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CALCULATION OF PRESSURE AND TEMPERATURE FROM EXPLOSIONS
IN CONFINED SPACES.

by
E Strønsøe

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CALCULATION OF PRESSURE AND TEMPERATURE
FROM EXPLOSIONS IN CONFINED SPACES

by

E Strömme

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CALCULATION OF PRESSURE AND TEMPERATURE FROM EXPLOSIONS IN CONFINED SPACES

1 INTRODUCTION

In a previous report (1) estimates were made of the post-detonation pressure and temperature when TNT charges detonate in a closed chamber at loading densities varying from 0.2 to 270 kg/m³. An important simplifying assumption was that reaction products other than C, CO, CO₂, H₂, H₂O and N₂ could be neglected. For TNT this introduces no serious error as long as the post-detonation temperature remains below about 2900 K, i.e. for all loading densities except the range 0.3 to 1.2 kg/m³, where oxygen balance is nearly obtained. For explosives with a higher detonation energy (eg RDX and PETN) this simplification is advisable only for loading densities well below those corresponding to oxygen balance.

The objective of the present report is to present a refined and more general approach to this problem, particularly in the sense that many more explosion products are considered.

2 ASSUMPTIONS

The following assumptions are made:

- The detonation and subsequent afterburning take place in a closed, rigid and thermally insulated chamber so that energy loss can be neglected
- The explosion gases can be described by the ideal gas law
- Chemical equilibria will be established within the time considered

- For C-H-N-O explosives these explosive products are considered: C(s), CO(g), CO₂(g), H₂(g), H₂O(g), O₂(g), N₂(g), OH(g), NO(g), H(g), O(g), NH₃(g), CH₄(g). For aluminized explosives ~~the~~ additional products ^{are} Al₂O₃(s/l), Al₂O(g), AlO(g), Al₂O₂(g), Al(g)
- The air composition is approximated by 21 per cent (by volume) O₂ and 79 per cent N₂
- The initial temperature and pressure are 298 K and 1.013 bar respectively

3 CALCULATION PROCEDURE

The details of the calculation procedure have been described elsewhere (2). The main steps are:

- a) Assume preliminary values for p (pressure) and T (temperature)
- b) Calculate composition of explosion products from material balances and chemical equilibria, and also n = total number of gaseous moles
- c) Find ΔH (enthalpy change) from enthalpy data for explosives and products
- d) Transfer enthalpy to energy (ΔE , constant volume) by adding the term $\Delta n RT$, where Δn is the increase of the number of gaseous moles and R is the gas constant
- e) Use ΔE and c_v -data (heat capacity at constant volume) to find T
- f) Use gas law to find p from T and n
- g) Compare calculated values of p and T with assumed values. If necessary, assume new values for p and T and repeat sequence b-g.

The thermochemical data have been taken from ref (3-5).

* This means that use has been made of the convention that the energy change is positive for an exothermic reaction.

4 RESULTS

Calculations have been performed for three C-H-N-O high explosives:

- TNT $C_7H_5N_3O_7$
- RDX $C_3H_6N_6O_6$
- PETN $C_5H_8N_4O_{12}$

and for two commonly used compositions containing alumin

- H-6 (45% RDX, 30% TNT, 20% Al, 5% wax)
- HBX-3 (31% RDX, 29% TNT, 35% Al, 5% wax)

The results (temperature and pressure as function of load density) for these are shown in figures 4.1 - 4.2. More detailed results, giving the composition of the explosive products, are presented in tables 4.1 - 4.2.

In order to study the effect of aluminium in more detail calculations were further performed for compositions of TNT/Al with Al-content ranging from 10 to 40%. The results are shown in figures 4.3 - 4.4.

Finally four fuel-air explosives (FAE) were studied:

- | | | |
|----------------------------|----------------|-----------|
| - Methane CH_4 | energy content | 50.2 kJ/g |
| - Acetylene C_2H_2 | " | 48.3 " |
| - Ethylene oxide C_2H_4O | " | 27.8 " |
| - Propane C_3H_8 | " | 46.5 " |

The results are shown in figures 4.5 - 4.6.

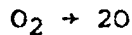
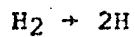
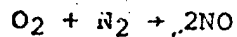
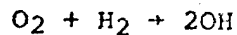
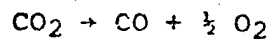
It should be noticed that both temperatures and pressures are presented as absolute values.

