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Research article

A practical method for predicting and analyzing the consequences of ammonium nitrate explosion accidents adjacent to densely populated areas

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ABSTRACT

Several catastrophic ammonium nitrate (AN) explosion accidents have been reported during the last decades. Previous studies have been mainly focused on investigating adverse effects caused by the AN explosion, while only a few systematically analyzed the consequences and impacts of AN explosions. This study collects data from three typical AN explosions (accidental explosion of the US fertilizer plant in 2013; an accidental explosion of China's Tianjin port in 2015, and a recent explosion (2020) of the Beirut port in Lebanon). The consequences of accidental explosions were analyzed by mathematical equations that further provide scientific explanations for AN explosions. Based on the explosives' properties on-site, these accidental explosions were caused by condensed phase explosives. Comparison with the conditions at the explosion site indicated that blast overpressure was the primary factor in the loss of life and damage to the building, while ground shock was a secondary factor. The severity of loss of life and building damage from explosions decreased with increasing distance. These distances could be calculated by the scaling law, which was replaced by the equivalent TNT mass of the explosive and the damage scale's overpressure boundary value. In addition, mapping the damaged area on a map helped in the visual presentation of the consequence assessment. The long-term environmental and ecological impact due to the explosions was also an important issue that could not be ignored. Overall, this study establishes a simple and easy-to-use method to rapidly predict and assess the consequences of an explosion, and provides technical guidance for future emergency response to similar large-scale accidents.

1. Introduction

Ammonium nitrate (AN) [CAS 6484-52-2], also known as NH_4NO_3, is a colourless, odourless, clear crystal or white crystal and is widely used as an agricultural and industrial chemical. Because of its high nitrogen content, high fertilizer efficiency, and low production cost, it is commonly used as a high-quality agricultural fertilizer in agricultural production [1,2]. Although AN is a stable compound at room temperature, it readily decomposes at high temperatures (>210 °C) and produces toxic gases such as nitrates, nitrites, ammonia (NH_3), nitrogen oxides (NO_x), in addition to pure oxygen (O_2) that may ignite and explode [3]. In addition, it is also used as an oxidizing agent and can be detonated under certain conditions including, but not limited to, elevated temperatures, the

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Table 1
Incidents involving AN storage or transport facilities, not including incidents involving ANFO, nor ones with involvement of explosives other than AN.

Date	Location of incident	Incident	Fire	Explosion
April-1920	Barksdale, WI	Warehouse fire with barrels of AN	Yes	No
14-April-1920	Brooklyn NY	Steamer Hall fried, poss. due to contamination	Yes	No
21-September-1921	Oppau, Germany	an explosion involving 450 tons of AN based fertilizer occurred when workers tried to disaggregate caked fertilizer mixture with industrial explosives.	Yes	Yes
4-April-1925	Muscle Shoals, AL	Rail cars with barrels of AN, poss. due to wood material of barrels	Yes	No
3-May-1925	Muscle Shoals, AL	Rail cars with barrels of AN, poss. due to wood material of barrels	Yes	No
April-1940	Gibbstown, NJ	Fire destroyed a large quantity of bagged and drummed AN, no explosion. Fire was at a manufacturing establishment, but in the warehouse, not production.	Yes	No
16-April-1947	Texas City, TX, USA	S.S. Grandcamp was in port and its cargo of AN ignited. This ignited neighboring buildings and also the ship S.S. High Flyer. Both ships detonated, but some AN warehouses on shore only burned.	Yes	Yes
28-July-1947	Brest, France	S.S. Ocean Liberty carrying AN detonated after a fire in the cargo hold	Yes	Yes
1947	USA	Truck fire due to cellulosic rope contacting AN cargo; cargo was hot	Yes	No
14-October-1949	Independence, KS	Fire in Air Force warehouse involved AN, but no explosion	Yes	No
23-January-1953	Red Sea	S.S. Tirrenia. Fire in AN, followed by explosion. Poss. role of paper goods next to AN in hold.	Yes	Yes
1957	USA	Truck suffered collision, fire ignited gasoline, ignited AN which exploded	Yes	Yes
1958	USA	Truck fire burned AN, no explosion	Yes	No
1959	USA	Rail car fire ignited AN, but was extinguished	Yes	No
10-May-1960	Boron, CA	Fire in warehouse of AN, but no explosion	Yes	No
17-December-1960	Traskwood, AR, USA	Rail car derailed, bagged AN ignited due to mixing with other chemicals, detonated	Yes	Yes
February-1963	Traskwood, AR, USA	Rail car derailed, AN burned, but no explosion	Yes	No
9-November-1966	Mount Vernon, MO	A fire started in an production facility, but the detonation was due to fire engulfing a 50 T pile bags of AN in their storage area	Yes	Yes
24-November-1966	Peytona, WV	Fire was in an explosives factory, and fire impinged on AN stored in a truck trailer and a rail car, no explosion	Yes	No
24-October-1967	Potosi, WI	Rail car with bagged AN ignited, no explosion	Yes	No
30-August-1972	Taroom, Australia	Truck carrying LD AN ignited, burned, detonated	Yes	Yes
1972	UK	Truck with bagged AN ignited, poss. due to contamination	Yes	No
17-January-1973	Pryor Creek, OK	Fire in Cherokee Ammonia manufacturing plant, but stored AN caught fire and fire was not in production machinery. Major detonation due to fire.	Yes	Yes
1976	France	Truck with bagged AN ignited, fire extinguished	Yes	No
1977	USA	Rail car derailed, causing ignition of AN	Yes	No
1978	Rocky Mountain, NC	Warehouse fire, stored AN burned up completely but no explosion	Yes	No
1979	Australia	Bagged AN ignited in truck	Yes	No
1981	Australia	Bagged AN ignited in truck	Yes	No
1982	Australia	Bagged AN ignited in truck	Yes	No
October-1982	UK	AN storage ignited and led to major fire; explosions occurred, but deflagration and not detonation.	Yes	No
1984	Australia	Fire in engine of truck ignited bagged AN	Yes	No
1989	France	Truck carrying AN ignited, extinguished	Yes	No
1991	France	Truck carrying AN ignited, extinguished	Yes	No
1991	Australia	Fire in truck carrying AN due to collision	Yes	No
1991	UK	Small fire in truck carrying AN	Yes	No
April-1992	UK	Fire in warehouse storing AN, no detonation	Yes	No
1993	Australia	Fire in truck carrying bagged AN, cargo burned up	Yes	No
19-December-1994	Port Neal, IA, USA	The explosion was initiated by “an accelerated thermal decomposition reaction as ‘a direct result of unsafe operating procedures and conditions’ at the plant”.	Yes	Yes
March-1997	Spain	Fire in drums involving AN; appears minor	Yes	No
July-1997	Brazil	Fire and collision of trucks carrying AN and gasoline; LD AN ignited and detonated	Yes	Yes
4-January-1998	Maysville, OH	Fire in Cargill Farm Service Center, involved AN. Probably electrical fire in nature. Propane tanks exploded, but AN did not.	Yes	No
28-June-2000	Duette, FL	Fire and collision of trucks carrying AN and gasoline	Yes	No
21-September-2001	Toulouse, France	AN contamination with chloride was determined to be the root cause of this incident.	Yes	Yes
February-2003	USA	Warehouse fire storing AN	Yes	No
2003	USA	AN fire in a farm supply store, poss. minor	Yes	No
2-October-2003	Saint-Romain-en-Jarez, France	AN fire in a small agricultural storage facility leading to a detonation	Yes	Yes
October-2003	UK	Fire involving AN in a small farm store	Yes	No
18-February-2004	Neyshabur, Iran	Major train derailment, caused a fire to ignite; AN burned and exploded	Yes	Yes
9-March-2004	Barracas, Spain	Truck collision, leading to fire and AN detonation	Yes	Yes

