A-P-T RESEARCH, INC.
AN EMPLOYEE-OWNED COMPANY

AMMONIUM NITRATE MODELING IN THE AN MODULE OF IMESAFR

Michael M. Swisdak, Jr. (A-P-T Research, Inc.)
William B. Evans (A-P-T Research, Inc.)

OUTLINE

- Background
- Initiation mechanisms
- Event frequencies
- AN airblast
  - Data sources
  - Composite airblast
  - Inert mass effects
- Other software changes
- Sample problem
- Summary/conclusions

BACKGROUND

- Billions of pounds of ammonium nitrate (AN) are used annually in the global commercial explosives industry
- This means very large manufacturing sites (some producing more than a billion pounds of AN per annum)
- It also means tens of millions of pounds of AN transported/handled/used daily and hundreds of millions of pounds in storage inventories every day
- AN is hazard classified for transport as an HD 5.1 oxidizer in most countries
  - This transport classification tends to be the “universal” classification
- A 5.1 classification for, e.g., storage means that there are no quantity-distance (QD) requirements to members of the public
  - This would also be true for related and unrelated workers, inventories of explosives, etc.

BACKGROUND

- AN is close to the perfect oxidizer in explosives formulations:
  - Low cost/high manufacturing efficiency and rates
  - High energy density
  - Very stable/safe
- While there are no known events with AN during handling or in storage under "normal" conditions
  - Worldwide, there have been many events, i.e., explosions, of AN both in high-temperature/pressure-processing conditions and in fire scenarios
  - This is explicitly recognized in the UN classification definition for AN

BACKGROUND

- It was recognized that there was a need in the AN manufacturing and commercial explosives business for an appropriate tool to quantify the risk of AN operations
- IMESAFR, the risk assessment software sponsored by the Institute of the Makers of Explosives (IME), is such a tool
- The standard version of IMESAFR handles AN by converting it to TNT, through a TNT equivalence factor, then assuming a TNT explosion
  - This is a very conservative approach
- Because of this conservatism and the desire to obtain more realistic answers, the IME approved the development of an AN Engine for the IMESAFR software

IME
institute of makers of explosives

INITIATION MECHANISMS/ EVENT FREQUENCIES

- The development of the AN Module was the joint effort of A-P-T Research, Inc. (APT), the IMESAFR Development Team, the IME AN Working Group, plus input from IME member companies
- The review of available published information indicated that the SAFEX AN Workgroup had already been working in this area and had generated recommendations for some of the required input values, e.g., event frequencies, that were required
- The SAFEX AN Workgroup had published these values in the Good Practice Guidelines (GPG) for the Storage of Technical-Grade AN (TGAN)
  - The GPG recognized three initiation mechanisms for stored AN inventories, along with relevant yields and event frequencies
  - The SAFEX AN Working Group review had been exhaustive and thorough, so the IME Groups decided to accept the event frequencies, initiation mechanisms, and yields as published in the GPG

INITIATION MECHANISMS/ EVENT FREQUENCIES

- The table below shows initiation mechanisms with the relevant yields and event frequencies proposed in the SAFEX GPG and adopted in the AN Module

Mechanism	Fire	Contamination	Shock/Projectile
Event Frequency	2.34 E-06	1.17 E-06	1.17 E-06
Yield	10%	50%	100%

FIRE

- The event frequency is based on historical data
- The % yield is also based on historical data
  - The low yield is largely driven by the very low likelihood that large stores of AN, which the SAFEX Group was mostly interested in, could be engulfed in fire
- Assumptions
  - Only AN directly engulfed in fire is likely to explode
  - Propagation not expected to occur