5 DISCUSSION5.1 C-H-N-O high explosives

The thermodynamic data used for these explosives are thought to be highly reliable. Also the assumptions made in chapter 2 are fairly realistic for the loading densities considered here. For higher values of the loading density, resulting in pressures of the order of 100 bars or more, real gas effects can no longer be neglected.

Experimental data presented by Weibull (6) and by James and Rowe (7) are in fair agreement with the present results.

Previous calculations (1, 8) have usually neglected various endothermic reactions, which become increasingly more important for temperatures exceeding about 2500 K:



Consequently, energies, temperatures and pressures are overestimated. For TNT the simple methods are fairly accurate, the greatest deviation for the pressure is about 10% in the range near oxygen balance. For RDX and PETN pressure deviations of 20% or more can easily be obtained when the composition is estimated by simplified methods.

It has been claimed (ref 8, figure 7) that fair agreement with experimental data has been obtained by simple methods at high loading densities for RDX/wax. It seems likely that this apparent agreement is due to two counteracting effects, neglect of endothermic reactions and ideal gas assumption.

5.2 Aluminized high explosives

The thermodynamic data for the various aluminium oxides (Al_2O_3 , Al_2O , AlO and Al_2O_2) are probably less reliable than corresponding data for explosion products from C-H-N-O explosives. For instance, estimates of the boiling point for Al_2O_3 vary from 3250 K (9) to 3770 K (5). Ref (3, 4) which are the main sources for the present report, do not contain data for Al_2O_3 (l) for higher temperatures than 3500 K so for these temperatures extrapolation was necessary.*

One should therefore not have the same confidence in the results for aluminized explosives as in the results for C-H-N-O explosives. This is particularly true at the highest temperatures.

The computer programme does not provide for aluminium in a condensed phase as a possible reaction product. This means that in the case of an appreciable negative oxygen balance calculations have not been carried out below the boiling point for aluminium, 2767 K.

The comparison of H-6 and HBX-3 is of some interest since it has been suggested that HBX-3, because of the afterburning effect might have a greater damage potential in confined explosions. Figure 4.2 shows that the pressure for HBX-3 is slightly higher than that for H-6 at loading densities below 0.8 kg/m^3 . With increasing loading density the HBX-3 performance rapidly becomes quite inferior. However, this comparison is not very realistic, since the explosion products of HBX-3 contain an appreciable amount of latent energy which may become available for mechanical work on expansion and cooling. A more useful approach would probably be to compare the Helmholtz free energy after the explosion products have expanded to ambient values of pressure and temperature. This would then require an estimate of the temperature at which the chemical equilibria become frozen.

*Also other Al-compounds, such as AlN , AlH and Al_4C_3 , have been suggested as explosion products. Cook (5), however, has shown that none of these can be important.

5.3 Fuel-air explosives

Fuel-air explosives are of considerable interest, both from a military and a civilian point of view.

Figures 4.5 - 4.6 show that maximum pressure and temperature occur at higher concentrations than the stoichiometric mixture, particularly for acetylene and ethylene oxide. It is further noteworthy that methane with the highest energy content shows the poorest performance in a confined space, whereas ethylene oxide with the lowest energy content gives the highest pressure at stoichiometric mixture. This phenomenon is of course connected with the oxygen requirement for complete combustion, which for methane is more than twice as high as for ethylene oxide.

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(9)

- Handbook of Chemistry and Physics, The Chemical Rubber Co, 45 Ed, Cleveland, Ohio (1964)

Explosion products	Loading density, kg/m ³								
	0.25			1.00			4.00		
	TNT	RDX	PETN	TNT	RDX	PETN	TNT	RDX	PETN
C	-	-	-	-	-	-	0.44	-	-
CO	0.67	-	-	25.10	4.71	2.67	122.85	36.68	27.85
CO ₂	7.04	3.37	3.95	5.72	8.80	12.95	0.01	17.38	35.40
H ₂	0.04	-	-	4.00	0.83	0.36	43.73	10.17	4.18
H ₂ O	2.55	3.36	3.15	6.55	11.50	11.42	0.03	38.70	41.68
O ₂	2.69	6.75	7.71	0.02	3.11	5.63	-	2.13	7.61
N ₂	33.60	35.54	33.80	38.85	44.99	37.80	58.73	84.95	55.70
OH	0.30	0.04	0.02	0.33	1.96	1.60	-	6.67	7.71
NO	0.71	0.28	0.16	0.11	1.64	1.65	-	2.80	3.80
H	0.02	-	-	0.60	0.39	0.16	0.38	3.69	1.76
O	0.10	-	-	0.03	0.56	0.43	-	1.41	1.92
CH ₄	-	-	-	-	-	-	0.05	-	-
NH ₃	-	-	-	-	-	-	-	-	-
T, K	2634	1956	1762	2986	3104	2934	2512	3521	3396
p, bars	10.45	8.02	7.15	20.18	20.25	18.26	47.15	59.89	52.98