(*continued on next page*)

Table 1 (*continued*)

Date	Location of incident	Incident	Fire	Explosion
22-April-2004	Ryongchon, North Korea	Train carrying AN collided with truck carrying oil; resulted in fire and explosion	Yes	Yes
24-May-2004	Mihăileşti, Romania	Truck carrying bagged AN overturned, fire resulted, then detonation	Yes	Yes
August-2004	USA	Fire in a dry bulk blending and distribution center that held AN	Yes	No
June-2006	France	Fire on a truck hauling bagged AN; extinguished by fire service	Yes	No
22-September-2006	Suisun City, CA	Fire involved E.B. Stone & Son facility as an exposure from a grass fire	Yes	No
6-March-2007	Pernik, Bulgaria	Truck carrying AN caught fire and exploded	Yes	Yes
30-July-2009	Bryan, TX, USA	Fire at El Dorado Chemical Co. started by welder in warehouse, burned down warehouse	Yes	No
8-August-2009	Mt. Isa, Australia	Truck carrying AN caught fire	Yes	No
21-January-2012	Mariveles, Philippines	Fire destroyed an warehouse at a shipyard	Yes	No
17-April-2013	West, TX, USA	The subject fire	Yes	Yes
29-May-2014	Athens, TX, USA	Fire at East Texas Ag Supply warehouse involving AN; no detonation, building burned up	Yes	No
5-September-2014	Charleville, Australia	A double-trailer truck carrying 52 tonnes of AN overturned, ignited, and exploded	Yes	Yes
12-August-2015	Tianjin, China	Due to the loss of wetting agent, the nitrocellulose appears locally dry, accelerating decomposition and exotherm under high temperature and other factors, accumulating heat and spontaneous combustion, resulting in the explosion of AN.	Yes	Yes
4-August-2020	Beirut, Lebanese	Welding sparks ignited the warehouse explosives, which in turn led to the explosion of ammonium nitrate in another warehouse.	Yes	Yes

presence of impurities and containment [4,5]. Thereby, the main hazards associated with AN are classified as explosion, fire and self-sustained decomposition [6,7]. Based on the properties, it is also used as explosive and even terrorist use, usually mixed with fuel, known as AN fuel oil (ANFO) [8].

The most catastrophic explosions in history have often been associated with industrial accidents [9]. Even more unfortunately, chemical explosions can occur at all stages of the supply chain worldwide, from the production of materials to their transportation and storage. The storage of large quantities of hazardous chemicals in urban areas inevitably increases the safety risks in the immediate area. Urban warehouses and storage facilities for dangerous cargoes are characterized by their large number, wide distribution and high risk. These factors lead to increasing safety risks in operations and furthermore to a high incidence of safety management accidents. However, this is indeed the case. Over the past 100 years, there have been several severe AN explosions in warehouses adjacent to densely populated urban areas. The risk of AN explosions exists at all stages in both developed and developing countries. Most accidents occurred in transportation (33%) and storage (29%), with the latter accidents more likely to have serious consequences [10]. The accidents listed in Table 1 involve a variety of circumstances, locations, and storage or transportation methods [11–13]. But they share one basic characteristic: 100% of the explosions were caused by uncontrollable fires. Whether the source of the fire is in a warehouse, truck, railcar or ship, there will be no explosion and no loss of life unless the fire breaks out and is not contained [13].

The destructive effects accompanying a chemical explosion include mainly air-blast shock waves and ground shock [14,15]. When an explosive occurs, a high-temperature and high-pressure gas is formed that instantly occupies the original space. This cloud of gas violently pushes against the surrounding stationary air while generating a series of compression waves that propagate in all directions, with the individual compression waves eventually superimposing to form a shock wave. Shock wave effects are primarily based on overpressure compression and dynamic pressure impacts, causing internal or external injuries, fractures, concussions and other injuries through crushing and throwing. In addition, when the explosion occurs on the ground, the blast energy propagates directly through the ground, introducing both directly induced and crater-induced ground motions [15]. Ground shock further exacerbates the loosening of the building, thus potentially causing secondary injuries to the populations.

Scientists have been engaged in research to establish methods for predicting and analyzing the consequences of explosions, but most of these studies have focused on the military field, with fewer civilian applications. One of the more common methods is to use the equivalence factor for trinitrotoluene (TNT) to describe the explosive force of an explosive. Another common approach to calculating the explosive force is not to distinguish between types of explosion, but to base it on an analytical assessment of the consequences of the explosion, which is then compared with the consequences of a TNT explosion [16], such as seismic wave data extrapolation [17], explosion formation crater characterization [18] and building damage estimation [19,20]. However, these methods often involve relatively complex formulae calculations, limiting their application and the need for rapid assessment in the field of sudden-onset accidents. The aim of our study is to infer blast power from traceable features developed in three typical AN explosions and to validate the assessment of the consequences of the accident, thereby establishing a simple and easy-to-use rapid prediction and assessment method with a view to providing the corresponding technical support for future emergency response to similar large-scale accidents. Meanwhile, through these three AN explosion accidents, we extract lessons from them to prevent the recurrence of similar accidents in the future.

2. Three typical an explosion accidents

2.1. *The explosion of the West fertilizer plant in the USA*

On April 17, 2013, AN explosion occurred in chemical storage and distribution facility in West, Texas, USA. The center of the explosion generated 28.3 m wide and 3 m deep crater. The explosion destroyed a middle school, nursing home, numerous residences, and businesses. Fifty structures were significantly damaged, while 100 structures were slightly damaged. In addition, an apartment complex was destroyed [21]. Debris was found up to 2.5 miles from the plant. Fifteen people died, and 228 people were recovered to the hospital, among whom 46 were admitted. Fifteen people were killed, among whom ten were firefighters, two were civilians who tried to extinguish the fire, and three were civilians who lived in a close-by residential area [21]. West fertilizer claimed to have in storage 540,000 pounds of AN, 110,000 pounds of anhydrous ammonia, 540 pounds of Grazonnext (herbicide), 60 pounds of Reclaim (herbicide), 192 pounds of Remedy Ultra (herbicide), 29.75 pounds of Surmount (herbicide), and 400 pounds of Yuma (insecticide) [21]. The investigations suggested that the explosion at the West fertilizer plant was triggered by an intense fire caused by 30 tonnes of AN in wooden crates, but no conclusions were provided as to the ignition source or what other factors played a role in the explosion [22].