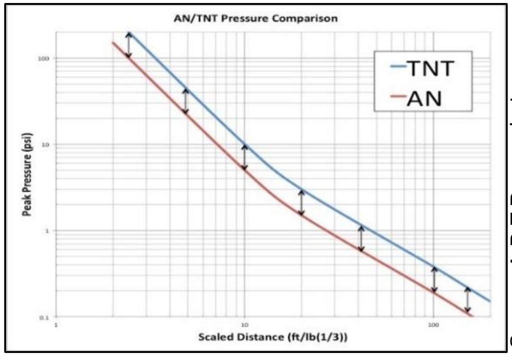
CONTAMINATION

- Very few contaminants can cause AN to spontaneously explode
  - Some chloro-organic compounds can
- Many contaminants can have some effect on the autoignition temperature of AN but not cause direct explosive decomposition
- A few compounds, e.g., nitrites, will cause AN to decompose, but not explosively
- The very low event frequency is based on most contamination being innocuous, at least from an explosive decomposition perspective
- The yield is based on a single event — Toulouse

SHOCK/PROJECTILE IMPACT

- Most regulators treat AN inventories within the “AN distance” of explosives as certain to explode at full yield if the explosives are initiated
  - This is a direct shock and/or projectile initiation of AN from the explosives event
  - There are no data to show this is incorrect, so a yield of 100% was accepted at half the event frequency of fire initiation

THREE LEVELS OF MODELING

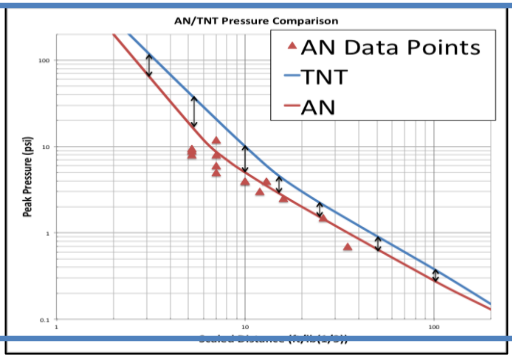


Source: A-P-T Research, Inc.

Level 1 (Lowest Detail)

- Scale to AN effects based on a single value for TNT equivalence.
- TNT Equivalence values are independent of charge weight and distance.
- Same equivalence used to scale both Pressure and Impulse.

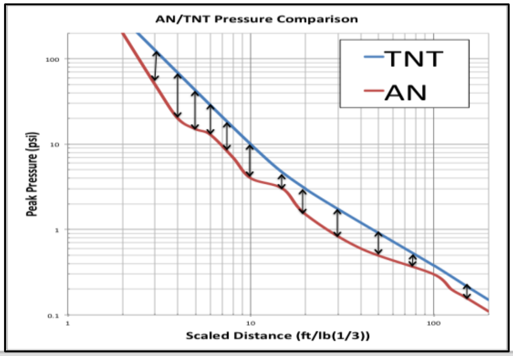
Level selected for AN Module



Source: A-P-T Research, Inc.

Level 2 (Middle Detail)

- Create curve fits for AN pressure and impulse from available test data and modeling.
- Pressure and Impulse models are not necessarily the same



Source: A-P-T Research, Inc.

Level 3 (Highest Detail)

- This would be the true AN waveform.
- Calculated value of P and I as a function of charge weight and distance.
- Pressure and Impulse models would be independent.

DATA SOURCES

- Reverse engineering from accidents and incidents
- Previous testing programs
- Numerical simulations

EMPIRICAL DATA SOURCES

- Reverse engineering from accidents/incidents
  - Required information often missing
  - Requires numerous assumptions regarding the source
    - Was the event a true detonation?
    - Did all of the AN detonate?
    - If all of the material did not detonate, how much material reacted?
    - How much material was involved?
    - For the material that reacted, what was its TNT equivalence?
    - What was the shape of the AN stack just prior to reacting?
    - Did all of the material detonate?
  - Descriptions of damage often incomplete or missing

Limited effort expended here, decision made not to pursue

PREVIOUS TESTING PROGRAMS

- Previous testing programs
  - Limited availability due to distribution restrictions
  - Few in number with limited data
  - Limited use
    - Only TNT equivalences reported, not actual results (pressures and impulses) from airblast measurements
    - Charge shape not reported
  - Five sources located and used in the model development

