Model-based evaluation of major accident consequences and effects occurring during the transport of dangerous substances presents a great interest, because it allows derivation of relevant conclusions on the cause-effect close relationship. Such a numerical (in-silico) analysis helps to improve safety regulations for the transport of hazardous substances aimed at preventing dramatic accidents causing many deaths, injuries, and structural damage. By using the standard TNT equivalency math model, coupled with the Probit functions technique, the consequences and effects of an accidental blast have been estimated.\textsuperscript{1,2} The approached case study here refers to the accidental explosion of a truck while transporting 20 t of ammonium nitrate (AN) in the proximity of Mihăileşti village (Romania) on 24 May 2004. The model-based simulated accident consequences and effects match the data taken on the spot after the accident. Multiple simulations lead to deriving relevant conclusions of practiced value for improving the transport safety of hazardous substances.

**Key words:**
Mihăileşti accident consequences, ammonium nitrate, TNT equivalency model, estimated damage, Probit functions, fatalities percentage

**Introduction**

Ammonium nitrate (AN) is a substance of high interest due to its multiple applications, being currently produced in large quantities on an industrial scale (6.61 million tonnes in 2018).\textsuperscript{3} AN is widely used in the chemical industry, agriculture (fertilizer), as an explosive, or as a potential ingredient of solid propellants in space and military missions.\textsuperscript{4}

Although it acts as a source of ammonia and nitrate ion vital to plants in the form of nitrogen fertilizer, in explosives and propellants, the nitrate ion is a source of oxygen and its application is as an oxidizer.

Due to its composition and properties (see further), AN is the principal component of most industrial explosives. Several compositions of AN, such as ammonium nitrate–fuel oil (ANFO), amatol, etc., are well-known explosives.\textsuperscript{4} “However, its use in the field of propellants / pyrotechnics, unlike potassium nitrate, which is the principal constituent of black powder or gun powder and was used in the earliest solid rockets, or ammonium perchlorate (AP), which is the main oxidizer of modern solid propellants, is rather limited. Its principal use in propellants is restricted to its low-burning-rate, low-performance applications, such as gas generators for turbo-pumps of liquid propellant rocket engines or emergency starters for jet aircraft”\textsuperscript{4}.

Accidental explosions of large AN amounts have been proved to be catastrophic (see Table 1, and reviews\textsuperscript{5,6}).

If such an explosion takes place in the proximity of a (petro-)chemical plant / unit, then more dramatic consequences may occur through the so-called Domino effect\textsuperscript{1,7,11,14}.

**The Mihăileşti accident**

On May 24, 2004 (4:57 AM), a truck loaded with 20 t of AN rolled over and caught fire before exploding an hour later, killing 20 people and injuring 13 others, on the European road E-85 in the proximity of Mihăileşti village (Buzău county, Romania).\textsuperscript{8} The truck was loaded with AN in the form of (porous) granules, partly put in bags, and partly in bulk (which was illegal). Accident investigators advanced the idea that after the accident, the truck entered a ditch and tilted at 45\textdegree, so that the fuel tank...
rubbed the ground and hit a bridge head, and thus breaking. A short circuit in the truck’s battery may have ignited the truck’s plastic wrap. The plastic that caught fire could have ignited the driver’s cabin, and the fuel spilled from the truck’s tank, causing the AN explosion.19

The casualties included: the driver, 7 fire-fighters from two fire-trucks that had arrived at the scene 20 minutes later, 2 members of a TV-crew quickly that had arrived at the accident scene to film the fire for a TV-News-channel, and several curious villagers gathered around the accident site. After the truck had caught fire, the gasoline leaked from the broken tank, thus reaching the AN load of the overturned truck. One hour after the accident (at 5:47 AM) a small explosion took place in the cabin of the truck, followed 2 minutes later by a major explosion (Fig. 1a-b), killing 20 people, and injuring 13 others in a radius of ca. 30 m.8,19

Out of the 20 fatalities, 2 people had to be identified by means of DNA testing. The explosion left behind a 6.5 meter deep crater (Fig. 1a-b), scattered human remains and debris over a radius of several tens of meters, and caused material damage amounting to more than 100 000 (€).

