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A. L. Kuhl, K. Balakrishnan, J. B. Bell, V. E. Beckner

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Evolution of Thermodynamic States and Species in TNT Explosions

Allen L. Kuhl[1], Kaushik Balakrishnan[2], John B. Bell[2] & Vincent E. Beckner[2]

[1] *Lawrence Livermore National Laboratory*
7000 East Avenue, Livermore, California USA 94551

[2]*Lawrence Berkeley National Laboratory*
1 Cyclotron Road, Berkeley, California, USA 94720

Abstract

Evolution of thermodynamic species and states found in TNT explosions is described. These include species along the CJ isentrope and p=1 isobar of the expanded detonation products, and the species corresponding to stoichiometric combustion of the TNT products with air. These are used to predict the species waveforms in the detonation wave, in the initial expansion of the blast wave, and in the turbulent combustion cloud of a 1-kg TNT explosion. Combined with the temperature field, these species allow one to predict the optical emissions from TNT fireballs.

1. Introduction

The wave structure of explosion field from 1 spherical TNT charge is presented in Fig. 1. The Contact Surface: CS separating the Detonation Products: DP from the air expands at 6 km/s, driving a strong shock: S into the surrounding air. This induces a shock IS which implodes and changes the entropy of the detonation products gases. We label these regions by

- *Region I:* isentropic expansion field of the DP gases
- *Region II:* variable-entropy region of the DP
- *Region III:* re-shocked (~isobaric) field of the DP
- *Region IV:* shock-heated air
- *Region V:* combustion products, centered on the CS (not shown in Fig. 1)

The thermodynamic states and species in the regions are presented in the next section. All states were calculated by the thermodynamic equilibrium code Cheetah [1].

2. Thermodynamic Analysis

2.1 Detonation Products

The fundamentals of the process are represented by the locus of thermodynamic states in the Le Chatelier plane of specific internal energy: u versus temperature T. One starts at the Chapmann-Jouguet point: *CJ* and expands down the isentrope to room temperature, thereby

spawning the function $u(T,S_{CJ})$. This locus is accurately fit by a quadratic function of T, as shown in Fig. 2. The pressure dependence is expressed by a perfect-gas version of JWL function $p = f(\rho,T)_{JWL-PG}$, which accurately fits the values along the CJ isentrope, as shown in Fig. 3.

The species composition along the CJ isentrope: $C_i = f_i(T,S_{CJ})$ is depicted in Fig. 4. As the detonation products expand, an embedded shock implodes and then explodes—thereby changing the entropy of the detonation products (DP) gases [2]. Soon thereafter the DP gases relax to atmospheric pressure; the corresponding species composition $C_i = f_i(T,p=1)$ along the $p=1$ isobar is depicted in Fig. 5.

2.2 Air

The Le Chatelier diagram for air, for temperatures up to 24,000 K is shown in Fig. 6. The curves are fit by the function: $\log(E_i - E_0) = a_i + b_i \cdot (\log T)^{\alpha_i}$. The fitting constants are listed in the following table:

i	ρ/ρ_0	a_i	b_i	α_i
1	10	0.798	0.106	2.37
2	1	0.623	0.128	2.30
3	0.1	0.0595	0.246	1.98

Given the internal energy, this curve fit provides the temperature; pressure is then evaluated from the perfect gas relation.

The species composition of dry air is shown in Fig. 7 as a function of temperature. At 1 electron volt, one can find monatomic nitrogen and oxygen, nitrous oxide along with ions N^+ and NO^+ and the corresponding electron concentrations.

2.3 Combustion Products

The Le Chatelier diagram for combustion of TNT detonation products with air is presented in Fig. 8. Stoichiometric conditions: $\alpha_s = 3.16667$ are assumed. The combustion products species are depicted in Fig. 9. Due to the stoichiometric ratio of ~3, they consist primarily of diatomic nitrogen (~21 moles/kg); combustion products are primarily carbon dioxide, water vapor and carbon monoxide.

3. TNT Explosion Fields

Next we considered a spherical TNT charge; we assumed that the charge was consumed by a constant velocity detonation propagating at the CJ velocity—creating a self-similar wave

structure [3]-[5]. The species concentrations in the detonation wave are shown in Fig.10; species waveforms in the expanding blast wave are presented in Fig. 11. Note the preponderance of carbon graphite and carbon dioxide in the wave. Species profiles in the 1 mm-thick shock-heated air layer are depicted in Fig. 12; these species may be opaque, blocking the emissions from the fireball gases at early times.

Soon the detonation products mix with the shock-heated air forming combustion products gases [6]; a visualization of the turbulent combustion cloud is shown in Fig. 13. Pressure distributions in the fireball are shown at three different times, near the implosion time of ~ 0.9 ms/kg$^{1/3}$ in Fig. 14. The corresponding temperature distributions are shown in Fig. 15. Temperature oscillations are caused by fuel-air pockets burning at the adiabatic flame temperature of ~2,400 K, surrounded by regions of cold air. They are an inherent feature of TNT fireballs; to predict them one needs a direct numerical simulation of the combustion field (i.e., a RANS model will not capture such features).

Profiles along the *x*-axis, of the major species in the turbulent fireball are shown in Fig. 16 at $t = 1.1\, ms/kg^{1/3}$. Concentration fluctuations often follow temperature fluctuations due to combustion. In the outer shell of the fireball ($75 < x(cm/kg^{1/3}) < 150$) at this time, one finds carbon dioxide, water vapor and carbon monoxide. It is these species that will be radiating photons—forming the emission spectrum of the fireball at this time. In the inner shell $x(cm/kg^{1/3}) < 75$), one can observe graphite and carbon dioxide, which are remnants of the detonation process.

