PREDICTING COALESCENCE OF BLAST WAVES *
FROM SEQUENTIALLY EXPLODING AMMUNITION STACKS

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ABSTRACT

The current requirement that quantity-distance computations for air blast limitations be based on the total weight of all mass-detonating explosives at a storage site may be excessively restrictive. Therefore, a computer program called BWACO, which is intended to estimate pertinent aspects of the blast environment associated with sequentiality detonating. spatially distributed ammunition stacks, was developed. This paper explains the assumptions used and documents the evolution of BWACO on the Cray following its initial implementation. Comparison of preliminary results with experimental data obtained by Zaker led to replacement of the standard initially used for the description of blast waves with a new standard based on experimental data. Application to a number of problems representative of typical ammunition storage configurations are detailed. The results indicated that regions of significant pressure associated with the coalescence of blast waves from distributed ammunition stacks may be less extensive than corresponding regions associated with the blast wave produced by a single stack having the combined weight of the distributed stacks. An advantage associated with the distribution of ammunition into smaller subdivisions was also demonstrated. BWACO has been adapted for the personal computer with enhanced graphical representations. As currently configured, BWACO provides a means of assessing the blast environment associated with the sequential detonation of an arbitrary arrangement of ammunition stacks. The limitations imposed by the assumptions have not been assessed in realistic configurations.

BACKGROUND

Army Regulation 38544 requires that quantity-distance computations for air blast limitations be based on the total weight of all mass-detonating explosives at a storage site unless it can be shown that barriers between storage subdivisions (ammunition stacks) prevent propagation of detonation between them.[1] This requirement is made under the assumption that the blast waves emanating from the stacks as they sequentially detonate will coalesce with one another before their arnplitudes become negligible. The regulation provides a crude criterion, based on initiation delay, for determining when such coalescence will occur for the explosion of any two closely spaced stacks. This criterion has not been verified for complicated ammunition storage arrangements and may be overly restrictive, particularly where significant spatial separation of stacks exists.

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Experience with the quantity-distance requirements has shown that they are often difficult to meet, and waivers have been issued. Significant advantage might result if the actual coalescence pattern from a complex array of ammunition stacks could be estimated. In principle, this could be accomplished by numerical simulation of the blast environment in the region of interest. However, this approach requires immense computer resources, even for the simplest arrangements, and is beyond the reach of the typical user. Alternatively, applicable resources based on simplified analyses have been developed in the nuclear blast community.

APPROACH

Algorithms found in the DNA Nuclear Blast Standard[2] (1 KT)a computer program which describes the blast environment produced by a 1-KT nuclear explosion and the Low Altitude Multiple Burst (LAMB) models computer program which describes the blast environment produced by multiple nuclear explosions of arbitrary yield—are applicable.

We originally intended to adapt these to our present purposes. However, direct use of the LAMB program required the performance of many unnecessary, time-consuming computations. Therefore, we developed a new application called BWACO, intended to estimate pertinent aspects of the blast environment associated with sequentially detonating, spatially distributed ammunition stacks.

In its initial implementation, BWACO made significant use of 1-KT Standard and LAMB algorithms. However, as we investigated the performance of the code, these were gradually abandoned in favor of new algorithms. The main development effort was conducted using ARL's Cray X(MP 48 because graphics were readily available. However, once a Fortran-callable graphics package was obtained, the code was converted for use on the IBM Personal Computer (PC) or compatible machines.

This paper explains the assumptions used and documents the evolution of BWACO on the Cray following its initial implementation. Application to a number of problems representative of typical ammunition storage configurations are detailed and examples showing features added in the PC version are given.

BWACO ASSUMPTIONS

Sequential detonations are assumed to occur as a result of propagation of detonation from one stack to another. The first stack of any such pair to detonate is called the donor and the second is called the acceptor. The first of all the stacks to detonate is referred to as the initial donor. Detonation propagation is assumed to occur at a velocity which is a property of the donor. This is consistent with a fragment impact mechanism at least over distances short enough to preclude significant deceleration of the fragments. It may be consistent with other mechanisms as well. In the case of fragment impact, the velocity used should be that of the fastest fragment produced by munitions in the stack augmented to account for focussing effects.

Classical blast wave structure is assumed. The blast wave consists of a shock wave and positive overpressure phase followed by a negative overpressure phase (when sufficiently far from the source). The usual scaling laws are assumed to apply and are used to determine required blast wave characteristics with reference to a standard. BWACO requires shock and zero-overpressure arrival times at specified stations. The 1-KT Standard gives the shock and zero-overpressure radii as functions of time based on fits to analytical solutions. These functions may be inverted using Newton's method to obtain the arrival times. We developed alternative fits to experimental data for a somewhat different standard which provides the shock arrival time and positive phase duration as functions of position. These can be used directly to compute shock and zero-overpressure arrival times.

The ground plane is assumed to be perfectly flat and rigid and to effectively double the explosive weight of a stack Waves from multiple sources are assumed to propagate independently from one another and coalescence is assumed to occur wherever and whenever the shock associated with one blast wave encroaches into the positive overpressure phase associated with another blast wave.

Under these assumptions, regardless of the spatial and temporal separation between the sources, at sufficiently large distances from the charges, coalescence will be predicted. Blast waves from actual detonating stack arrangements do not exhibit this property because they do not propagate independently. Rather, some of them propagate in air processed by their predecessors. An overtaking wave may first encounter the negative overpressure phase of the wave being overtaken causing it to decelerate. The overtaking wave must be somewhat stronger than the wave being overtaken or it will not be able to penetrate the negative overpressure phase and coalescence cannot occur. Once this phase has been penetrated and the overtaking wave has entered the positive phase of the wave being overtaken, coalescence is assured but occurs only after some additional propagation. For these reasons, the BWACO coalescence algorithm can be expected to predict coalescence where, in actuality, it does not occur. This provides a margin of safety.