Following this event, safety regulations in Romania for the transport of hazardous chemical substances were improved, and AN was classified as a hazardous chemical compound. Several managers from two companies involved in the transport of AN without safety measures were charged with homicide by negligence and destruction of property. All were found guilty and sentenced to jail as well as the payment of compensation to the victims’ families. More details can be found in the media of that time.8

Due to its hazardous properties (discussed further herein), AN is difficult to transport and store in perfect safety. This explains the large number of accidents involving AN. Some of them are presented in Table 1, and in a review.5

The aim of this paper was to simulate, using a standard math model from the literature, this AN truck accident/explosion which took place at Mihailești in 2004. The results of multiple simulations were compared with the accident scene data, and used to derive some useful conclusions and suggestions concerning safety measures to be taken during long-distance road transport of AN worldwide.

**AN properties**

AN is a substance with \( \text{NH}_4\text{NO}_3 \) formula. It is a crystalline colorless salt, highly soluble in water. Although it is hygroscopic, it does not form hydrates. It is also soluble in alcohol, acetic acid, and nitric acid. AN dissolves in liquid ammonia to form what is known as Divers’ solution, and can be used to strip ammonia from gases. AN has a negative heat of solution in water, and can therefore be used to prepare freezing mixtures. The chemical reactivity of AN has been well documented in literature.9 The boiling point of the pure material is around 210 °C at 11 mmHg, and it distills without decomposition. “It decomposes around 230 ºC at 760 mmHg, and above 325 °C it deflagrates. If confined, AN may explode between 260 and 300 °C.”4,6,17 Data on
Fig. 1 – (a) Accident site after the explosion of the truck with AN near Mihăilești village (Romania) on 2004. [Top left corner] A view of the explosion taken from a distance by an amateur (20 t AN exploded). [Top right corner] A view of some debris at the accident scene. Source: https://adevarul.ro/locale/buzau/video-foto-explozia-mihailesti-plaseaza-buzau-istoria-catastrofelor-romania-tc_51be2982c7b835f3569aca3e/index.html

(b) Accident site map next to Mihăilești village (Romania). The explosion centre is marked with a yellow star (placed on the E-85 European road). Google-map Source: https://www.google.com/maps/@44.9137626,26.6905546,1953m/data=!3m1!1e3
solubility, vapor pressure, boiling point, specific heat of aqueous AN solutions, and many other properties, especially those relevant to its use as a component of explosive mixtures, are well documented. AN has attracted the attention of researchers in different disciplines due to some of its interesting properties. Firstly, the intrinsic phase transitions of this solid have been studied in the field of solid-state physics in order to examine the details of such transformations. The phase transitions of the solid state takes place near ambient temperatures (20–30 °C) contributing to its agglomeration (an unwanted phenomenon). Some properties of AN are displayed in Table 2. The transition between the five (I-V) different phases of AN has important consequences on practical applications. Thus, it was observed that AN composite propellant grain cracks on storage at room temperature due to IV-to-III transition (32–85 °C). While being stable in the lower temperature range, however, when heated above 190 °C (e.g., by gasoline fire, as in the present case study) auto-ignition and explosion may take place, due to the catalytic effects of the impurity on the decomposition of AN. Technical grade AN is always impure, because in the process of its manufacture, storage, transport, and use, AN is often contaminated by impurities, such as inorganic acid, organic oil, and others.

AN is an hazardous substance mainly because its decomposition (following a complex mechanism) leads to a large amount of gases in a very short time (ms). The ANFO (AN mixed with fuel oil) combustion and self-sustained decomposition follows the overall reaction:

\[
3 \text{NH}_2\text{NO}_3 + \text{CH}_2[\text{hydroc.}] \rightarrow 3\text{N}_2 + 7\text{H}_2\text{O} + \text{CO}_2 + 4017 \text{kJ kg}^{-1}
\]

where “CH2[hydroc.]” denotes fragments of hydrocarbons.

The AN self-sustained thermal decomposition follows a complex reaction mechanism. When heated above 170 °C, the following exothermic reactions take place:

\[
\begin{align*}
\text{NH}_4\text{NO}_3 & \rightarrow \text{N}_2\text{O} + 2\text{H}_2\text{O} + 59 \text{kJ mol}^{-1} \\
\text{NH}_4\text{NO}_3 & \rightarrow 0.5\text{N}_2 + \text{NO} + 2\text{H}_2\text{O} + 257 \text{kJ mol}^{-1} \\
\text{NH}_4\text{NO}_3 & \rightarrow 0.75\text{N}_2 + 0.5\text{NO}_2 + 2\text{H}_2\text{O} + 944 \text{kJ mol}^{-1} \\
\end{align*}
\]