4. Conclusions

Species Composition in a TNT fireball depends strongly on time & space. At detonation wave breakout, optical emissions come from: $C_{graphite}, H_2O, CO_2, CO \,\&\, CHNO$. During the initial expansion wave, optical emissions come from the shock-heated air: N_2, O, N, NO. After the shock-heated air becomes transparent, emissions come expanded detonation products: $C_{graphite}, CO_2, CO \,\&\, CH_4$. When the detonation products mix with air, emissions come from combustion products: N_2, O_2, CO_2, H_2O. Given adequate spatial & temporal & spectral resolution, measurements should be able to measure such species concentrations.

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References

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[2] Brode, H.L.: A calculation of the blast wave from a spherical charge of TNT, Rand Report **RM-1965** (1957).
[3] Taylor, G. I., The Dynamics of the Combustion Products behind Plane and Spherical Detonation Fronts in Explosives, *Proc. Royal Society A*, **200**, (1950) pp. 235-247.
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[5] A. L. Kuhl et al. On the structure of self-similar detonation waves in TNT charges, 35th Int. Combustion Symposium, (submitted).
[6] A. L. Kuhl, J. B. Bell, V. E. Beckner, K. Balakrishnan, A. J. Aspden, Spherical combustion clouds in explosions, *Shock Waves* (2013) 23: 233-249.

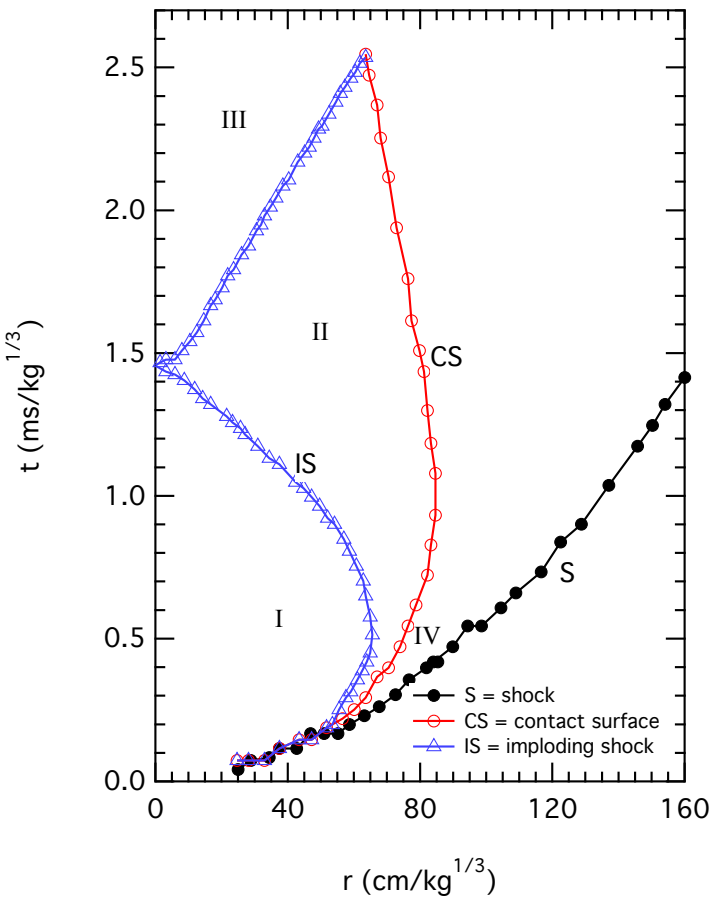

Figure 1. Time-distance diagram for a TNT explosion (Brode, 1957); Region I: isentropic expansion field of DP gases; Region II: variable-entropy region of DP; Region III: re-shocked (isobaric) field of DP; Region IV: shock heated air.

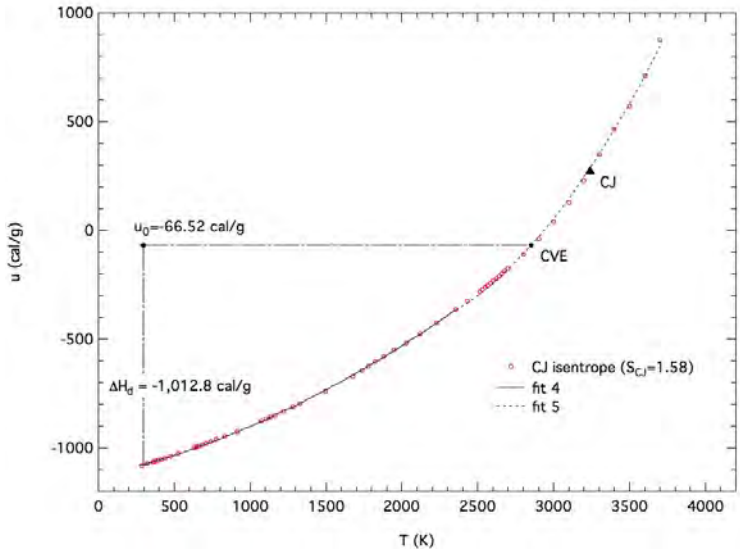

Figure 2. Locus of states of the TNT detonation products expansion along the CJ isentrope in the Le Chatelier plane. Quadratic curve fit are:

- Fit 4: $u(T) = 6.9982 \times 10^{-5} \cdot T^2 + 0.16051 \cdot T - 1{,}131$
- Fit 5: $u(T) = 35.227 \times 10^{-5} \cdot T^2 - 1.2316 \cdot T + 579$

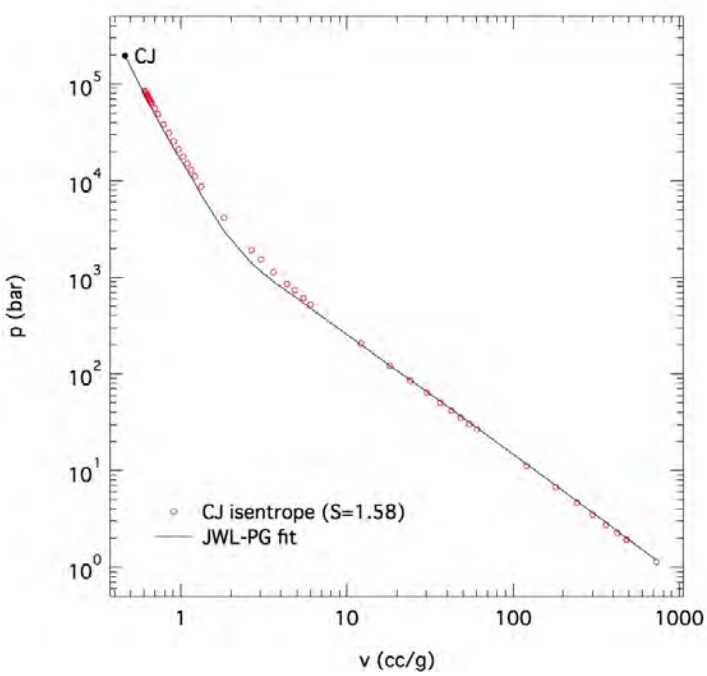

Figure 3. Pressure-Volume diagram for TNT detonation products gases. A perfect gas version of the JWL function was used to fit the computed points:

$$p(\rho,T)_{JWL-PG} = A'\left(1-\frac{\omega\cdot\rho}{R_1\cdot\rho_0}\right)e^{-R_1\cdot\rho_0/\rho} + B\left(1-\frac{\omega\cdot\rho}{R_2\cdot\rho_0}\right)e^{-R_2\cdot\rho_0/\rho} + \rho R_u T / M_{DP}$$

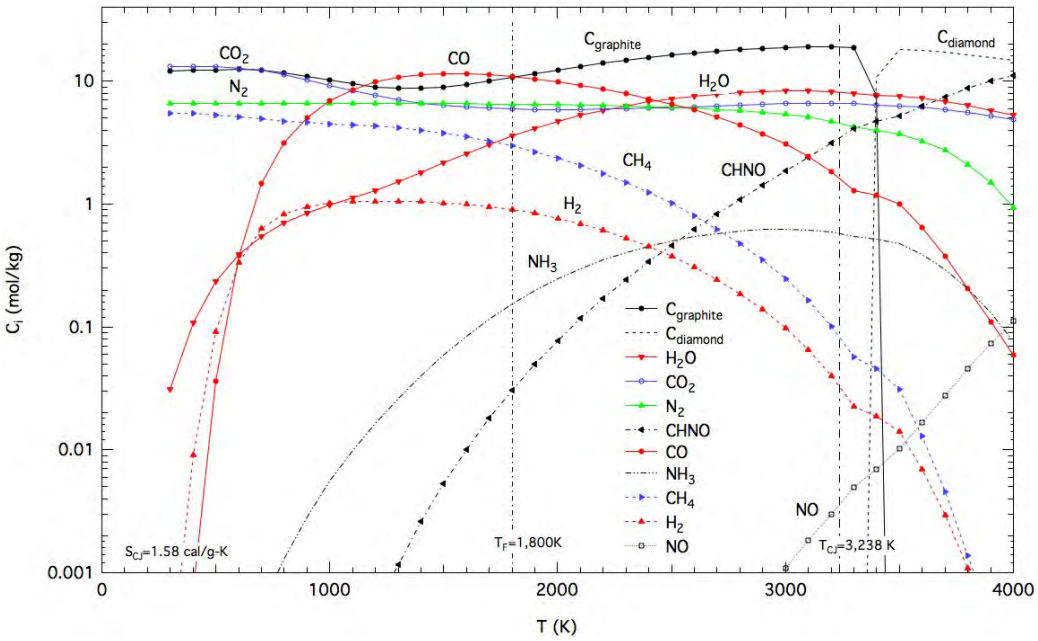

Figure 4. TNT detonation products species along the CJ isentrope.

