# Pressure Diagnostics of Combustion Following an Explosion

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The exothermic process of combustion following a detonation of an explosive charge in a closed vessel filled with air generates a significant amount of pressure. The task of pressure diagnostics is to solve an inverse problem: deduction of the effectiveness with which fuel was utilized in the course of the dynamic stage of combustion engendering the pressure, and the concomitant changes in the thermodynamic state of the system and its components, from pressure transducer records. The paper presents the chemical and thermodynamic background and numerical solution of such an inverse problem, evaluated on the basis of measured pressure profiles and mass spectroscopic data obtained from preliminary tests of explosion in nitrogen, instead of air, to establish the chemical composition of fuel. Specifically, the data for the case at hand were provided by explosion tests involving a charge of ~0.9 kg of TNT in an ~17 $m^3$ enclosure filled with air.

## Chemical background

The tests for pressure diagnostics were carried out with 875 gm of TNT, contained in a cylindrical vessel 16.6 $m^3$ in volume, filled with 20 kg of air at a pressure of ~1 bar and a temperature of ~300K. The chemical composition of fuel was determined from preliminary tests carried out with nitrogen, instead of air, by mass spectroscopic measurement of the products of TNT explosion in such an inert atmosphere. Data of this kind are, as a rule, incomplete, in that they do not include the concentrations of C, $H_2O$ and $N_2$. Their mass fractions have to be deduced, therefore, from a stoichiometric balance for chemical reactions taking place in the course of explosion. Its global expression is as follows:

$$C_7H_5N_3O_6 + \nu_nN_2 = \nu_1CO_2 + \nu_2CO + \nu_3CH_4 + \nu_4H_2 + \nu_5O_2 + \nu_6N_2 + \nu_7C + \nu_8H_2O \tag{1}$$

or, in terms of the measured mole fractions, $X_{oi}$,

$$C_7H_5N_3O_6 + \nu_nN_2 = \alpha\,[X_{o1}CO_2 + X_{o2}CO + X_{o3}CH_4 + X_{o4}H_2 + X_{o5}O_2] + \nu_6N_2 + \nu_7C + \nu_8H_2O \tag{2}$$

Atom balances of (2) yield four equations:

O: $$[2X_{o1} + X_{o2} + 2X_{o5}]\alpha + \nu_8 = 6 \tag{3}$$

H: $$[4X_{o3} + 2X_{o4}]\alpha + 2\nu_8 = 5 \tag{4}$$

C: $$[X_{o1} + X_{o2} + X_{o3}]\alpha + \nu_7 = 7 \tag{5}$$

N: $$2\nu_6 = 3 + 2\nu_n \tag{6}$$

yielding the values of $\alpha$, together with those of $\nu_6$, $\nu_7$ and $\nu_8$, whence $\nu_i = \alpha\, X_{oi}$ for i = 1-4, and, concomitantly, $X_i = \nu_i / \Sigma\nu_i$.

## Thermodynamic background[1]

An exothermic process of combustion is carried out in three steps:

1. initiation by ignition or compression, devoid of a productive pressure rise
2. dynamic stage, when the exothermic effects prevail over the endothermic energy losses, manifested by a monotonic pressure rise furnishing the potential for work
3. decay, dominated by molecular and thermal diffusion, associated with energy loss due to heat transfer, terminating the productive pressure rise.

Of primary relevance to the dynamic features of combustion is, of course, the second stage, forming, therefore, the main subject of our studies. In its course, reactants, R, of fuel, F, and air, A, are converted into products, P, whose composition is specified by its thermodynamic equilibrium. It takes place in a

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[1] The background for this section was laid down by our previous publications on the thermodynamic method of approach to the analysis of closed combustion systems, in particular: [1] Oppenheim, A.K. & Kuhl, A.L., *Archivum Combustionis*, vol. 19, no. 1-4, pp. 15-65, 1999: [2] Oppenheim, A.K. & Kuhl, A.L., *Progress in Energy and Combustion Science,* vol. 26, pp. 533-564, 2000

thermodynamic system, defined as the working substance contained within an impermeable boundary; in this case the walls of the test vessel.