Table 4.1 Composition of explosion products (moles/m³) at various loading densities, TNT, RDX and PETN

Explosion products	Loading density, kg/m ³							
	0.4		0.8		1.2		1.6	
	H-6	HBX-3	H-6	HBX-3	H-6	HBX-3	H-6	HBX-3
CO	3.82	4.90	13.22	13.01	21.75	19.98	29.81	26.72
CO ₂	3.75	1.78	1.90	0.35	0.93	0.06	0.43	0.01
H ₂	0.53	0.85	3.95	5.20	9.59	11.20	15.97	16.87
H ₂ O	3.91	2.46	4.58	1.16	3.35	0.28	1.89	0.03
O ₂	1.44	0.90	0.21	0.02	0.03	-	-	-
N ₂	34.99	34.20	38.45	37.07	41.85	39.62	45.16	42.07
OH	1.10	1.22	1.31	0.52	0.78	0.04	0.32	-
NO	1.07	1.08	0.59	0.22	0.25	0.01	0.08	-
H	0.39	0.93	2.37	4.30	4.45	3.28	5.43	1.25
O	0.49	0.79	0.46	0.25	0.21	0.01	0.06	-
Al ₂ O ₃	1.48	2.59	2.95	4.57	4.31	4.65	5.31	3.66
Al ₂ O	-	-	-	0.25	0.04	1.96	0.29	5.03
AlO	-	-	0.02	0.16	0.06	0.07	0.08	0.01
Al ₂ O ₂	-	-	-	-	-	-	-	-
Al	-	-	0.01	0.59	0.14	2.27	0.59	3.33
T, K	3186	3448	3529	3756	3624	3438	3593	2978
p, bars	13.64	14.08	19.68	19.70	26.38	22.52	29.91	23.60

Table 4.2 Composition of explosion products (moles/m³)
at various loading densities, H-6 and HBX-3