2.2. *The explosion of the Tianjin port in China*

On August 12, 2015, an explosion occurred at a container terminal in Tianjin Binhai New Area [23,24]. The explosion was caused by flammable and explosive materials inside the container. At the explosion scene, there was a mushroom cloud tens of meters high, accompanied by projective combustion. The center of the explosion generated a very large crater-like hole with a width of 97 m and 2.7 m deep. One hundred sixty-five people were killed (including 24 firefighters in active service, 75 firefighters in Tianjin port, 11 police officers, 55 employees, and residents of enterprises where the accident happened and surrounding enterprises), 8 people were gone missing (including 5 firefighters in Tianjin, 3 employees of surrounding enterprises and family members of firefighters in Tianjin Port), 798 people were injured (58 seriously injured and 740 slightly injured), 304 buildings, 12428 commercial vehicles and 7533 containers were damaged [23,24]. According to reports, 72 kinds of dangerous goods (4840.42 tons) were stored on-site, including 800 tons of AN, 360 tons of sodium cyanide, 48.17 tons of nitrocellulose, nitrocellulose solution, and nitro lacquer [23,24]. The high summer temperatures led to the spontaneous combustion of the highly flammable nitrocellulose. This led to the explosion of approximately 800 tonnes of AN stored near the port of Tianjin [25].

2.3. *The explosion of the Beirut port in Lebanon*

On the afternoon of August 4, 2020, a huge explosion occurred in the port area of the Lebanese capital, Beirut, forming a bucket-shaped crater with a diameter of about 140 m. In addition to the large crater on the ground, the explosion produced a huge cloud of orange-red smoke and dust surrounded by a white mushroom cloud. At the origin of the explosion epicenter, most of the buildings within 2 km were destroyed. The sound and shock waves were felt in Cyprus, 180 km away. Two explosions, which occurred in the early evening on Aug 4, after a warehouse caught fire on Beirut's northern industrial waterfront, resulted from the detonation of 2750 tons of AN that has been improperly stored for six years. At least 220 people were killed, and more than 12,000 were injured of which 8643 were registered in emergency rooms and 1056 were admitted to the hospital [9]. The explosion left 300000 people homeless and caused up to $15 billion in damage. Also, 50000 houses, 9 large hospitals, and 178 schools were damaged [26]. Due to the strength of the blast, the explosion was considered as one of the largest recorded in modern history [27]. The investigation revealed gross negligence in the management of warehouse 12 at the port of Beirut, as it contained a large quantity of fireworks and firecrackers in addition to the 2750 tonnes of ammonium nitrate in which the explosion occurred.

3. Accident analysis

3.1. *Explanation of an explosive phenomenon*

Pure AN is relatively stable at room temperature. Yet, when exposed to high temperature, high pressure, oxidizing substances and electric spark, it can explode. Three AN explosions mentioned above confirmed that uncontrolled fires were the leading root cause for the majority of AN detonation incidents. At the theoretical level, AN undergoes the following changes when exposed to heat. The chemical equations are as follows:

$$\text{At } 110\ ^{\circ}\text{C} : NH_4NO_3 = NH_3 + HNO_3 \tag{1}$$

$$\text{At } 185\ ^{\circ}\text{C}\sim_{200}\ ^{\circ}\text{C} : NH_4NO_3 = N_2O + 2H_2O \tag{2}$$

$$\text{Above}^{\circ}\text{C} : 2NH_4NO_3 = 2N_2 + O_2 + 4H_2O \tag{3}$$

$$400\ ^{\circ}\text{C} : 4NH_4NO_3 = 3N_2 + 2NO_2 + 8H_2O \tag{4}$$

Equations (1)–(4) show that AN has different decomposition products at different temperatures. The above reaction is basically the "ideal" explosive decomposition reaction of AN. At 300 °C, the decomposition of AN already has the characteristics of explosive decomposition. At the same time, AN explosion produces a large number of toxic gases, such as nitrogen dioxide, ammonia, nitric acid, etc. This indicates that the surrounding population should be evacuated in a timely manner as well as good personal protective measures.

According to the above Equation (4), AN decomposes and explodes when the temperature exceeds 400 °C. The explosion of 270 tons, 800 tons, and 2750 tons of AN produced about 121.6 tons, 360.2 tons and 1238.3 tons of water, 77.6 tons, 230.0 tons and 790.4 tons of nitrogen dioxide, and 70.9 tons, 210.0 tons and 721.8 tons of nitrogen, respectively. However, due to the complexity of the explosion reaction, the amount of these products generated may be stoichiometric, which will lead to some discrepancies with reality. Because the molecular weight of water is only 39.1% of nitrogen dioxide, water's kinetic energy is higher, and the propagation distance is farther. However, nitrogen dioxide has little kinetic energy and can only be lifted into the air under the pressure of an explosion's epicenter. This explains why a huge white gas wave was formed during explosions, following a reddish-brown cloud from the explosion center. The first huge white wave was actually a large amount of high-temperature and high-pressure steam produced by AN explosion. It has also been found that the explosion caused by solid or liquid explosives is a condensed phase explosion [28]. The condensed phase explosive process is usually initiated by thermal pulse, mechanical pulse, or direct action of detonator or booster. Detonation is usually caused by thermal pulses, after which it goes through an unstable combustion stage [28]. It was reported that there were many dangerous chemicals stored in the warehouse in three accidents. The thermal pulse generated by warehouse fire can provide continuous energy for all kinds of condensation hazardous chemicals, thus leading to the intense explosion of condensation explosives. Therefore, it is believed that the three explosions were caused by condensed phase explosives.