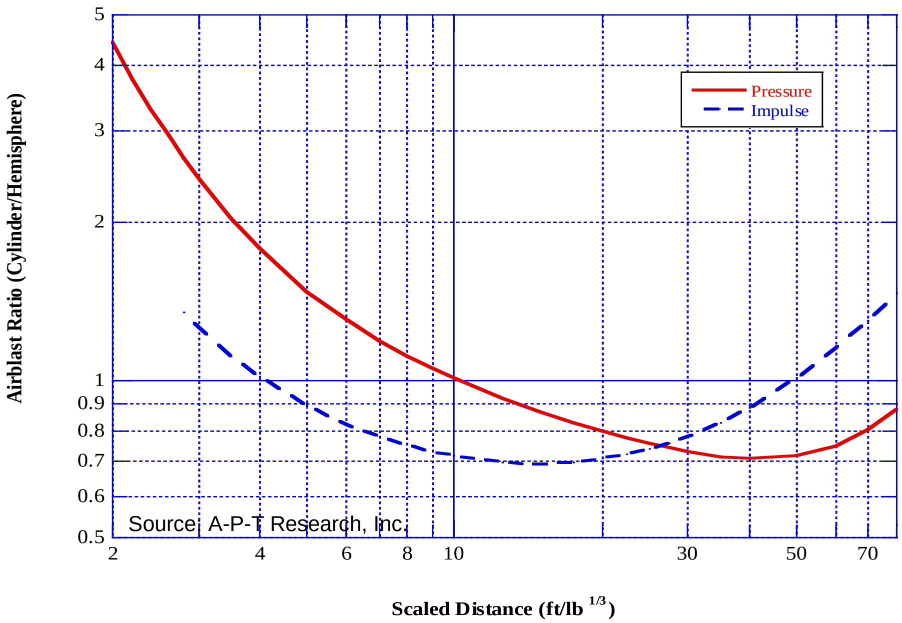
NUMERICAL SIMULATIONS

- VEXDAM
  - Vapor cloud model
  - Explosion strength (ES) parameter within VEXDAM was varied to simulate differing confinement levels provided by the inert mass
  - VEXDAM software only calculates peak pressure and does not consider impulse
  - Model run by Dr. David Dillehay at UAB
- FEFLO
  - Computational Fluid Dynamic Model
  - Model simulations performed by Karagozian & Case, Inc.
  - Following model inputs were used:

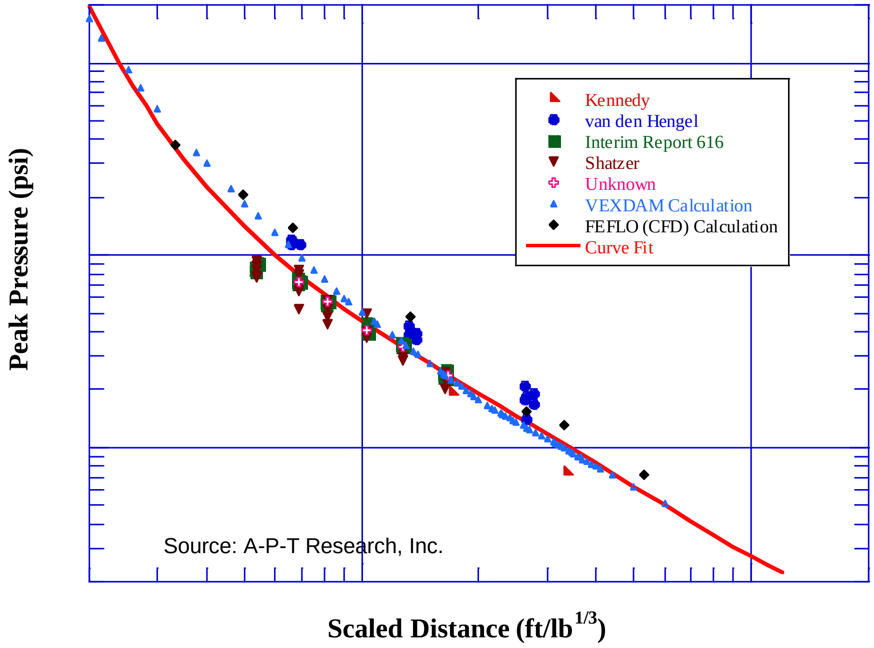
Energetic Material	Properties	JWL Equation of State	Container	Initiation
TGAN	Mass: 3,496 kg Density: 0.82 g/cm^3 Heat of Detonation: 1712 KJ/Kg Detonation Velocity: 3.0 km/s Detonation Pressure: 1.845 Gpa	A: 49.46 Gpa B: 1.891 Gpa R1: 3.907 R2: 1.118 ω: 0.33	Shape: Cylinder Material: Cardboard Wall thickness: 3cm Height: 4m Diameter: 1.165m	Plane Wave across upper surface

