



# Thermochemistry of the combustion of gas phase and condensed phase detonation products in an explosive fireball



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## ABSTRACT

This paper uses the thermochemical behaviour of reacting species to differentiate between the combustion of gas phase and condensed phase detonation products in the fireball of an explosion. Experiments were carried out involving the detonation 15 g charges of C-4 and Detasheet-C explosives in a closed vessel. The initial partial pressure of oxygen in the vessel was varied in order to control the extent of the secondary afterburn reactions, and the total heat release was measured using the calorimeter that contained the closed vessel. A simple model that independently describes the evolution of heat from the gas phase and condensed phase detonation products as a function of oxygen consumption was developed, and was used to show that condensed phase products react much more effectively in the fireball than gas phase reactions, because the transport properties of particulates entrained in a turbulent flow gives them an advantage when it comes to the manner in which they mix with the surrounding air. An additional set of trials employing the entrainment of an external combustible material further confirms the importance of particle combustion in explosive fireballs.

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## 1. Introduction

When high explosives are detonated, they often produce energetic, secondary fireballs. In many cases, the proportion of the total combustion energy released, assuming the detonation products could react completely with air, could exceed what would be liberated during the initial detonation. For example, with C-4, the heat of detonation is only 44% the total heat of combustion, and for Detasheet-C, it is only 32% [1].

$$\Delta H_{c,x} = \Delta H_{d,x} + \Delta H_{ab,x} \quad (1)$$

The mechanical energy carried away by the blast has been the traditional focus of explosives research, because it is this portion that does the useful work in civil, mining, or military applications. However, with the advent of thermobaric charges and enhanced blast weapons, where the afterburn reactions that occur behind the initial shock wave can sustain the duration of the positive impulse phase of a blast, the phenomena associated with the fireball have become increasingly important [2].

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Considerable advances have been made in recent years in describing the dynamic energy release that occurs in the fireball. In the work by Balakrishnan [3,4], in particular, modern computational techniques have been applied in order to describe the fireball mechanics in 3 dimensions, building on previous work by Brode [5], Ansimov and Zeldovich [6], and Kuhl et al. [7]. Frost et al. [8] also attempted to model the expansion, instabilities, and turbulent mixing of the fireball while investigating heterogeneous explosives, where reactive particulates were suspended in an explosive matrix and detonated.

However, in terms of homogeneous explosives, the interrelationship between transport and chemical reaction, and how they may differ between different types of reacting species, has largely been neglected. The complex mixing models developed by Balakrishnan, for example, have largely assumed that the afterburn is entirely transport-controlled, with infinitely fast reaction kinetics and no differentiation between different chemical species [3,4]. McNesby et al. [9], on the other hand, considered the kinetics of the afterburn reactions, but modelled them as a spatially homogeneous system without taking into account mixing and transport, and with no mention of the behaviour of the condensed phase carbonaceous soot.

In either case, the important distinction between the combustion of gas phase species (e.g., CO, H<sub>2</sub>, CH<sub>4</sub>, NH<sub>3</sub>, etc.), and condensed phase species (e.g., carbonaceous soot), has not been taken into account, and the present work aims to show that