If AN is suddenly heated up at temperatures higher than 170 °C, there will be explosive decompositions following the very exothermic reactions:

\[
\begin{align*}
2\text{NH}_2\text{NO}_3 & \rightarrow 2\text{N}_2 + \text{O}_2 + 4\text{H}_2\text{O} + 1057 \text{kJ mol}^{-1} \\
8\text{NH}_2\text{NO}_3 & \rightarrow 5\text{N}_2 + 4\text{NO} + 2\text{NO}_2 + 16\text{H}_2\text{O} + 600 \text{kJ mol}^{-1} \\
\end{align*}
\]

Due to the aforementioned reasons, AN is difficult to transport and store in perfect safety. This explains the large number of accidents involving AN (see Table 1, and review).

### TNT equivalency model

As mentioned previously, once the temperature exceeds 170 °C, and reaches 230 °C, due to the fuel / plastics fire (in the present case), AN decomposition starts and, above 325 °C, it detonates.

To simulate an AN explosion, the TNT model has successfully been used as reported in the literature, e.g., to simulate the Beirut AN catastrophic explosion, or to evaluate the safety distance in land use planning.

### The basic model

When a large amount of a flammable liquid, or a substance likely to decompose rapidly, a vapour cloud forms and disperses with the surrounding air. In the present case study, AN was rapidly heated by the fuel fire which happened in the same place. If the cloud is ignited / detonated before the cloud is diluted below its lower flammability limit (LFL), or its lower detonation limit (LDL) respectively, a VCE (vapour cloud explosion) will occur. To simulate a VCE, several mathematical models can be applied, i.e.: i) TNT equivalency model; ii) TNO multi-energy model, and iii) modified Baker model.
In the present study, the TNT equivalency model was applied, as being more intuitive, sufficiently accurate, and more often used to simulate AN explosions of different sizes.\textsuperscript{10,17}

The TNT model includes three main computational steps (Steps 1–3 presented in Table 3). The basic idea of the model was to estimate the amount of TNT (denoted by $W$) which, by exploding, produces blast consequences equivalent to those produced by the explosion of the analysed substance quantity. Based on the equivalent $W$ (computed with the relationship in Table 3), the model was then able to estimate the blast parameter vector $f = [p_0, ip, td, ta]$ (defined in the notation list), for a given distance $R$ from the explosion centre, by using a couple of algebraic empirical functions, in the following form:

$$
\log_{10}(\phi) = \sum_{i=0}^{n} c_i \left( a + b \cdot \log_{10}(Z) \right)^i 
$$

(1)

Step 4. Evaluate the Probit variable ($Y$) using the following recommended empirical relationships:

$Y = -77.1 + 6.91 \cdot \ln (p_0)$, for human receptors

$Y = -23.8 + 2.92 \cdot \ln (p_0)$, for structures (buildings, industrial plants, etc.)

Step 5. Evaluate the probability or percentage of affected receptors at a given distance $R$, using the Probit variable ($Y$), with the recommended relationship:

$$
P_f = 50 \left[ 1 + \frac{Y - 5}{\sqrt{Y - 5}} \text{erf} \left( \frac{Y - 5}{\sqrt{2}} \right) \right], \text{ (also denoted as P%).}
$$

In Eq. (1), the scaled distance “$Z$” defined for a given distance $R$ from the explosion centre to a defined receptor is given by the following relationship, Table 3:

$$
Z = \frac{R}{\sqrt[3]{W}}
$$

(2)

The empirical coefficients $[a, b, c(i)]$ for the blast parameter functions in (1) are given in Table 4.

Once the overpressure “p0” was evaluated, it was possible to estimate the explosion damages (effects), expressed in both human losses (P% fatalities), and P% structural losses, by using the Probit functions method. Based on the blast overpressure dose (p0) received by a receptor located at a defined distance “$R$”, a Probit variable ($Y$) was evaluated using the empirical relationships of Step 4 displayed in Table 3. Irrespective of the accident type (toxic dose, overpressure dose, or thermal radiation dose), the Probit variable ($Y$) is related to the probability or percentage of affected receptors (P%) by the relationship defined in Step 5 of Table 3. More details on the Probit functions method can be found in the literature.\textsuperscript{1} More specific damages for common structures due to the blast overpressure are given in Table 6.

