonic velocity upper  
511 limit. Meanwhile, the flame speed in case No. 5 reaches the lower limit of supersonic flame  
512 speed of 1500 m/s.

513 In order to accurately model turbulence and flame development between two tanks with a  
514 separation gap, in the SETUP file, a keyword of KEYS="PS1=01" is used as a criterion in  
515 FLACS to ensure the maximum speed exceeding the sonic speed during combustion is taken  
516 into account.



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(a) 5.5 diameter tank of explosion No. 1 in Table 3

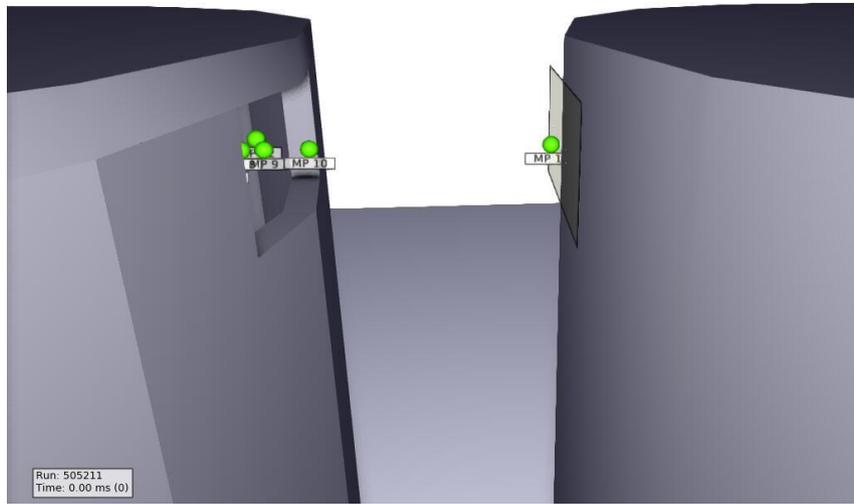


(b) 7.5 diameter tank of explosion No. 5 in Table 3

**Fig. 19 3D view of flow velocity at 0.9s and 1.2s for two different vented gas explosions**

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In FLACS, external pressures are recorded by the external monitor on the pressure-accepting tank wall. The external monitor is allocated directly opposite the vent as seen in Fig. 20. In addition to the monitor on the pressure-accepting tank, a passive panel to record the averaged external pressures is also used. The passive panel in FLACS is an inactive panel that does not affect the numerical simulation in any respect but records variables (e.g. pressure data). The area size of the passive panel is set to 0.6 m<sup>2</sup> to get the averaged pressure. The location of the panel is fixed in the simulations in this study for investigation of pressure decay and the subsequent parametric simulations of the separation distance effect on pressure mitigation. As shown in Fig. 20, the pressure-time data starting from the vent is also recorded by the vent-pressure monitor located in the middle of the vent. The vent-pressure monitor and external-pressure monitor are on the same axis perpendicular to the vent.

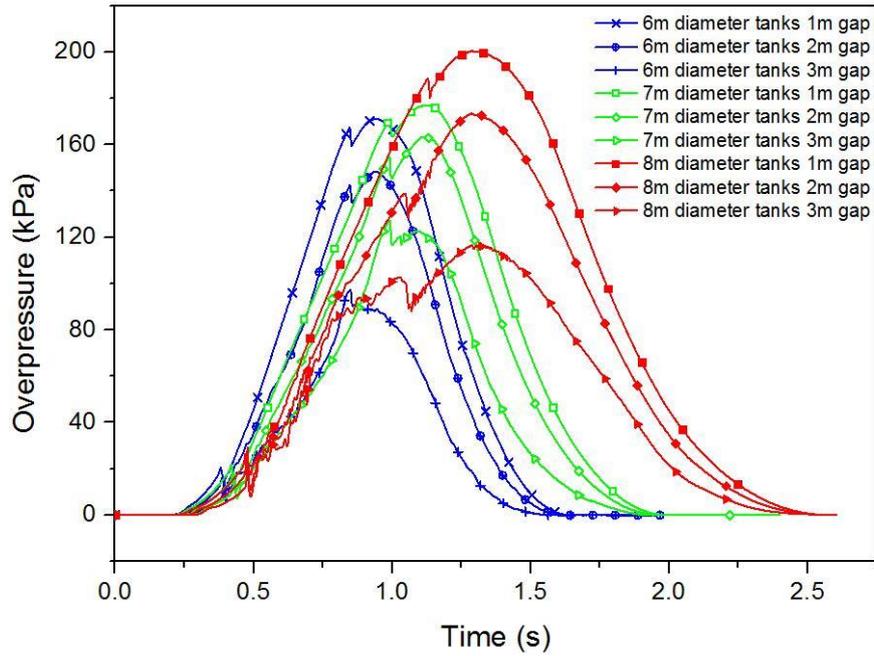


**Fig. 20 3D view of monitors near the vent of the donor tank and data recording panel on the acceptor tank in FLACS simulation**

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Although a new approach by (Hansen et al., 2010; Hansen and Johnson, 2015) has been proposed to improve the far-field pressure prediction accuracy of FLACS, overpressures predicted by FLACS in the far field may still decay too quickly. Especially if the external pressures are recorded at a far distance more than twice of the tank diameter and when the CFLC and CFLV parameters are not small enough (e.g. CFLC = 5 and CFLV = 0.5). Due to such simulation limitation and high computational cost (if CFLC and CFLV are decreased further) in FLACS, the distance between two tanks chosen in this study is decided to vary in a small range of 1m to 3m. In practice, if separation distance is more than 3 m, the pressure on the adjacent tank is expected to be smaller than that when the separation distance is 3 m.