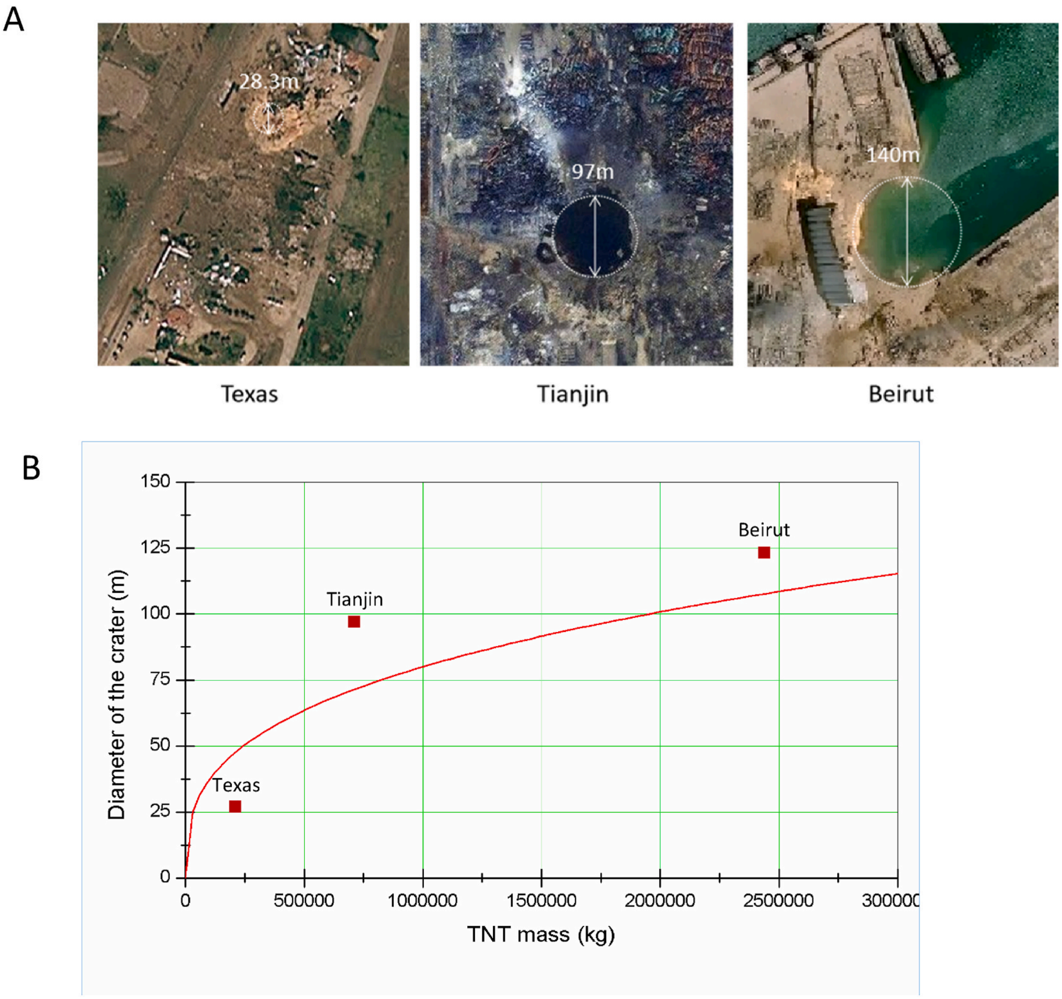

Fig. 1. Comparison between the predicted and actual value of crater diameter in three explosion accidents. (A) A map of the crater size of the actual explosion. The double-arrowhead line represented the crater diameter. **(B)** Prediction curve and actual value of crater diameter. The Black Square represents the actual crater value.

3.2. Analysis of crater diameter caused by an explosion

Based on TNT experiments and previous literature, Ambrosini et al. validated the empirical equation of Kinney and Graham that relates the diameter of the crater (D) to the TNT mass (Q_{TNT}) for an explosion at ground level and which is expressed below with mass in kg and distance in meters [21,29]. Following this correlation, we calculated the diameter of the crater caused by the explosion of TNT.

$$D = 0.8(Q_{TNT})^{\frac{1}{3}} \tag{5}$$

For other types of explosives, they are converted to TNT equivalent by similar energy. The conversion formula is the following.

$$Q = \frac{q_i}{q_{TNT}} Q_i \tag{6}$$

where Q is the TNT explosive equivalent, kg; Q_i is the explosive quantity of certain explosive, kg; q_i is the detonation heat of certain explosive, kJ/kg; q_{TNT} is the detonation heat of TNT explosive, kJ/kg.

The detonation heat released by 1 kg TNT explosive is 4230–4836 kJ/kg, and the average detonation heat is 4500 kJ/kg generally. AN is calculated with H_2O liquid as a reference, and the detonation heat of AN is 2479 kJ/kg [30].

Fig. 1 shows the theoretical and actual crater diameters calculated by using Equations (5) and (6) above for the three accidental explosions, respectively. As shown in Fig. 1A, the crater's diameter formed by the 270 ton AN explosion in the USA was 28.3 m, which is much smaller than the predicted diameter of 42.4 m (Fig. 1B). By comparison, 800 tons of AN explosion in China formed a crater with a diameter of 97 m (Fig. 1B), but the theoretical diameter calculated by the formula was 60.9 m (Fig. 1A), which was slightly smaller than the actual crater diameter. Similarly, the predicted value of a crater with a diameter of 91.9 m formed by the explosion of 2750 tons of AN in Lebanon was also smaller than the actual diameter of 140 m (Fig. 1). Bull and Woodford pointed out that the crater's deviation can reach 30–40% [31]. AN has an excellent crater effect, which may lead to underestimation of crater diameter based on TNT mass estimation. Moreover, the AN effectiveness reported in the literature varies from 0.25 or 0.3–0.55, to 0.84 [21,32]. Some studies suggested the use of 0.346 as a standard because it corresponds to the ratio of explosion heat of AN to that of TNT. Therefore, choosing a higher effective factor will make the quality assessment closer to the actual value. Combined with the prediction of crater diameter in these accidental explosions, we speculated that only when the AN mass reaches certain height, a better crater effect will appear, which may result in underestimation of the crater diameter. Based on the above results, we confirmed that the formula should be modified with reference to the empirical validity so as to better predict the actual diameter of the crater caused by an explosion.

3.3. Impact of shock wave overpressure on casualties

Understanding the common types of injuries associated with blasts is essential to developing an appropriate emergency response and treatment plan. AN explosion releases a large number of high-temperature and high-pressure explosion products, which impact the surrounding air at high speed and increase the pressure, density, and temperature, forming air-blast shock wave. According to the Chinese national standard “safety regulations for blasting” (GB6722-2014) [33], the shock wave overpressure is calculated according to the following formula under the condition of flat terrain.

$$\Delta p = 14\frac{Q}{R^3} + 4.3\frac{Q^{\frac{2}{3}}}{R^2} + 1.1\frac{Q^{\frac{1}{3}}}{R} \tag{7}$$

where ΔP is the shock wave overpressure, $\times 10^5$ Pa; R is the distance between protecting objects and blasting points, m; Q is the explosive quantity equivalent to TNT in one blasting, the total quantity is the simultaneous blasting, and the maximum quantity is the delayed blasting, kg. For other types of explosives, TNT equivalent can also be converted according to the above listed formula (6).

In Table 2, four levels of casualties caused by shock wave overpressure are defined: mild injury, moderate injury, severe injury, and extremely severe injury [34]. The shock wave overpressure values at different distances from the explosion epicenter can be obtained by formula calculation. Fig. 2A shows the overpressure variation trend with the distance of the explosion epicenter for 270 kg, 800 kg, and 2750 kg AN, respectively. It can be seen from the figure that there is a functional relationship between the shock wave overpressure and the charge amount, and the distance from the explosion epicenter. Higher explosive production generates a higher overpressure of the shock wave (Fig. 2A). As is generally accepted, the overpressure values of shock waves produced by different equivalent explosions decreased gradually with the increase of the distance from the epicenter; nevertheless, the overpressure values of

Table 2
Relationship between casualties and air-blast overpressure.

Overpressure (10^5Pa)	Injury level	Injury situation
0.2–0.3	Mild	Minor contusion
0.3–0.5	Moderate	Eardrum injury, moderate contusion, fracture, etc.
0.5–1.0	Severe	Severe internal bruising and even death
>1.0	Extremely severe	Death