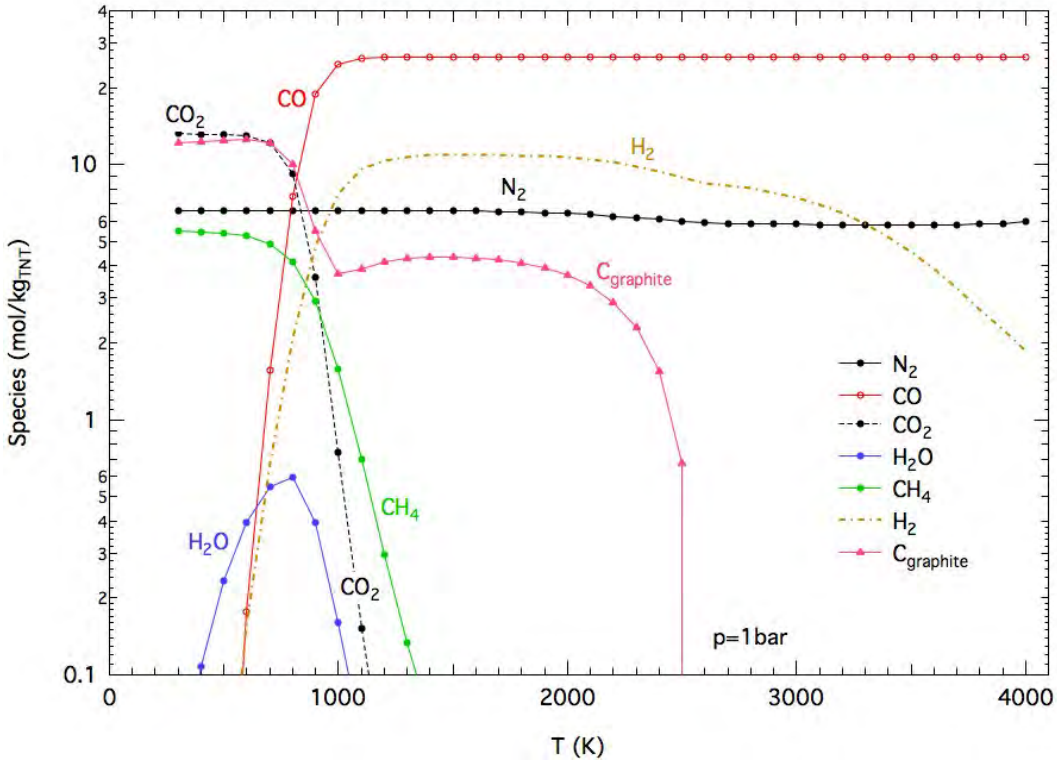

Figure 5. TNT detonation products species along the p = 1 isobar.

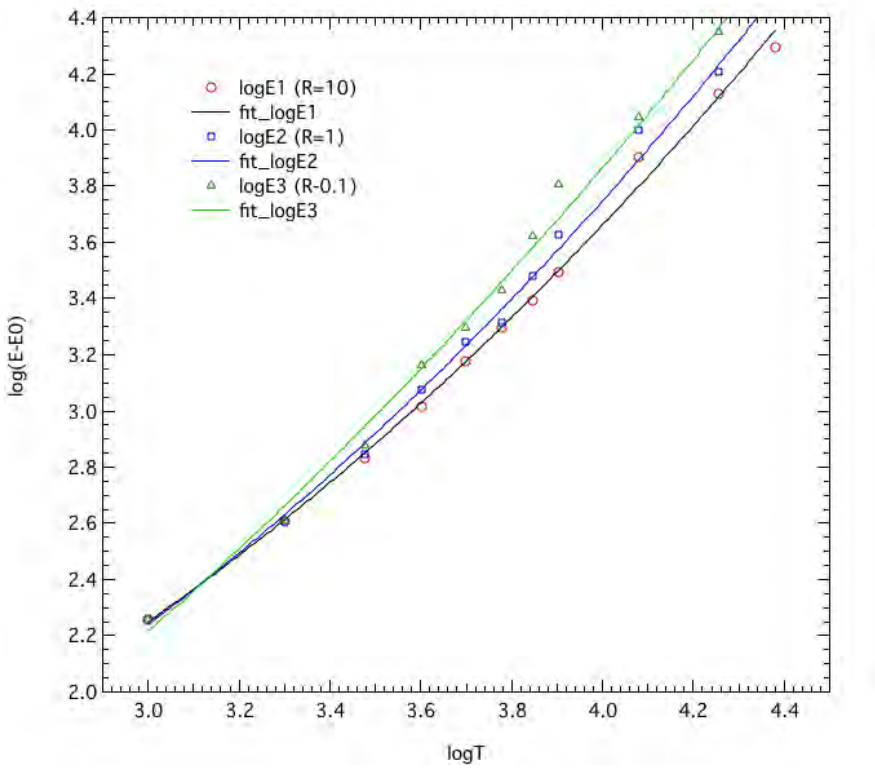

Figure 6. Le Chatelier diagram for air up to 24,000 K (Gilmore 1957); curve fit:

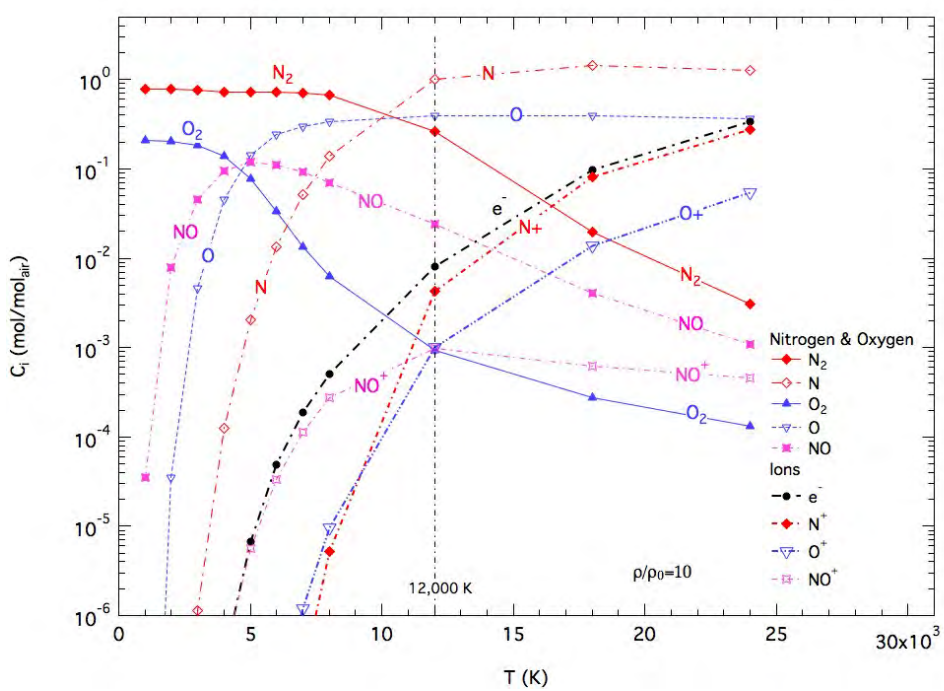

Figure 7. Equilibrium composition of dry air as a function of temperature.

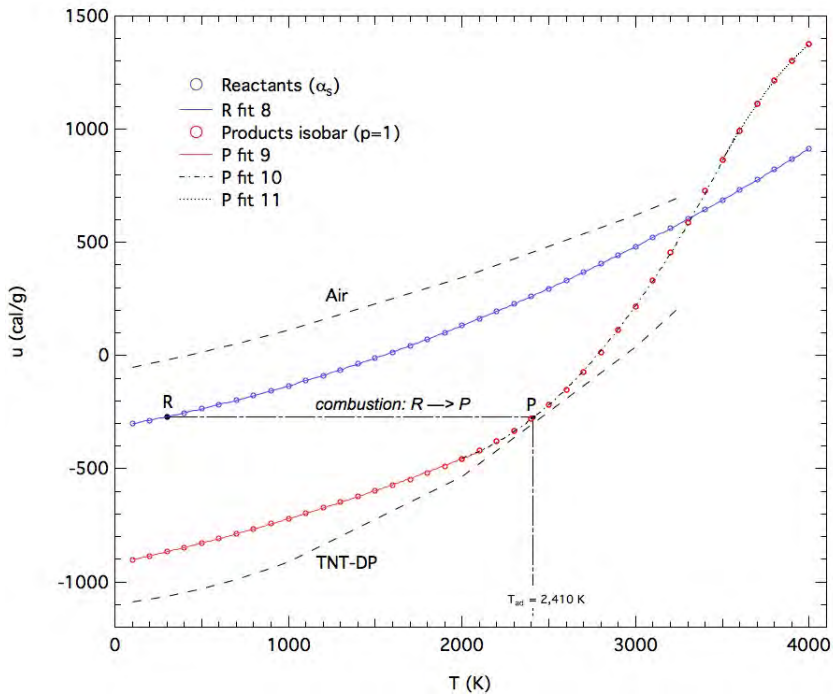

Figure 8. Le Chatelier diagram for combustion of TNT products in air under stoichiometric conditions ($\alpha_s = 3.16667$) at one atmosphere. Quadratic curve fits are:

- Fit 8: $u(T) = -315.89 + 0.1401 * T + 4.1885 \times 10^{-5} * T^2$
- Fit 9: $u(T) = -919.17 + 0.16435 * T + 3.35910^{-5} * T^2$
- Fit 10: $u(T) = 619.75 - 1.3427 * T - 0.000403 * T^2$
- Fit 11: $u(T) = -12{,}838 + 6.4407 * T - 0.000722 * T^2$

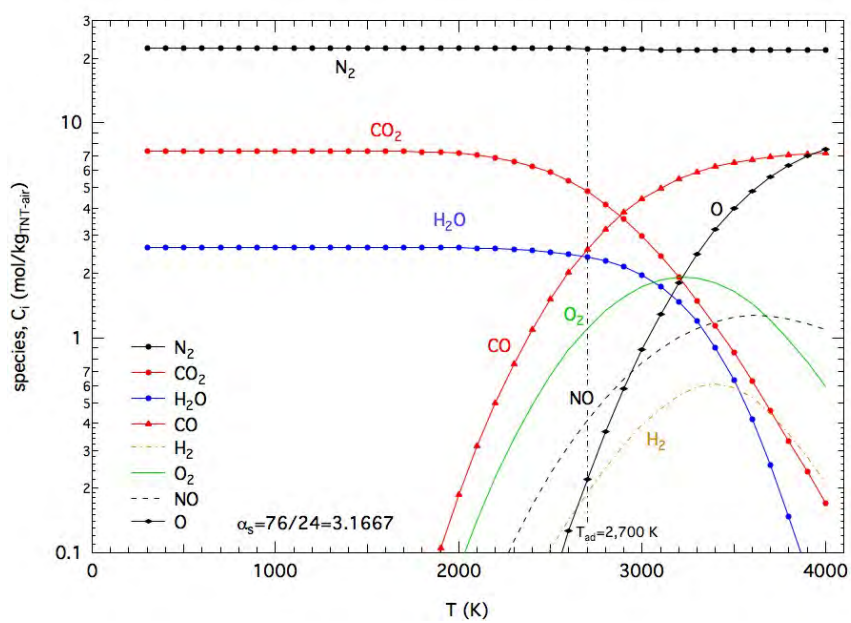

Figure 9. TNT-air combustion products species under stoichiometric conditions α_s & $p = 1$ bar.