The external pressure decay between two tanks is then investigated by conducting FLACS simulation and the results are compared with the far-field pressures estimated by using the dimensionless correlations from the authors' previous study (Li and Hao, 2018). The explosion No. 2, No. 4 and No. 6, which are tanks with diameters of 6m, 7m and 8m (tank height is 4m as a constant value) are chosen for the external pressure study.



552  
 553 **Fig. 21 External pressure-time data recorded by external monitors on pressure-accepting tanks**  
 554

555 In FLACS, the external pressures in 9 cases (i.e. 3 different tank volumes and 3 different  
 556 separation distances) are recorded by the external monitors on the pressure-accepting tanks as  
 557 shown in Fig. 21. It is apparent to see larger tank cases has greater overpressure peaks and  
 558 longer durations of the pressure-time histories. By increasing the separation distance, the  
 559 overpressure peaks decrease, which is due to the turbulence interruption within the separation  
 560 gap, as well as geometric attenuation of explosion wave.

561 Overpressure peaks from FLACS in Fig. 21 are extracted and summarized in Table 5 along  
 562 with tanks' geometry details. The external pressure data are used for the investigation of  
 563 pressure decay by using the correlations for external pressure calculation.

564 **Table 5 External pressure data and tank geometry details for pressure decay calculation**

Tank diameter (m)	Separation (m)	Tank volume (m <sup>3</sup> )	Pressure near vent (kPa)	Pressure on external monitor* (kPa)
6.0	1.0	113.1	102.1	171.2
6.0	2.0	113.1	100.4	148.4
6.0	3.0	113.1	97.4	97.6
7.0	1.0	153.9	108.4	177.2
7.0	2.0	153.9	107.1	163.3
7.0	3.0	153.9	105.5	122.3

<b>8.0</b>	1.0	201.1	114.2	200.4
<b>8.0</b>	2.0	201.1	111.9	172.2
<b>8.0</b>	3.0	201.1	108.8	118.6

565 \*The pressures from external monitors on tank wall are reflected pressures.

566 The initial mechanical energy from the vent is calculated by:

$$567 \quad E_g = \frac{\Delta p_v (V - mb)}{\gamma - 1} \quad (10)$$

568 where  $b$  is a co-volume constant, which is 0.04278 L/mol, or 0.002674 m<sup>3</sup>/kg for methane gas,

569  $V$  and  $m$  are the volume and mass of gas inside the tank. The ratio of specific heat  $\gamma$  is 1.32

570 for methane at 20 degrees Celsius.  $\Delta p$  is the overpressure near vent.

571 The explosion energy from the vent is then used to calculate the overpressure in far field with

572 a distance of  $R$  in the dimensionless equation as shown below:

$$573 \quad \frac{\Delta P_e}{P_o} = 1.1 \cdot \frac{\Delta p_v}{P_o} \cdot e^{-\left(0.011 \cdot \frac{\Delta p_v}{P_o} + 0.4\right) \frac{R}{(\alpha E_g / P_o)^{1/3}}} \quad (11)$$

574 where  $\Delta P_e$  is the external overpressure peak,  $P_o$  is the ambient atmospheric pressure,  $\alpha$  is the

575 mechanical energy coefficient (Molkov and Kashkarov, 2015). For the vented explosion from

576 the side wall, it is assumed there is no reflection of blast wave from the fully-opened vent.

577 Therefore,  $\alpha=1.0$  is used in this study.  $R$  is the distance from the vent opening to the pressure

578 monitor point in meters.

579 By using Equation (10) and (11), initial mechanical energies from the vent and external

580 overpressure peaks are determined and given in Table 6. It is worth noting that the overpressure

581 peaks predicted by FLACS in Table 5 are about twice of the analytically calculated

582 overpressure peaks. The difference between these two sets of data is because the dimensionless

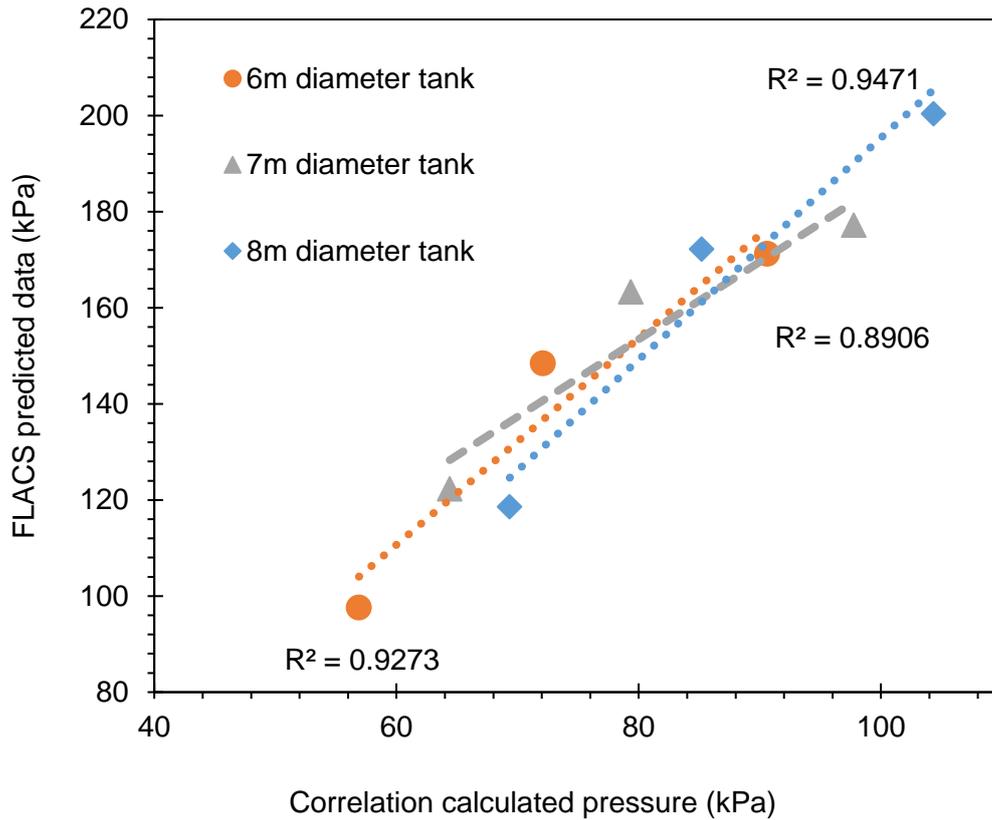
583 correlations by the authors were derived based on the single tank experiments, and the pressure

584 decaying were obtained in open space, i.e., not the reflected pressure. Whereas in this study,  
 585 twin tanks are used in the numerical simulation, simulations are conducted within the region  
 586 where blast wave propagates from the pressure donor tank to the pressure acceptor tank.  
 587 Pressure wave is reflected from the wall of pressure-accepting tank.