We considered several methods of combining peak overpressures from coalesced waves. These include simple superposition, the full LAMB algorithm, or use of the pressure produced by the total explosive weight associated with the coalesced waves combined at their center of charge.

USING BWACO

In order to run BWACO, the user supplies a description of the distributed ammunition stacks (position and equivalent explosive weight) and, if desired, of the region of interest. If no region is specified, BWACO selects a region limited to the area in which the total equivalent weight of the explosive in all the stacks produces peak blast overpressures above the inhabited-building limit, unless similar considerations for the individual stacks dictate a larger region. The program divides the region into discrete stations. It is recognized that, generally, any stack may act as the initial donor and it is necessary to determine the worst-case loading (highest combined peak overpressure) at each station considering all initial donors. For each initial donor, BWACO determines the timing of detonation of each of the other stacks. It then applies the coalescence criterion and computes both the total equivalent weight of the explosive in the stacks contributing to the blast and the peak overpressure at each station. It retains the values associated with the highest peak overpressure for any initial donor. The results are reported in graphical form.

User specifications are supplied by means of an appropriately formatted input file. Each ammunition stack is defined by specifying its coordinates in a user-defined Cartesian system, its net equivalent explosive weight, a propagation velocity for communication of mass detonation to neighboring stacks, and whether or not the stack may act as an initial donor. Any convenient Cartesian coordinate system may be used with distances specified in meters. The explosive weight for the TNT equivalent, in pounds, of all the explosive in the stack is required, as is the propagation velocity in m's. Usually, in order to allow determination of the worst-case blast loading, all of the stacks should be allowed to act as initial donors. However, this input option provides the flexibility required to address special problems such as those with known donors. The extent of the region of interest is specified using the same coordinate system defined for the stacks or, if unspecified, computed using maximum permissible overpressure conditions. The program then positions 3,600 stations within the region.

BWACO cycles through all possible initial donors as specified by the user. For each initial donor, using the given propagation velocities, it computes the times at which the other stacks detonate. It applies the coalescence criterion and, if necessary, combines the peak overpressures at each station.

BWACO provides different graphical representations of the results depending on the version used. The coalescence map is a plot showing areas of coalescence within the region of interest and indicating, in the Cray version, the number of waves which have coalesced or, in the PC version, the total equivalent explosive weight contributing to the blast. The peak overpressure map, available only in the PC version, is a contour plot showing the worst-case peak overpressure from the blast in the region of interest. The contour intervals correspond to the permissible exposure levels defined in AR 38564.

EVOLUTION OF THE BWACO MODEL

REVIEW OF EXPERIMENTAL RESULTS

In 1969, Zaker reported results of an extensive analytical and experimental study of the coalescence of blast waves produced by pairs of sequentially detonating Composition C-4 charges having a total weight of two pounds. In the analysis, the charges were assumed to be located at the same point, while in the experiments they were separated by ten inches and a steel barrier to prevent sympathetic detonation. Pressure was measured along a lateral line equidistant from the charges and along an axial line. The analysis was assumed to be applicable to the experiments along the lateral line. The axial values measured depend on the separation between the charges and are affected by the presence of the barrier while the lateral values are approximately independent of the separation and are predicted by the analysis.

Zaker considered charge weight ratios for successively detonated charges of 1:2, 1:1 and 2:1 and nominal initiation delay times ranging from 0.8 to 5.7 ms corresponding to 0.60 to 4.11 ms/lb$^{1/3}$ using conventional blast scaling. From this it can be inferred that an equivalent TNT weight of about 2.62 pounds was used in the scaling. The blast environment was monitored using pressure gauges on the axis of charge centers and in the lateral direction perpendicular to this axis at the center of charge to a distance of approximately 58 feet (42 ft/lb$^{1/3}$). This distance is a little shorter than that at which the overpressure from the combined charges decays to about 0.9 psi, which represents the smallest permissible exposure level (which applies to inhabited buildings) defined in AR 385-64.

Pressure records showing the coalescence process were presented by Zaker. These indicate that substantial propagation, covering most of the field of observation, may occur as coalescence progresses. He observed that the peak overpressures associated with coalesced waves were essentially the same as those produced by single charges of the same total explosive weight.

For two charges of equal mass, Zaker found that a "tendency" to coalescence in the lateral direction occurs for delays of less than 4.3 ms (3.2 ms/lb$^{1/3}$). The term "tendency' was not clearly defined but it may be assumed to mean observation of decreasing intervals between wave peaks with increasing distance from the charge center. This is actually very similar to the BWACO criterion. He observed a tendency to coalescence in the axial direction with all of the delays considered (up to 5.7 ms or 4.1 ms/lb$^{1/3}$). By comparing lateral and axial data, he estimated that the effect of the charge separation and the barrier on the interval between peaks in the axial direction is equivalent to an additional delay of 1.8 ms (1.3 ms/lb$^{1/3}$). Thus, axial coalescence may be assumed to occur for delays less than 6.1 ms (4.5 ms/lb$^{1/3}$). This result may include significant effects of the barrier.

For charges of unequal mass, Zaker observed that coalescence persists at longer delays with a weight ratio of 1:2 and vanishes at shorter delays with a weight ratio of 2:1 compared to equal charges. (Thus, the criterion given in AR 385-64 uses more conservative values of 4.0 and 5.6 ms/lb$^{1/3}$ respectively.) Zaker also performed some experiments with three equal charges. He observed that the third pulse tends to overtake the second before the second overtakes the first.

