# Estimating Equivalency Of Explosives Through A Thermochemical Approach

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## Abstract

The Cheetah thermochemical computer code provides an accurate method for estimating the TNT equivalency of any explosive, evaluated either with respect to peak pressure or the quasi-static pressure at long time in a confined volume. Cheetah calculates the detonation energy and heat of combustion for virtually any explosive (pure or formulation). Comparing the detonation energy for an explosive with that of TNT allows estimation of the TNT equivalency with respect to peak pressure, while comparison of the heat of combustion allows estimation of TNT equivalency with respect to quasi-static pressure. We discuss the methodology, present results for many explosives, and show comparisons with equivalency data from other sources.

## Introduction

The question of TNT equivalency arises when considering blast effects of different explosives, such as in calculating the maximum quantity of different explosives allowed in a firing chamber designed for a specified quantity of TNT, or rating shipping containers for different explosives.

The definition of TNT equivalency is complex. There are many experimental bases for comparison of explosives, such as heat of combustion (more relevant for quasi-static pressure in confined volumes); heat of detonation (more relevant for peak pressure); detonation energy as measured by brisance, fragmentation tests, plate dent tests, cavity-volume-producing tests, ballistic pendulum tests, or cylinder tests; detonation energy calculated from detonation velocity and density; or detonation and afterburn energy measured by blast pressure. Unfortunately, data to compare many different explosives are not available for most of these tests, and in many cases where data are available the comparisons are not always consistent. An example of this inconsistency is found in Table 3.8 of Cooper[1] where data for the sand crush test, ballistic mortar test, plate dent test, and heat of explosion give TNT equivalencies of C-4 as 116, 130, 115, and 147% respectively.

Because there are so many aspects of TNT equivalency, we must be careful to define the context in which a TNT equivalency value is stated. For the purposes of this work, we will consider two aspects of TNT equivalency:

1) TNT equivalency with respect to peak pressure (short time scale)
2) TNT equivalency with respect to quasi-static pressure in a confined volume (long time scale)

The peak pressure is directly related to the energy released in the detonation, so TNT equivalency with respect to peak pressure can be estimated by comparing the detonation energy of a particular explosive to that of TNT. These energies are not available for many materials, particularly new materials or combinations of materials. The quasi-static pressure in a confined volume is related to the total energy released during complete reaction of the explosive components during detonation and ensuing combustion of detonation products. Therefore the TNT equivalency with respect to quasi-static pressure can be estimated by comparing heats of combustion.

Our considerations of TNT equivalency have been developed primarily in the context of explosions in confined systems such as a firing chamber or a shipping container. Application of the concepts outlined here to other situations such as far-field air blast appear valid, but may require further study.

## Application of Cheetah

As described above, it is difficult to compare detonation energies based on the very limited available empirical data. In addition, although calculation of heat of combustion is conceptually straightforward, the actual calculation may be somewhat involved. We instead turn to the thermochemical code Cheetah [2] to provide this information. The Cheetah code performs thermochemical calculations to evaluate the detonation properties of explosives, such as detonation velocity and pressure and detonation energy as may be measured in a cylinder test; it also calculates the heat of combustion of the explosive. The code contains most standard explosives, and others can be readily added. Cheetah 3.0, recently released by LLNL, does not use any detonation data to calibrate the code, but instead relies on accurate and known chemical and physical properties in calculating the detonation properties. The accuracy of the code for explosives where data exist is about 3%. Since the code does not rely on detonation data, the accuracy for other explosives is expected to be similar. This accuracy is significantly better than the agreement between the different experimental methods outlined above. In addition to this high accuracy, the use of Cheetah also provides a consistent method for comparing different explosives. The combination of accuracy and general applicability to any explosive makes Cheetah attractive for TNT equivalency evaluations. Technical details on the thermochemical calculations used in Cheetah are given in the Cheetah manual. [2]

Cheetah calculates two energy values for a detonation – the "mechanical energy of detonation" and the "thermal energy of detonation", the sum of which gives the "total energy of detonation". The "mechanical energy of detonation" is the energy released during expansion of the detonation products to atmospheric pressure. The "thermal energy of detonation" is the energy remaining in the hot products at atmospheric pressure, and is typically negligible except for situations where there is a high level of solid product formation. To evaluate which is the proper energy to use in TNT equivalencies, we must consider whether the thermal energy remaining in the hot solid products can be released fast enough to feed energy into the blast wave. For detonations in a firing chamber with diameter of a few meters, evaluation of the time scale for thermal energy release from solid products shows that the thermal energy will contribute

to the blast wave (see Appendix A). Therefore, it is appropriate to use the Cheetah "total energy of detonation" in assessing TNT equivalencies.