Model implementation and preliminary checks

The TNT model is part of a large number of commercial software (see the literature reviews).\textsuperscript{2,12,13} Instead, a “home-made” routine including the TNT model was developed using the Matlab\textsuperscript{TM} package facilities. To validate our software, two solved case studies exemplifying the TNT model have been used (i.e., those of pp. 174–176 of a reference book from literature).1 Based on the positive validation / check of our routine, we concluded that our developed Matlab\textsuperscript{TM} code to simulate VCE-s using the standard TNT model, proved to be satisfactorily accurate. Consequently, this coded TNT model has been used to solve the approached case study, by in-silico (model-based) estimation of the Mihăileşti accident consequences /
Table 4 – The explicit blast parameter functions defined by Eq. (1), i.e., \([p_0, ip, td, ta]\). Adapted from AIChE1 by courtesy of AIChE.

Remark: the 14-digit correlation coefficients have been truncated to only 4-digits. Notation: \(\text{Lg} = \log_{10}\).

| Parameter | Correlation |
|-----------|-------------|
| \(p_0\)   | Valid for \(0.0674 \leq Z \leq 40\) \[\text{Lg}(p_0) = 2.7807 - 1.6958 \cdot \text{ABP} - 0.1541 \cdot \text{ABP}^2 + 0.5140 \cdot \text{ABP}^3 + 0.0988 \cdot \text{ABP}^4 - 0.2939 \cdot \text{ABP}^5 - 0.0268 \cdot \text{ABP}^6 + 0.1090 \cdot \text{ABP}^7 + 0.0016 \cdot \text{ABP}^8 - 0.0214 \cdot \text{ABP}^9 + 0.0001 \cdot \text{ABP}^{10} + 0.0016 \cdot \text{ABP}^{11}\]; Where \(\text{ABP} = (-0.2143 + 1.3503 \text{Lg}(Z))\) |
| \(ip(1)\)  | Valid for \(0.0674 \leq Z \leq 0.955\) \[\text{Lg}(ip) = 2.5245 - 0.5029 \cdot \text{ABIP} + 0.1713 \cdot \text{ABIP}^2 + 0.0450 \cdot \text{ABIP}^3 - 0.0118 \cdot \text{ABIP}^4 - 0.0066 \cdot \text{ABIP}^5 - 0.0028 \cdot \text{ABIP}^6 + 0.0013 \cdot \text{ABIP}^7\]; Where \(\text{ABIP} = (2.0676 + 3.0760 \text{Lg}(Z))\) |
| \(ip(2)\)  | Valid for \(0.955 \leq Z \leq 40\) \[\text{Lg}(ip) = 1.6728 - 0.3845 \cdot \text{ABIP} - 0.0260 \cdot \text{ABIP}^2 + 0.0059 \cdot \text{ABIP}^3 + 0.0145 \cdot \text{ABIP}^4 - 0.0066 \cdot \text{ABIP}^5 - 0.0028 \cdot \text{ABIP}^6 + 0.0013 \cdot \text{ABIP}^7\]; Where \(\text{ABIP} = (-1.9470 + 2.4069 \text{Lg}(Z))\) |
| \(td(1)\)  | Valid for \(0.178 \leq Z \leq 1.01\) \[\text{Lg}(td) = -0.6142 + 0.1301 \cdot \text{ABTD} + 0.1348 \cdot \text{ABTD}^2 + 0.0391 \cdot \text{ABTD}^3 - 0.0047 \cdot \text{ABTD}^4 - 0.0042 \cdot \text{ABTD}^5 + 0.0056 \cdot \text{ABTD}^6 + 0.0001 \cdot \text{ABTD}^7 - 0.0066 \cdot \text{ABTD}^8\]; Where \(\text{ABTD} = (1.9294 + 5.2509 \text{Lg}(Z))\) |
| \(td(2)\)  | Valid for \(1.01 \leq Z \leq 2.78\) \[\text{Lg}(td) = 0.3154 - 0.0297 \cdot \text{ABTD} + 0.0306 \cdot \text{ABTD}^2 + 0.0183 \cdot \text{ABTD}^3 - 0.0173 \cdot \text{ABTD}^4 - 0.0010 \cdot \text{ABTD}^5 + 0.0056 \cdot \text{ABTD}^6 + 0.0001 \cdot \text{ABTD}^7 - 0.0066 \cdot \text{ABTD}^8\]; Where \(\text{ABTD} = (-2.1249 + 9.2969 \text{Lg}(Z))\) |
| \(td(3)\)  | Valid for \(2.78 \leq Z \leq 40\) \[\text{Lg}(td) = 0.6869 + 0.0933 \cdot \text{ABTD} - 0.0005 \cdot \text{ABTD}^2 - 0.0022 \cdot \text{ABTD}^3 - 0.0002 \cdot \text{ABTD}^4 + 0.0014 \cdot \text{ABTD}^5 + 0.0056 \cdot \text{ABTD}^6 + 0.0001 \cdot \text{ABTD}^7 - 0.0066 \cdot \text{ABTD}^8\]; Where \(\text{ABTD} = (-3.5362 + 3.4634 \text{Lg}(Z))\) |
| \(ta\)     | Valid for \(0.0674 \leq Z \leq 40\) \[\text{Lg}(ta) = -0.0591 + 1.3570 \cdot \text{ABTA} + 0.0524 \cdot \text{ABTA}^2 - 0.1965 \cdot \text{ABTA}^3 - 0.0601 \cdot \text{ABTA}^4 + 0.0696 \cdot \text{ABTA}^5 + 0.0216 \cdot \text{ABTA}^6 - 0.0161 \cdot \text{ABTA}^7 + 0.0023 \cdot \text{ABTA}^8 + 0.0014 \cdot \text{ABTA}^9\]; Where \(\text{ABTA} = (-0.2024 + 1.3778 \text{Lg}(Z))\) |