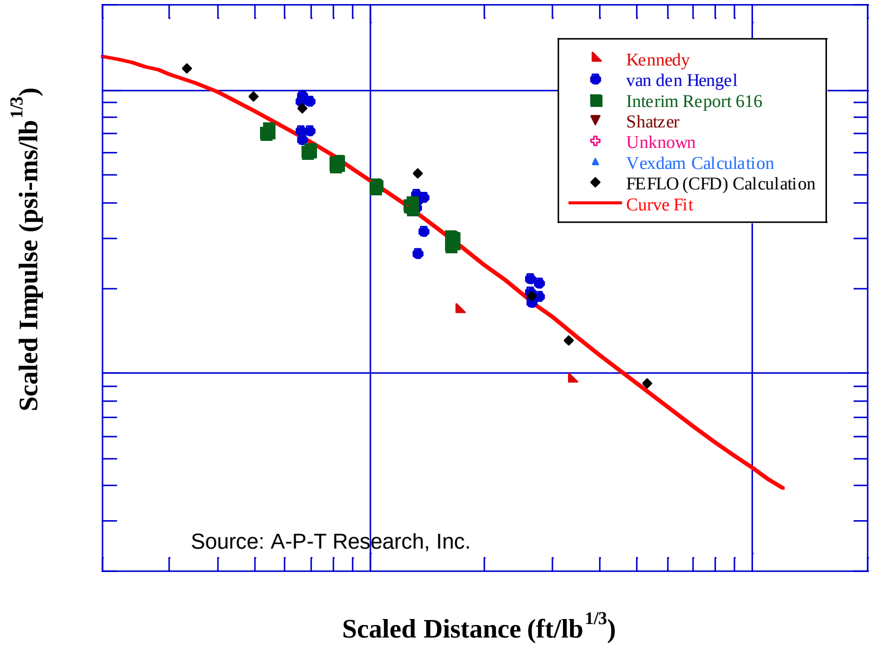
CHARGE SHAPE

- IMESAFR assumes all energetic material is hemispherical in shape
- All test data and numerical simulations were 4:1 right circular cylinders
- Correction factor necessary to convert cylindrical data to hemispherical shape



