

Combustion of TNT Products in a Confined Explosion

A. L. Kuhl
Lawrence Livermore National Laboratory
Livermore, California, USA 94550

R. E. Ferguson
Krispin Technologies Inc.
Rockville, Maryland, USA 20850

R. Spektor & A. K. Oppenheim
University of California
Berkeley, California, USA 94720

Effects of turbulent combustion induced by explosion of a 875-g cylindrical charge of TNT in a 16.6 m³ chamber filled with air, are investigated. The detonation wave in the charge transforms the solid explosive ($C_7H_5N_3O_6$) to gaseous products, rich (~20% each) in carbon dust and carbon monoxide. The detonation pressure (~210 kb) thereby engendered causes the products to expand rapidly, driving a blast wave into the surrounding air. The interface between the products and air, being essentially unstable as a consequence of the strong acceleration induced by the blast wave, evolves into a turbulent mixing layer—a process enhanced by shock reflections from the walls (Fig. 1). Under such circumstances rapid combustion takes place where the expanded detonation products play the role of fuel. Its dynamic effect is manifested by the experimental measurement of a 3-bar pressure increase in the chamber, in contrast to a 0.8-bar increase for a TNT explosion in nitrogen (Fig. 2). Such pressure enhancements are consistent with a “*Heat of Combustion*” = 3575 Cal/g versus a “*Heat of Detonation*” = 1093 Cal/g, as measured in a bomb calorimeter by Ornellas^[1].

The experiments were modeled as turbulent combustion in an unmixed system at large Reynolds, Peclet and Damköhler numbers.^[2,3,4] The three-dimensional CFD solution was obtained by a high-order Godunov scheme^[5] using an Adaptive Mesh Refinement—AMR^[6] to trace the turbulent mixing on the computational grid in as much detail as possible. The calculated pressure histories were in good agreement with the measurements (vid. Fig. 2)—thereby demonstrating that model faithfully reflects the controlling mechanism of exothermic energy deposition: turbulent mixing.

The evolution of the calculated mass fraction of fuel consumed by combustion is presented in Fig. 3. It starts with a finite burning rate (associated with the finite area of the fuel surface) followed by an exponential decay. Fuel consumption is well approximated by the “*Life Function*”^[7] (also known as a “*Vibe Function*”^[8]):

$$\mathbf{x}(t; \lambda, n, T) = \frac{e^{\zeta(t)} - 1}{e^{\lambda/(n+1)} - 1} \quad (1)$$

where $\zeta(t) = \lambda[1 - (1 - t/T)^{n+1}]/(n+1)$. Regression analysis was used to establish the fitting parameters that gave a good approximation to the calculated burning curve $\{\lambda = 46; n = 49; T = 300 \text{ ms}\}$.

The corresponding burning rate is:

$$\mathbf{x}'(t; \lambda, n, T) = \frac{\lambda (1 - t/T)^n e^{\zeta(t)}}{T e^{\lambda/(n+1)} - 1} \quad (2)$$

which represents the “Kinetic Equation” for the turbulent combustion process^[9].

The results reveal the dynamics of a combustion process in which the exothermic energy deposition is controlled by fluid-mechanic transport (convective mixing) in a highly-turbulent field^[10], in contrast to the conventional reaction-diffusion mechanism of laminar flames as proposed by Zel’dovich & Frank-Kamenetzki^[11] in 1938.

References

- [1] Ornellas, D. L., *Calorimetric Determination of the Heat and Products of Detonation for Explosives: October 1961 to April 1982*, Lawrence Livermore National Laboratory, **UCRL-52821**, Livermore, CA, 1982.
- [2] Zel'dovich, Ya. B., Barenblatt, G. I., Librovich, V. B., and Makhviladze, G. M., *The Mathematical Theory of Combustion and Explosions*, trans. by D. H. McNeill, Consultants Bureau of Plenum Publishing, New York 1985, xxi + 597 pp {vid. esp. Ch. 6: "Gasdynamics of Combustion", pp. 450-452}.
- [3] Shchelkin, K. I., and Troshin, Ya. K., *Gasdynamics of Combustion*, trans. by B. W. Kuvshinoff and L. Holschlag, Mono Book Corp., Baltimore, MA 1965, x + 222 pp.
- [4] Kuhl, A. L., Ferguson, R. E., and Oppenheim, A. K., "Gasdynamic Model of Turbulent Exothermic Fields in Explosions", *Advances in Combustion Science—in Honor of Ya. B. Zel'dovich*, edited by A. N. Merzhanov, L. DeLuca and W. A. Sirignano, *Prog. in Astro. & Aero. Series*, **173**, AIAA, Wash., DC 1997, pp. 251-261.
- [5] Colella, P. and Glaz, H. M., "Efficient Solution Algorithms for the Riemann Problem for Real Gases", *J. Computational Physics*, **59** (2), 1985, pp. 264-289.
- [6] Bell, J. B., Berger, M., Saltzman, J., Welcome, M., "Three-Dimensional Adaptive Mesh Refinement for Hyperbolic Conservation Laws," *SIAM Journal on Scientific and Statistical Computing*, **15** (1), 1994, pp. 127-138.
- [7] Oppenheim, A. K., and Kuhl, A. L., "Life of Fuel in an Engine Cylinder", SAE paper **980780**, Society of Automotive Engineers, 10 pp., 1998.
- [8] Vibe, I. I., "Semi-Empirical Expression for Combustion Rate in Engines", *Proceedings of Conference on Piston Engines*, USSR Academy of Sciences, Moscow, pp. 185-191, 1956.
- [9] Oppenheim, A. K., Spektor, R., and Kuhl, A. L., "Thermostatics and Thermokinetics of Closed Combustion Systems", *17th ICDERS Book of Abstracts*, University of Heidelberg, 1999.
- [10] Kuhl, A. L., and Oppenheim, A.K., "Turbulent Combustion in the Self-Similar Exothermic-Flow Limit", *Advanced Computation and Analysis of Combustion*, Edited by G. D. Roy, S. M. Frolov and P. Givi, ENAS Publishers, Moscow, 1997, pp. 388-396.
- [11] Zel'dovich, Ya. B., and Frank-Kamenetzki, D. A., "A Theory of Thermal Propagation of Flame", *ACTA Physico-Chimica URSS*, **9** (2), 1938, pp. 341-350.