588 **Table 6 Calculation of mechanical energy and external overpressure peak by correlations in**  
 589 **different cases**

<b>Tank condition</b>	<b>Mechanical energy (MJ)</b>	<b>Correlation-calculated pressure (kPa)</b>	<b>Different between correlation-calculated data and FLACS estimated data</b>
<b>6m diameter tanks with 1m gap</b>	36.1	90.6	188.9%
<b>6m diameter tanks with 2m gap</b>	35.5	72.1	205.8%
<b>6m diameter tanks with 3m gap</b>	34.4	56.9	171.5%
<b>7m diameter tanks with 1m gap</b>	52.1	97.8	181.2%
<b>7m diameter tanks with 2m gap</b>	51.5	79.4	205.8%
<b>7m diameter tanks with 3m gap</b>	50.7	64.4	189.9%
<b>8m diameter tanks with 1m gap</b>	71.7	104.3	192.1%
<b>8m diameter tanks with 2m gap</b>	70.3	85.2	202.1%
<b>8m diameter tanks with 3m gap</b>	68.3	69.4	171.0%

590  
 591 Despite the reflection factor (in the range of 1.7 to 2.1), the pressure decaying trend simulated  
 592 by FLACS in large-scale tanks agrees well with the pressure decreasing trend estimated by  
 593 correlations, as seen in Fig. 22. By increasing the separation distance from 1m to 3m, the  
 594 overpressure peaks proportionally decrease. In the comparison of two sets of data from 9  
 595 different cases, the R-square values are between 89% and 94.7%. Therefore, it can be  
 596 concluded that the correlations used for far-field/external pressure calculation by (Li and Hao,  
 597 2018) can accurately predict the external pressure decay between two large tanks. However, an  
 598 appropriate pressure reflection factor (1.7 to 2.1 in this study) should be used for the calculation  
 599 of external pressure reflected from tank wall.



600  
601 **Fig. 22 Comparison of FLACS predicted pressures and correlation-calculated data**  
602

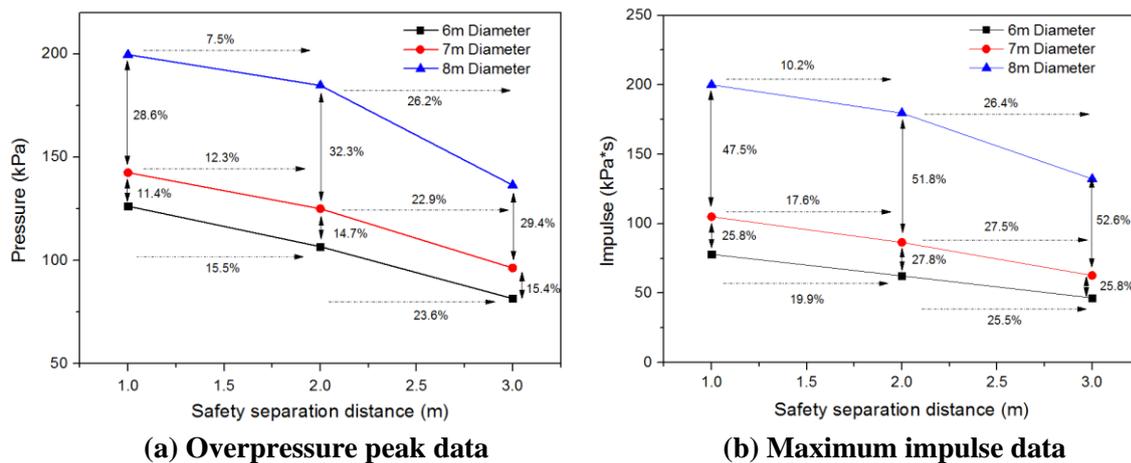
603 **4. Parametric study**

604 In section 3, the grid sensitivity study on large-scale twin tank explosion has been conducted.  
605 A series of FLACS simulations by using the chosen grid mesh have been carried out. It is  
606 proven that FLACS predicted pressures from these large-scale explosions are in good  
607 agreement with the data by using the analytical correlations with correct scaling. A more  
608 detailed parametric study is performed in this section to investigate the effect of separation  
609 distance between adjacent tanks on pressure and impulse mitigation by using these large-scale  
610 twin tanks. The interaction between the separation distance and various tank parameters is  
611 discussed.

612 **4.1 Effect of separation distance on pressure and impulse from explosions of**  
613 **tanks of different diameters**

614 To investigate the effect of separation distance on vented gas explosion mitigation, pressure  
 615 and impulse data recorded from the pressure-accepting tanks are used. Meanwhile, since the  
 616 pressures and impulses are not strictly uniform on a curved tank wall surface, an  
 617 inactive/passive panel (as seen in Fig. 20) is used to average all data.