AN COMPOSITE AIRBLAST

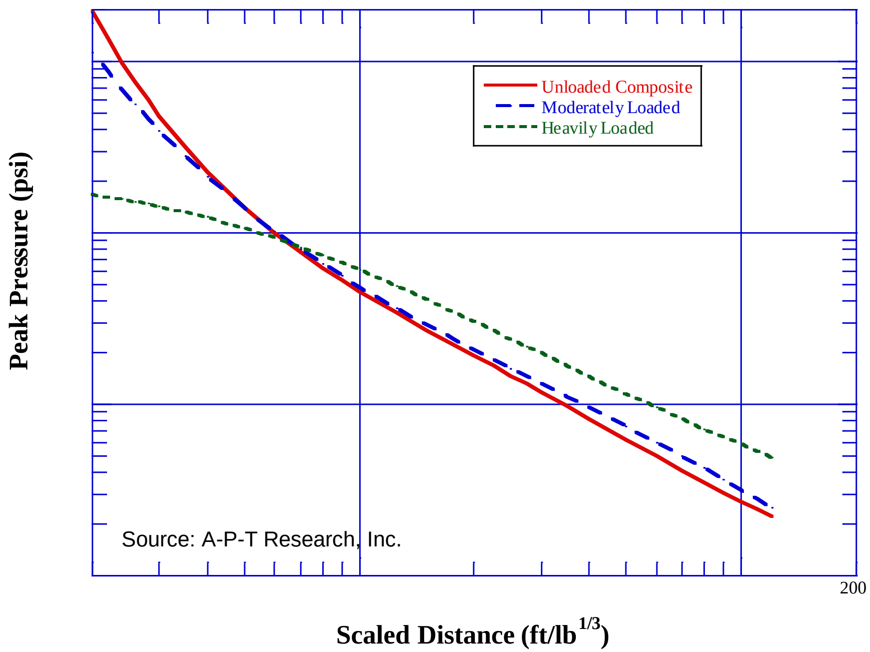


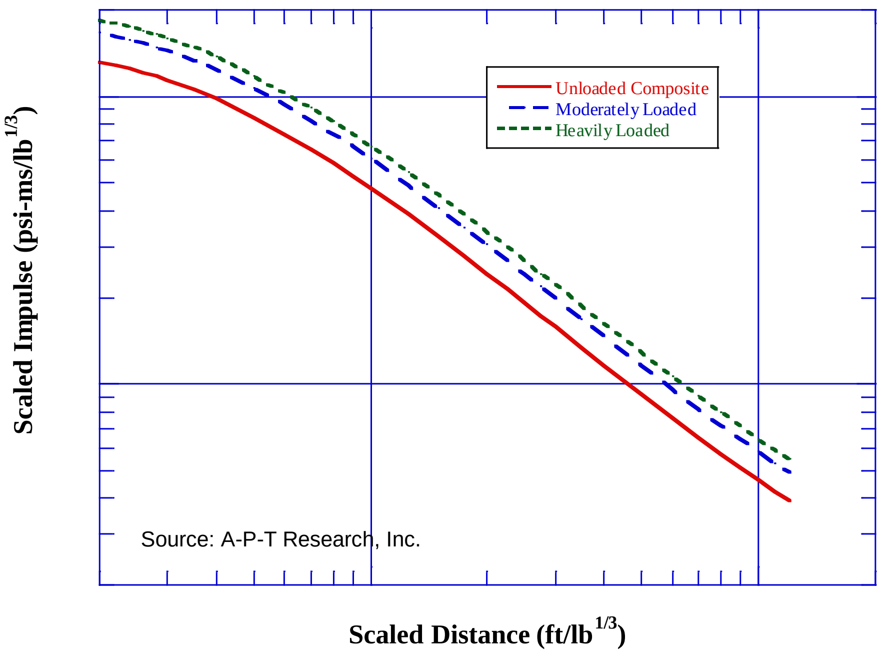


INERT MASS EFFECT

- Inert mass effect discussed by Porzel
  - Porzel, F. B., “Introduction To A Unified Theory of Explosions,” NOLTR 72-209, 4 September 1972
  - Porzel, F. B., “Damage Potential From Real Explosions: Total Head and Prompt Energy,” Minutes of 16th Explosives Safety Seminar, August 1974
- The effect of inert mass is to depress the pressure near the charge (less than a scaled distance of about 10 ft/lb$^{1/3}$) and increase the pressures beyond this point
- The effect of inert mass is assumed to increase the impulse at all ranges
- Three inert mass loading regimes identified:
  - Unloaded
    - Corresponding to a reaction of 70-100% of the AN available
    - Produced by projectile/shock initiation
  - Moderately Loaded
    - Corresponding to a reaction of 30-70% of the AN available
    - Produced by contamination initiation
  - Heavily Loaded
    - Corresponding to a reaction of < 30% of the AN available
    - Produced by fire initiation