Salient features of the progress of an exothermic process, taking place in the course of its dynamic stage, are exhibited by the diagram of components of Fig. 1, in terms of their mass fractions considered as the vectors of components. Their variation, taking place in the course of the dynamic stage of combustion, is expressed as functions of the progress parameter, *x*, the sole independent variable. Thus, as evident from Fig. 1,

$$y_{\mathrm{P}} = \mathrm{Y}_{\mathrm{R}} x \tag{7}$$

where, with $\sigma \equiv \mathrm{Y}_{\mathrm{A}} / \mathrm{Y}_{\mathrm{F}}$, $\mathrm{Y}_{\mathrm{A}} = (1+\sigma)\mathrm{Y}_{\mathrm{F}}$, while, with K = A, F,

$$y_{\mathrm{K}} = \mathrm{Y}_{\mathrm{K}}(1-x) \tag{8}$$

Loci of states for A, F, R, and P, refereed to as state polars, are portrayed on the diagram of states of Fig. 2. The coordinates of this diagram identify the vectors of states, expressed in terms of $z_K = w_K, u_K$. The components of the state vector of the system are determined then by scalar products of the vectors of components and those of their states, so that

$$\mathbf{z} \cdot \mathbf{y} = z_{\mathrm{F}} y_{\mathrm{F}} + z_{\mathrm{A}} y_{\mathrm{A}} + z_{\mathrm{P}} y_{\mathrm{P}} + z_{\mathrm{B}} y_{\mathrm{B}} = z_{\mathrm{S}} \tag{9}$$

whence, in view of (7) and (8),

$$z_{\mathrm{F}} \mathrm{Y}_{\mathrm{F}} + z_{\mathrm{A}} \mathrm{Y}_{\mathrm{A}} + z_{\mathrm{B}} \mathrm{Y}_{\mathrm{B}} + (z_{\mathrm{P}} \mathrm{Y}_{\mathrm{R}} - z_{\mathrm{F}} \mathrm{Y}_{\mathrm{F}} - z_{\mathrm{A}} \mathrm{Y}_{\mathrm{A}}) x = z_{\mathrm{S}} \tag{10}$$

or, in terms of the vector of charge, whose composition is fixed by initial conditions, while the thermodynamic parameters vary between their initial and final values,

$$z_{\mathrm{C}} \equiv z_{\mathrm{A}} \mathrm{Y}_{\mathrm{A}} + z_{\mathrm{F}} \mathrm{Y}_{\mathrm{F}} + z_{\mathrm{B}} \mathrm{Y}_{\mathrm{B}} \tag{11}$$

while

$$z_{\mathrm{R}} \mathrm{Y}_{\mathrm{R}} \equiv z_{\mathrm{F}} \mathrm{Y}_{\mathrm{F}} + z_{\mathrm{A}} \mathrm{Y}_{\mathrm{A}} \tag{12}$$

Thus, the state vector of the system can be expressed simply as

$$z_{\mathrm{S}} = z_{\mathrm{C}} + (z_{\mathrm{P}} - z_{\mathrm{R}}) \mathrm{Y}_{\mathrm{R}} x \tag{13}$$

The state coordinates of F and A are prescribed by their initial chemical composition, while those of the reacting mixture, R, are calculated on the basis of (12), so that

$$z_R = \frac{\mathrm{Y}_{\mathrm{F}} z_F + \mathrm{Y}_{\mathrm{A}} z_A}{\mathrm{Y}_{\mathrm{R}}} = \frac{z_F + \sigma_{\mathrm{R}} z_A}{1 + \sigma_{\mathrm{R}}} \tag{14}$$

