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NUMERICAL PREDICTION OF BLAST EFFECTS CAUSED BY LARGE-SCALE EXPLOSION OF LOX/LNG FUEL

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SUMMARY

In this study we propose a quantitative prediction of blast wave properties caused by a large-scale accidental explosion of a huge quantity of LOX/LNG fuel at more than 1 kilometer from the explosion point. The two cases of 17 and 5 tonnes of fuel total mass are considered. We carried out basically one-dimensional spherical symmetric numerical simulations by using a multi-material Euler solver of the hydrocode ANSYS® AUTODYN®. Overpressures and impulses of the blast wave were measured numerically at several locations at the distances of less than 3 kilometers. On the other hand, practical down-scaled experiments for the explosion of gram order gaseous fuel were conducted for validation of the numerical simulations. These results were summarized by using the scaling law for explosions. Numerical relationships between scaled blast wave properties and scaled distances were qualitatively in good agreement with experimental ones. The applicability of the scaling law to the large-scale explosions of tonne order explosive substances was demonstrated.

1. INTRODUCTION

When we examine the safety of the environment around plants or storage facilities of explosive substances in case of accidental explosion, quantitative understanding of the safety distance is one of important matters. In order to estimate the safety distance as exact as possible, it is necessary to obtain the detonation property of the explosive substance and to predict the influence of a blast wave caused by the explosion. In this study, we assume a large-scale accidental explosion in two cases of 17 and 5 tonnes of the LOX(Liquid Oxygen)/LNG liquid fuel. It is assumed that the fuel reacts completely in an extremely short duration in gaseous or liquid phases respectively, which affect the amount of its total energy to release into the atmosphere. In this condition, blast wave influences at more than 1 kilometer from the explosion point should be investigated.

It is practically impossible that such a large-scale explosion of tonne order explosive substances is experimentally reproduced in the comparable scale. We conduct numerical simulations of the blast wave caused by the explosion and quantitatively obtain peak overpressures and impulses measured at several gauges located from the explosion point to the maximum 3 kilometers. A spherical symmetric numerical model in the one-dimensional geometry is applied to the numerical region in the range from the explosion point to the maximum 3 kilometers by using a multi-material Euler solver of the hydrocode ANSYS® AUTODYN®. On the other hand, practical down-scaled experiments for the explosion of gram order methane-oxygen mixture gas were conducted in the open air testing ground [Kim et al, 2008] for validation of the numerical simulations. We simulate the experiment by applying the two-dimensional axisymmetric model to it in order to take account of the shock wave reflection by the ground. A series of peak overpressures and impulses obtained numerically and experimentally is summarized by using the scaling law for explosions. Then, the relationships between scaled blast wave properties and scaled distance are obtained. Finally the validity of numerical predictions of blast wave influences caused by the large-scale explosion is evaluated.

2. NUMERICAL SIMULATION

2.1 Analysis case

Analysis cases are shown in Table 1. In the cases from 1 to 4, we assume two cases of 17 and 5 tonnes of the fuel mass, and two cases of gaseous and liquid phases of the fuel condition, respectively. The mass of the methane including in 17 and 5 tonnes of the fuel is calculated to be 3.4 and 1.0 tonnes on the assumption of the stoichiometric ratio respectively. In the case of a gaseous phase, as the release energy for explosion is the largest when the equivalent ratio is 1.4, the mass of the methane-oxygen mixture gas to contribute to the explosion is approximately 13 and 3.9 tonnes respectively. On the other hand, in the case of a liquid phase, as the energy is a maximum when the equivalent ratio is 1.0, the mass of the mixture liquid corresponds to that in the initial condition, 17 and 5 tonnes, respectively.

The down-scaled experiment was performed in several conditions of the mixture gas to change the mass and the mixing ratio of the mixture gas. In the case 5, we conducted the numerical simulation only for one of the conditions, 5.8 grams of the mixture gas in the stoichiometric ratio.