Table 5 – Simulated Mihăilești case study input data

| Parameter                              | Value     | Remarks                  |
|----------------------------------------|-----------|--------------------------|
| Ammonium nitrate mass                  | \(M = 20\) t | Mihăilești (Romania) accident\(^{1,6}\) |
| Analysed surface radius around the explosion | \(R = 150\) m | adopted                  |
| Unittest empirical explosion efficiency | \(\eta = 0.05\) | recommended\(^{1,7}\) |
| Heat of combustion NH\(_2\)NO\(_3\)   | \(E_c = 1447.7\) kJ kg\(^{-1}\) | from\(^1\) |
| Heat of combustion of TNT              | \(E_{\text{TNT}} = 4652\) kJ kg\(^{-1}\) (i.e. 2000 Btu lbf\(^{-1}\)) | from\(^1\) |
effects, to eventually predict / recommend safety requirements when transporting large amounts of AN by truck over long distances. Damages due to truck fragments \(^{18}\) were not considered in our numerical analysis.

**Simulation of explosion consequences and effects**

*Mihăileşti accident (20 t. AN blast)*

By using the here presented TNT math model, Tables 3–4, and the input data in Table 5, the Mihăileşti AN blast consequences and effects were simulated. The results are presented in Figs. 2–4. The analysis of the obtained blast parameters led to the following conclusions:

i.- P% fatalities of humans and structures are practically 100 % within a radius of 30 m around the explosion centre, Fig. 2 and Fig. 4, but negligible (or much smaller) outside this area. Human P% fatalities are negligible outside an area of a 30 m radius, while P% structure fatalities are negligible outside an area of a 50 m radius according to the plot in Fig. 2. Such a result is in complete agreement with the data collected from the accident site (Fig. 1a).

ii.- The overpressure displayed in Fig. 3 indicates high values up to 570 atm inside the circle of 30 m radius, i.e., in the area where the blast crater formed, and where the truck, and adjacent cars were destroyed and scattered in pieces (see Fig. 1a), and where 100 % human fatalities had been reported. Such a result is also in agreement with the consequences predicted by Table 6 for the structural damage produced by the overpressure.