## TNT equivalency from Cheetah

We ran Cheetah calculations for many common explosives, all calculated at 100% of theoretical maximum density (this is a worst case estimate, and one could use the actual densities for a less conservative analysis). The results are tabulated in Table 1, where we list the calculated total energy of detonation on a volumetric basis and the heat of combustion for each explosive. Also shown are the TNT equivalencies for peak pressure and quasi-static pressure, calculated from:

$$\text{TNT equivalency}_{\text{peak P}} = \frac{\left(\dfrac{\text{HE total energy of detonation, kJ/cc}}{\text{HE density, g/cc}}\right)}{\left(\dfrac{\text{TNT total energy of detonation, kJ/cc}}{\text{TNT density, g/cc}}\right)} \qquad \text{Eq. (1)}$$

and

$$\text{TNT equivalency}_{\text{quasi-static P}} = \frac{\text{HE heat of combustion, cal/g}}{\text{TNT heat of combustion, cal/g}} \qquad \text{Eq.(2)}$$

The TNT equivalencies for peak pressure in Table 1 are reasonably consistent with those in the Department of Defense Explosives Safety Board (DDESB) Blast Effects Computer spreadsheet,[3] and with those in Cooper.[1] The Cheetah code therefore provides a method for estimating TNT equivalency for any explosive that is consistent and repeatable. We note that the TNT quasi-static-pressure equivalencies for the explosives in Table 1 are all less than 1. TNT is carbon-rich, and releases a relatively large amount of energy during combustion as compared to detonation. This results in other explosives with a better oxygen balance showing less combustion, and a lower quasi-static-pressure equivalency. The situation is quite different for aluminized explosives, as described below, which are designed for strong quasi-static-pressure loading.

Two additional points. First, Equations (1) and (2) are written in terms of TNT equivalency. However, using another explosive (e.g. PETN) as a basis for comparison may be done simply by using the properties of that explosive instead of those of TNT in the denominator of the equations. Second, the use of the latest version of Cheetah is suggested (version 3 at this time), since the latest version should have the most accurate calculational algorithms.

## Aluminized explosives

The application of the Cheetah methodology to explosive formulations containing aluminum or other reactive metals may result in an overestimation of the TNT equivalency. This arises because Cheetah assumes complete reaction of the metal in calculating the energy of detonation. In actuality the reaction rate of aluminum in gaseous detonation products may be sufficiently slow (depending on composition and

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temperature of the gaseous products and on particle size and morphology of the aluminum) that the energy from its reaction does not contribute to the intensity of the blast wave. This effect may be accounted for in Cheetah calculations by defining part of the aluminum reactant as inert aluminum.

Calculated TNT equivalencies for several aluminized explosives with different extents of aluminum reaction are shown in Table 2. In many cases the actual extent of the reaction of aluminum is not known. To assess these cases, it is conservative to first assume that all aluminum reacts and contributes to the blast, and to calculate the corresponding TNT equivalency. In most cases this will give a very high TNT equivalency. If experimental blast or performance data are available for a particular explosive, it may be used to estimate the actual extent of aluminum reaction. These results may then be used for related explosives to estimate extent of aluminum reaction and therefore TNT equivalencies, with careful consideration of factors such as the detonation product composition and temperature. Such an analysis is shown in Appendix B using Department of Defense Explosives Safety Board data for aluminized explosives to develop an estimation method for TNT equivalency with respect to peak pressure, based on oxygen balance of the explosive. As data become available, we expect to find that the TNT equivalencies based on quasi-static pressure are significantly higher than those based on peak pressure, since the aluminum is expected to contribute to the final quasi-static pressure but not to the peak pressure of detonation.

## Conclusions

For estimation of TNT equivalency of different explosives with respect to peak pressure or quasi-static pressure, the use of Cheetah to calculate detonation energy for non-aluminized explosives should provide a suitably accurate value of the TNT equivalency. For aluminized explosives, Cheetah calculations assuming full aluminum reaction significantly over-predict the TNT equivalency, and an estimation method such as in Appendix B is needed for improved accuracy.