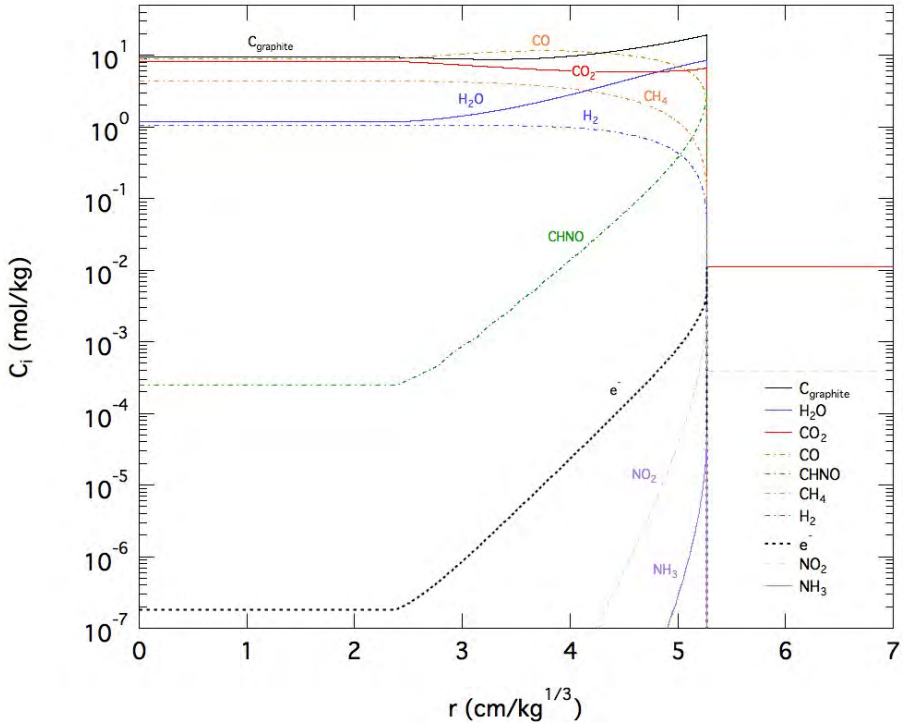

Figure 10. Species concentrations in the detonation wave of a spherical TNT charge.

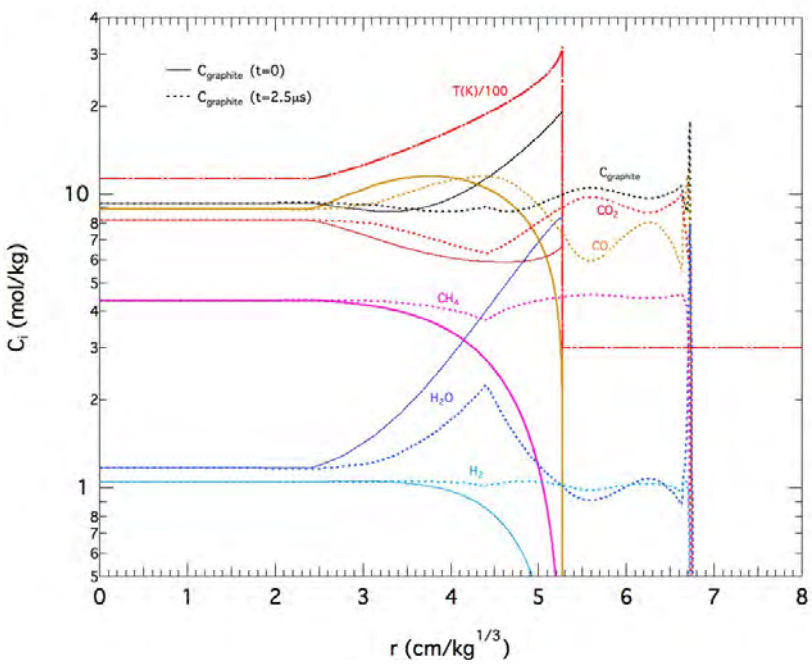

Figure 11. Species waveforms in the TNT detonation products gases at $t = 0$ and 2.5 μs in a spherical detonation.