| Pressure  | Damage                                                                 |
|-----------|------------------------------------------------------------------------|
| atm | kPa | |
| 0.0014 | 0.14 | Annoying noise (137 dB if of low frequency 10–15 Hz)                   |
| 0.0021 | 0.21 | Occasional breaking of large glass windows                              |
| 0.0028 | 0.28 | Loud noise (143 dB), sonic boom, glass failure                         |
| 0.0069 | 0.69 | Breakage of small windows under strain                                  |
| 0.01 | 1.03 | Typical pressure for glass breakage                                    |
| 0.02 | 2.07 | “Safe distance” (probability 0.95 of no serious damage below this value); projectile limit; damage to house ceiling; 10 % window glass broken |
| 0.027 | 2.76 | Limited minor structural damage                                           |
| 0.033–0.068 | 3.4–6.9 | Large and small windows usually shattered; occasional damage to window frames |
| 0.047 | 4.8 | Minor damage to house structures                                        |
| 0.068 | 6.9 | Partial demolition of houses, made uninhabitable                        |
| 0.068–0.136 | 6.9–13.8 | Corrugated asbestos shattered; corrugated steel or aluminium panels, fastenings fail, followed by buckling; wood panels (standard housing) fastenings fail, panels blown in |
| 0.088 | 9.0 | Steel frame of clad building slightly distorted                         |
| 0.136–0.204 | 13.8–20.7 | Concrete or cinder block walls, not reinforced, shattered            |
| 0.156 | 15.8 | Lower limit of serious structural damage                                |
| 0.17 | 17.2 | 50 % destruction of brickwork of houses                                |
| 0.204 | 20.7 | Heavy machines (3000 lb) in industrial building suffered little damage; steel frame building distorted and pulled away from foundations |
| 0.204–0.272 | 20.7–27.6 | Frameless, self-framing steel panel building demolished; rupture of oil storage tanks; cladding of light industrial buildings ruptured |
| 0.34–0.475 | 34.5–48.2 | Almost complete destruction of houses; loaded train wagons overturned |
| 0.475–0.543 | 48.2–55.1 | Brick panels, 8–12 inches thick, not reinforced fail by shearing or flexure |
| 0.612 | 62.0 | Loaded train boxcars completely demolished                             |
| 0.68 | 68.9 | Probable total demolition of buildings; heavy machine tools (7000 lb) moved and badly damaged; very heavy machine tools (12,000 lb) survive |
| 20.41 | 2068 | Limit of crater lip
iii.- The blast wave arrival time is very short (up to 50 ms, in Fig. 2), in the analysed area of a 150 m radius. By contrast, the overpressure duration time is high (ca. 0.5 s, in Fig. 2) in a small area (below 10 m) around the explosion centre.

iv.- TNT model predictions for this case (20 t AN blast) corresponds to an equivalent $W = 0.35$ t TNT blast, meaning a considerable amount.

Detect the AN truck load that can improve the transport safety

Such major and tragic consequences/effects of the AN blast when large quantities are transported by truck, require a supplementary model-based analysis to detect the larger amount of AN which can be transported by truck to fulfil two requirements:
(A) It is sufficiently large for an economical transport, and
(B) It is sufficiently small to improve transport safety. In other words, in the case of an accidental explosion, small (limited) consequences to occur.

There are different measures to express transport safety. In the present study, we chose a certain upper limit of P% system fatalities. That was because simulations using a wide range of AN amounts (1 to 20 t, not presented here) indicated the area of 50 m radius around the explosion location as being the place where maximum damage occurs. In all tested cases, the human P% fatalities were practically negligible outside an area of a 30 m radius.

These AN explosion repeated simulations with varying the AN quantity, indicated the best compromise between the two criteria (A-B). The best result was found for a 5-t AN truck load. Truck loads smaller than 5 t were considered non-economic, while truck loads larger than 20 t lack safety requirements. Thus, in the case of AN explosion, such an accident is expected to produce even more catastrophic consequences compared to those of Mihăilești. Simulated consequences of a hypothetical explosion of a 5 t AN load are presented in Figs. 5–6). This truckload quantity seems to be the best choice, because: (a) it is reasonably large for an economical transport, and (b) if an accident occurs, its consequences would be significant, but less tragic compared to those of a 20-t AN blast.

Thus, the results obtained by simulating a 5 t AN load hypothetical explosion, led to the following conclusions:

a) P% fatalities of humans / structures are practically 100% within a smaller radius of 15 m/20–30 m, (Fig. 5), for the 5 t exploded AN compared to 25 m/50 m in the Mihăilești accident (20 t exploded AN), but negligible outside this area. Such a conclusion concerning the “critical” AN mass is strengthened by Fig. 7 that illustrates the dependence of P% fatalities of structures (buildings, adjacent cars, etc.) on the exploded mass of AN, at the same distance of 30 m from the explosion source. It clearly appears that explosions of AN amounts larger than 5 t lead to practically total destruction of structures located in the vicinity of the explosion.

b) The overpressure (not displayed here in circular plots, but only in Fig. 5) indicates a high value of 198 atm (at the explosion centre), which gradually decreases inside a circle of 15 m radius until an overpressure of 0.24 atm (at 30 m), i.e., in the area where the blast crater will be formed and where the truck will be destroyed, as predicted by the data displayed in Table 6. Outside the circular area of 30 m radius, the overpressure is small (below 0.1 atm).

c) The blast wave arrival time is very short (up to 20 ms, in Fig. 5), in a circular area of 50 m radius. By contrast, the overpressure duration time is much smaller (less than 5 ms in Fig. 5 compared to 0.5 s in the case of a 20 t AN blast) in a small area (below 10–20 m) around the explosion centre.