Table 1 Analysis case

Case #	Fuel mass	Fuel condition
1	13 tonnes	Gas
2	3.9 tonnes	Gas
3	17 tonnes	Liquid
4	5.0 tonnes	Liquid
5	5.8 grams	Gas

2.2 Numerical model

We used the multiple solver hydrocode ANSYS® AUTODYN®, which has efficient solvers of Lagrangian, three types of Eulerian, ALE, SPH, shell and beam. In this study, we applied the multiple material Eulerian and ALE solvers to the air and the explosive substance. In the cases from 1 to 4, the spherical region with the maximum radius of 3 kilometers from the explosion point was modeled by using the two-dimensional (2D) axisymmetric wedge model nearly identical to the one-dimensional (1D) spherical symmetric model as shown in Fig. 1. The mixture is positioned spherically at the center of the numerical region filled with the atmospheric air. For the measurements of pressure histories of the propagating blast wave, numerical gauges were positioned at several locations from the explosion point. A uniform mesh size of 0.2 meter is used. In order to simulate the ground explosion by using the 1D spherical symmetric model, twice the mass of charge weight was given to the source of the explosion in consideration of symmetry on

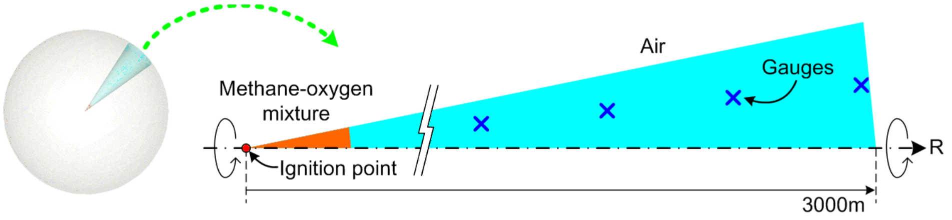


Figure 1 Two-dimensional axisymmetric wedge model nearly identical to the one-dimensional spherical symmetric model

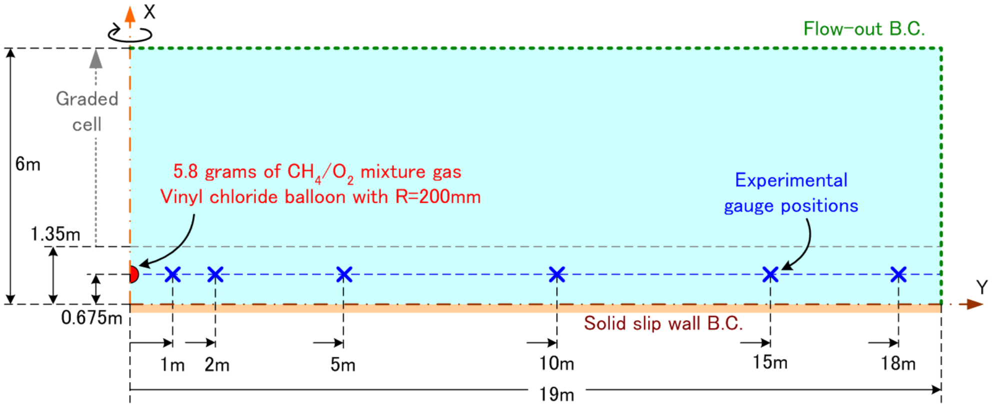


Figure 2 Two-dimensional axisymmetric model equivalent to the practical experimental setup

calculation.

In the case 5, the axisymmetric region of 19 meters in radius from the explosion point and 6 meters in height from the ground equivalent to the practical experimental setup was modeled by using the 2D axisymmetric model as shown in Fig. 2. The rigid wall boundary condition was applied to the ground surface. The flow-out boundary condition was applied to the he upper and side interfaces of the numerical region. A mesh size was fixed to be 7.5 millimeters in the region to the horizontal direction and up to the 1.35 meters from the ground. In the region over the height, a mesh size was graded upward gradually. The extra region was for the purpose that the numerical disturbances generated at the upper interface were prevented from affecting the blast wave propagating along the ground. 5.8 grams of the mixture gas was filled in the spherical vinyl chloride balloon with a radius of 200 millimeters. The balloon was located at the height of 675 millimeters from the ground and was ignited at the center in the experiment. In the experiment, it was observed by high speed camera that the mixture gas was deflagrated [Kim et al, 2008]. However, for the purpose of reference, we considered two numerical assumptions of an instantaneous combustion in a constant volume and a detonation for the reaction of the mixture gas. Gauges were positioned at 675 millimeters in height and at 1 meter interval from the center of the balloon.