618 The tanks with diameter of 6m, 7m and 8m are firstly used for the investigation of the effect of  
 619 separation distance on mitigation of pressure and impulse from vented explosions of tanks with  
 620 different diameters. The diameters of pressure donor tank (tank filled with gas cloud) and  
 621 pressure-accepting tank vary simultaneously from 6m to 8m. The tank height is fixed at 4m,  
 622 vent area is  $0.6\text{m}^2$ , and the separation gap is in the range of 1m to 3m.



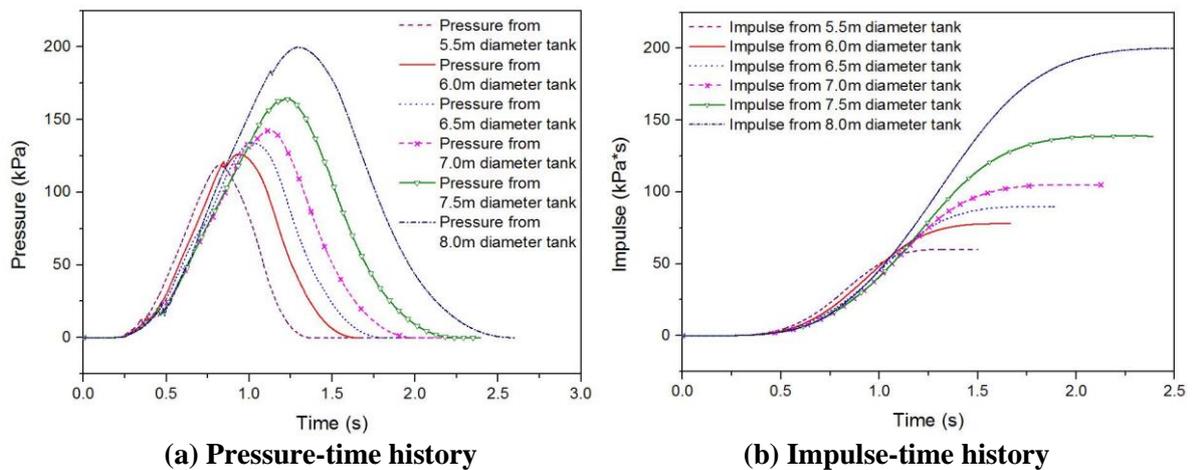
623 (a) Overpressure peak data (b) Maximum impulse data  
 624  
 625 **Fig. 23 Pressure and impulse data from pressure-accepting tanks with 3 different diameters and**  
 626 **3 different separation distances**

628 The overpressure peaks and maximum impulses from these 9 cases are extracted and shown in  
 629 Fig. 23. The dashed horizontal arrows represent the level of pressure decrease when the  
 630 separation distance increases 1m. The solid vertical arrows are the pressure differences between  
 631 two different tank diameter cases. From the dashed horizontal arrows, it is seen that the pressure  
 632 mitigation level is higher when the separation distance is bigger. For instance, the mitigation  
 633 percentages are 26.2%, 22.9% and 23.6% (corresponding to 8m, 7m, and 6m diameter tanks)  
 634 when the separation distance increases from 2m to 3m, whereas they are only 7.5%, 12.3 and  
 635 15.5% when the separation distance increases from 1m to 2m (Fig. 23(b)). The similar decaying

636 tendencies are seen in the impulse data of Fig. 23(b). In other words, the effect of increasing  
 637 the separation distance on pressure and impulse mitigation is more obvious when the distance  
 638 is large.

639 In terms of the solid vertical arrows, it is observed that the pressure and impulse decrease level  
 640 (about 30% decrease and 50% decrease for pressure and impulse, respectively) are much more  
 641 significant if the tank diameter reduces from 8m to 7m, while the pressure and impulse show  
 642 about 14% and 26% decrease when the tank diameter shrinks from 7m to 6m. In other words,  
 643 the decays in pressure and impulse are nonlinearly related to the reduction in tank diameter  
 644 from the vented gas explosions.

645 In order to thoroughly investigate the tank diameter effect on external pressure and impulse,  
 646 tank diameters ranging from 5.5m to 8.0m (6 different explosion cases) are considered. The  
 647 separation distance is fixed as 1m and the results are shown in Fig. 24.

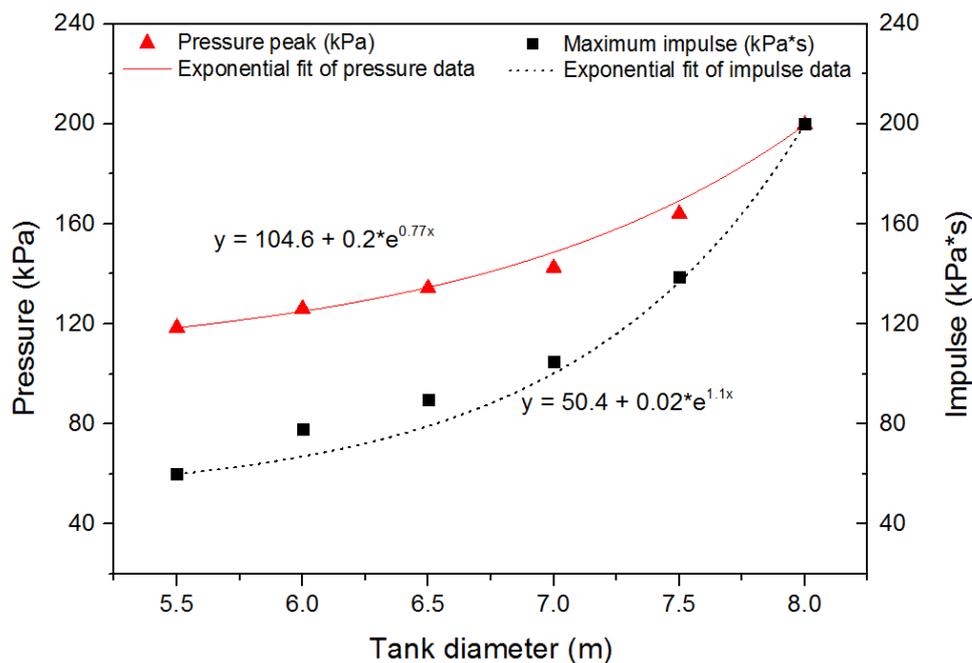


648  
 649 **(a) Pressure-time history**  
 650 **(b) Impulse-time history**  
 651 **Fig. 24 Pressure and impulse on the pressure-accepting tanks with different diameters**