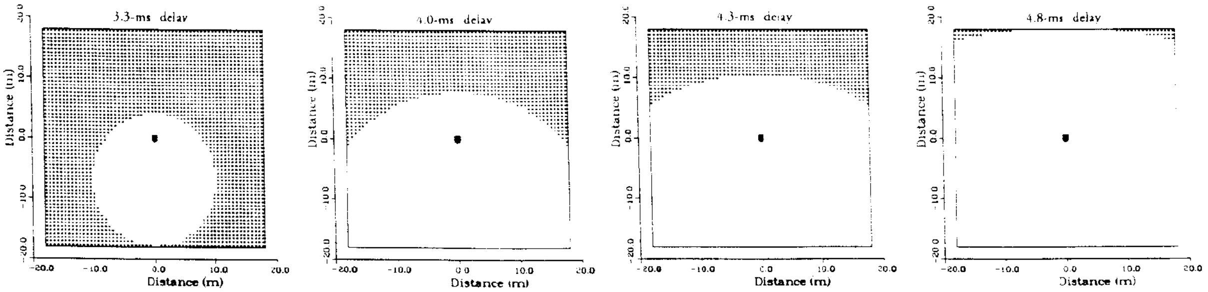
SIMULATION OF THE EXPERIMENTS USING THE 1-KT STANDARD

In order to simulate Zaker's equal-charge experiments, we made BWACO computations for two 1.31-lb stacks separated by 0.254 m, specifying only one possible initial donor. Specific delay times were obtained using appropriate values of the propagation velocity. The region of interest was specified as extending to 18.0 m from the center of charge in each direction, corresponding to the region of experimental observation. The delay times associated with the vanishing of coalescence at the edges of the region may be compared with experimental values.

Coalescence maps for various delay times are plotted in Figure 1. Regions of coalescence are shaded with dots. For delays less than 3.3 ms, coalescence within the region of interest is predicted in all directions. For delays greater than 4.0 ms coalescence in the lateral direction vanishes. Thus, with a delay of 4.3 ms (Zaker's limit for lateral coalescence), coalescence in the lateral direction is not predicted. Coalescence in the axial direction persists until the delay exceeds 4.7 ms. This may be compared to Zaker's value of 6.1 ms. The difference between the delays for which coalescence vanishes in the axial and radial directions respectively is only 0.7 ms, which is much less than Zaker's value of 1.8 ms.

In each direction, vanishing of coalescence is predicted at shorter delays than observed in or estimated from the Zaker experiments. The discrepancy is most significant in the axial direction. This result contradicts our expectations for the bias in BWACO's coalescence algorithm and is unacceptable. It suggests that the 1-KT Standard is inaccurate.

Figure 1.
Coalescence Maps for Zaker Experiment Simulations Using the 1 -KT Standard.



ALTERNATIVES TO THE 1-KT STANDARD FITS

Kingery has reported air blast parameters, including shock arrival time, positive phase duration and peak overpressure, versus distance for large-scale hemispherical TNT surface bursts. This data provides a basis for evaluating the applicability of the 1-KT Standard. Comparison with the 1-KT Standard is shown in Figure 2. There is close agreement for the shock arrival time except in a tiny region very near the source. Comparison with the 1-KT Standard positive phase duration shows that the values from the standard are generally too short at distances of interest. This would tend to suppress the prediction of coalescence, as we observed. Comparison with the 1-KT Standard peak overpressure and Zaker's small-scale results indicates that the 1 -KT Standard pressures are generally lower than the measured values.

Alternative fits which give shock arrival time and positive phase duration as functions of distance were developed. These retain the appropriate asymptotic behavior at large distances from the source. The fit for shock arrival time is of the form

EQUATION

$$t_a = a_a\left[r - b_a \tanh\left(\frac{r}{r_a}\right)\right],$$

where a_a, b_a and r_a are constants.

The fit for positive phase duration is of the form

EQUATION

$$\Delta t_+ = a_+\left(1 - \frac{b_+}{r^{c_+}}\right)\left[\ln\left(r^2 + r_+^2\right)\right]^{1/2},$$

where a_+, b_+, c_+ and r_+ are constants.

This fit is not used for very small values of r, for which the value of the positive phase duration is frozen. Kingery (1964) provided a fit for peak overpressure. These fits are also plotted in Figure 2 and provide improved agreement with measurements in each case.

Figure 2. Comparison of the 1-KT Standard with the Alternate Standard.