2.3 Material model

Assuming that the methane-oxygen mixture gas in the cases of 1, 2 and 5 is an ideal gas, the ideal gas EOS described as follows was applied.

$$P = (\gamma - 1)\rho e \tag{1}$$

where, P is the pressure, γ is the coefficient of expansion, ρ is the density, e is the internal energy per unit mass, respectively. The detonation parameters of the methane-oxygen mixture gas at the equivalent ratio 1.4 are shown in Table 2. The constant volume combustion parameters of the mixture gas at the equivalent ratio 1.0 are shown in Table 3. These values were calculated by using the method of Gordon-McBride, the CET93 program [Gordon et al, 1994].

For the methane-oxygen mixture liquid in the cases of 3 and 4, the JWL EOS described as follows was applied.

$$P = A\left(1-\frac{\omega\eta}{R_1}\right)\exp\left(-\frac{R_1}{\eta}\right) + B\left(1-\frac{\omega\eta}{R_2}\right)\exp\left(-\frac{R_2}{\eta}\right) + \omega\eta\rho_{ref}e \tag{2}$$

where, $\eta = \rho/\rho_{ref}$, ρ_{ref} is the reference density, A, B, R_1, R_2, ω are the material constants, respectively. The detonation parameters of the methane-oxygen mixture liquid at the equivalent ratio 1.0 are shown in Table 4. These values were calculated by using the detonation properties calculation program, KHT2003 [Tanaka, 2003]. We assume that the detonation velocity in explosive substances is constant in the cases from 1 to 4.

For the air, the ideal gas EOS with a reference density of 1.225 kg/m^3 and the specific heat ratio of 1.4 were applied.

Table 2 Detonation parameters of methane -oxygen mixture gas at the equivalent ratio 1.4.

Variable	Unit	Value
Reference Density	kg/m^3	1.135
Specific internal energy	MJ/m^3	13.41
Detonation velocity	m/s	2662
C-J pressure	MPa	3.525
Coefficient of expansion	-	1.138

Table 3 Constant volume combustion parameters of methane-oxygen mixture gas at the equivalent ratio 1.0.

Variable	Unit	Value
Reference Density	kg/m^3	1.165
Specific internal energy	MJ/m^3	11.43
Initial pressure	MPa	2.029
Coefficient of expansion	-	1.130

Table 4 Detonation parameters of methane -oxygen mixture liquid at the equivalent ratio 1.0.

Variable	Unit	Value
Reference Density	kg/m^3	861.6
Constant A	GPa	223.4
Constant B	GPa	5.735
Constant R_1	-	5.599
Constant R_2	-	1.324
Constant ω	-	0.1541
Specific internal energy e	MJ/m^3	10.14
Detonation velocity	m/s	5825
C-J pressure	MPa	8.366

3. RESULTS AND DISCUSSION

3.1 The scaling law for explosion

We applied the scaling law for explosion [Baker, 1973, Saito et al, 2007] to peak overpressures and impulses obtained numerically and experimentally. These are described as follows:

$$\bar{p} = \frac{p - p_0}{p_0} \tag{3}$$

$$\bar{I} = \frac{I\, c_0}{E^{1/3}\, {p_0}^{2/3}} \tag{4}$$

$$\bar{R} = \frac{R}{(E/p_0)^{1/3}} \tag{5}$$

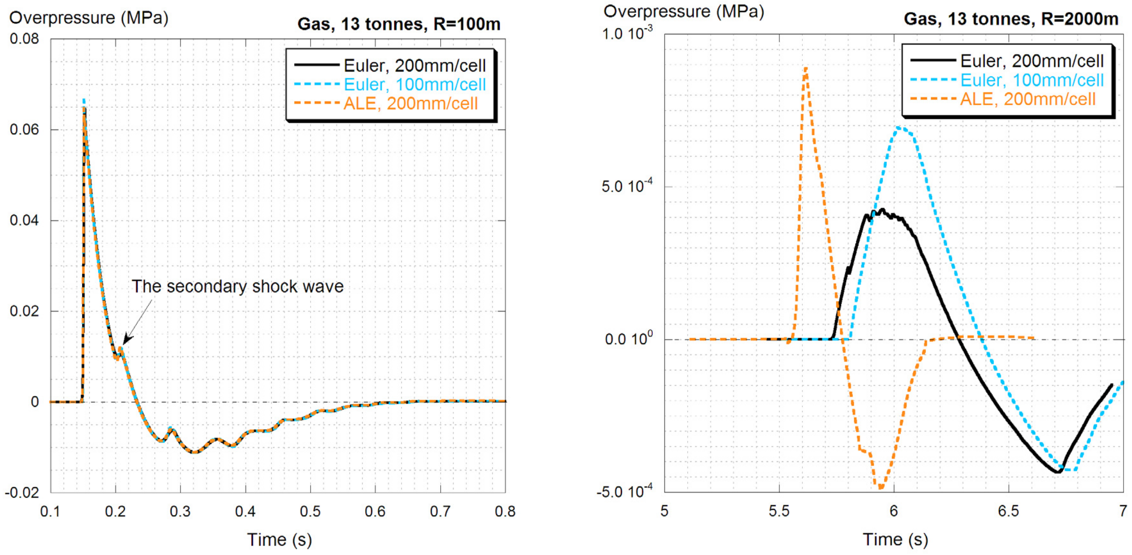
where, $\bar{p}$ is the scaled pressure, p is the peak overpressure, p_0 is the atmospheric pressure, $\bar{I}$ is the scaled impulse, I is the impulse, c_0 is the sound speed in the atmospheric air, E is the energy released into the atmospheric air, $\bar{R}$ is the scaled distance, R is the distance from the explosion point, respectively.

3.2 Numerical and experimental results

Figure 3 shows overpressure histories at 100 and 2000 meters from the explosion point in the case of 13 tonnes of the mixture gas. For the purpose of reference, two numerical results of the ALE (Arbitrary Lagrangian Eulerian) solver and the Euler solver with the mesh size of 0.1 meter were plotted by the blue and orange dotted lines, respectively. The ALE solver allows the numerical mesh to move with the material as a Lagrangian mesh and also to move in an arbitrarily specified manner to prevent it from distorting.

In Fig. 3 (a), the overpressure profile at 100 meters rises steeply and the generation of the secondary shock wave can be observed. The profiles are completely identical at the distance in all cases of the Euler solvers with two mesh sizes and the ALE solver. However, in Fig. 3 (b), the profiles of both Euler solvers become smoothed at 2000 meters, that is, each peak value becomes lower and the loading time interval in the positive pressure region of each profile is extended longer comparing with the ALE solver. It may be caused by the accumulation of numerical diffusion and the mesh size dependency of the Euler solver. In the case of ALE solver, the cell size in the vicinity of the peak of the blast wave is effectively finer than the initial one, because it becomes small depending on its compression. The numerical diffusion generated by the ALE solver is very trivial because it is not necessary to calculate the advection term between neighboring cells. Hence, the pressure profile of the ALE solver becomes hardly smoothed even at relatively distance from the explosion point. The profiles in other cases of tonne order fuel has a similar tendency to this case. On the other hand, it is found that a finer mesh size of the Euler solver suppresses the reduction of the peak overpressure at relatively long distances from the explosion point.

Figure 4 shows pressure contours obtained by the numerical simulation for the down-scaled explosion experiment of 5.8 grams of the methane-oxygen mixture gas. The maximum and minimum values of the color contour scale in Figs. 4 (a), (b) and (c) are not fixed. In Fig. 4 (a), we can observe two spherical blast waves: the primary wave propagating directly from the explosion point; the reflected wave from the ground. These waves interacts each other to generate the Mach stem propagating along the ground surface. The reflection pattern is called as Mach reflection. It can be observed in the pressure contours that the propagating blast wave along the ground has a positive pressure region and the following slight