652 It is shown in Fig. 24 that by increasing the tank diameter from 5.5m to 8.0m, the overpressure  
 653 peaks increase monotonically (Fig. 24(a)). The duration of pressure-time curve also increases,  
 654 which is due to the longer combustion time inside the larger tank. It is known that impulse is  
 655 the integral of pressure-time history. As both the overpressure peak and combustion time  
 656 increase, the impulse increases more prominently than overpressure peak. Fig. 25 well

657 demonstrates the above observations. The maximum impulse versus tank diameter relationship  
 658 curve has a more rapid increment rate than the overpressure peak curve.

659 The relationships among tank diameter, overpressure peak and impulse in Fig. 25 are expressed  
 660 by two exponential growing curves, indicating both the pressure and impulse increase with the  
 661 tank diameter exponentially.



662 **Fig. 25 Relationships among tank diameter, overpressure peak and maximum impulse**

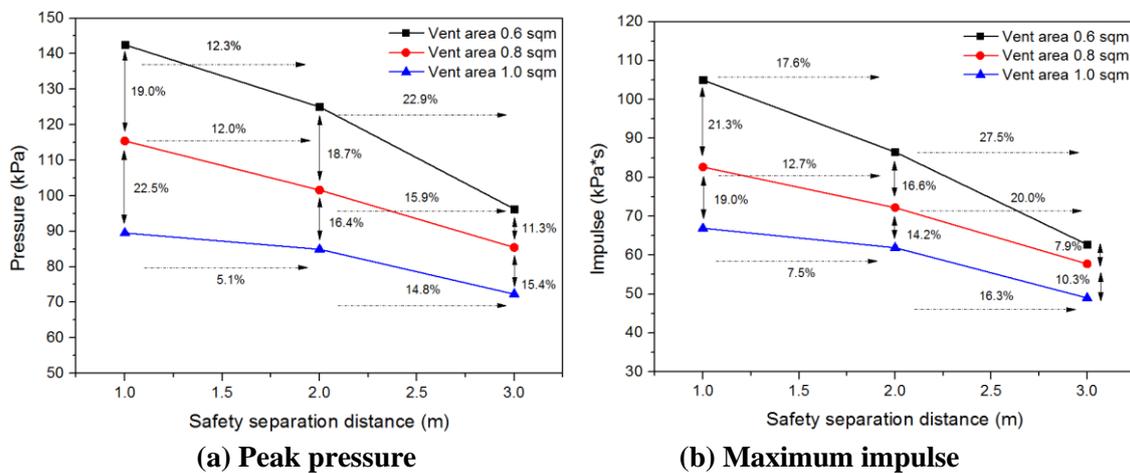
663  
 664  
 665  
 666 **4.2 Effect of separation distance on explosion pressure and impulse from tanks of**  
 667 **different vent area sizes**

668 The separation distance effect on explosion pressure and impulse from tanks with different vent  
 669 area sizes is investigated in this section. The 7m diameter and 4m height tank, which is the tank  
 670 in the middle range of all tanks in section 4.1, is chosen for the study. The vent arrangement is  
 671 the same as shown in Fig. 14. In the parametric study, vent area sizes of 0.6m<sup>2</sup>, 0.8m<sup>2</sup> and  
 672 1.0m<sup>2</sup> are considered.

673 As seen in Fig. 26 (the dashed horizontal arrows), increasing the separation distance between  
 674 tanks from 1m to 3m results in overpressure peak decrease for all vent area cases. Similar to

675 those observed in section 4.2, the pressure shows a larger reduction rate when the separation  
 676 distance is larger. The reason is that the pressure decays more severely when pressure wave  
 677 propagates in open space. Larger separation distance leads to more pressure decay and more  
 678 energy dissipation in the air.

679 Although it is well known that larger vent area results in smaller vented explosion pressure,  
 680 from the solid vertical arrows, it is interesting to see that increasing the vent area from  $0.6\text{m}^2$   
 681 to  $0.8\text{m}^2$ , the pressure decreases 19.0% for the 1m separation case, while the pressure decreases  
 682 11.3% when the separation distance between adjacent tanks is 3m. Similarly, increasing the  
 683 vent area from  $0.8\text{m}^2$  to  $1.0\text{m}^2$ , the pressure decreases 22.5% in the 1 m separation case,  
 684 whereas the pressure decreases 15.4% in the case with separation gap of 3m. These results  
 685 indicate the pressure decrease ratio is inversely proportional to the separation distance. In other  
 686 words, if the separation distance is larger, the pressure decrease less with the same increase in  
 687 vent area.