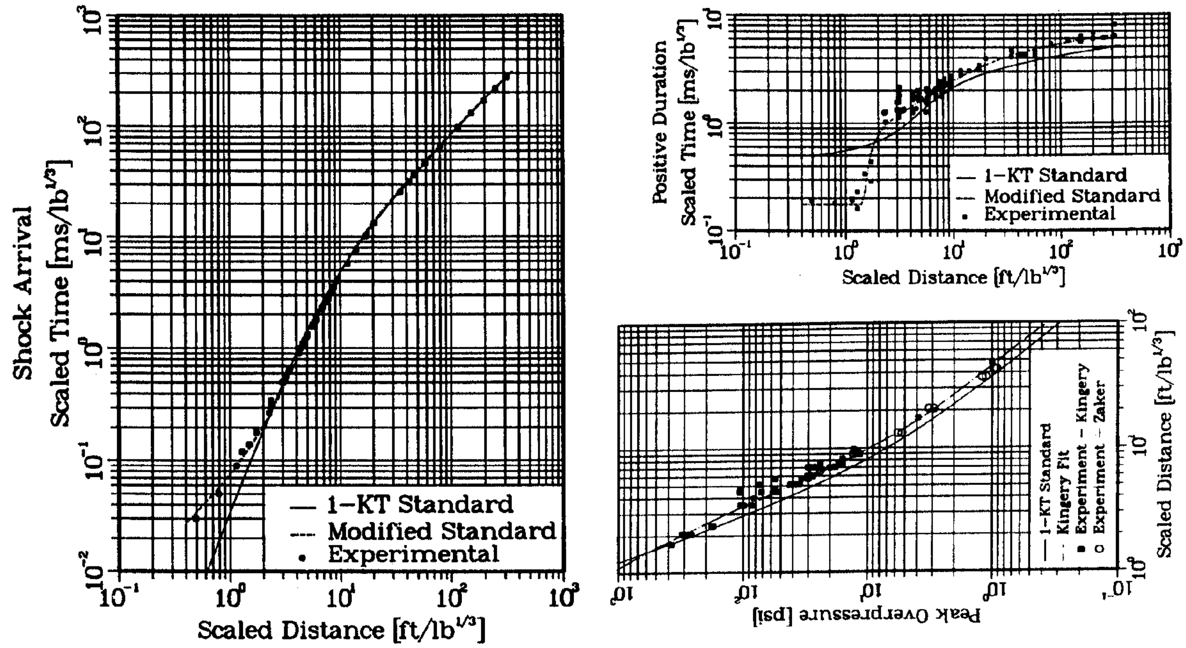


Figure 2. Comparison of the 1-KT Standard with the Alternate Standard.

Figure 3. Coalescence Maps for Zaker Experiment Simulations Using the Alternate Standard.

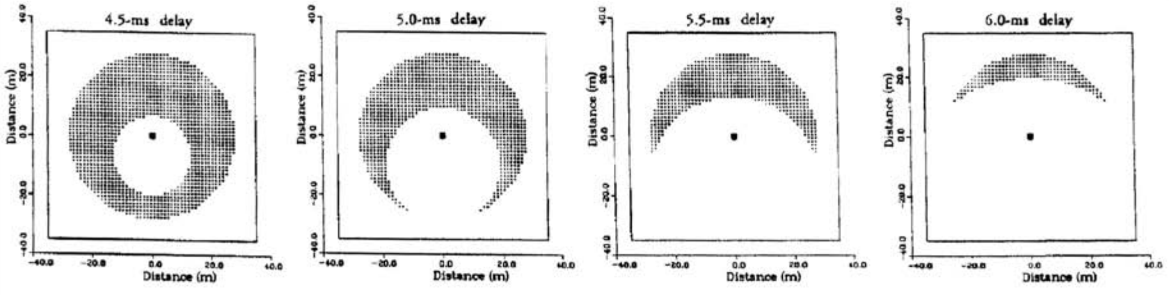


Figure 3. Coalescence Maps for Zaker Experiment Simulations Using the Alternate Standard.

SIMULATION OF THE EXPERIMENTS USING THE ALTERNATE STANDARD

Coalescence maps obtained using the alternate standard are shown in Figure 3. BWACO was configured to suppress identification of coalescence in the far field where the combined peak overpressure is below the maximum permissible exposure level for inhabited buildings. It appears that the pressures combined using simple superposition are somewhat high, as the extent of the region of significant pressure is considerably greater than that associated with a single charge of the same total weight (as used in Figure 1). As a result of the expanded extent, coalescence is observed at somewhat longer delays than those associated with the experimental region of significant pressure specified in the earlier computations.

EFFECT OF PRESSURE COMBINATION ALGORITHMS

In order to assess the effect of the pressure combination algorithms on the extent of the region of significant pressure. We made computations with from two to ten stacks, located at the same point, with the same total equivalent explosive weight (2.62 lb). The ratio of the radius of the region of significant pressure produced by the detonation of n stacks to that produced by the detonation of one stack is plotted as a function of n in Figure 4. Contrary to Zaker's observation, this shows substantial increase in the extent of the region of significant pressure with increasing number of stacks even though the total explosive weight remains constant.

The results obtained with the LAMB algorithm (also shown in Figure 4) are virtually identical to those obtained using simple superposition. The LAMB algorithm has been shown to produce correct results for the head-on collision of two equal blast waves and overestimates the pressure in other cases (Hikida and Needham, Brode). In the case of overtaking waves the magnitude of the overestimate appears significant.

As an alternative, we computed the combined pressure by first combining the stacks which produce the coalesced wave into a single stack positioned at the center of charge. This approach, suggested by Zaker's observation, is applicable where the angles between coalescing waves are small, as occurs at any point whose distance from the stacks significantly exceeds the distance between stacks. It automatically produces regions of significant overpressure which do not increase with the number of stacks. This is also shown in Figure 4.

SIMULATION OF THE EXPERIMENTS USING THE ALTERNATE STANDARD AND PRESSURE COMBINATION ALGORITHM

The way in which the alternate pressure combination algorithm modifies the results obtained with two equal charges is shown in Figure 5. As expected, the region of significant pressure is reduced in comparison to that shown in Figure 3. The delays at which coalescence vanishes are slightly increased compared with those associated with the analysis shown in Figure 3 because the region of significant pressure is larger than the region of experimental observation. Lateral coalescence vanishes for delays exceeding about 5.3 ms, which is significantly greater than Zaker's observation of 4.3 ms. In the axial direction coalescence vanishes for delays of 6.1 ms or greater, agreeing with Zaker's estimate of 6.1 ms. There is no significant change in the difference between the axial and radial values. It is still less than half that determined by Zaker. The remaining discrepancies between the BWACO predictions and the Zaker experiments may be due to contributions of the barrier to delaying coalescence in the axial direction. The predictions obtained with the alternate standard and pressure combination algorithm do not miss regions of coalescence and are acceptable.