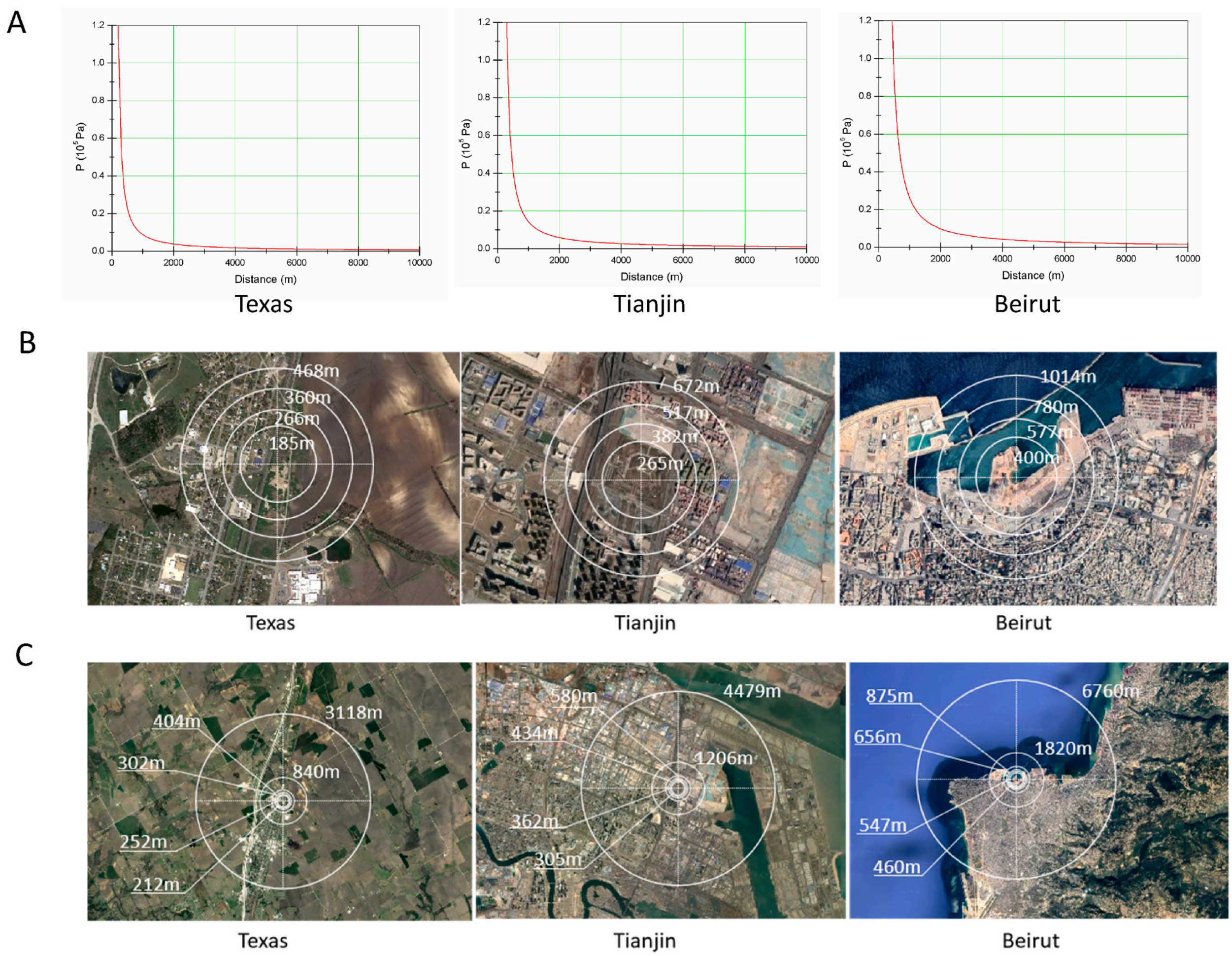

Fig. 2. The influence of different distances on the change of air-blast overpressure and the predicted damage scale zones of casualty and building damage induced by air-blast overpressure. (A) The curve of air-blast overpressure varying with the distance from the epicenter of the explosion. **(B)** The predicted damage scale zones of casualties caused by air-blast overpressure. **(C)** The predicted damage scale zones of buildings caused by air-blast overpressure. (map data © 2013 Google).

the shock waves were sharply reduced until a certain distance (about 1000 m) was reached (Fig. 2A). Therefore, the range and degree of casualties and building damage caused by shock wave overpressure could be calculated theoretically according to the variation of shock wave overpressure in different areas.

Fig. 2B showed the predicted zones of casualties caused by shock wave overpressure in the three explosions. The global positioning system (GPS) satellite images and aerial views were collected through an online search. By formula calculation, after the AN explosion, the shock wave overpressure zone of more than 1×10^5 Pa was formed at 185 m, 265 m, and 400 m away from the respective explosion epicenter (Fig. 2B). Referring to Table 2, the results showed that within 185 m, 265 m, and 400 m of respective explosion epicenter, high shock wave overpressure would cause death in these areas. Within 185–266 m, 265–382 m, and 400–577 m, the shock wave overpressure was $(0.5–1) \times 10^5$ Pa, which could cause severe internal bruising and even death. In addition, in the zones of 266–360 m, 382–517 m, and 577–780 m, the shock wave overpressure was $(0.3–0.5) \times 10^5$ Pa, which could lead to eardrum injury, moderate contusion, and fracture. However, in the zones of 360–468 m, 517–672 m, and 780–1014 m, the shock wave overpressure was reduced to $(0.2–0.3) \times 10^5$ Pa, which could only cause a slight contusion. Due to the lack of accurate information on casualties in three explosion accidents, this study could not accurately compare the theoretical prediction with the actual casualties. Still, the calculated zones of casualties were basically consistent with the media reports.

3.4. Impact of the shock wave overpressure on buildings

In Table 3, seven damage scales for the severity of the blast-induced damages for buildings are defined: Damage Scale 1 (DS1) almost no damage, Damage Scale 2 (DS2) minor damage, Damage Scale 3 (DS3) mild damage, Damage Scale 4 (DS4) moderate damage, Damage Scale 5 (DS5) severe secondary damage, Damage Scale 6 (DS6) severe damage, and Damage Scale 7 (DS7) complete

Table 3
Relationship between damage degree of buildings and air-blast overpressure.

Damage scale		DS1	DS2	DS3	DS4	DS5	DS6	DS7
		Almost no damage	Minor damage	Mild damage	Moderate damage	Secondary severe damage	Severe damage	Complete destruction
Overpressure (10^5 Pa)		<0.02	0.02–0.09	0.09–0.25	0.25–0.40	0.40–0.55	0.55–0.76	>0.76
Damage description	Glass	Accidently damaged	A small portion was broken chunks; most were small	Most pulverized to break into small pieces	Break up	–	–	–
	Wooden doors and windows	No damage	The window sash is slightly damaged	A large number of window sashes are damaged, and doors, windows, and window frames the destruction	The window sash fell or fell inside, and the window frame and door leaf were damaged.	Doors and window sashes are destroyed, and window frames fall	–	–
	Brick facade	No damage	No damage	There are small cracks, the width is less than 5 mm, and it is slightly inclined	Large cracks appear, the width of the joint is 5–50 mm, obviously inclined, small cracks appear in the brick stack	Large cracks larger than 50 mm appear, severely inclined, large cracks appear in the brick stack	Partially collapsed	Most to all collapsed
	Wooden roof	No damage	No damage	The wooden house panel is deformed, occasionally tearing apart	Wooden house roof panels and wooden purlins are demolished, and wooden roof trusses are loose	The wooden purlins are dismantled, the wooden roof truss members occasionally break, and the supports are misaligned	Partially collapsed	All collapsed
	Tile roof	No damage	A small amount of movement	Most appeared to move	A mass move to all tilt	–	–	–
	Steel reinforced concrete roof	No damage	No damage	No damage	Small cracks less than 1 mm appear	There are small cracks with a width of 1–2 mm, which can be used after repair	Cracks larger than 2 mm appear	The load-bearing brick walls all collapsed, and the steel-reinforced concrete load-bearing columns were destroyed
	Ceiling	No damage	A small amount of plaster falling	A large number of plaster falling	Wooden keel partially destroyed sagging seam	Collapse	–	–
	Inner wall	No damage	Plastering of slatted walls drops a little	Plastering of slatted walls fell heavily	Small cracks in the brick wall	Large cracks in the brick wall	Serious cracks in the internal brick wall to a partial collapse	Most of the brick wall collapsed
	Steel reinforced concrete column	No damage	No damage	No damage	No damage	No damage	Tilt	Large tilt

destruction [33]. Since DS1 and DS2 cause slight damage to buildings, Fig. 2C showed only the predictable zones of the other five damage scales (DS3-DS7). These distances represent the boundaries for the zones of the fiver damage scales. It can be seen from the figure that the shock wave overpressure was more than 0.76×10^5 Pa within the range of 212 m, 305 m, and 460 m away from the respective explosion epicenter; buildings within this range were expected to be completely damaged (DS7). In the range of 212–252 m, 305–362 m, and 460–547 m away from the respective explosion epicenter, the explosion overpressure was $(0.55–0.76) \times 10^5$ Pa, and the buildings in this area were seriously damaged (DS6) (Fig. 2C). In addition, buildings within 252–302 m, 362–434 m, and 547–656 m away from each explosion epicenter suffered serious secondary damage (DS5); buildings within 302–404 m, 434–580 m, and 656–875 m moderate damage (DS4), and buildings within 404–840 m, 580–1206 m and 875–1820 m a slight damage (DS3) (Fig. 2C). These results show that buildings within the three explosion epicenters of 840 m, 1206 m, and 1820 m were damaged in different degrees by the shock wave overpressure.