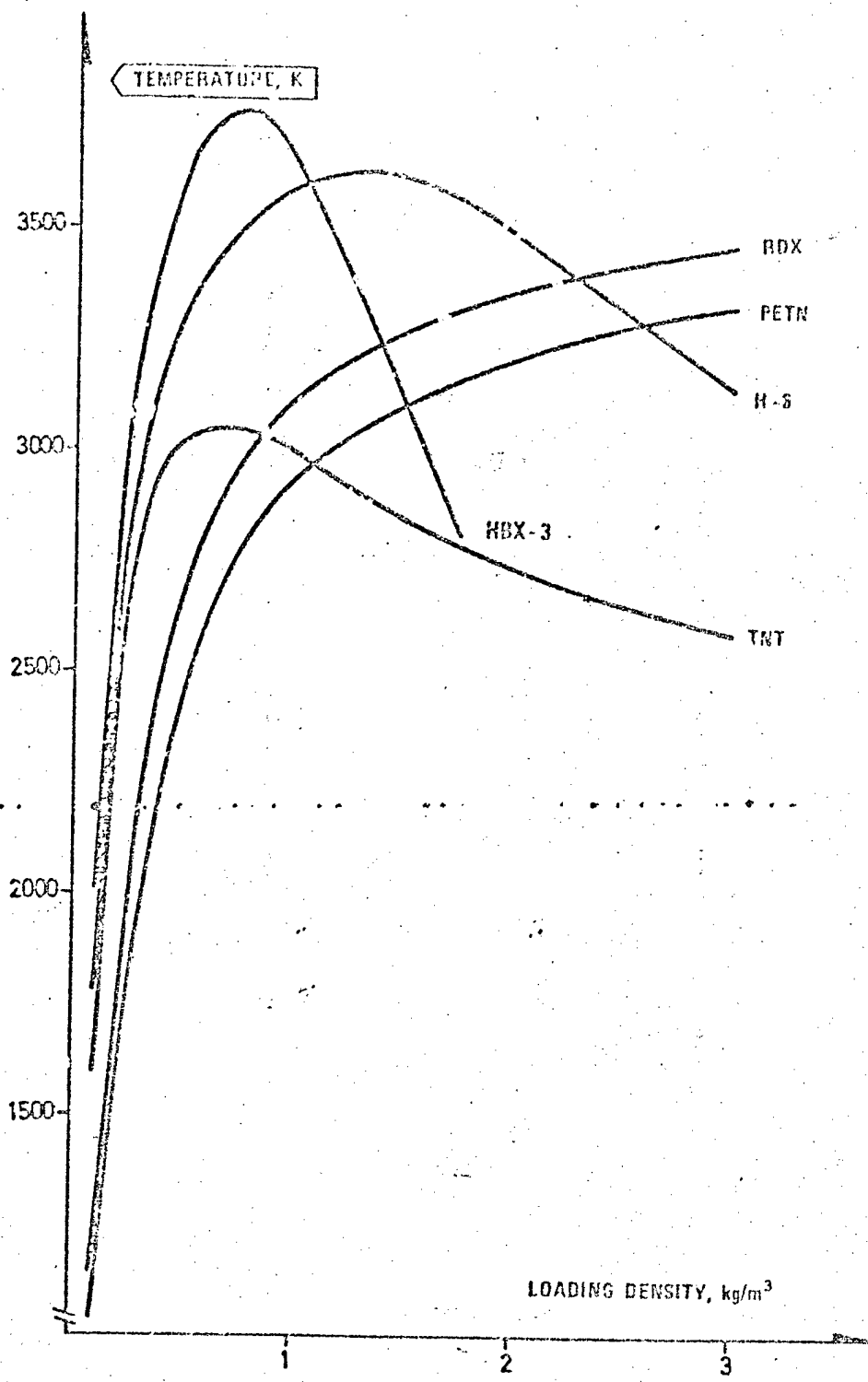


Figure 4.1 Post-detonation temperature for confined explosion