The analyses in this note were initially developed for consideration of TNT equivalency for dynamic stressing of firing chambers. To extend this methodology to other circumstances, additional considerations must be made:

- For detonations in very small vessels, the time for thermal energy to contribute to detonation energy is reduced, and the use of Cheetah "mechanical energy of detonation" instead of "total energy of detonation" should be re-evaluated using the methodology of Appendix A. For chamber dimensions larger than a few centimeters in diameter, the "total energy of detonation" appears appropriate.

- When short-range airblast without time for afterburn to contribute significantly to blast energy is the concern, the peak pressure equivalency should be appropriate.

- When airblast at long ranges is the concern, there is time for air to mix into detonation products with resultant afterburn and additional energy production. Here the quasi-static pressure equivalency should be appropriate.

## Acknowledgements

## References

1. P.W. Cooper and S.R. Kurowski, *Introduction to the Technology of Explosives*, Wiley-VCH, New York (1996).

2. L.E. Fried, W.M. Howard, P.C. Souers and P.A. Vitello, "Cheetah v 3.0", Lawrence Livermore National Laboratory, UCRL-CODE-2001-010 (2001).

3. M.M. Swisdak, "DDESB Blast Effects Computer Version 4.0", Department of Defense Explosives Safety Board, July 1, 2000.

4. B.M. Dobratz and P.C. Crawford, "LLNL Explosives Handbook: Properties of Chemical Explosives and Explosive Simulants", Lawrence Livermore National Laboratory, UCRL-52997 change 2 (January 31, 1985).

5. T.N. Hall and J.R. Holden, "Navy Explosives Handbook, Explosion Effects and Properties - Part III Properties of Explosives and Explosive Compositions", NSWC, NSWC MP 88-116 (October 1998).

6. H.S. Carslaw and J.C. Jaeger, *Conduction of Heat in Solids*, Clarendon Press, Oxford (1959).

7. R.C. Weast, *CRC Handbook of Chemistry and Physics, 65th edition*, CRC Press, Inc, Boca Raton, FL (1984).

Table 1. TNT equivalencies, based on peak pressure and on quasi-static pressure, for several common explosives as calculated from Cheetah detonation energy and heat of combustion results. The main energetic materials in each formulation are shown in parentheses, details are in the LLNL and Navy Handbooks. [4, 5]

| Compound | Density, g/cc | Total energy of detonation, from Cheetah, kJ/cc | Heat of combustion, from Cheetah, cal/g | TNT equivalency, based on peak pressure (Eq. 1) | TNT equivalenc quasi-static ṛ (Eq. 2 |
|---|---|---|---|---|---|
| TNT | 1.654 | 7.403 | 3474 | 1.00 | 1.00 |
| CL-20 | 2.044 | 12.53 | 1897 | 1.37 | 0.55 |
| PETN | 1.778 | 10.574 | 1823 | 1.33 | 0.52 |
| HMX | 1.905 | 10.995 | 2117 | 1.29 | 0.61 |
| RDX | 1.816 | 10.338 | 2132 | 1.27 | 0.61 |
| TATB | 1.937 | 8.504 | 2734 | 0.98 | 0.79 |
| Explosive D (amm. pic.) | 1.720 | 7.048 | 2627 | 0.92 | 0.76 |
| LX-19 (95% CL-20) | 1.972 | 11.392 | 2103 | 1.29 | 0.61 |
| LX-16 (96% PETN) | 1.781 | 10.052 | 1851 | 1.26 | 0.53 |
| LX-10 (95% HMX) | 1.902 | 10.658 | 2139 | 1.25 | 0.62 |
| C-4 (91% RDX) | 1.728 | 9.348 | 2510 | 1.21 | 0.72 |
| Comp B (63% RDX, 36% TNT) | 1.732 | 8.952 | 2698 | 1.15 | 0.78 |
| A-3 (91% RDX) | 1.621 | 8.352 | 2880 | 1.15 | 0.83 |
| PBX-9502 (95% TATB) | 1.941 | 8.282 | 2674 | 0.95 | 0.77 |
| LX-17 (92.5% TATB) | 1.943 | 8.171 | 2644 | 0.94 | 0.76 |
| ANFO (94% AN) | 1.627 | 6.443 | 962 | 0.88 | 0.28 |