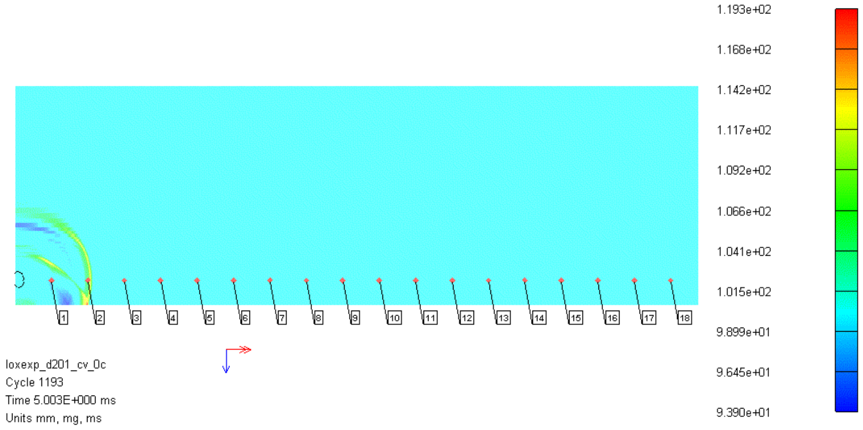


(a) 100 meters (b) 2000 meters

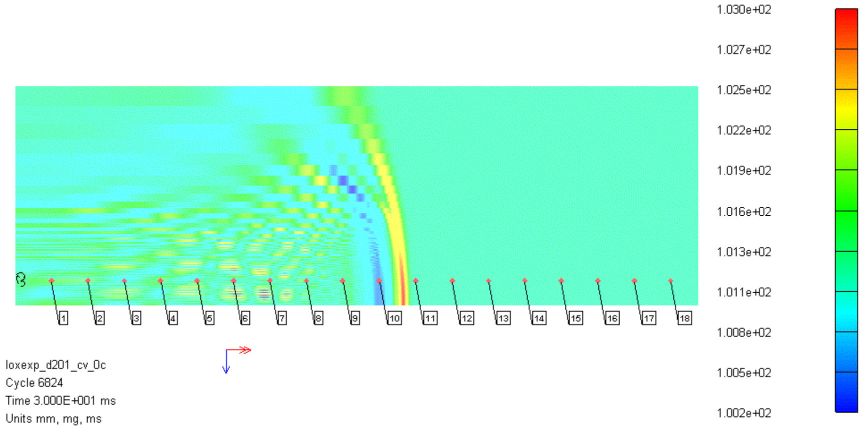
Figure 3 Overpressure histories at 100 and 2000 meters from the explosion point in the case of 13 tonnes of the methane-oxygen mixture gas

negative pressure region under the atmospheric pressure. We can also observe that weak disturbances are generated from the upper boundary and spread over the whole numerical region. However, as the waves can not clearly catch up with the blast wave propagating along the ground, it is out of interest.

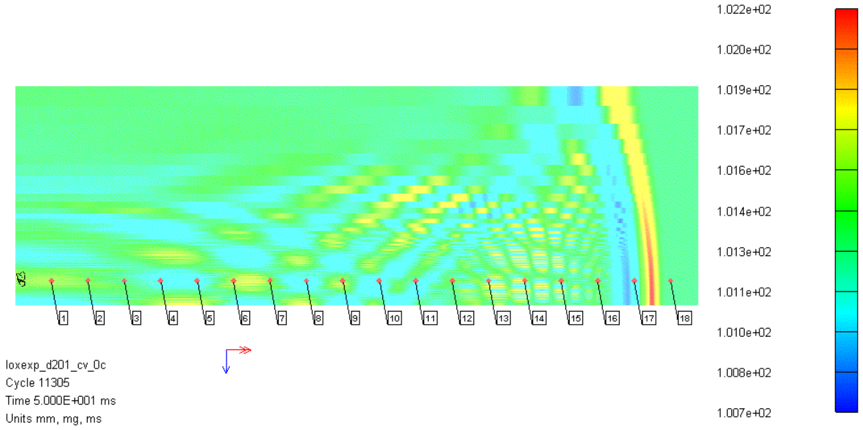
Figure 5 shows comparisons of numerical and experimental overpressure histories at 2, 5, 10 and 18 meters from the explosion point in the case of 5.8 grams of the methane-oxygen mixture gas. There is the time difference of the blast wave arrival between numerical and experimental results. The reason may be that the combustion speed is much slower in the experiment than that of the assumption in the