For the calculation of overpressure of blast air shock wave, the commonly used empirical formulas in the early stage are the national standard “safety regulations for blasting” (GB 6722-2014), Henrych formula, Sadovsky formula, and Brode’s formula [35]. Many scholars applied those formulas for calculation, but these empirical formulas were mainly based on the experimental data and theoretical analysis results. Because of the short history of the explosion, the accuracy of experimental results is often affected. With the rapid development of computer technology, numerical simulation methods have been developed for studying explosion effects in recent years. Many scholars have carried out a series of studies on shock wave overpressure by combining explosion tests with numerical simulation. This study collected and sorted out buildings’ actual damage through the Internet and literature reports and described the damage with different distances around the explosion epicenter (Tables 6–8). These tables provide the comprehensive damage conditions of the buildings in different damage scale zones. The actual damage, the damage degree, and scope caused by the three explosion accidents (USA, China, and Lebanon) were basically consistent with the theoretical prediction. The air blast shockwave from three explosion accidents did contribute to the structural damages of the buildings. Moreover, the predicted range of this formula was in good agreement with the actual damage observed in most buildings. For some buildings, such as building A5 and C2, the severity of the damage was more like the moderate damage scale (DS4). Nevertheless, these buildings were actually located in the DS3 (mild damage) zone (Tables 6 and 8), which was not consistent with the results. In addition, the damage to building B6 could be almost classified as no damage level (DS1) when the building is actually located in the DS2 (minor damage) zone (Table 7). These phenomena could not be explained by the air-blast incident overpressure.

3.5. Ground shock caused by an explosion

Although the seismic wave caused by the AN explosion can not destroy the original solid rock, it generates vibration or shaking of all objects on the ground near the explosion source. When the blasting vibration reaches a certain intensity, the buildings (structures) around the blasting area are damaged. According to the national standard “safety regulations for blasting” (GB6722-2014) [33], the safe permissible distance of blasting vibration can be calculated according to the following formula.

$$R = \left(\frac{K}{V}\right)^{\frac{1}{\alpha}} \cdot Q^{\frac{1}{3}} \tag{8}$$

The ground shock can be calculated according to the conversion formula below.

$$V = \frac{K}{\left(\frac{R}{Q^{\frac{1}{3}}}\right)^{\alpha}} \tag{9}$$

where V is the ground vibration peak particle velocity (PPV) at the location of the protected object, cm/S; R is the distance between the protected object and the blasting point, m; Q is the explosive quantity, the total quantity is for the simultaneous blasting, and the maximum quantity is for the delayed blasting, kg; K and α are the coefficients and attenuation indexes related to the terrain and geological conditions between the blasting point and the calculated protected object. It can be selected according to Table 4 [33] or determined by field test. Considering the geological and topographical conditions of the explosion site, we chose soft rock parameters, $K = 350$, and $\alpha = 1.8$.

The relationship between seismic intensity and vibration physical quantity is shown in Table 5 [36]. According to the calculation results of the relationship between PPVs and distances, combined with Table 5 and the Chinese Seismic Intensity Scale (GB/T17742-2020), and by taking class III buildings as an example (the explosion affecting civil buildings and the structure was Class III buildings), we calculated and analyzed the impact caused by ground shock. Fig. 3 shows that after 270 tons, 800 tons, and 2750 tons of AN explosion, within 160 m, 229 m, and 346 m from each explosion epicenter, respectively, the seismic intensity was more than 10°,

Table 4
K and ɑ values of different rock properties.

Rock properties	K	ɑ
Hard rock	50–150	1.3–1.5
Medium hard rock	150–250	1.5–1.8
Soft rock	250–350	1.8–2.0

Table 5
Relationship between seismic intensity and physical quantities of vibration.

Seismic intensity	Natural earthquake			Maximum vibration speed of blasting (cm/s)
	Acceleration (cm/s^2)	Speed (cm/s)	Displacement (mm)	
VII	50–100	4.1–8.0	21.-4.0	6.0–12.0
VIII	100–200	8.1–16.0	4.1–8.0	12.0–24.0
IX	200–400	16.1–32.0	8.1–16.0	24.0–48.0
X	400–800	32.1–64.0	16.1–32.0	>48

Table 6
Damage to surrounding buildings caused by the explosion of the West fertilizer plant in the United States.

Serial number	Building name	Distance to epicenter (m)	Damage to buildings	Damage scale
A1	2-story wood light-frame apartment complex	166	Roofs complete blow out. East wall surface: collapsed completely; west wall surface: collapsed partially (the second story collapsed); north and south surfaces: façade collapsed completely, wall panels severely damaged. Wood framing destructed completely.	DS7
A2	A regular-shaped single-story residential house	174	A large area of Collapse. East surface destructed completely; a large area of façade collapse and wall panel destruction (south surface). East surface wall framing destroyed; large amount of roof truss failure.	DS7
A3	A single-family residential house	256	Very large deflections; several big holes. A large area of façade collapses (south surface). Failure of several roof trusses.	DS6
A4	A residential house	442	Shattering of all window glass on the east surface. Destruction of the garage door; several small-sized roof shingle torn offs.	DS4
A5	A residential house	526	All window glass is broken or Shattered. Destruction of garage door; small area of brick facade collapse (north surface).	DS4
A6	A school	827	There are small areas where the brick façade wall collapsed, corrugated wall panels and the garage door slightly buckled, and a few window glasses were broken. For the interior of the building, a lot of ceiling materials, e.g., boards, grids, and insulation materials, collapsed.	DS3

Table 7
Damage to surrounding buildings caused by an explosion in Tianjin Port, China.

Serial number	Building name	Distance to Epicenter (m)	Damage to buildings	Damage scale
B1	Tianjin Port Public Security Bureau	400	There are only frames left in the 5-story office building	DS6
B2	Harbour City Community	800	The glass was shattered instantly, and the door frame and anti-theft door were damaged	DS3
B3	Tianbin Apartment	1000	The glass windows were all shattered, and the ceiling outer layer fell off	DS3
B4	TEDA Football Stadium	2000	Damaged external steel structure, glass, doors and windows	DS2
B5	China Automobile Research Institute Tianjin Branch	4000	The house was slightly damaged	DS2
B6	Jinmo Technology Company	5000	Office area was slightly damaged	DS1

Table 8
Damage to surrounding buildings caused by an explosion in Beirut Port, Lebanon.