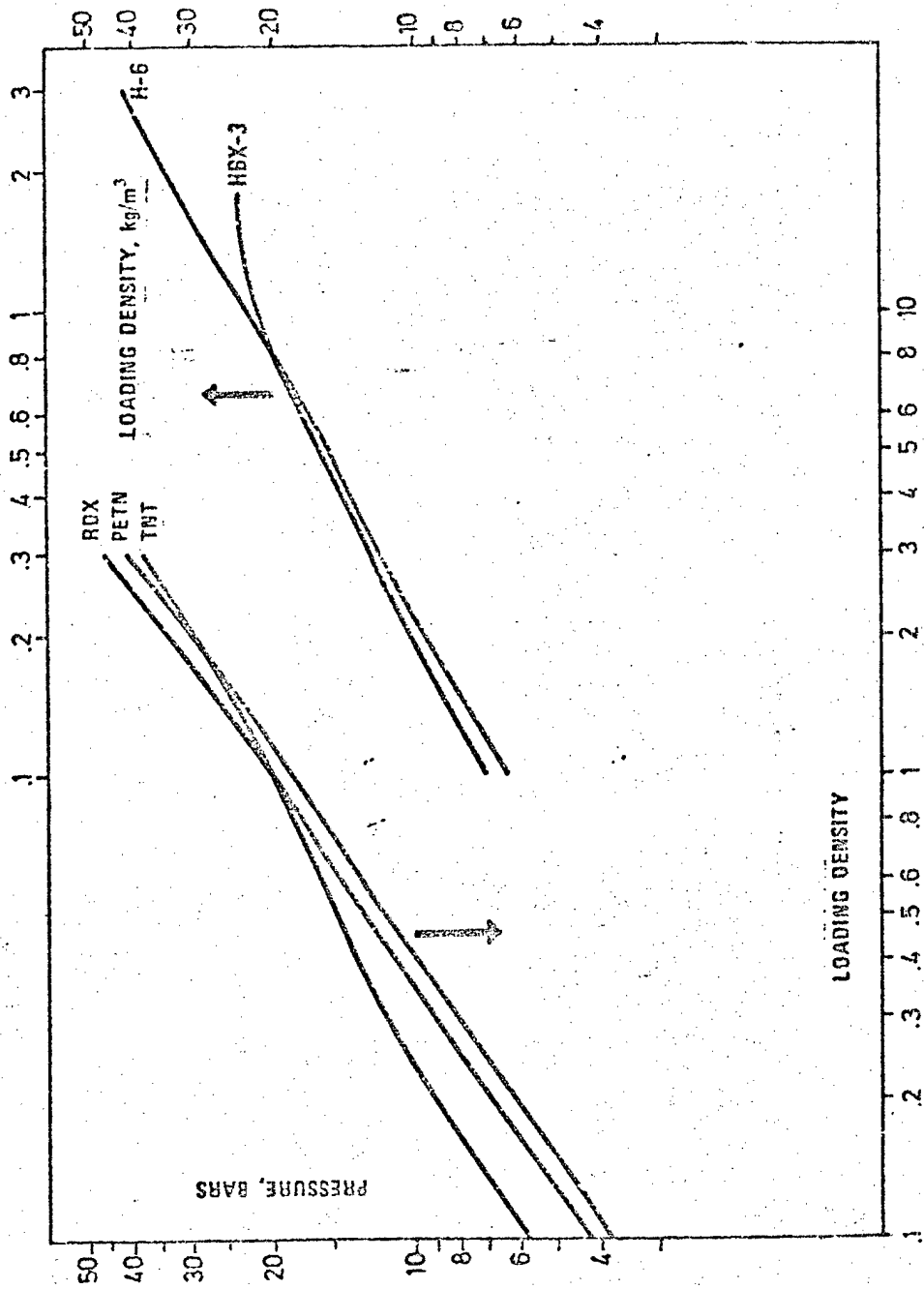


Figure 4.2 Post-detonation pressure for confined explosions