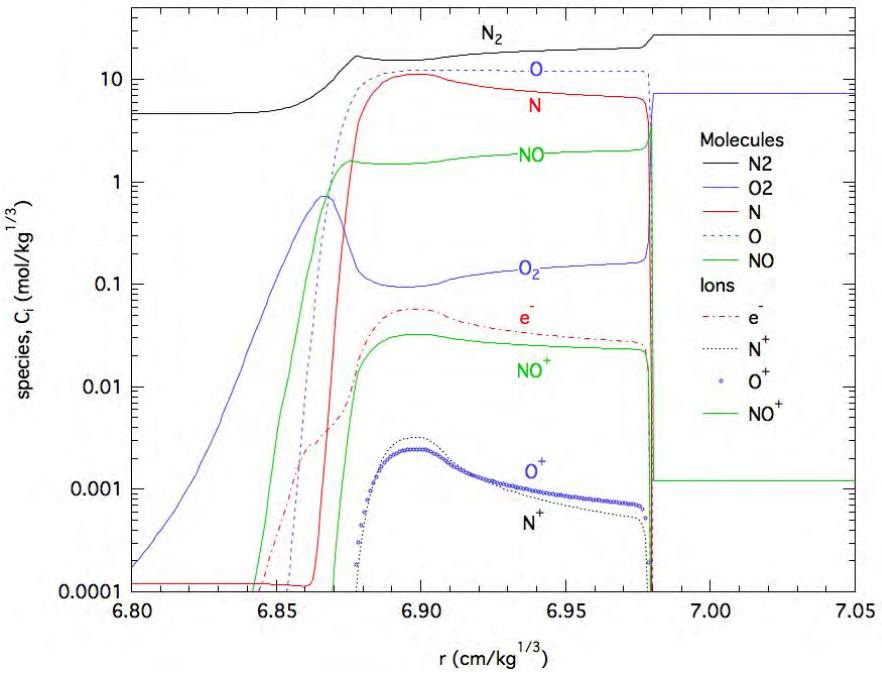

Figure 12. Species profiles in the shock-heated air region at $2.5\ \mu s$.

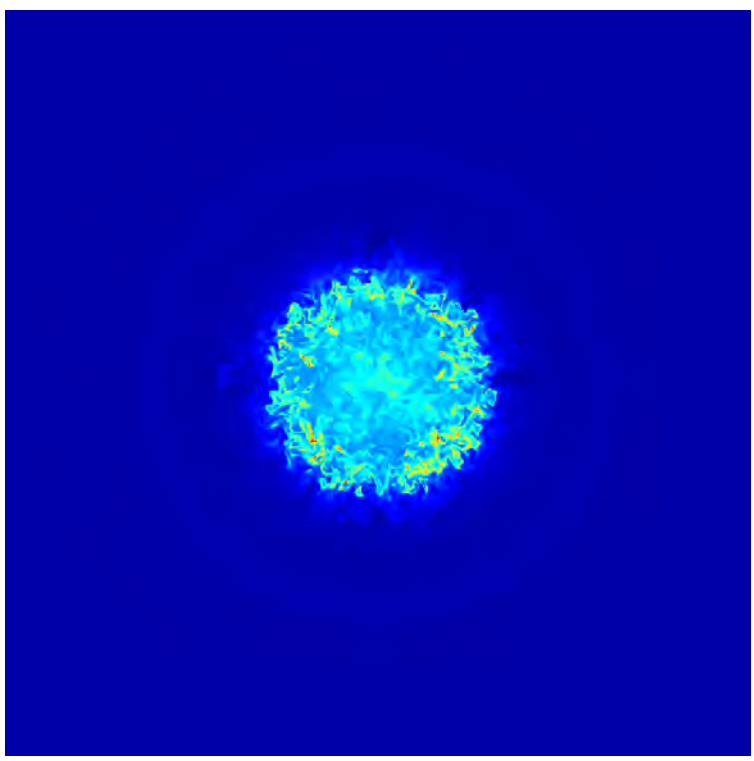

Figure 13. Visualization of the turbulent combustion cloud in a TNT explosion ($D \sim 3$ m).

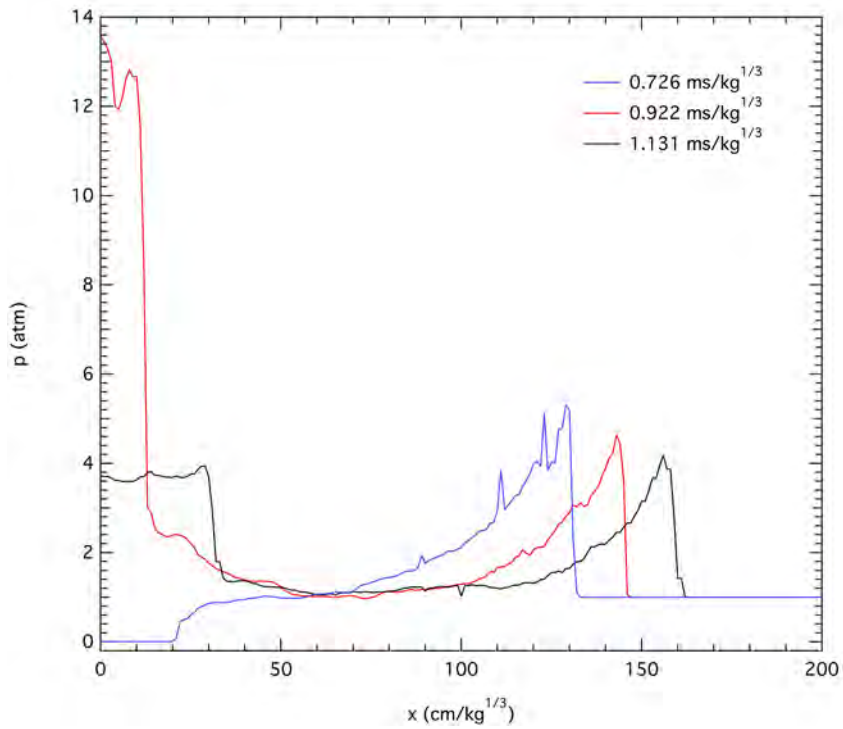

Figure 14. Pressure distributions in the turbulent combustion fireball of a TNT explosion near the implosion time: $t \sim 0.9\ ms / kg^{1/3}$.