Serial number	Building name	Distance to epicenter (m)	Damage to buildings	Damage scale
C1	Marfa Modern Art Gallery	600	Almost completely destroyed	DS6
C2	Hotel Le Gray	1500	The huge force generated by the explosion blew through the walls of the hotel, the hotel furniture was also filled with shards of glass, and the carpet was scattered with glass slag.	DS4
C3	Lebanese Prime Minister's Office	1600	All doors and windows fell to the ground by the explosion	DS3
C4	Four Seasons Hotel Beirut	1850	The hall is full of dumped furniture and construction materials	DS3
C5	"Little China" Chinese Restaurant	3000	Damaged store	DS2
C6	Embassy of South Korea	7300	Two broken windows	DS2

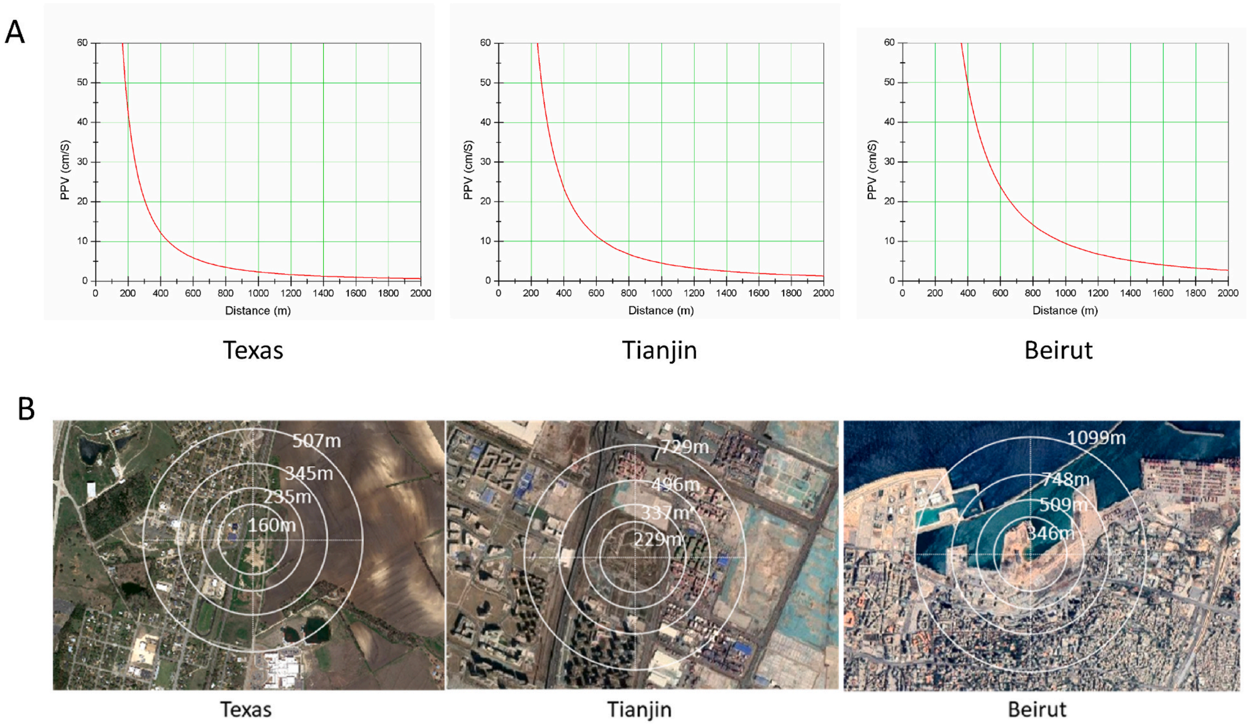

Fig. 3. The influence of different distances on the change of ground shock and the predicted damage scale zones of casualty and building damage induced by ground shock. (A) The curve of ground shock varying with the distance from the epicenter of the explosion. **(B)** The predicted damage scale zones of buildings caused by ground shock. (map data © 2013 Google).

and most of the class III buildings were toppled. The PPVs within the range of 160–235 m, 229–337 m, and 346–509 m from each explosion epicenter were equivalent to 9° of seismic intensity, and these areas were severely damaged (Fig. 3A and B). In addition, the building structure was severely damaged and partially collapsed. The PPVs generated within a range of 235–345 m, 337–496 m, and 509–748 m from the epicenter of the respective explosions were equivalent to 8° of seismic intensity, and these areas were moderately damaged, and the structure of the building was damaged and would need to be repaired before it could be used. In the range of 345–507 m, 496–729 m, and 748–1099 m away from each explosion epicenter, the PPVs were equivalent to the seismic intensity of 7° (Fig. 3A and B). These areas suffered mild damage, partial house damage or cracking, and required minor repair or no repair at all. Thus, it was concluded that in the three explosion accidents, buildings within 507 m, 729 m, and 1099 m from the respective epicenter of the explosion could suffer varying degrees of damage due to the ground shock caused by the explosion. Results also showed that the ground-shock reduced as the standoff distance increases.

Previous studies have found that buildings' roof collapse may be a typical sign of building damage related to ground shock. In addition, with the increase of the distance between the explosion epicenter and the buildings, the contribution of the ground shock to the structural damage is more obvious. In the explosion in Texas, USA, many local buckling damages were observed on the collapsed roof truss, which can not be explained by the air-blast overpressure [37]. Their results also showed that in the destructive failure and hazardous failure zones, very few damage characteristics caused by ground shock could be identified. In these zones, the ground shock-induced damages were overwhelmed by the air-blast incident overpressure-induced damages. In the repairable moderate damage zone, the vertical cracks appear. These results suggested that the damage observed on-site could be more accurately explained by considering the influence of ground shock. Thus, it was proved that the AN explosion accident's overpressure was the leading factor of building damage. Although ground shock was a secondary factor, it still plays an important role. In a future analysis of the consequences of such accidents, the influence of air blast overpressure and ground shock should be considered comprehensively so that the relationship between explosion load and building damage could be accurately obtained.

3.6. Environmental pollution caused by an explosion

The chemical explosions caused long-term environmental and ecological contamination. Although there are limited follow-up reports and information on the three AN explosions, the residual chemicals and secondary contaminants from the explosions may have exceeded 100 or more, causing varying degrees of contamination of the air, water and soil environment in the central area of the accident and the surrounding area. Liu et al. collected different soil samples from the Tianjin accident site and calculated the contamination at different depths. They found a nitrate concentration of nearly 1000 mg/L at a depth of 5.0 m, which is well above the maximum lethal level reported in the study data [38]. In addition, residual chemicals from the explosion continued to contaminate the atmosphere, potentially endangering human lives. The Chinese Ministry of Environmental Protection reported that on the eighth day after the explosion, the maximum concentration of toxins was 356 times above the acceptable limit [39]. On the one hand, it reduced immune function in children, increased the incidence of chronic pharyngitis and bronchial asthma, and increased the incidence of eye and respiratory diseases in the elderly. The Beirut port explosion occurred during the ongoing COVID-19 pandemic. The explosion caused the air in the area to be filled with particulate matter, making people more susceptible to serious respiratory diseases, including COVID-19 infections. The official website for Beirut reported a dramatic increase in positive COVID-19 cases among the local population in the 10 days following the explosion [40]. On the other hand, the toxic gases produced by AN decomposition can affect the human nervous system and be fatal to humans. For example, in the accident in the Escombreras Valley, Cartagena, Spain, the fertilizer consisted mainly of monoammonium phosphate, AN and potassium chloride, the decomposition of which produced a toxic cloud formed by NO_X [41].