The coordinates of products, P, are determined, thereupon, by the condition of thermodynamic equilibrium attained from any state point of R, corresponding, in accordance with the phase rule, to two specified parameters of state, such as (p,T), (h,p), or (u,v), the latter of no relevance here since it applies only to the case a single component system. For a dynamic system, (13) provides the key to the balances of volume and energy. The first is obtained for *z* = *w*, whence

$$w_{\mathrm{S}} = w_{\mathrm{C}} + (w_{\mathrm{P}} - w_{\mathrm{R}}) \mathrm{Y}_{\mathrm{R}} x \tag{15}$$

The second corresponds to *z* = *u*, so that

$$u_{\mathrm{S}} = u_{\mathrm{C}} - (u_{\mathrm{R}} - u_{\mathrm{P}}) \mathrm{Y}_{\mathrm{R}} x \tag{16}$$

while the energy balance for a closed system means simply that

$$u_S = \mathrm{u}_{\mathrm{Si}} - u_e \tag{17}$$

where $u_e$ denotes the energy expenditure consisting of work performed by the system and heat transferred from it to the surroundings. For an isochoric and adiabatic case under consideration, $u_{\mathrm{e}} = 0$, so that

$$(u_{\mathrm{R}} - u_{\mathrm{P}}) \mathrm{Y}_{\mathrm{R}} x = (\mathrm{u}_{\mathrm{Si}} - u_{\mathrm{C}}) \tag{18}$$

To complete the analysis, internal energy, *u*, has to be related to the reference parameter, *w*. This is accomplished by linear representation of the relatively short sectors of state polars between state points i and f, as depicted in Fig. 2. Of particular service for this purpose are the slopes, $\mathrm{C}_{\mathrm{K}}$ and the ordinates of their tangents at w = 0, $\mathrm{u}_{\mathrm{Ko}}$ (K = R, P), whence $\mathrm{q} = \mathrm{u}_{\mathrm{Ro}} - \mathrm{u}_{\mathrm{Po}}$. The transition between the linear polars for the reactants and the products, expressed by q, is then just a geometric factor, rather then "heat release" - a well-established terminology that often leads to confusion. Perhaps a better term would be "exothermic energy," but, irrespectively how it is called, its basic nature is that of a distance between two points on the axis of ordinates in the diagram of states. The transition from a state point on R to one on P is then *de facto* a difference between their polar vectors.

Thus,

$$u_R = C_R w_R \qquad \text{while} \qquad u_P = C_P w_P - q \tag{19}$$

whence

$$u_C - u_{Si} = C_R (w_C - w_{Si}) \tag{20}$$

while

$$u_R - u_P = C_R w_R - C_P w_P + q \tag{21}$$

For an isochoric and adiabatic enclosure, the energy balance of (18) becomes then

$$(C_R w_R - C_P w_P + q) Y_R x = C_C (w_C - w_{Si}) \tag{22}$$

and, upon eliminating of $w_P$ by the virtue of (15),

$$[q - (C_P - C_R) w_R] Y_R x = C_P (w_S - w_C) - C_C (w_C - w_{Si}) \tag{23}$$

whence,

$$x = \frac{1}{Y_R} \frac{C_P (w_S - w_{Si}) + C_C (w_C - w_{Si})}{q_R - (C_P - C_R) w_R} \tag{24}$$

or, in a form normalized with respect to $w_{Si}$, while the process of compression is expressed by a polytrope, according to which, in terms of $P \equiv p / p_i$, $w_S / w_{Si} = P$, $w_C / w_{Si} = w_{R_D} / w_{Si} = P^{\alpha}$, where, with n denoting the polytropic index, $\alpha \equiv 1 - n^{-1}$, while $Q \equiv q/w_{Si}$,

$$x = \frac{1}{Y_R} \frac{C_P (P - 1) - (C_P - C_C)(P^{\alpha} - 1)}{Q - (C_P - C_R)\ P^{\alpha}} \tag{25}$$

- an expression providing the key to pressure diagnostics: the determination of the progress of the dynamic stage of combustion from the measured pressure transducer record.

**Solution**[*]

The inverse problem we addressed was to deduce data specifying the evolution of the dynamic stage of combustion from mass spectroscopic measurements of the composition of the detonation products and the transducer records of pressure profiles.