Table 2. TNT equivalencies, based on peak pressure and on quasi-static pressure, for several aluminized explosives as calculated from Cheetah detonation energy results. The extent of aluminum reaction is varied for each explosive. The main energetic materials in each formulation are shown in parentheses, details are in the LLNL and Navy Handbooks. [4,5]

| Compound | Density, g/cc | Percent aluminum reacted in detonation | Total energy of detonation, from Cheetah, kJ/cc | Heat of combustion, from Cheetah, cal/g | TNT equivalency, based on peak pressure (Eq. 1) | TNT equiv; quasi-static |
|---|---|---|---|---|---|---|
| HBX-3 (31% RDX, 29% TNT) | 1.852 | 100% | 18.573 | 4790 | 2.24 | |
| HBX-3 | 1.852 | 50% | 11.224 | 3491 | 1.35 | |
| HBX-3 | 1.852 | 0% | 5.934 | 2193 | 0.72 | |
| Tritonal (70% TNT 70/30) | 1.872 | 100% | 18.571 | 4660 | 2.22 | |
| Tritonal | 1.872 | 50% | 10.524 | 3547 | 1.26 | |
| Tritonal | 1.872 | 0% | 6.099 | 2434 | 0.73 | |
| H-6 (45% RDX, 30% TNT) | 1.762 | 100% | 12.802 | 4009 | 1.62 | |
| H-6 | 1.762 | 50% | 9.363 | 3261 | 1.19 | |
| H-6 | 1.762 | 0% | 6.977 | 2525 | 0.88 | |
| HBX-1 (40% RDX, 38% TNT) | 1.732 | 100% | 11.553 | 3958 | 1.49 | |
| HBX-1 | 1.732 | 50% | 8.933 | 3327 | 1.15 | |
| HBX-1 | 1.732 | 0% | 6.980 | 2696 | 0.90 | |
| Minol-2 (40% AN, 40% TNT) | 1.826 | 100% | 11.753 | 3019 | 1.44 | |
| Minol-2 | 1.826 | 50% | 8.952 | 2277 | 1.10 | |
| Minol-2 | 1.826 | 0% | 6.493 | 1535 | 0.79 | |
| PBXN-109 (64% RDX) | 1.662 | 100% | 11.818 | 4310 | 1.59 | |
| PBXN-109 | 1.662 | 50% | 8.714 | 3568 | 1.17 | |
| PBXN-109 | 1.662 | 0% | 6.433 | 2826 | 0.86 | |

## Appendix A. Analysis of contribution of thermal energy from detonation to blast energy

To assess if thermal energy from detonation can contribute to overall blast, we need to determine if the release of thermal energy is fast enough to contribute to the blast wave as the blast wave travels to the chamber wall. We will consider a shot in the 10-kg spherical tank in the High Explosive Application Facility at LLNL as an example.

### 1. Time constant for thermal energy transfer from hot solids to detonation products

The rate of heat transfer from heated solids to a cooler fluid has been analytically evaluated in H.S. Carslaw and J.C. Jaeger.[6] The behavior in dimensionless form is shown in the figure below, figure 30 on page 241. This analysis considers only the heat transfer within the sphere, assuming that heat transfer to the gas and within the gas is rapid. This is reasonable given the highly turbulent nature of detonation products surrounding the solid detonation product particles.
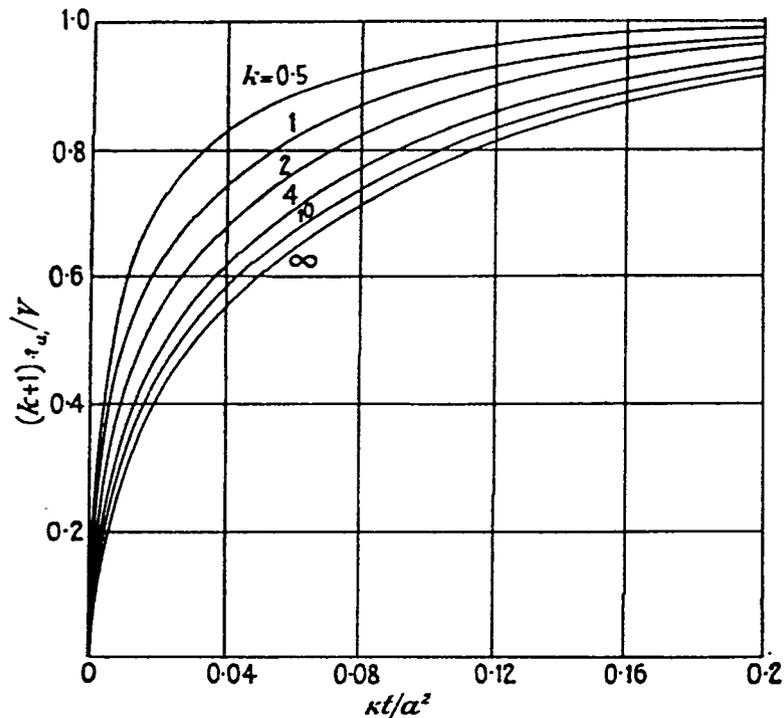
Fig. 30. The rise in temperature of fluid in a calorimeter when a spherical solid is introduced.