EFFECT OF UNREACTED MATERIAL





NEW PES

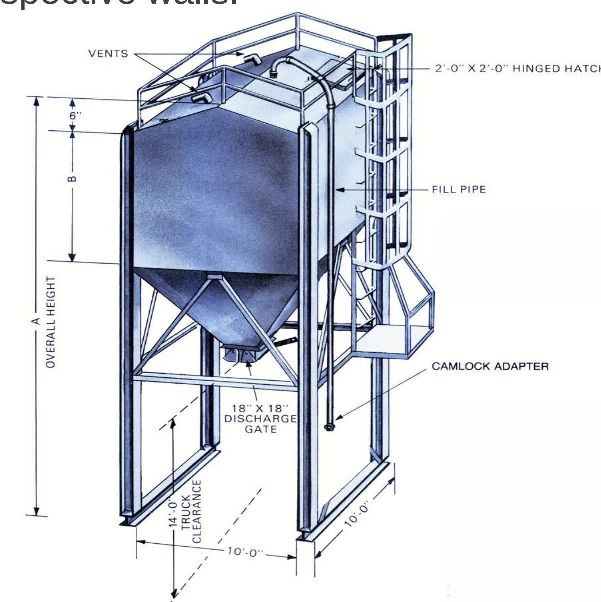
Rail Car

- Typical Dimensions:
  - Length: 58′ (17.7 m)
  - Width: 10′8″ (3.3 m)
  - Height: 15′6″ (4.7 m)
- Weight:
  - 62,000 lb (28,112 kg)

- IMESAFR ignores the mass of the bogies (or assumes they aren't thrown)
- Floor mass is not thrown

Overhead Silo

- 60 ton silo modeled.
- Total weight:
  - 16,500 lb (7,484 kg)
- 33% of each leg will be considered when calculating the amount of debris thrown.
- The considered leg mass is accounted for in the respective walls.



DYNAMIC MASS DISTRIBUTION UPDATED

- As with the airblast model, the explosives properties of AN were considered in detail, primarily the detonation velocity.
- In the AN Engine, the dynamic mass distribution process accounts for the reduced energy available to break the PES apart.
- The ranges of potential loading densities were also considered.
  - The TNT model currently ranges from 0.00162 to 21.1 lb/ft^3.
  - AN can have a loading density as high as 50 lb/ft^3 for a completely full silo or rail car.

AN MASS DISTRIBUTION TABLES

- The loading densities for the AN tables are assigned to the existing test data as shown in the table below.
- The three highest theoretical data rows are not used in the AN Engine.
- The dynamic model functions the same, “hinging” around the ISO-4 data. For this reason, this data row is still considered as the “nominal” for the model.
- Mass distribution for example PES component.

AN loading density (lb/ft^3)	TNT loading density (lb/ft^3)	Source data	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10
0.5	0.00162	Theoretical	94.30%	2.40%	1.70%	1.00%	0.50%	0.30%	0.00%	0.00%	0.00%	0.00%
2	0.0162	Theoretical	93.80%	2.40%	1.70%	1.10%	0.60%	0.30%	0.00%	0.00%	0.00%	0.00%
5	0.162	KG ISO	63.30%	8.70%	5.90%	5.50%	4.50%	3.70%	3.30%	2.50%	1.30%	1.30%
10	0.97	Theoretical	39.60%	13.60%	9.10%	9.00%	7.60%	6.30%	5.80%	4.50%	2.20%	2.20%
20	1.6	ISO-4	33.00%	15.00%	10.00%	10.00%	8.50%	7.00%	6.50%	5.00%	2.50%	2.50%
50	6.5	ISO-2	14.20%	8.30%	7.00%	9.50%	10.30%	14.50%	9.80%	8.50%	8.10%	10.00%
Not used	11.3	Theoretical	7.10%	3.20%	4.70%	5.90%	9.00%	11.20%	18.50%	12.90%	12.10%	15.40%
Not used	16.2	Theoretical	2.50%	1.20%	0.80%	3.80%	5.70%	10.50%	14.10%	23.50%	17.80%	20.10%
Not used	21.1	Theoretical	0.00%	0.00%	0.80%	1.90%	3.60%	5.30%	7.00%	15.80%	27.90%	37.90%

INITIAL VELOCITY

- The initial velocity (IV) of secondary fragments is scaled in the AN Engine to represent the potential of AN to throw fragments at lower IVs than TNT.
- The default option is 0.77. The user can select a less conservative factor of 0.59.
  - The 0.77 factor is based on the ratio of the impulse of AN and TNT.
  - The 0.59 factor is based on the ratio of detonation velocities between AN and TNT.
- The cut-off values used in the TNT Engine are scaled by whichever factor is chosen by the user in the same manner as the IVs themselves are scaled.
- Example: AN Shed PES Initial Velocity Cut-offs:
  - TNT Engine: 3,000 ft/s
  - AN Engine, 0.77: 2,310 ft/s
  - AN Engine, 0.59: 1,770 ft/s