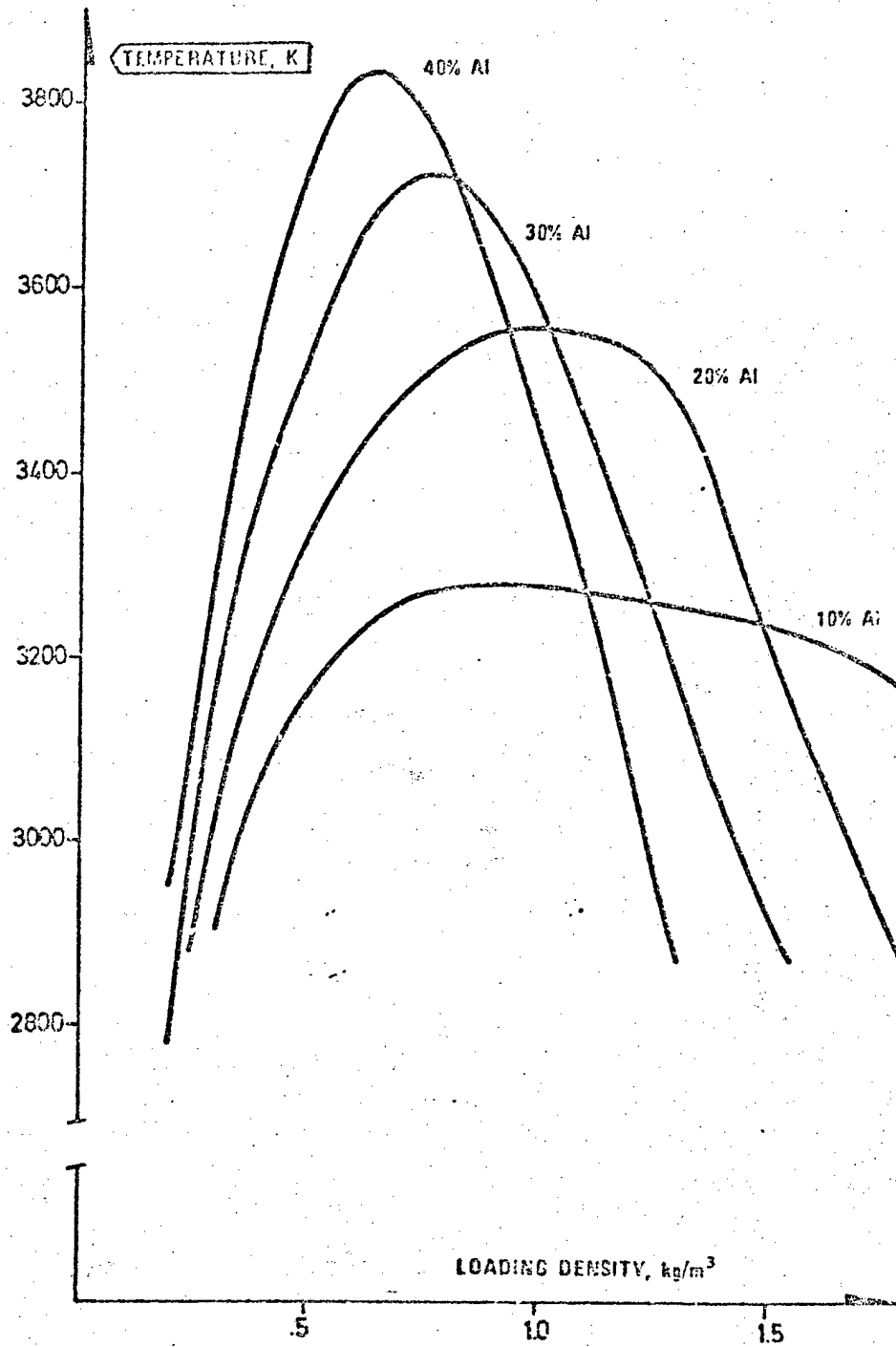


Figure 4.3 Post-detonation temperature for confined explosion.