Figure A-1. Heat flow from heated solid into cooler surrounding fluid. From Carslaw and Jaeger.[6]

The ordinate represents the dimensionless temperature in the fluid which is being warmed by heat transfer from the hot solid. This dimensionless temperature is proportional to the total energy transferred to the fluid from the solid. The abscissa is defined as $\kappa t/a^2$, where $\kappa$ is the thermal diffusivity of the solid, a is the radius of the solid, and t is the time for the

heat transfer to occur. The thermal diffusivity is defined as $\kappa = \lambda / (\rho\, C_p)$, where $\lambda$ is the thermal conductivity, $\rho$ the density, and $C_p$ the specific heat of the solid.

A representative time constant for heat transfer from solid to gas is the time for 50% of the energy to be transferred from the hot solid to the gaseous products and hence into the blast wave. The figure above shows that the corresponding abscissa value ranges from < 0.01 to ~ 0.04, depending on the value of k, the ratio of specific heat of the fluid to the specific heat of the solid. For the purpose of this analysis, we use the abscissa value representing the slowest heat transfer (longest time), and therefore will evaluate the time where the parameter $\kappa\, t/a^2 = 0.04$ as the time required to deliver 50% of the thermal energy into the gaseous detonation products.

For the case of aluminized explosives, the predominant solid products are carbon (graphite) and aluminum oxide. The relevant properties of these solids are shown in Table A-1.[7] We use room temperature properties as representative, since this analysis is only an approximation. Using these properties, we calculate the time constant for heat transfer from solid to gas, using the relationship $\kappa\, t/a^2 = 0.04$. The results are shown for several particle sizes of graphite and aluminum oxide in Table A-2.

Table A-1. Properties of solid detonation products

| Material | Density, g/cc | Specific heat, J/mole K | Atomic/ molecular weight, g/mole | Thermal conductivity, W/cm K | Thermal diffusivity, cm²/s |
|---|---|---|---|---|---|
| Graphite | 2.3 | 8.8 | 12 | 0.01-0.1 | 0.06 |
| Aluminum oxide | 3.7 | 84 | 102 | 0.07 | 0.02 |

Table A-2. Time to deliver 50% of thermal energy from hot solids into gaseous products

| | Particle diameter | | |
|---|---|---|---|
| Material | 1 μm | 10 μm | 100 μm |
| Graphite | 0.002 μs | 0.2 μs | 20 μs |
| Aluminum oxide | 0.005 μs | 0.5 μs | 50 μs |

From the results in Table A-2, we see that a time of ~ 50 μs is sufficient for effective energy delivery from large solid particles, with much shorter times being required for smaller particles.

## 2. Time constant for thermal energy to contribute to blast energy

Energy from the hot solids is deposited into the gaseous products for ~ 50μs after the detonation. This energy will contribute to the blast intensity up until the time that the blast wave hits the side of the confinement. For the 10-kg spherical tank, the tank diameter is about 16 feet. The speed of sound in air at one atmosphere and room

temperature is ~ 1100 ft/sec, so the time for the blast wave to reach the tank wall is 8/1100 = 0.007 seconds = 7000 $\mu$s. Therefore, energy released during several thousand microseconds after detonation will contribute to the blast energy received by the tank wall.

## 3. Conclusion
The time for release of thermal energy from hot solids into gaseous detonation products is less than 50 $\mu$s. The time for released energy to contribute to blast energy is over 100 times longer. Therefore, there is sufficient time for all thermal energy in hot solid products of detonation to be converted to blast energy.

## Appendix B. Analysis of TNT equivalencies of aluminized explosives

As discussed in the main text, the evaluation of TNT equivalency of aluminized explosives requires an estimation of the extent of aluminum reaction during the relevant time period. The extent of aluminum reaction should be governed by many variables, including aluminum morphology (particles with high surface-to-volume ratio burn faster), detonation temperature (higher temperatures lead to faster burn) and oxygen balance (more oxygen in detonation products leads to greater reaction extent).