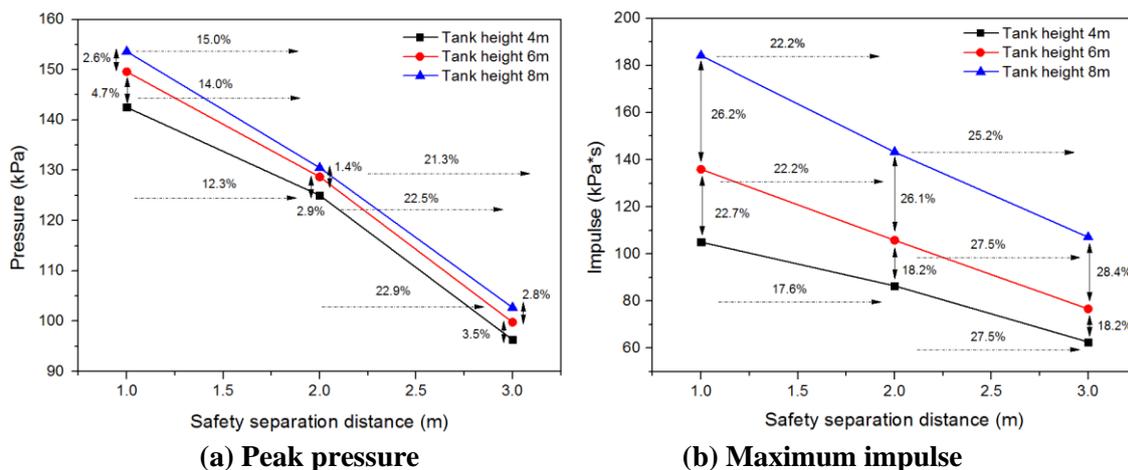
688  
 689 **(a) Peak pressure** **(b) Maximum impulse**  
 690 **Fig. 26 Pressure and impulse data from pressure-accepting tanks with 3 different vent areas and**  
 691 **3 different separation distances**

692  
 693 Similar observations regarding the effect of separation distance on explosion impulse as shown  
 694 in Fig. 26(b) can be drawn. As shown the impulse lines are even closer to each other on the  
 695 right hand side of the figure. It is known that changing the vent area is an effective way to  
 696 mitigate pressure and impulse. These results indicate that when the separation distance is large,

707 vent area effect on pressure and impulse mitigation becomes less prominent. Therefore, beside  
 708 increasing the vent area, providing a large separation distance is also effective on pressure and  
 709 impulse mitigation. When the separation distance is sufficiently large, increasing the vent area  
 700 becomes less effective in mitigating the pressure and impulse.

701  
 702 **4.3 Separation distance effect on explosion pressure and impulse for tanks of**  
 703 **different heights**

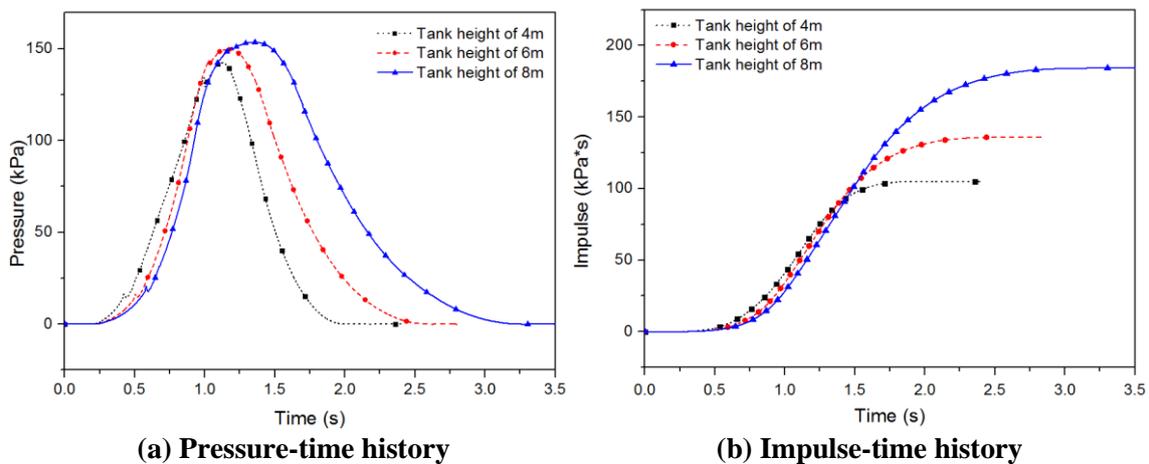
704 In this section, the separation distance effect on pressure and impulse mitigation is examined  
 705 for tanks with different heights. The tank diameter is kept as 7m, vent area size is 0.6m<sup>2</sup>.  
 706 Separation distances considered are 1m, 2m and 3m. Tank heights are 4m, 6m and 8m. In total,  
 707 9 cases are simulated.



708  
 709 **(a) Peak pressure** **(b) Maximum impulse**  
 710 **Fig. 27 Peak pressure and impulse from pressure-accepting tanks of 3 different heights and 3**  
 711 **different separation distances**

712  
 713 Fig. 27 shows the peak pressure and impulse with respect to the different separation distances  
 714 from tanks of three different heights. As shown at least 12.3% and 17.6% pressure and impulse  
 715 reduction by increasing the separation distance from 1m to 2m can be achieved. The  
 716 corresponding mitigation levels increase to 17.8% and 25.2% if the separation distance is  
 717 increased from 2m to 3m. It is again proven that providing large separation distance is effective  
 718 for mitigating pressure and impulse from vented explosions in adjacent tanks.

719 As shown in the figure (the solid vertical arrows), the differences in peak pressures from tanks  
 720 of different heights are considerably smaller (between 1.4% and 4.7%) than the corresponding  
 721 differences shown in Fig. 23 and Fig. 26, indicating tank diameter and vent area size are more  
 722 influential parameters than tank height on explosion pressure. However, in Fig. 27(b), the  
 723 differences between two vertical data are over 18.2%, which means reducing tank height is  
 724 more effective in impulse mitigation than pressure reduction. Fig. 28 demonstrates the  
 725 observations on tank height effect on pressure and impulse more thoroughly. As can be seen,  
 726 overpressure peaks are marginally increased from explosions in the 4m height tank to the 8m  
 727 height tank, while the maximum impulses are significantly increased. The reason is that the  
 728 impulse is the integral of pressure over time, since the combustion duration is increased by  
 729 extending the tank height, the final impulse value is therefore considerably increased as well.