The analytical gas mass spectroscopy measurements of the products of preliminary explosion tests in nitrogen yielded the volumetric fractions, $X_{oi}$, in terms of: 0.72 $CO_2$, 0.84 CO, 0.05 $CH_4$, 0.26 $H_2$, 0.02 $O_2$, and 98.11 $N_2$. On this basis, (3)-(6) yielded $\alpha = 1.879$, as well as $\nu_6 = 178.5$, $\nu_7 = 4.12$ and $\nu_8 = 1.86$, so that, according to (2),

$$C_7H_5N_3O_6 + 177N_2 \Rightarrow 1.29CO_2 + 1.5CO + 0.09CH_4 + 0.46H_2 + 0.04O_2 + 4.12C + 1.86H_2O + 178.5N_2$$

for which $\sigma_N = 3.17$. The composition of the fuel for the ensuing process of combustion, thus determined, was found to be in a satisfactory agreement with the results of the computations made by the use of CHEETAH[2]. The latter were carried out for isentropic expansion of detonation products from the Chapman-Jouguet state to initial conditions of the dynamic stage of combustion. The state coordinates of F and A, as well as of P, were evaluated then by the use of STANJAN[3], while those of S and R were deduced from the data for F and A by means of (14).

The pressure records were obtained from four test runs in air and four in nitrogen. The latter provided the base line for the pressure profile of the dynamic stage of combustion in the shock compressed air re-

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[*] As appropriate for an abstract, provided here are only highlights of the results we obtained. Their complete set and numerical background, as well as answers to any questions an interested reader may pose, are readily obtainable by demand addressed to ako@me.berkeley.edu

[2] Fried, L.E., *Cheetah 1.22*, LLNL Publication, 185 pp.,1995

[3] Reynolds, W.C., *STANJAN,* Department of Mechanical Engineering, Stanford University, 48 pp., 1986

corded by the former. In both cases, they were obscured initially by high amplitude fluctuations due to the oscillating shock fronts, produced by the blast wave generated by the explosion of the TNT charge. Upon a relatively short period of this noise, the rest of the data were time-averaged. The results are presented in Fig.3, where t = 0 marks their extrapolated start. As evident there, the initial point was then determined by the intersection of the pressure profile of the dynamic stage and its level base.

The experimental test was carried out with an initial (for explosion) TNT/air mass ratio, $\sigma_M = 18.5$. The initial pressure for combustion following the explosion was $p_i = 1.74$ atm, at a temperature of $T_i = 444$K, while the maximum pressure was recorded at a level of $p_f = 3.75$ atm, as displayed in Fig. 3. The corresponding state diagram of the system and its components in w-u coordinates is presented in Fig. 4. Provided thus are thermodynamic coordinates for two cases: (1) a completely mixed system, M, and (2) a completely unmixed system, N. According to the pressure levels specified above, P = 2.16. Thus it was found that $q_M = 0.59$ kJ/g, $C_{R_M} = 2.66$ and $C_{P_M}$ 3.08, while $\alpha_M = 0.27$ ($n_M = 1.37$) and $Y_{R_M} = 0.84$, whereas $\sigma_N = 3.17$, $q_N = 2.85$ kJ/g, $C_{R_N} = 2.91$ and $C_{P_N} = 4.60$, while $\alpha_N = 0.20$ ($n_N = 1.25$) and $Y_{R_N} = 0.24$. Thus, to generate the measured pressure rise, 84% of the charge would have been consumed if the system were completely mixed, while only 24% would suffice if it were completely unmixed.

The time profile of the progress parameter was then expressed in terms of the life function - a kinetic expression for the evolution of the dynamic stage of combustion introduced in our previous publications cited in the footnote on page 1, according to which,

$$x = \frac{e^{\zeta} - 1}{e^{\zeta_f} - 1} \qquad \text{where} \quad \zeta = \frac{\alpha}{\chi + 1}[1 - (1 - \tau)^{\chi + 1}] \qquad \text{while} \quad \tau \equiv \frac{t - t_i}{t_f - t_i}, \tag{26}$$

The results of our computations were found corresponding to $\alpha = \chi = 1.5$. The mass fraction and rate of fuel consumption, thus evaluated, are displayed in Fig. 5, while the concomitant profiles of temperatures and densities are depicted on Fig. 6.