**Nomenclature**

<b>A</b>	matrix relating reaction extent vector to vector of oxygen-weighted and energy-weighted total reaction extents	<i>Greek</i>	
<i>a</i>	ratio of oxygen stoichiometry coefficients	$\eta$	energy-weighted total reaction extent
<i>b</i>	ratio of heats of reaction	$\nu$	stoichiometric coefficient
$C_c$	Cunningham slip correction factor	$\xi$	individual reaction extent
$D$	diffusivity ( $\text{m}^2 \text{s}$ )	$\xi$	vector containing individual reaction extents
$d_p$	particle diameter	$\mu$	dynamic viscosity (Pa s)
$E_r$	total rotational kinetic energy of a turbulent eddy (J)	$\rho$	density ( $\text{kg m}^{-3}$ )
<i>f</i>	fractional rate at which oxygen is consumed in gas phase reactions	$\tau$	relaxation time of a particle
$f_m$	mass fraction of combustible detonation products	$\chi$	oxygen-weighted total reaction extent
$\Delta H_{ab}$	heat of afterburn ( $\text{kJ mol}^{-1}$ )	$\omega$	angular velocity of a turbulent eddy ( $\text{rad s}^{-1}$ )
$\Delta H_c$	heat of combustion ( $\text{kJ mol}^{-1}$ )		
$\Delta H_d$	heat of detonation ( $\text{kJ mol}^{-1}$ )	<i>Subscript</i>	
$\Delta H_r$	heat of reaction ( $\text{kJ mol}^{-1}$ )	<i>c</i>	condensed phase
<i>j</i>	mass flux ( $\text{kg m}^{-2} \text{s}^{-1}$ )	<i>crit</i>	critical transition point
$k(\ell)$	specific turbulent kinetic energy at length scale $\ell$ ( $\text{m}^2 \text{s}^{-2}$ )	<i>d</i>	molecular diffusion
$\ell$	length scale (m)	<i>dt</i>	duct tape
<i>n</i>	moles of reacting species (mol)	<i>g</i>	gas phase
$\Delta n$	moles consumed by reaction (mol)	<i>i</i>	initial
<i>Q</i>	heat release (kJ)	<i>k</i>	Kolmogorov
<i>R</i>	radius of curvature for a circulating flow (m)	<i>meas</i>	measured
<i>r</i>	rate of reaction ( $\text{mol s}^{-1}$ )	$\text{O}_2$	oxygen
<i>v</i>	effective interfacial mixing velocity ( $\text{m s}^{-1}$ )	<i>p</i>	particle
$v_t$	tangential velocity of a circulating flow ( $\text{m s}^{-1}$ )	<i>x</i>	explosives
		<i>Superscript</i>	
		*	at stoichiometry

nuances in the way that particulates mix in the turbulent flow gives them an advantage that allows them to react with oxygen at considerably higher rates than gas phase species.

## 2. Gas-particle mixing in a turbulent environment

In a turbulent flow, as would be encountered in a fireball, the gases mix together because of turbulent shear. High shear at the interface between detonation product gases and air makes the flow unstable, and causes mixing analogous to a Kelvin-Helmholtz instability [10]. This results in circulation between the two interfaces. For the gas phase reactions to occur, intimate molecular contact between species is required, and on the micro-scale the only way to achieve this is through molecular diffusion. Bulk phase mixing occurs, and the gas phase reactions would, of course, occur along the interface between gases, but the ingress of species into the opposite phase, and therefore the thickness of the reaction zone, would be limited by molecular diffusion.

Particulates, on the other hand, have a mass, and have inertia relative to the gas in which they are suspended, and in an accelerating flow (i.e., when the gas flow makes a turn), they will deviate from the streamlines of the flow based on their relaxation time,  $\tau = \rho_p d_p^2 C_c / 18 \mu$  [11,12]. This means that particulates can get thrown out of the carrier gas, and cross fluid–fluid boundaries as illustrated in Fig. 1. In turbulent flow fields, particles are known to be strongly influenced by small scale turbulence, and can exhibit erratic flow paths and be subject to intense accelerations as a result [13]. As the gases mix together, particles will escape from the detonation products and cross into the air. This allows them to come into contact more efficiently with oxygen compared to molecular diffusion, which allows for a much thicker reaction zone, and thus enhances the rate at which they are consumed.

To express this in more formal terms, the radial velocity of a particle in a circulating fluid is based on the tangential velocity of the gas, as well as the radius of curvature of the circulation [11,12]. This defines the speed at which particles deviate from the streamlines of the gases, and as such the speed at which they can ingress into more oxygen-rich regions.

$$v_p = \tau \frac{v_t^2}{R} \quad (2)$$

The relaxation time,  $\tau$ , contains all of the information about the particle transport properties, including particle size and density, drag, and fluid viscosity. The circulation of the fluid is a manifestation of the turbulence of the flow, and so one would expect the particulates' radial velocities to be a function of both the turbulent kinetic energy and turbulent length scale. To get an idea of the general behaviour of particulates in turbulence, consider an aerosol-laden cylindrical eddy rotating like a rigid body with an angular velocity  $\omega$ . The outward radial velocity of the particulates could then be expressed by:

$$v_p = \tau R \omega^2 \quad (3)$$

The rotational kinetic energy of the cylindrical eddy, with radius  $R$  and length  $h$  would therefore be:

$$E_r = \frac{\pi}{4} \rho_g h R^4 \omega^2 \quad (4)$$

The turbulent kinetic energy of a fluid is contained in the rotational energy of individual eddies rotating over a spectrum of different length scales, and so normalizing Eq. (4) by the mass of the cylindrical eddy would essentially give its contribution to the turbulent kinetic energy for an eddy of a particular size.

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