730  
 731 (a) Pressure-time history (b) Impulse-time history  
 732 **Fig. 28 Pressure and impulse data for 3 different tank height cases with 1m separation distance**  
 733

734  
 735 Therefore, according to the parametric studies of the effect of separation distances on  
 736 mitigation of large-scale explosion pressure and impulse, it can be concluded that providing a  
 737 large separation distance is very effective on pressure and impulse mitigation from adjacent  
 738 tank explosions. When the separation distance is large, application of vent on explosion  
 739 mitigation become less effective. Compared to the other two parameters, tank diameter is a  
 740 more influential parameter than tank height on peak pressures recorded on adjacent tank wall.

741 However, reducing the tank height for a vented explosion can lead to significant reduction in  
742 pressure impulse on adjacent tank wall although its effect on mitigating the peak pressure is  
743 insignificant.

744

## 745 **5. Conclusion**

746 In this study, numerical and analytical study of vented gas explosion between large-scale twin  
747 tanks is conducted. The large-scale explosion simulations are carried out by using CFD  
748 software FLACS. Experimental data are used for the validation of FLACS simulation accuracy.  
749 The FLACS predicted data agree well with all experimental results in this study. Sensitivity  
750 study for the selection of correct meshing grids is performed for the large-scale models.

751 In the analytical study, the internal pressure and external pressure from vented gas explosion  
752 in a cylindrical tank are investigated. It is proven in this study the authors' previously proposed  
753 correlations are applicable for large-scale vented gas explosion overpressure peak prediction.  
754 However, two scale-up factors are required for the adjustment of correlations.

755 According to the parametric study results, providing separation between tanks is effective on  
756 reducing the pressure and impulse on adjacent tanks. The effectiveness of vent on explosion  
757 mitigation is weakened when the separation distance is large. The larger diameter is the tank,  
758 the higher are the explosion pressure and impulse. The peak pressure and impulse increase  
759 exponentially with the tank diameter. Reducing tank height is effective in reducing the impulse  
760 but has insignificant effect on the peak pressure acting on adjacent tanks.

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765 **References**

- 766 API-650. 2007. Welded Steel Tanks for Oil Storage. *American Petroleum Institute, 11th*  
767 *Edition.*
- 768 Arntzen, B.J., 1998. Modelling of turbulence and combustion for simulation of gas  
769 explosions in complex geometries. Thesis. The Norwegian University
- 770 Bao, Q., Fang, Q., Zhang, Y.D., Chen, L., Yang, S.G., Li, Z., 2016. Effects of gas  
771 concentration and venting pressure on overpressure transients during vented explosion  
772 of methane-air mixtures. *Fuel.* 175, 40-48.
- 773 Bauwens, C.R., Chaffee, J., Dorofeev, S., 2010. Effect of Ignition Location, Vent Size, and  
774 Obstacles on Vented Explosion Overpressures in Propane-Air Mixtures. *Combust Sci*  
775 *Technol.* 182 (11-12), 1915-32.
- 776 Bauwens, C.R., Chao, J., Dorofeev, S.B., 2012. Effect of hydrogen concentration on vented  
777 explosion overpressures from lean hydrogen-air deflagrations. *Int J Hydrogen Energ.*  
778 37 (22), 17599-605.
- 779 Bjerketvedt, D., Bakke, J.R., Van Wingerden, K., 1997. Gas explosion handbook. *J Hazard*  
780 *Mater.* 52 (1), 1-150.
- 781 Bradley, D., Mitcheson, A., 1978. The venting of gaseous explosions in spherical vessels.  
782 II—Theory and experiment. *Combustion and Flame.* 32, 237-55.
- 783 Cammarota, F., Di Benedetto, A., Russo, P., Salzano, E., 2010. Experimental analysis of gas  
784 explosions at non-atmospheric initial conditions in cylindrical vessel. *Process Safety*  
785 *and Environmental Protection.* 88 (5), 341-49.
- 786 Catlin, C.A., 1991. Scale Effects on the External Combustion Caused by Venting of a  
787 Confined Explosion. *Combustion and Flame.* 83 (3-4), 399-411.
- 788 Cen, K., Song, B., Huang, Y., Wang, Q.S., 2017. CFD Simulations to Study Parameters  
789 Affecting Gas Explosion Venting in Compressor Compartments. *Math Probl Eng.*
- 790 Ferrara, G., Di Benedetto, A., Salzano, E., Russo, G., 2006. CFD analysis of gas explosions  
791 vented through relief pipes. *J Hazard Mater.* 137 (2), 654-65.
- 792 Ferrara, G., Willacy, S.K., Phylaktou, H.N., Andrews, G.E., Di Benedetto, A., Salzano, E.,  
793 Russo, G., 2008. Venting of gas explosion through relief ducts: Interaction between  
794 internal and external explosions. *J Hazard Mater.* 155 (1-2), 358-68.
- 795 Gexcon. 2017. FLACS v10.7 User's Manual, Norway.
- 796 Hansen, O.R., Hinze, P., Engel, D., Davis, S., 2010. Using computational fluid dynamics  
797 (CFD) for blast wave predictions. *J Loss Prevent Proc.* 23 (6), 885-906.
- 798 Hansen, O.R., Johnson, D.M., 2015. Improved far-field blast predictions from fast  
799 deflagrations, DDTs and detonations of vapour clouds using FLACS CFD. *J Loss*  
800 *Prevent Proc.* 35, 293-306.
- 801 Harrison, A.J., Eyre, J.A., 1987. External Explosions as a Result of Explosion Venting.  
802 *Combust Sci Technol.* 52 (1-3), 91-106.
- 803 Hisken, H., 2018. Investigation of instability and turbulence effects on gas explosions:  
804 experiments and modelling (Thesis). University of Bergen.
- 805 Hjertager, B.H., 1984. Computer-Simulation of Turbulent Reactive Gas-Dynamics. *Model*  
806 *Ident Control.* 5 (4), 211-36.
- 807 Hjertager, B.H., 1993. Computer Modeling of Turbulent Gas-Explosions in Complex 2d and  
808 3d Geometries. *J Hazard Mater.* 34 (2), 173-97.
- 809 Kasmani, R.M., Ancirews, G.E., Phylaktou, H.N., 2013. Experimental study on vented gas  
810 explosion in a cylindrical vessel with a vent duct. *Process Safety and Environmental*  
811 *Protection.* 91 (4), 245-52.