Figure 4. Comparison of the Effects of the Pressure Combination Algorithm on the Region of Significant Pressure as a Function of the Number of Charges

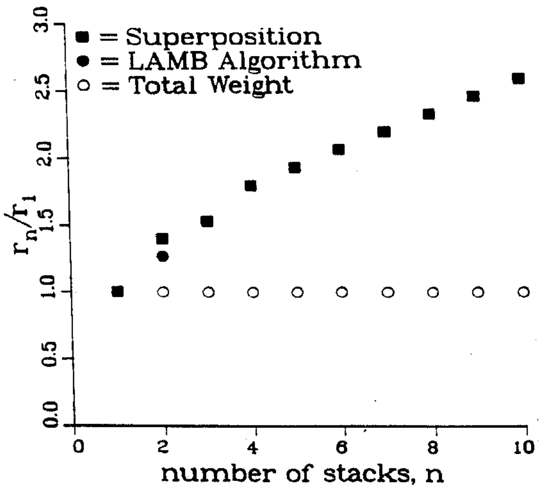


Figure 4. Comparison of the Effects of the Pressure Combination Algorithm on the Region of Significant Pressure as a Function of the Number of Charges

Figure 5. Coalescence Maps for Zaker Experiment Simulations Using the Alternate Standard and Pressure Combination Algorithm.

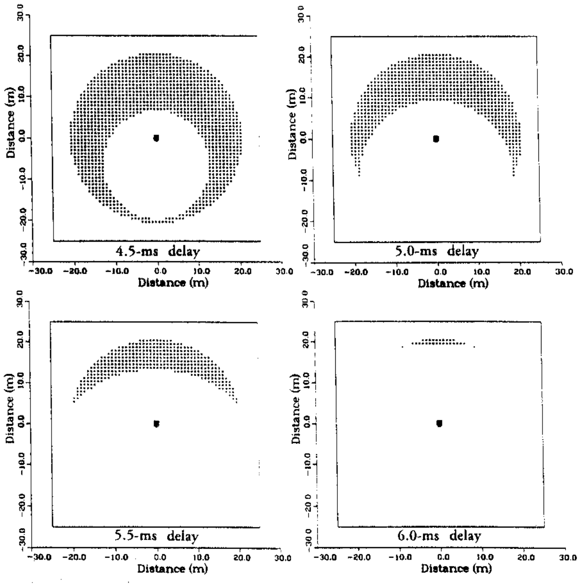


Figure 5. Coalescence Maps for Zaker Experiment Simulations Using the Alternate Standard and Pressure Combination Algorithm.

We also made computations with unequal charges in ratios of 1:2 and 2:1 with a constant total equivalent weight of 2.62 pounds. Figure 6 compares results from each of these cases with the equal-charge case at two different delays. This shows that the persistence of coalescence decreases as the ratio of the donor weight to the acceptor weight increases. The result is consistent with Zaker's observations.

Figure 7 shows coalescence maps obtained in a simulation of Zaker's three-charge experiment. The size of each shading dot is proportional to the number of waves coalesced at the corresponding station. However, it cannot be ascertained which waves have coalesced. For short delays, coalescence of all three waves is predicted in all directions, although two-wave coalescence occurs first. As the delay is increased, three-wave coalescence begins to vanish, starting in the negative axial direction. Two-wave coalescence persists for longer delays. The results are consistent with Zaker's observation that the third pulse tends to overtake the second before the second overtakes the first. The region over which significant pressures are predicted is larger than for two charges of the same total weight.

SIMULATIONS OF REPRESENTATIVE LARGE-SCALE CONFIGURATIONS

In the large-scale scenarios that BWACO is intended to treat, initiation delay is dependent on the separation between stacks. The simulations described in the following paragraphs were intended to illustrate the effects of the separation between stacks and the distribution of explosive weight among stacks when all stacks act as initial donors. They were made using a total equivalent weight of 100,000 pounds distributed over two or more stacks. The velocity of propagation between stacks was fixed at 2,500 m's. As an added feature, the region of significant pressure produced by a single 100,000-pound stack is outlined as a broken circle in the coalescence maps. This is the region that must be considered under present regulations. The results may be interpreted by comparing the extent of the region of significant pressure predicted by BWACO with the circle.

Figure 6. Coalescence Maps for Zaker Experiment Simulations with Weight Ratios of 1:2,1:1 and 2:1.