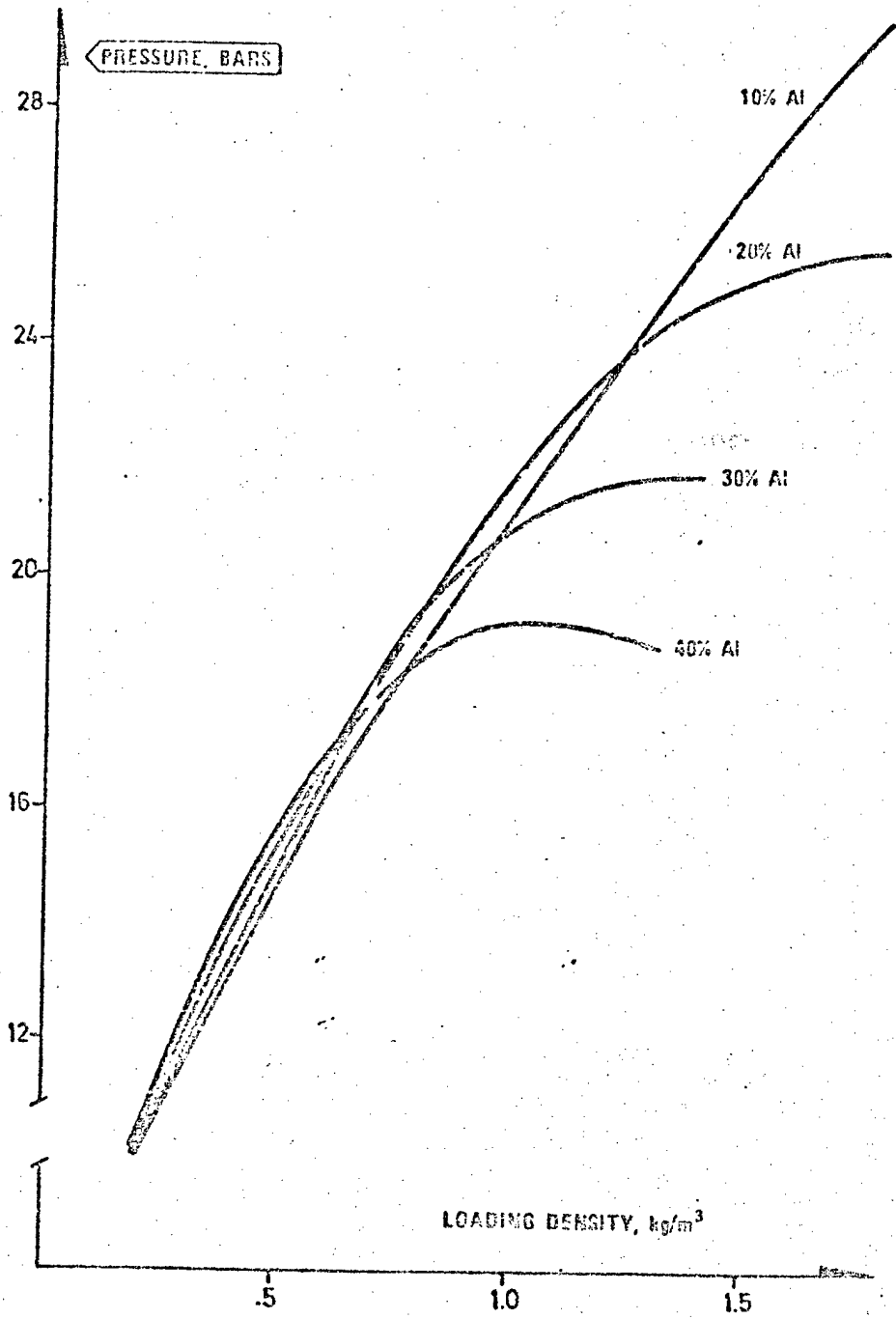


Figure 4.4 Post-detonation pressure for confined explosions

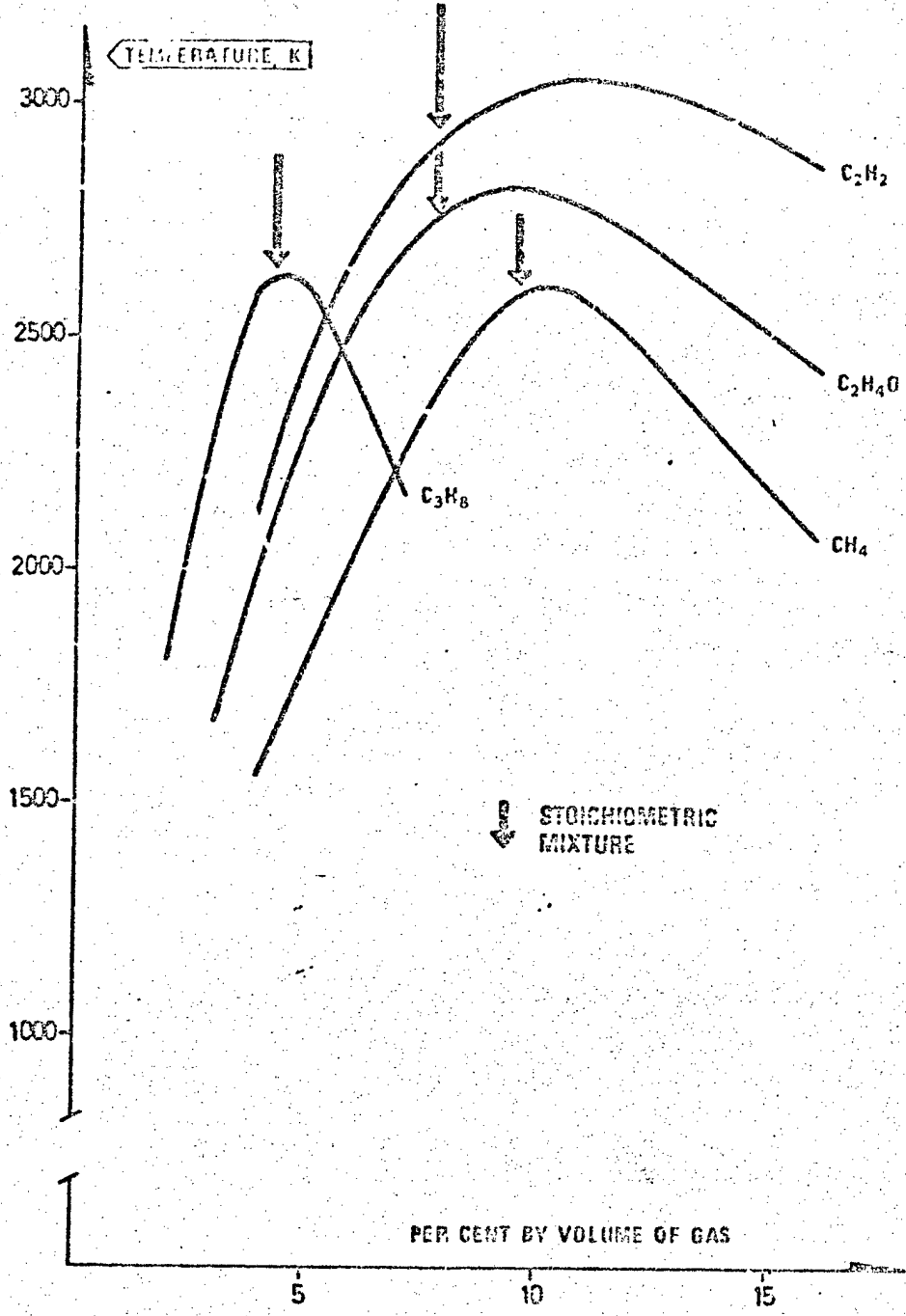