## Résumé

Presented here is a solution of an inverse problem: evaluation of the progress of an exothermic process of combustion, following an explosion of a TNT charge in air from pressure transducer records. Thereupon, time profiles of all the thermodynamic parameters of the system were obtained in both its completely mixed and completely unmixed cases.

### Nomenclature

| | |
|---|---|
| $C_K$ | slope of a locus of states |
| $p$ | pressure |
| q | $\equiv u_{Ro} - u_{Po}$ |
| $t$ | time |
| $T$ | temperature |
| $u_K$ | internal energy |
| $v_K$ | specific volume |
| $w_K$ | $\equiv p_K v_K$ |
| $x$ | progress parameter |
| X | mole fraction |
| $y_K$ | variable mass fraction |
| $Y_K$ | fixed mass fraction |
| $\mathbf{z}_K$ | $= \boldsymbol{w}_K, \boldsymbol{u}_K$ |
| $\alpha$ | stoichiometric variable, life function parameter, polytropic exponent |
| $\chi$ | life function parameter |
| $\nu$ | stoichiometric coefficient |
| $\rho$ | density |
| $\sigma_K$ | air/fuel mass ratio (K = M, N) |
| $\tau$ | time normalized with respect to lifetime |
| $\zeta$ | life function exponent |

*Designations*

| | |
|---|---|
| A | air |
| B | inert component |
| C | charge |
| F | fuel |
| f | final |
| i | initial |
| K | ≡ A, F, R, P, S |
| M | completely mixed system |
| N | completely unmixed system |
| R | reactants |
| P | products |
| S | system |