In the absence of definitive experimental data for TNT equivalency of aluminized explosives, we turn to the Department of Defense Explosives Safety Board (DDESB) for a set of equivalencies which at least carry the imprimatur of institutional acceptance and long practical application. The DDESB Blast Effects Computer, Version 4.0, dated July 1, 2000, lists TNT equivalencies for several aluminized explosives.[3] These values are shown in Table B-1, along with detonation temperature from Cheetah with complete aluminum reaction. Also included is the explosive oxygen balance (reacting the carbon to CO). No information on particle morphology is available, but it is reasonable to assume that all are standard military grade aluminum. Finally, the Cheetah equivalency assuming all the aluminum reacts is shown in Table B-1, as well as the percent of aluminum reacted in Cheetah to give the TNT equivalency of the DDESB Blast Effects Computer.

Table B-1. TNT equivalency data and related parameters for aluminized explosives

| Explosive | DDESB TNT equivalency | Detonation temperature, 100 % Al reacted (Cheetah), K | Oxygen balance (to CO), % | Cheetah TNT equivalency, 100% Al reacted | % Al reacted in Cheetah calculation to give DDESB TNT equivalency |
|---|---|---|---|---|---|
| HBX-3 | 1.14 | 4585 | 44 | 2.24 | 33 |
| Tritonal | 1.07 | 4594 | 48 | 2.22 | 32 |
| H-6 | 1.35 | 4587 | 67 | 1.62 | 69 |
| HBX-1 | 1.17 | 4425 | 69 | 1.49 | 53 |
| Minol-2 | 1.20 | 4302 | 109 | 1.44 | 65 |

In Table B-1 we see that the DDESB TNT equivalencies are significantly lower than those calculated by Cheetah with 100% aluminum reacted, as we expect. We further see a wide range of variation in the over-prediction, with Cheetah predicting high by 20 to 100% depending on the explosive.

The detonation temperature cannot explain the wide variation in the extent of Cheetah over-prediction, since the temperatures are similar for all these explosives. However, the oxygen balance does correlate with the extent of over-prediction, with the greatest over-prediction occurring for explosives with low oxygen balance. This is chemically reasonable, since in the detonation time frame the aluminum must react with oxygen produced by the detonating explosive. For oxygen-poor explosives there will be relatively little aluminum reaction and Cheetan with full aluminum reaction will greatly over-

predict the energy. For oxygen-rich explosives there will be relatively high aluminum reaction, bringing the Cheetah results more in line with the actual energy. This effect is quantified in the last column in Table B-1, which shows the extent of aluminum reaction in Cheetah that will give the DDESB TNT equivalency. We see that the aluminum reaction is calculated at around 1/3$^{rd}$ in explosives with low oxygen balance (< 50%) and around 2/3$^{rd}$ in explosives with high oxygen balance (> 50%).

From this (very limited) information, we can generate a crude rule of thumb to apply to other aluminized explosives.

> For explosives with oxygen balance > 50%, assume 2/3$^{rd}$ of the aluminum reacts.
> For explosives with oxygen balance < 50%, assume 1/3$^{rd}$ of the aluminum reacts.

We can check the validity of this approximation by comparing it with stress data in firing chamber walls from detonations with TNT and with Tritonal. Strain gauges mounted on the 10-kg spherical tank in HEAF were used to measure strains and calculate peak wall stresses – the data are shown below in Table B-2 (thanks to Roanne Lee of LLNL for providing the data). Also shown are the TNT equivalencies calculated from the stress data normalized by the explosives masses.

Table B-2. Wall stresses measured for explosives shots in the 10-kg spherical tank in HEAF. Stress values are rounded to two significant digits. TNT equivalency is calculated from the stress data and is rounded to 1 significant digit.

| Explosive | Mass, g | Shot date | Stress, strain gauge #1, psi | Stress, strain gauge #2, psi | Average stress, psi | TNT equivalency |
|---|---|---|---|---|---|---|
| TNT | 3008 | 1/8/02 | 13,000 | 15,000 | 14,000 | 100% |
| Tritonal | 3139 | 1/10/02 | 11,000 | 14,000 | 13,000 | 90% |

Tritonal has a low oxygen balance (48%), and our rule of thumb would predict that 1/3$^{rd}$ of the aluminum would react. Cheetah calculations with 1/3$^{rd}$ reactive aluminum and 2/3$^{rd}$ inert aluminum give a TNT peak pressure equivalency of 1.03 for Tritonal. Cheetah still over-predicts the TNT equivalency, but the predicted value is much closer to that determined by the stress data while remaining conservatively high.

An improved approximation will require more blast data. As these become available the above rule of thumb may be modified as appropriate.