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![Fig. 5 – Blast parameters and P% fatalities for humans and structures at various distances from the explosion location (case of 5 t AN explosion)](image-url)
It is understood that truck transport of an AN quantity in the range of 5 t-20 t (the analysed limits) will produce, in the case of an undesirable accident, much worse consequences/effects than those produced by a 5 t case, even if not as serious as for the 20 t explosion. Consequently, it seems that a 5 t AN truck transport is the best choice for both economic and safety reasons.

e) TNT model predictions for this case (5 t AN blast) corresponds to an equivalent of $W = 0.09$ t TNT blast, which is roughly 4x lower than the case of the exploded fully loaded 20 t AN truck, with corresponding much diminished negative consequences.

Conclusions

This study presents an in-silico (math model-based) method for rapidly determining the blast consequences and effects in a reasonable prediction area around the location where a truck loaded with AN accidentally caught fire and exploded. The approached case study (Mihăilești accident, Romania, 2004) allowed checking and validating the model predictions by comparing the simulated results with the data collected from the accident site after the explosion.

Here, the extracted simulation data, such as time of arrival, duration time, overpressure, and P% human and system fatalities, correlated with the distance from the explosion center (20 t of AN), shows a clear trend, being well represented by the established semi-empirical TNT model predictions for an equivalent 350 kg TNT blast. The TNT model predictions fit very well the data collected from the accident site, in terms of arrival time, duration, and P% fatalities.

In order to account for the uncertainties associated with determining precise locations and timings, the results have also been analyzed by taking a reasonable range of 5–20 t AN, and a maximum distance of 150 m from the explosion center. The lower limit for the truckload (5 t AN) was well represented by semi-empirical predictions for an equivalent 90 kg TNT blast.

Repeated simulations using the TNT model indicated that a 5 t AN transport by truck is the best choice for both economic and safety reasons. From this point of view, the TNT math-model proves to be a valuable tool for accurately predicting the risk involved in the transport of explosives.

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NOTE: The corresponding author confirms that our paper has no conflict of interest of any kind or nature.
Abbreviations and notations

\( a, b, c(i) \) – Empirical constants in the blast parameter functions (given in Table 2)

\( E_c \) – Heat of combustion of the explosive compound, \( \text{kJ kg}^{-1} \)

\( E_{\text{TNT}} \) – Heat of combustion of TNT, \( (4437–4765 \text{ kJ kg}^{-1}) \)

\( \text{ip} \) – Overpressure impulse, \( \text{Pa s} \)

\( M \) – Mass of the explosive compound, kg

\( p_0 \) – Peak side-on overpressure, kPa

\( Pf, P\% \) – Probability or percentage of affected receptors at a given distance \( R \), –

\( R \) – Distance from the explosion location to the receptor, m

\( \text{ta} \) – Arrival time of the shock-wave to the receptor, ms

\( \text{td} \) – Positive phase duration time of the pulse to the receptor, ms

\( W \) – Equivalent mass of TNT, kg

\( Y \) – Probit variable, –

\( Z \) – Scaled analysis range for a given distance \( R \), \((\text{m kg}^{-1/3})\)

Greeks

\( \eta \) – Unitless empirical explosion efficiency (recommended 0.05 in literature)

Abbreviations

AN – Ammonium nitrate

ANFO – AN mixed with fuel oil

AP – Ammonium perchlorate

References

1. AIChE, Guidelines for chemical process quantitative risk analysis, 2nd ed., Center for Chemical Process safety of the American Institute of Chemical Engineers, New York, 2000, pp. 159–165, 174–176, 246–248, 275.

2. Maria, G., Chemical process quantitative risk analysis and modelling of accident consequences, Printech Publ., Bucharest, 2007 (in Romanian).

3. Knoema, Ammonium nitrate production, Knoema Co., Technical report, URL: https://knoema.com/atlas/topics/Agriculture/Fertilizers-Production-Quantity-in-Nutrients/Ammonium-nitrate-production?type=maps (20.11.2020)

4. Chaturvedi, S., Dave, P. N., Review on thermal decomposition of ammonium nitrate, J. Energ. Mater. 31 (2013) 1. doi: https://doi.org/10.1080/07370652.2011.573523

5. Saker, A., 2020 Beirut explosion, Report Contract No. DE-AC02-06CH11357, U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, Washington, 2020.