(a) 5 milliseconds

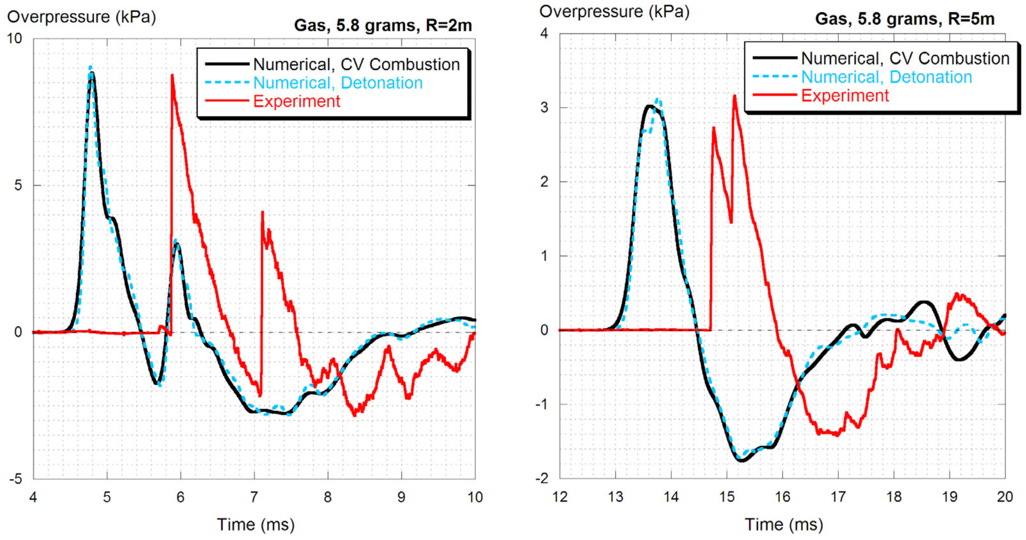


(b) 30 milliseconds

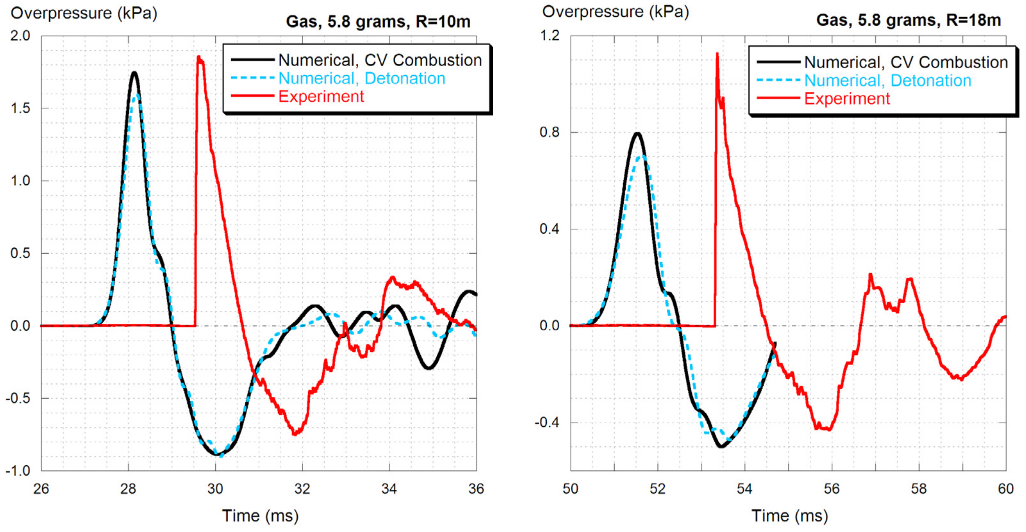


(c) 50 milliseconds

Figure 4 Pressure contours obtained by the numerical simulation for the down-scaled explosion experiment of 5.8 grams of the methane-oxygen mixture gas. The maximum and minimum values of the color contour scale in these figures are not fixed.



(a) 2 meters (b) 5 meters



(c) 10 meters (d) 18 meters

Figure 5 Comparisons of numerical and experimental overpressure histories at 2, 5, 10 and 18 meters from the explosion point in the case of 5.8 grams of the methane-oxygen mixture gas

numerical simulation because the deflagration of the mixture gas was deflagrated in practice. Numerical pressure profiles in the cases of the constant volume combustion and the detonation are almost identical. Therefore, the blast wave properties at relatively long distances may be independent of the ignition conditions of the mixture gas. In Fig. 5 (a), we can find two pressure peaks of the primary wave and the reflected wave from the ground surface. The two waves gradually approached each other as shown in Fig. 5 (b) and then overlapped as shown in Fig. 5 (c). In comparison of the numerical and experimental pressure profiles, numerical one becomes gradually smoothed down with the distance becoming longer in the same manner of the tonne order of explosions.

3.3 Relationship between blast wave properties and distance

Figures 6 and 7 show the relationships between the scaled peak overpressures and impulses and the scaled distances. The solid and dotted lines indicate the experimental and numerical results, respectively. The experimental results not only of 5.8 grams but also of 21 grams of the mixture gas were plotted.

