Combustion of TNT Products in a Confined Explosion

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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]):

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

The corresponding burning rate is:

$$\mathbf{x}'(t;\lambda,n,T) = \frac{\lambda}{T} \frac{(1-t/T)^n e^{\zeta(t)}}{e^{\lambda/(n+1)} - 1}$$
(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-Kamenetzkii^[11] in 1938.

References

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Figure 1. AMR simulation of the explosion of a 875-g cylindrical TNT charge in a 16.6-m³ 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*.



Figure 2. Over-pressure history from the 3D-AMR simulation (run 1) of a TNT explosion and combustion in air compared with TNT experiments in air and nitrogen atmospheres.



Figure 3. Mass-fraction burned, μ , and burning rate, μ' , from 3D AMR simulations of turbulent combustion of TNT products in air (Δ = mesh size, δ = initial charge perturbation, $\lambda \& n$ are parameters of the Life Function **x**).