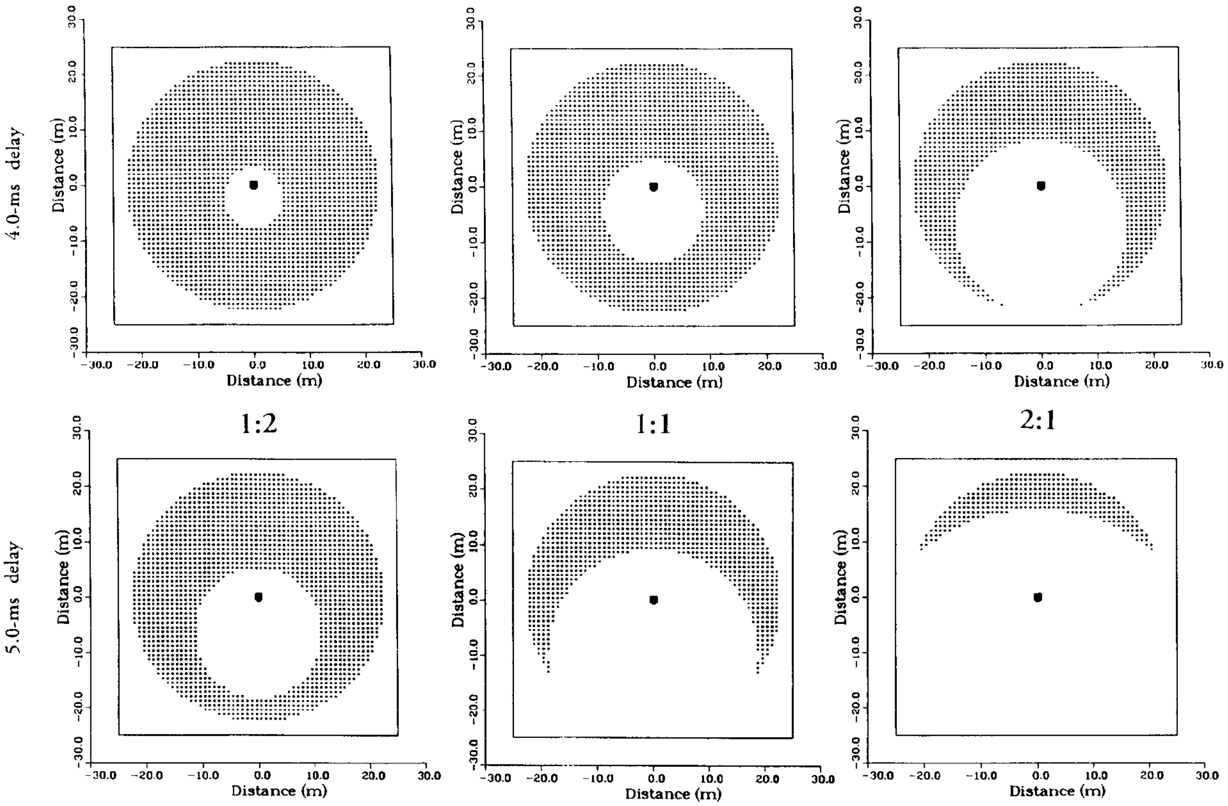


Figure 6. Coalescence Maps for Zaker Experiment Simulations with Weight Ratios of 1:2, 1:1 and 2:1.

Figure 7.
Coalescence Maps for Zaker Three-Charge Experiment Simulations.

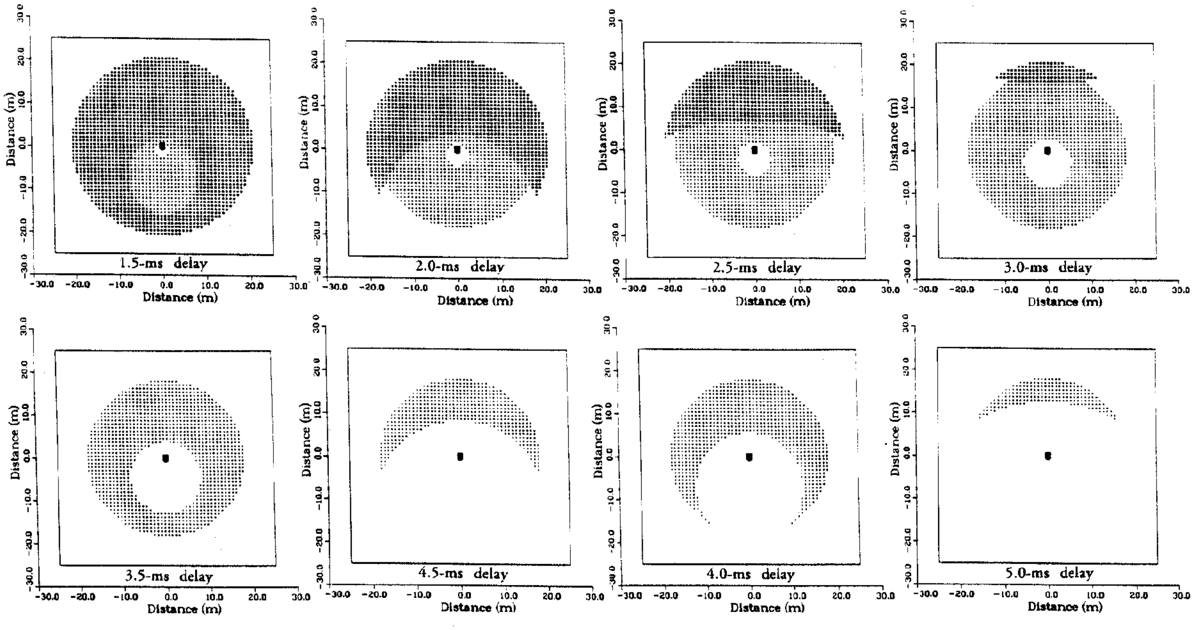


Figure 7. Coalescence Maps for Zaker Three-Charge Experiment Simulations.

Figure 8.
Coalescence Maps for Large-Scale Simulations of Two 50,000-lb Stacks.

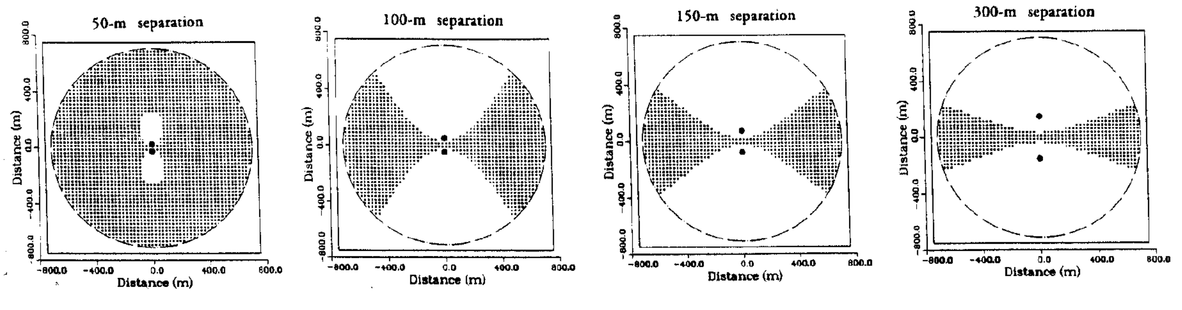


Figure 8. Coalescence Maps for Large-Scale Simulations of Two 50,000-lb Stacks.

Figure 9. Coalescence Maps for Large-Scale Simulations of Two Unequal Stacks with a 100,000-lb Total Weight.