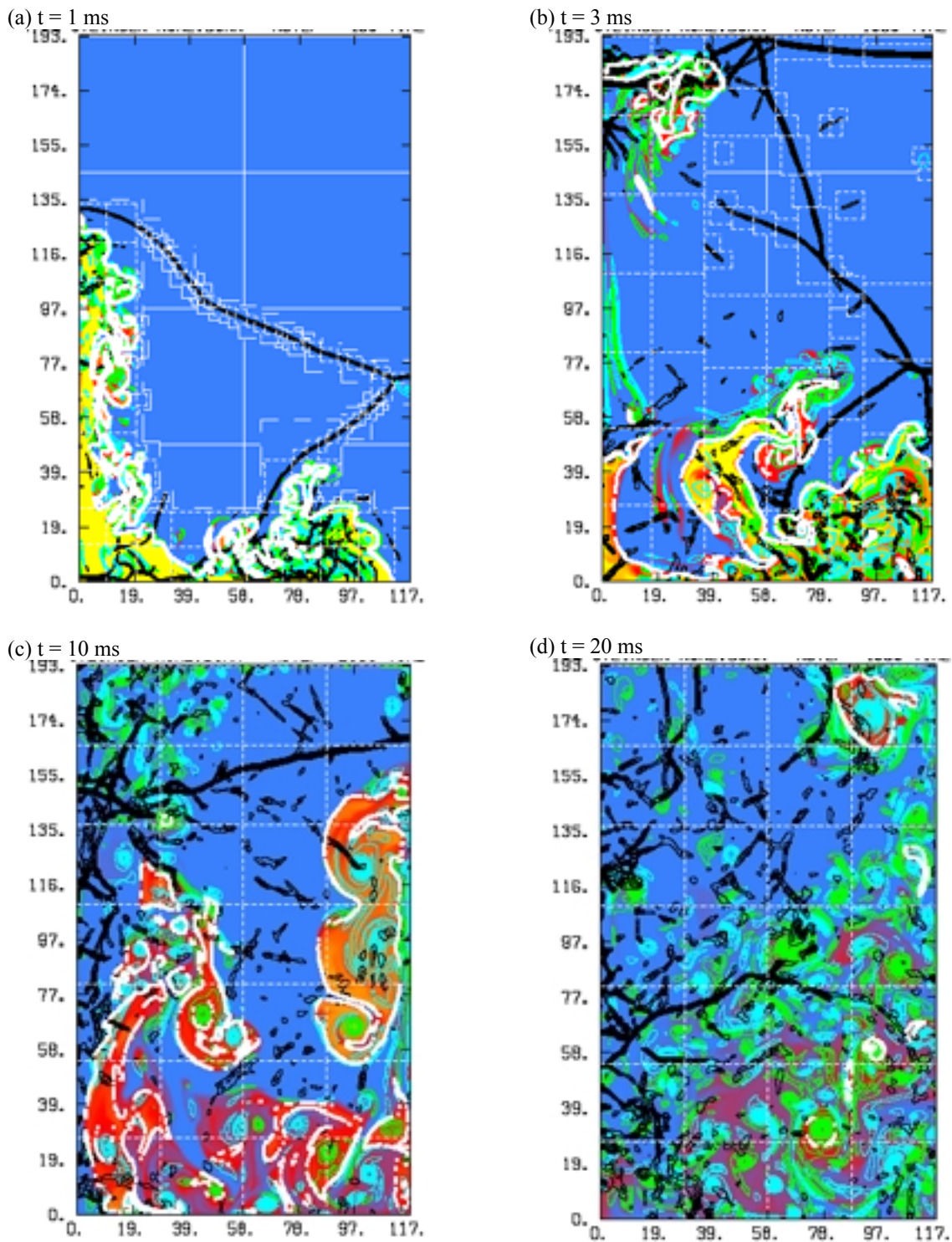


Figure 1. AMR simulation of the explosion of a 875-g cylindrical TNT charge in a 16.6-m^3 chamber filled with air at atmospheric pressure. TNT detonation products (shown in *yellow*), mix with air (depicted as *blue*) thereby forming combustion products (represented as *red*). Exothermic cells are marked by *white* dots. Vorticity contours are *green* (negative) and *turquoise* (positive), while dilatation contours are *black*.