Figure 4.5 Post-detonation temperature for confined explosion

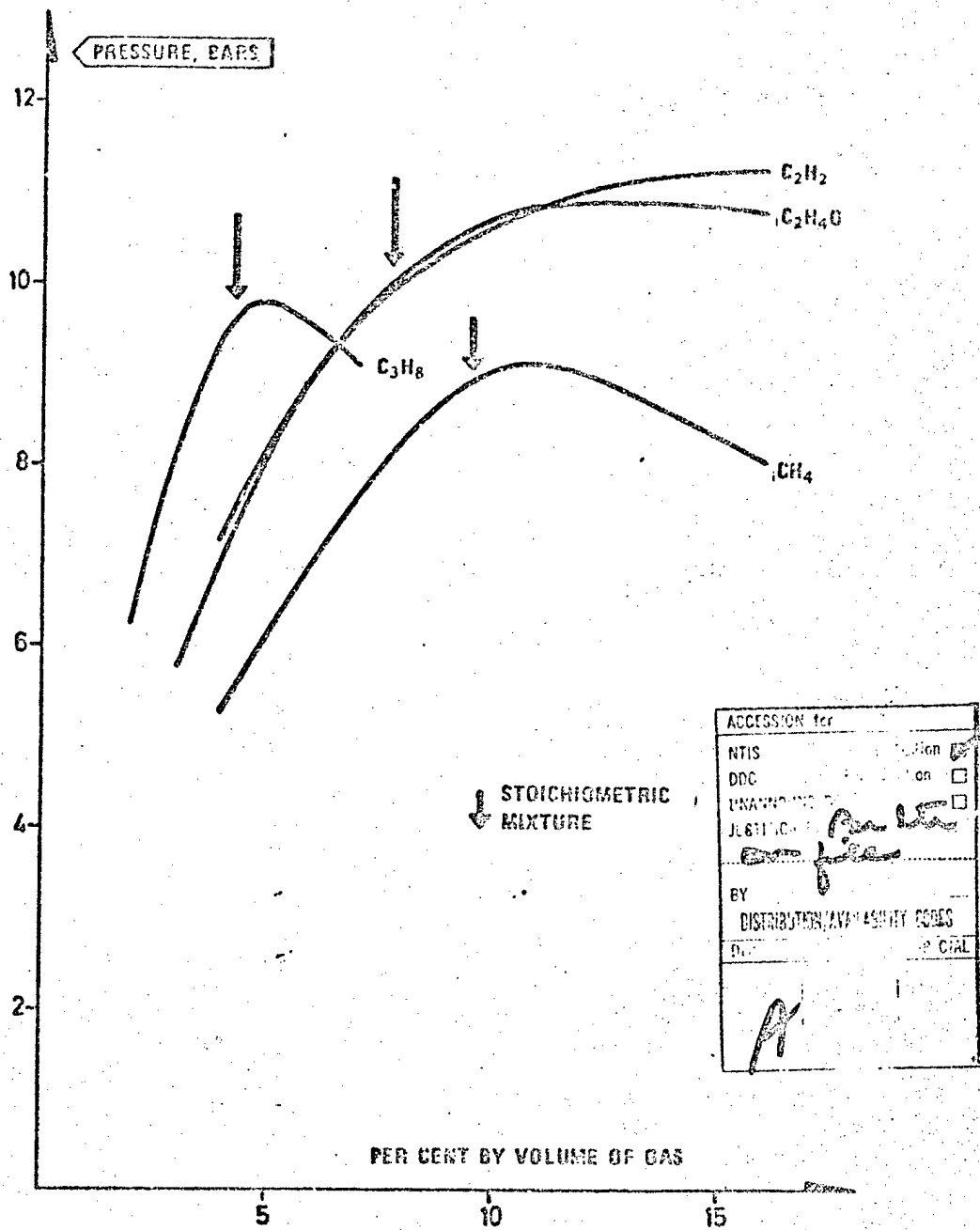


Figure 4.6 Post-detonation pressure for confined explosions