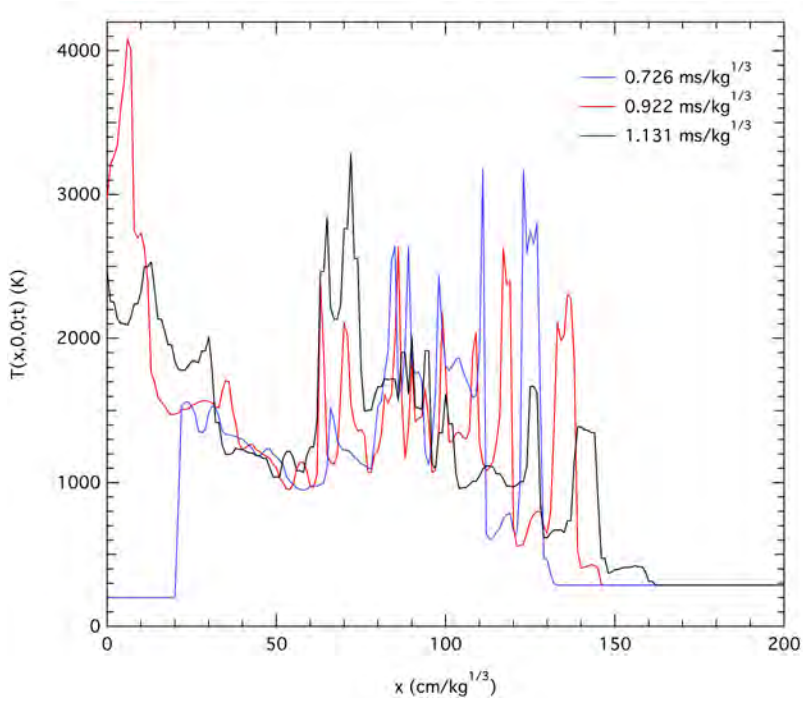

Figure 15. Temperature distributions in the turbulent combustion fireball of a TNT explosion near the implosion time: $t \sim 0.9\ ms / kg^{1/3}$.

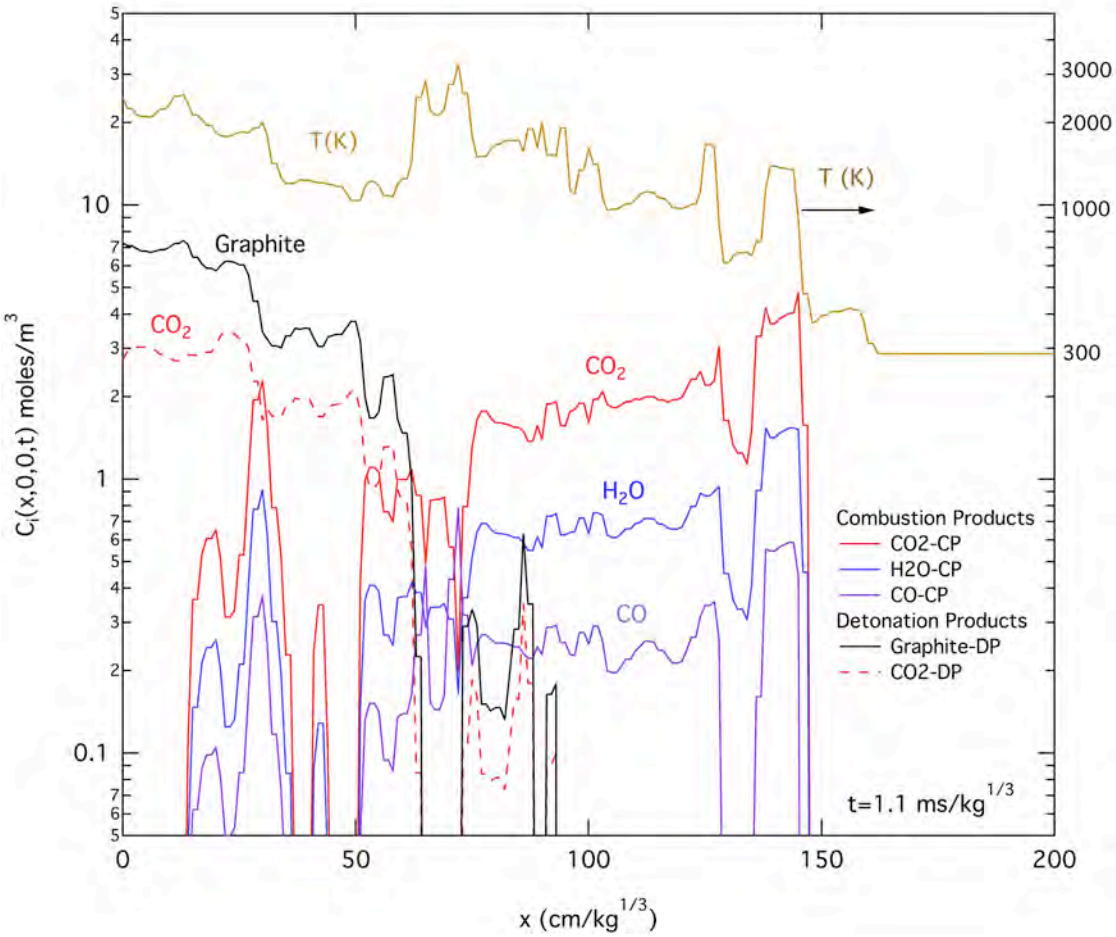

Figure 16. Major species profiles in the turbulent combustion fireball of a TNT explosion at $t = 1.1\ ms/kg^{1/3}$. Diatomic nitrogen and oxygen are also significant (~ 33 and ~ 9 moles/m^3), but are not presented in this figure, so as to focus on combustion species.