6. Han, Z., Thermal stability studies of ammonium nitrate, PhD thesis, Texas A&M University, Chem. Eng. Dept., 2016.

7. Khwayyir, H. H. S., Maria, G., Dinculescu, D., Influence of fireball coupled with a toxic puff release accident condition influence on consequences and possible Domino effect occurrence for two risky neighbouring chemical plants, Environ. Eng. Manag. J. 14 (2015) 2555.

8. Braileanu, R., Manzu, I., Tragedy of Mihăilești, Revista 22 (Bucharest), 735 (9 June 2004), (Last accessing 24 May 2011; in Romanian). Romanian electronic version at the URL: https://ro.wikipedia.org/wiki/Explozia_de_la_Mih%C4%83ile%83ti C8%99li (25.11.2020)

9. Mellor, J. W., A comprehensive treatise on inorganic and theoretical chemistry, vol.2, Longmans Green, London, 1992.

10. Rigby, S. E., Lodge, T. J., Aliotaibi, S., Barr, A. D., Clarke, S. D., Langdon, G. S., Tyson, A., Preliminary yield estimation of the 2020 Beirut explosion using video footage from social media, Shock Waves 30 (2020) 671. doi: https://doi.org/10.1007/s00193-020-00970-z

11. Maria, G., Dinculescu, D., Khwayyir, H. H. S., Proximity risk assessment for two sensitive chemical plants based on the accident scenario consequence analysis, Asia-Pac. J. Chem. Eng. 9 (2014) 146. doi: https://doi.org/10.1002/pace.1755

12. Phare, Planning for emergencies involving dangerous substances, Phare Project Report PM.00.11.01/HZ, NethConsult & BKH Consulting Engineers, Ljubljana (Slovenia), 2002. URL: https://www.gov.si/assets/ministrstva/MOP/Dokumenti/Industrijske-nesrece/c93c587d86/pripravljenost_na_nesrece.pdf (25.11.2020)

13. Lobato, J., Rodríguez, J. F., Jiménez, C., Llanosa, J., Márquez, A. N., Inarejos, A. M., Consequence analysis of an explosion by simple models: Texas refinery gasoline explosion case, Afinidad 66 (2009) 372. URL: https://www.raco.cat/index.php/afinidad/article/view/279547 (21.11.2020)

14. Cozzani, V., Gubinelli, G., Salzano, E., Escalation thresholds in the assessment of domino accidental events, J. Hazard. Mater. A129 (2006) 1. doi: https://doi.org/10.1016/j.jhazmat.2005.08.012

15. Van Dolah, R. W., Mason, C. M., Perzak, F. J. P., Hay, J. E., Forshey, D. R., Explosion hazards of ammonium nitrate under fire exposure, U. S. Dept. of the Interior, Bureau of Mines, Report 6773, Washington, 1966. URL: https://www.osmre.gov/resources/blasting/docs/USBM/R6773ExplosionHazardsAmmoniumNitrateUnderFireExposure.pdf (25.1.2021)

16. TNO, TNO Green Book, Methods for the determination of possible damages to people and objects resulting from the releases of hazardous materials, Report CPR 16E, The Director General of Labour, Voorburg (Netherlands), 1989. URL: https://ro.scribd.com/doc/61170131/Green-Book-Methods-for-the-Determination-of-possible-Dam-age-CPR-16E (25.11.2020)

17. Török, Z., Ozunu, A., Hazardous properties of ammonium nitrate and modeling of explosions using TNT equivalency, Environ. Eng. Manag. J. 14 (2015) 2671.

18. Alonso, F., Ferradas, E., Minarro, M., Aznar, A., Gimeno, J., Perez, J., Consequence analysis by means of characteristic curves to determine the damage to buildings from the detonation of explosive substance as a function of TNT equivalency, J. Loss Prev. Process Ind. 21 (2008) 74. doi: https://doi.org/10.1016/j.jlp.2007.08.002

19. BBC Romanian, Mihăilești explosion, BBC.romanian.com, 29 May 2004. http://www.bbc.co.uk/romanian/news/story/2004/05/040529_mihailesi_accident.shtml (17.1.2021)