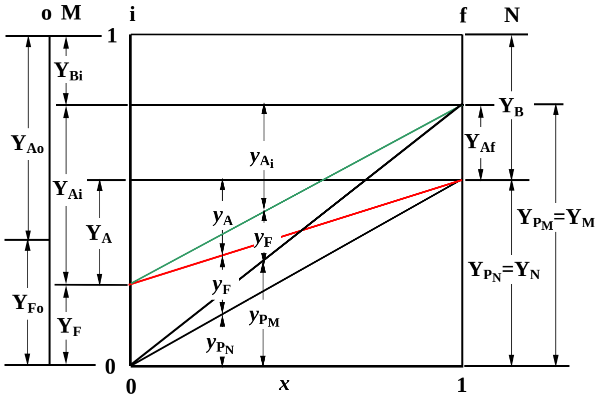

*Fig. 1.* Illustration of a diagram of components

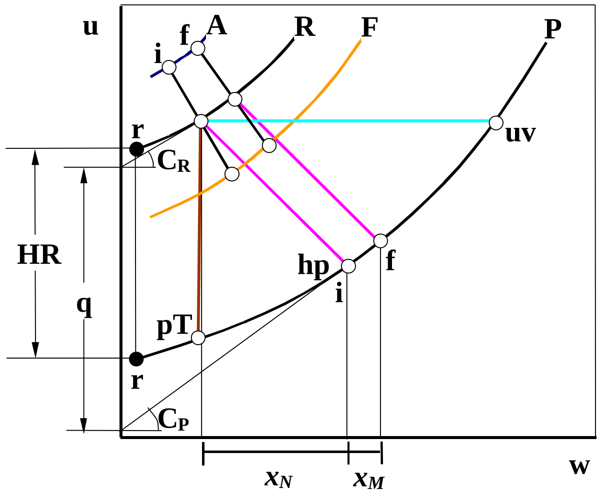

*Fig. 2.* Illustration of a diagram of states

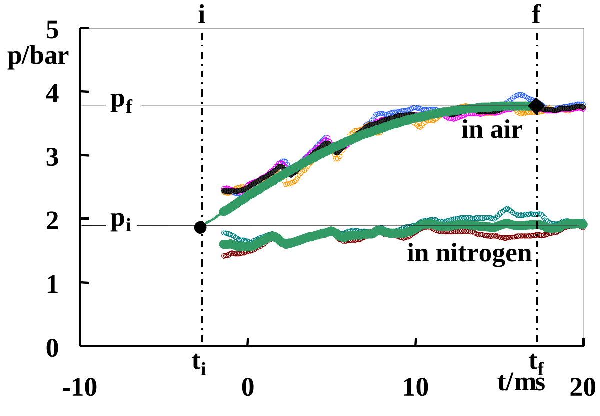

*Fig. 3.* Measured pressure profiles

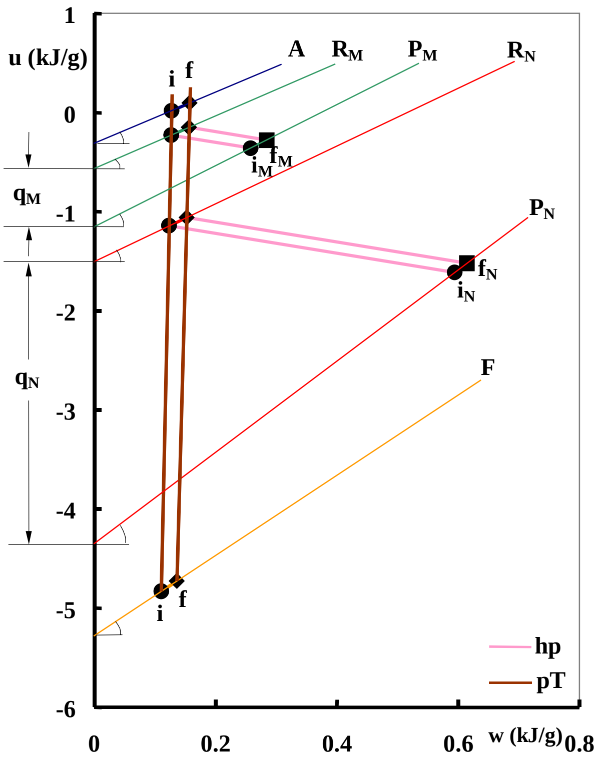

*Fig. 4.* Diagram of states

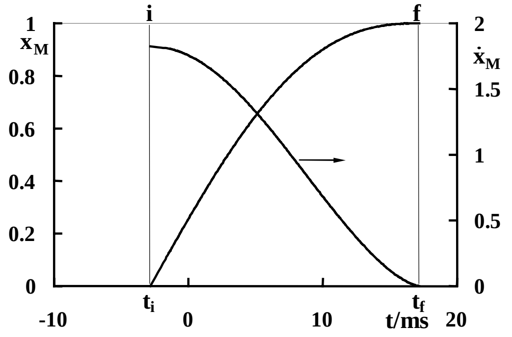

*Fig. 5.* Profiles of progress parameter, $x_M$ , and its rate, $\dot{x}_M$

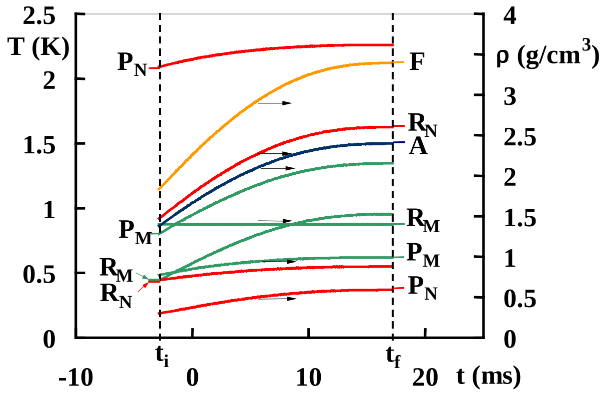

*Fig. 6.* Profiles of thermodynamic parameters