In Figs. 6 and 7, the curves in each case of tonne order mixture gas and liquid are almost identical, respectively. The values of the scaled peak overpressure and impulse are around 40 to 50 percent higher at any distances in the liquid cases than in the gaseous cases. At more than 8 of the scaled distance, the scaled peak overpressure decreases severely and the scaled impulse increases suddenly because of the smoothness of the pressure profile as discussed in the overpressure histories. The real distances corresponding to the effective scaled distance of 8 are approximately 600 and 1000 meters in the cases of 17 or 5 tonnes, respectively. In principle, it is desirable that only blast wave properties up to the effective scaled distance are used for the sake of safety evaluations. If the properties over the effective scaled distance are unavoidably required, it should be re-evaluated by using the correction factors taken account of smoothness of pressure profiles.

The curves in the cases of the experiments and its simulation increase around 2 to 5 of scaled distances respectively. The reason is that the reflected wave from the ground overlaps the primary wave as seen in Fig. 4. We regarded the curves in a part after the increase as the experimental result of the ground explosion and compared with numerical result in the cases of 5.8 grams mixture gas. Numerical scaled peak overpressure was evaluated to be approximately 70 percent of the experimental value at around 20 of the scaled distance. On the contrary, numerical scaled impulse was approximately 115 percent of the experimental value at the scaled distance. These differences are clearly due to the smoothness of pressure profiles at relatively long distances as shown in Fig. 5 (d).

We compare the curves in the cases of tonne order explosion with those in the cases of gram order in a part after the increase. The curves of the scaled peak overpressure in the cases of tonne order are lower than those in the cases of gram order over around 10 of the scaled distance. These were dramatically affected by the smoothness of pressure profiles due to mesh size dependency as well as by the shock wave reflection pattern from the ground surface. We should examine more carefully the validity of the scaling law for mixture gas explosions with respect to scaled peak overpressure. On the other hand, the curves of the scaled impulse in the cases of tonne order has the identical slope to that in the cases of gram order over around 4 of the scaled distance. Hence, these curves qualitatively agree well. This means that the amount of impulse of the blast wave does not change very much even if the pressure profile becomes slightly smoothed. We demonstrated the validity of the scaling law for mixture gas explosions with respect to scaled peak impulse.

The discussion above would be valid only in the situation that a blast wave propagates in a windless and static state. The peak overpressure at approximately 1 kilometer from the explosion point will be practically attenuated to be no more than the order of the sound pressure of approximately 1 kPa. Then, such a weak pressure wave can be hardly distinguished from various disturbances caused by practical winds and weather conditions. Moreover it is significantly affected by the ground geometry and ground surface condition such vegetation. Therefore, it should be discussed on the other study.

4. CONCLUSION

We conducted numerical simulations of a large-scale accidental explosion of two huge quantities of LOX/LNG fuel and obtained blast wave properties at more than 1 kilometer from the explosion point. Peak overpressures and impulses obtained by numerical simulations and practical down-scaled experiments were summarized by using the scaling law for explosions. Then, the relationships between scaled blast wave properties and scaled distance were obtained. The blast wave influence is approximately 50 percent higher at any distances in the liquid cases than in the gaseous cases. Concerning tonne and gram order mixture gas explosions, the scaled peak overpressures in the cases of tonne order were evaluated to be lower than those in the cases of gram order. The validity of the scaling law for explosions with respect to scaled peak impulse was demonstrated. This indicates that the numerical predictions can successfully give quantitative evaluations of the blast wave influences. This methodology would be useful for definitions of adequate safety area in case of large-scale accidental explosion.