812 Li, J., Hao, H., 2018. Far-field pressure prediction of a vented gas explosion from storage  
813 tanks by using new CFD simulation guidance. *Process Safety and Environmental*  
814 *Protection*. 119, 360-78.

815 Li, J., Hao, H., Shi, Y.C., Fang, Q., Li, Z., Chen, L., 2018. Experimental and computational  
816 Fluid Dynamics study of separation gap effect on gas explosion mitigation for  
817 methane storage tanks. *J Loss Prevent Proc*. 55, 359-80.

818 Li, J., Hernandez, F., Hao, H., Fang, Q., Xiang, H.B., Li, Z., Zhang, X., Chen, L., 2017.  
819 Vented Methane-air Explosion Overpressure Calculation—A simplified approach  
820 based on CFD. *Process Safety and Environmental Protection*. 109, 489-508.

821 Liu, Q.M., Zhang, Y.M., Niu, F., Li, L., 2015. Study on the flame propagation and gas  
822 explosion in propane/air mixtures. *Fuel*. 140, 677-84.

823 Mercx, W.P.M., Vanwingerden, C.J.M., Pasman, H.J., 1992. Venting of Gaseous Explosions.  
824 *Inst Chem E*. 130, 411-26.

825 Molkov, V., Dobashi, R., Suzuki, M., Hirano, T., 2000. Venting of deflagrations:  
826 hydrocarbon-air and hydrogen-air systems. *J Loss Prevent Proc*. 13 (3-5), 397-409.

827 Molkov, V., Kashkarov, S., 2015. Blast wave from a high-pressure gas tank rupture in a fire:  
828 Stand-alone and under-vehicle hydrogen tanks. *Int J Hydrogen Energ*. 40 (36), 12581-  
829 603.

830 NFPA-68. 2007. *Standard on explosion protection by deflagration venting* (National Fire  
831 Protection Association).

832 Nishimura, I., Mogi, T., Dobashi, R., 2013. Simple method for predicting pressure behavior  
833 during gas explosions in confined spaces considering flame instabilities. *J Loss*  
834 *Prevent Proc*. 26 (2), 351-54.

835 Pasman, H.J., 2015. *Risk Analysis and Control for Industrial Processes-Gas, Oil and*  
836 *Chemicals: A System Perspective for Assessing and Avoiding Low-Probability, High-*  
837 *Consequence Events* (Butterworth-Heinemann).

838 Pedersen, H.H., Middha, P., 2012. Modelling of Vented Gas Explosions in the CFD tool  
839 FLACS. *Chem Engineer Trans*. 26, 357-62.

840 REMBE. 2015. Explosion Safety Product Information.  
841 [http://www.rembe.com/fileadmin/produkte/explosionsschutz/EGV/Product\\_Information\\_EGV.pdf](http://www.rembe.com/fileadmin/produkte/explosionsschutz/EGV/Product_Information_EGV.pdf).  
842

843 Rodgers, S.A., Zalosh, R., 2013. NFPA 68 - New Gas Venting Equations. *AIChE 9th Global*  
844 *congress on process safety*.

845 Rota, R., Canu, P., Carra, S., Morbidelli, M., 1991. Vented Gas Deflagration Modeling - a  
846 Simplified Approach. *Combustion and Flame*. 85 (3-4), 319-30.

847 Russo, P., Di Benedetto, A., 2007. Effects of a duct on the venting of explosions - Critical  
848 review. *Process Safety and Environmental Protection*. 85 (B1), 9-22.

849 Solberg, D., Pappas, J., Skramstad, E., 1981. Observations of flame instabilities in large scale  
850 vented gas explosions. In *Symposium (International) on Combustion*. 1607-14.  
851 Elsevier.

852 Swift, I., 1989. Nfpa-68 Guide for Venting of Deflagrations - Whats New and How It Affects  
853 You. *J Loss Prevent Proc*. 2 (1), 5-15.

854 Toliás, I., Giannisi, S., Venetsanos, A., Keenan, J., Shentsov, V., Makarov, D., Coldrick, S.,  
855 Kotchourko, A., Ren, K., Jedicke, O., 2018. Best practice guidelines in numerical  
856 simulations and CFD benchmarking for hydrogen safety applications. *Int J Hydrogen*  
857 *Energ*.

858 Tomlin, G., Johnson, D.M., Cronin, P., Phylaktou, H.N., Andrews, G.E., 2015. The effect of  
859 vent size and congestion in large-scale vented natural gas/air explosions. *J Loss*  
860 *Prevent Proc*. 35, 169-81.

861 Tsuruda, T., Hirano, T., 1987. Growth of Flame Front Turbulence during Flame Propagation  
862 across an Obstacle. *Combust Sci Technol.* 51 (4-6), 323-28.

863 Vyazmina, E., Jallais, S., 2016. Validation and recommendations for FLACS CFD and  
864 engineering approaches to model hydrogen vented explosions: Effects of  
865 concentration, obstruction vent area and ignition position. *Int J Hydrogen Energ.* 41  
866 (33), 15101-09.

867 Vyazmina, E., Jallais, S., Krumenacker, L., Tripathi, A., Mahon, A., Commanay, J.,  
868 Kudriakov, S., Studer, E., Vuillez, T., Rosset, F., 2018. Vented explosion of  
869 hydrogen/air mixture: An intercomparison benchmark exercise. *Int J Hydrogen*  
870 *Energ.*

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873