The pollutants left in the air also caused other potential environmental pollution problems. The presence of NO_X pollutants in the air can be inferred from the red smoke produced by the three explosions. This substance is usually accompanied by the burning of various objects and continues for a long time, even continuing with multiple reactions, subsequently producing new, more toxic compounds that migrate through the soil and groundwater, seriously contaminating the ecosystem. Calculations suggest that the nitrates produced in the aftermath of the Tianjin port explosion will dissolve into the soil for over 100 m within five years, potentially posing a serious ongoing risk to nearby residents [38]. More importantly, NO_X, one of the most important ozone-producing substances, are closely linked to ozone concentrations and photochemical pollution, causing not only soil acidification, but also eutrophication of water bodies due to emissions of NO_X and sulphur dioxide into the atmosphere, as well as rainwater falling into rivers, lakes and oceans and entering groundwater, which in turn causes changes in soil chemistry, i.e. soil acidification and ecosystem imbalance. In addition, the effects of pollutants on marine organisms had been reported. Reports indicated that NH_3 was acutely toxic to 19 freshwater invertebrate species at concentrations ranging from 0.53 to 22.8 mg/L. In fish species, reported lethal concentrations (96-h LC_{50}) ranged from 0.083 to 1.09 mg/L for salmonids and 0.14–4.60 mg/L for non-salmonids [42]. In contrast, the actual values of nitrate contamination concentrations would be much higher than the lethal concentration (LC_{50}) values for amphibians and aquatic animals. Once nitrate is transferred to the sea under various hydraulic and climatic conditions, the main problem in coastal areas will be quite severe. Marine organisms, especially fish, can experience harmful results if they are exposed to high concentrations of these compounds for long periods of time.

3.7. Lessons learned from the explosion accidents

Trouble is often accumulated in negligence. Although these accidents occur with a certain degree of suddenness and chance, the analysis afterwards often originates from the details that are usually neglected or hidden in the daily inadvertent performance of duties. Thought paralysis is the most terrible hidden danger in safety production. Once neglected, it is easy to cause a serious disaster, resulting in irreparable damage to people's lives and property. Safety production is no small matter, we must further strengthen the concept of safety development, strengthen the supervision of safety production, and firmly guard the baseline of safety production.

With the rapid development of social economy, more and more port enterprises have come into being, and a large number of ports, terminals, warehouses, yards as well as dangerous chemical transport vehicles and transport vessels involving dangerous chemicals exist, which leads to the frequent problem of mixed safety management in the actual operation process. Thus, it is important to strengthen the safety management of dangerous goods port operations. For this reason, on the one hand, relevant government departments should not only fully consider the various risks they may face when building large facilities such as ports, but also increase infrastructure development efforts to ensure the long-term completeness of port infrastructure. On the other hand, the complex composition of the goods leads to increased security risks. A strict inspection system focusing on ports, terminals, logistics warehouses, chemical parks, etc. should be established, and strong laws and regulations should be formulated for all kinds of goods entering the region, as well as for the way dangerous goods are operated and stored. There should also be a professional team of personnel to implement and ensure the regular special inspection and rectification of hazardous chemical storage safety.

In addition, urban planning should be rationalized as much as possible to reduce the risk factors. There is also a point to reflect on in these explosions. These cities do not have sufficient safety barriers between residential areas and dangerous chemical storage warehouses. Therefore, urban planning should try to provide sufficient safety distances between residential areas and large infrastructures such as urban port terminals and hazardous sources, with buffer zones in between. In this way, in case of fire and explosion, a large number of casualties can be avoided and the degree of damage to residential houses and other facilities can be reduced. At the same time, effective information exchange of hazardous chemicals is also very important. Residents near hazardous chemical storage sites, first aid departments in the jurisdiction and other relevant parties must be clearly informed of the existence and specific conditions of hazardous sources so that residents and rescuers can quickly grasp the situation and carry out appropriate self-help and rescue work after a disaster occurs.

4. Conclusions

Through the systematic investigation and analysis of three typical AN explosions, a rapid prediction and assessment method has been developed and validated in our study. Combined with the scene situation of explosion accident and prediction analysis, the following conclusions are drawn:

(1) According to the explosives' properties on-site, these accidental explosions were caused by condensed phase explosives. Combined with the blasting site conditions and relevant data, the crater diameter could be calculated by explosive equivalent, but there was a certain deviation between the predicted value and the actual value. Consequently, the formula needs to be further modified.
(2) The severity of casualties and building damage caused by the explosion decreased with the increase of the standoff distances. The farther away the residents and buildings were, the fewer casualties and building damage occurred. These distances could be calculated by the scaling law, which was replaced by the equivalent TNT mass of the explosive and the damage scale's overpressure boundary value. The formula should be suitable for estimating blast-induced damage characteristics and damage scales or severities, and both the air-blast incident overpressure and ground-shock PPV in the field.
(3) Marking damaged areas on the map might be helpful for visualization. Moreover, the air-blast overpressure was typically the dominant factor for casualties and building damages. The ground shock was the secondary factor, but it was still important. Consideration of the ground-shock effects can lead to a more comprehensive and precise explanation of the buildings' field-observed damages.
(4) Attention should also be paid to the long-term environmental and ecological impacts of AN explosions. Explosions often involve a variety of species and large quantities of hazardous chemicals, and the toxic gases released could cause widespread air, water and ground contamination which affected the health and environmental safety of the local population. In addition, once the explosion was in port, then the impact of these pollutants on marine life was also a major issue.

However, this study also has some limitations. The consequence analysis based on crater size and damage supports other estimates of the order of magnitude of the number of AN detonated, but also indicates a high degree of uncertainty in that number. Furthermore, the fact that AN detonations are often a mixture of multiple compounds, even in some cases multiple detonations, may also lead to some discrepancies between our findings and the actual situation.

Based on the above resulting analysis, from the perspective of safe storage transportation of hazardous chemicals and emergency preparedness, this research can be applied to the following three aspects: first, the AN explosion has a devastating impact on nearby residents, mainly due to the lack of zoning or urban planning to create buffer zones between sites storing explosives and critical infrastructure. Through our mathematical model, we can help government departments to make more effective urban planning and guide the delimitation of "safe distance" and "exclusion zones". Secondly, this method can analyze the consequences of typical AN explosion accidents and predict the severity and influence range of the consequences of explosion accidents more accurately, providing a reliable basis for carrying out medical rescue in a timely and effective manner. Thirdly, it can provide sound advice on the emergency response to unexpected ecological and environmental events. For example, emergency environmental monitoring was carried out by mobilizing multiple forces to monitor the atmosphere, water and marine environment in and around the central area of the accident, and to monitor the soil outside the central area of the accident with grid-based sampling. For the sewage in and around the central area of the accident, the first time to adopt the "front blocking, back sealing and intermediate treatment" measures, including the construction of a high level fence around the central area of the accident and the blocking of drainage inlets, surface drains and rainwater discharge pipes. The sewage from the central area of the accident was closed and scientific, multi-channel sewage treatment was carried out according to the concentration level to achieve the standard discharge and minimize casualties and property damage.

Author contribution statement

Qiang Wang: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Lei Zhang: Performed the experiments; Analyzed and interpreted the data.

Lili Wang: Contributed reagents, materials, analysis tools or data.

Lijuan Bu: Analyzed and interpreted the data.

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Data availability statement

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Additional information

No additional information is available for this paper.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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