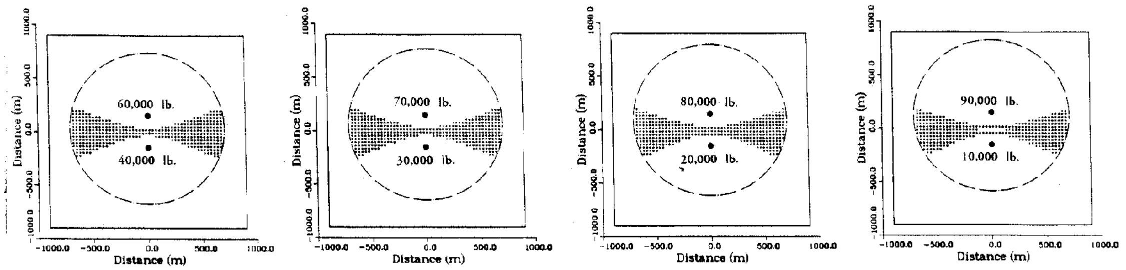


Figure 9. Coalescence Maps for Large-Scale Simulations of Two Unequal Stacks with a 100,000-lb Total Weight.

Results obtained with two stacks of 50,000 pounds each are shown in Figure 8. As the separation is increased, significant regions in which coalescence does not occur appear within the single-stack circle. In these regions, requiring consideration of the blast produced by the total explosive weight of both stacks is clearly too restrictive. At the larger separation distances, regions of coalescence persist only near the horizontal symmetry axis. Here, consideration of the total weight is necessary. The extents of these regions change little for separations greater than 200 m. We also simulated the effects of varying the distribution of explosive weight between two stacks separated by 300 m. The results, shown in Figure 9, indicate very little change in the coalescence region along the horizontal axis as the weight is redistributed.

The results observed with four 25,000-pound stacks are similar to those seen with two 50,000 pound stacks. They are shown in Figure 10. Coalescence of waves from all four stacks and from three of the four stacks is only exhibited at the 50-m separation distance. At the 100-m separation, only two-stack coalescence results. As the separation is further increased, this coalescence becomes limited to the vicinity of the vertical and horizontal symmetry axes. Again, the extent of these regions increase little for separations greater than 200 m. At the largest separation, the region of significant pressure extends somewhat beyond the single-stack circle. Thus, consideration of the total weight may be insufficient when the separation is large even though coalescence emanates from only two of the stacks.

The effect of the number of stacks was also investigated. If each stack in the four-stack arrangement is divided into four equal stacks which are positioned such that their center of charge lies at the position of the original stack while retaining a uniform separation, an arrangement of 16 stacks with half the original separation results. The coalescence maps produced are shown in Figure 11. Each map is comparable to the corresponding map in Figure 10. A significant advantage to smaller subdivisions is indicated.

Figure 10.
Coalescence Maps for Large-Scale Simulations of Four 25,000-lb Stacks.

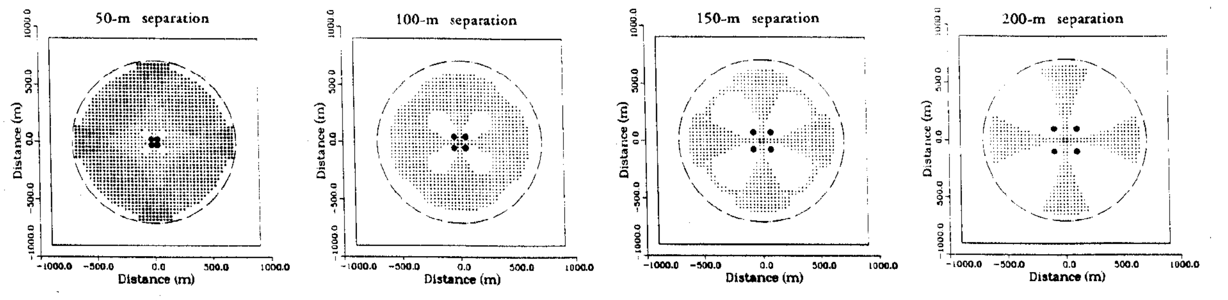


Figure 10. Coalescence Maps for Large-Scale Simulations of Four 25,000-lb Stacks.

Figure 11.
Coalescence Maps for Large-Scale Simulations of Sixteen 6,250-lb Stacks.

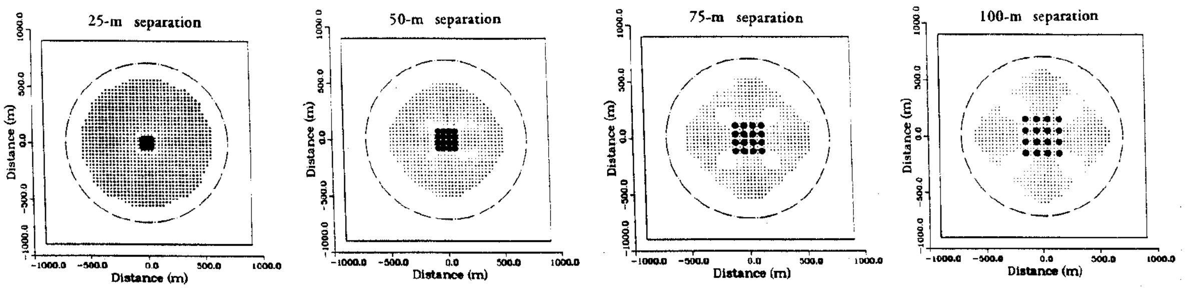


Figure 11. Coalescence Maps for Large-Scale Simulations of Sixteen 6,250-lb Stacks.

PERSONAL COMPUTER VERSION GRAPHICS

When BWACO was adapted for use on the personal computer, the coalescence map was enhanced with the addition of contours of the total explosive weight associated with the coalesced waves and a capability for producing peak overpressure contour plots was added. Examples of these maps for three previously considered problems with 200-m separation distances are shown in Figure 12. The maps may be obtained either on the PC display or in hard-copy form.