EXAMPLE

This example will show the difference in risk values calculated by the TNT and AN Engines for the same inputs

- The PES is a standard AN Shed
  - Inventory is 88,000 lb (40 tonnes) of AN
  - Activity is AN storage for full year
- The ES is a standard residence
  - Small stud wall house with standard roof and 15% glass
  - The ES is 2,300 ft (700 m) from the PES, on the normal
  - Occupied by a single person all year
- The comparison shown is for the TNT Engine vs. the AN Engine
  - The TNT Engine converts the AN to a TNT NEW
  - The AN Engine treats the AN as AN
    - But at different % yields for the three initiation mechanisms
    - Shock/projectile should be most similar to the TNT results

IMESAFR AN MODULE: EXAMPLE RESULTS

	TNT Engine	An Engine					
		Projectile/Shock Initiation		Contamination		Fire	
		Unreacted Mass Considered	Unreacted Mass Not Considered	Unreacted Mass Considered	Unreacted Mass Not Considered	Unreacted Mass Considered	Unreacted Mass Not Considered
Public Probability of Fatality (E_f)	3.41E-08	1.11E-09	1.11E-09	6.02E-10	6.01E-10	6.30E-10	6.30E-10
Individual probability of Fatality (P_f)	3.41E-08	1.11E-09	1.11E-09	6.02E-10	6.01E-10	6.30E-10	6.30E-10
Adjusted Probability of Event (P_e)	4.99E-06	1.25E-06	1.25E-06	1.20E-06	1.20E-06	2.34E-06	2.34E-06
P_f Overall Given Event	4.16E-03	5.43E-04	5.43E-04	3.06E-04	3.06E-04	1.65E-04	1.65E-04
Risk: Overpressure	2.07E-09	2.07E-09	2.07E-09	2.07E-09	2.07E-09	2.07E-09	2.07E-09
Risk: Glass	6.98E-06	4.46E-06	4.46E-06	6.47E-07	3.32E-07	1.00E-10	1.00E-10
Risk: Building Collapse	1.16E-10	1.16E-10	1.16E-10	1.16E-10	1.16E-10	1.16E-10	1.16E-10
Risk: Horizontal Debris	4.16E-03	5.37E-04	5.37E-04	3.04E-04	3.04E-04	1.64E-04	1.64E-04
Risk: Vertical Debris	8.11E-06	1.36E-06	1.36E-06	1.36E-06	1.36E-06	1.19E-06	1.19E-06

EXAMPLE RESULTS

- The risk values for the scenario are largely as expected.
  - The TNT Engine has the highest risk and highest individual risk contributors (Note that both overpressure and building collapse are at the floor values across the table).
  - The shock/projectile risk results are the highest for the AN Engine.
  - The fire and contamination risks are comparable, fire being lower on consequence but at a higher default event frequency.
  - At the relatively large distance, the unreacted AN mass has almost no effect, as expected.

SUMMARY/CONCLUSIONS

- AN Module is a novel advance in the modelling of AN events
- First non-TNT-based model for AN explosions due to fire, contamination, and shock/projectile impact
- AN engine based on test data and numerical simulation
- Two new PES types developed for IMESAFR
  - Railcar
  - Overhead Silo
- The AN Engine was developed to better model AN explosions
  - The expectation was that risk and consequences would be lower
  - Numerous comparative runs have shown this to be almost always true for consequences and always true for risk due to lower default event frequencies

OTHER IMESAFR-RELATED PAPERS

- Tatom, John W., *IMESAFR Overview*, Minutes of 2018 International Explosives Safety Symposium & Exposition, 6-10 August 2018, San Diego, CA
- McNeill, Shonn, *The IMESAFR Science Panel*, Minutes of 2018 International Explosives Safety Symposium & Exposition, 6-10 August 2018, San Diego, CA
- Hoffman, Joshua, *IME Derailed Debris Collection*, Minutes of 2018 International Explosives Safety Symposium & Exposition, 6-10 August 2018, San Diego, CA