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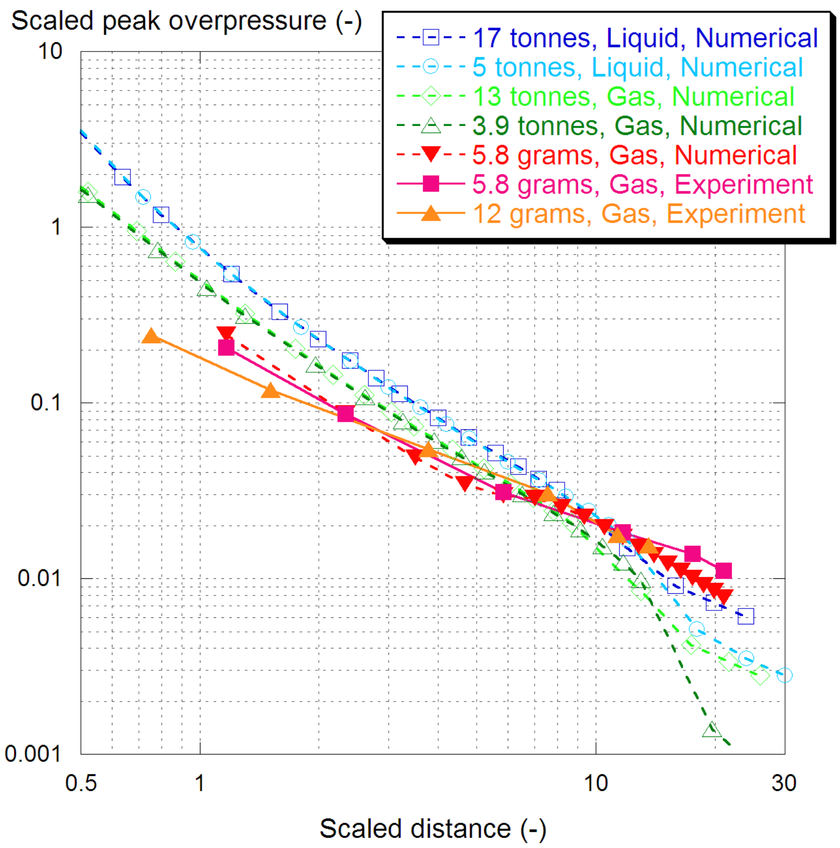

Figure 6 Relationship between the scaled peak overpressure and the scaled distance.

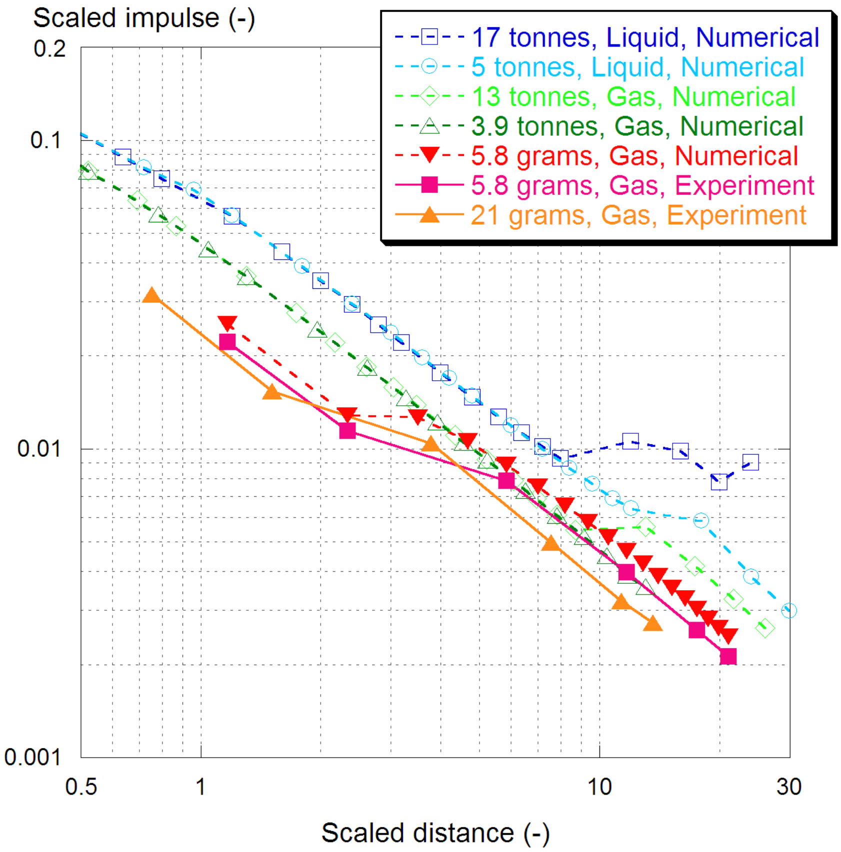

Figure 7 Relationship between the scaled impulse and the scaled distance.