Regions in which coalescence is detected are hatched in the coalescence map. Each contour is labeled to indicate the total explosive weight contributing to the worst-case blast environment within that contour. The outermost contour line follows the 0.9 psi overpressure limit for inhabited buildings.

In the peak overpressure map, contours are labeled to indicate the worst-case peak overpressure at each point within the region of interest. The contour levels are those specified in AR 385-64.

SUMMARY AND CONCLUSIONS

In this paper, we have explained the assumptions underlying the BWACO algorithms, documented the evolution of BWACO based on comparisons with available experimental data, and demonstrated the application of BWACO to typical large-scale ammunition storage configurations.

Assumptions were made in order to determine the order and timing of the detonation of the stacks following the detonation of any initial donor stack, to establish a criterion for detecting coalescence, and to determine the combined pressure associated with a number of coalesced waves at a point.

Figure 12.
Coalescence and Peak Overpressure Maps from the PC Version of BWACO.

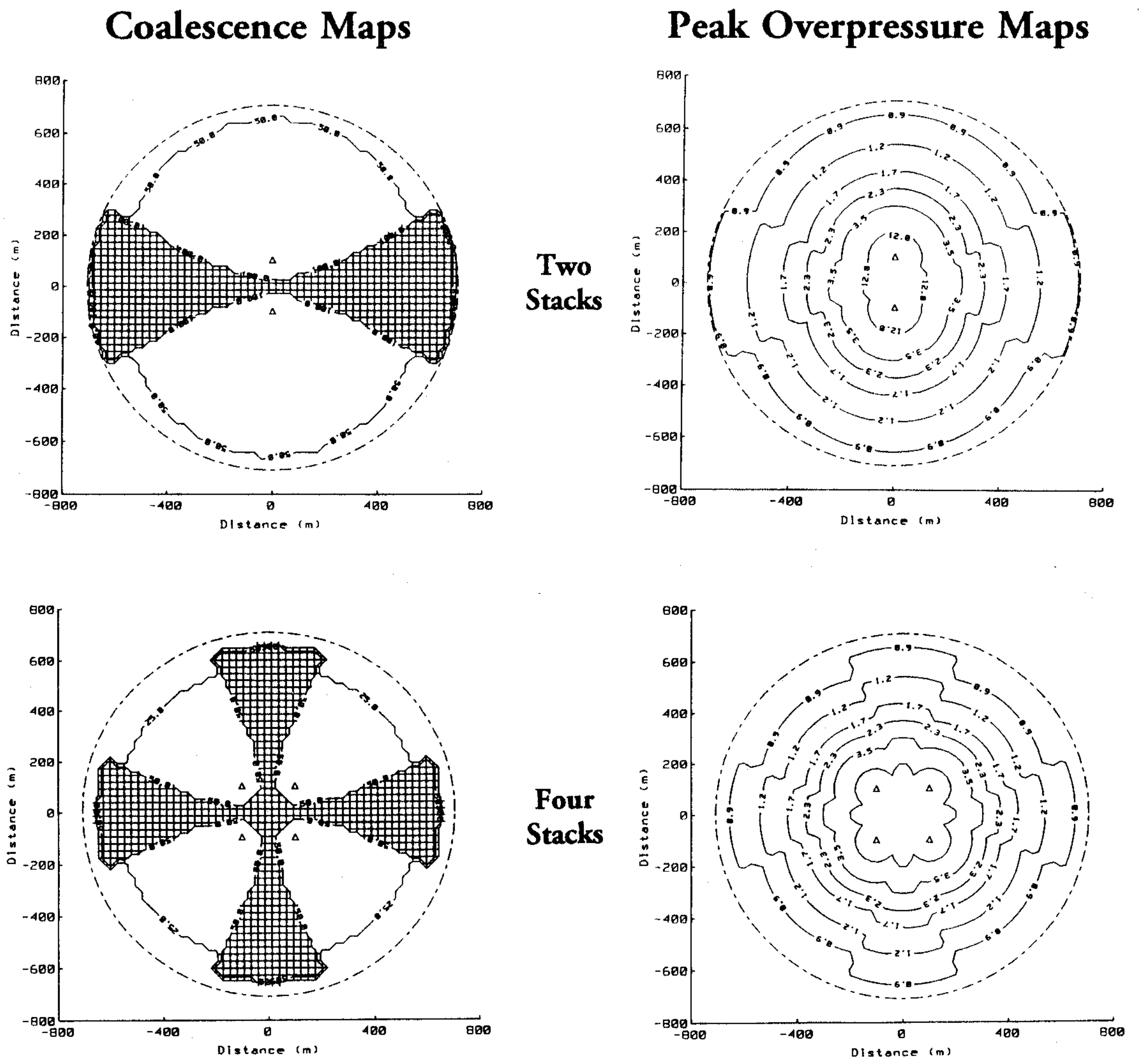


Figure 12. Coalescence and Peak Overpressure Maps from the PC Version of BWACO.

Comparison of preliminary results with experimental data obtained by Zaker led to replacement of the standards initially used for the description of blast waves. Use of the 1-KT Standard was found to produce predictions which tended to miss detection of coalescence where the experiments showed that coalescence occurred. It was replaced with a standard based on experimental data reported by Kingery.

Application to a number of problems representative of typical ammunition storage configurations were detailed. The results indicated that regions of significant pressure associated with the coalescence of blast waves from distributed ammunition stacks may be less extensive than corresponding regions associated with the blast wave produced by a single stack having the combined weight of the distributed stacks. An advantage associated with the distribution of ammunition into smaller subdivisions was also demonstrated.

BWACO has been adapted for the personal computer with enhanced graphical representations. As currently configured, BWACO provides a means of assessing the blast environment associated with the sequential detonation of an arbitrary arrangement of ammunition stacks. The limitations imposed by the assumptions have not been assessed in realistic configurations.

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