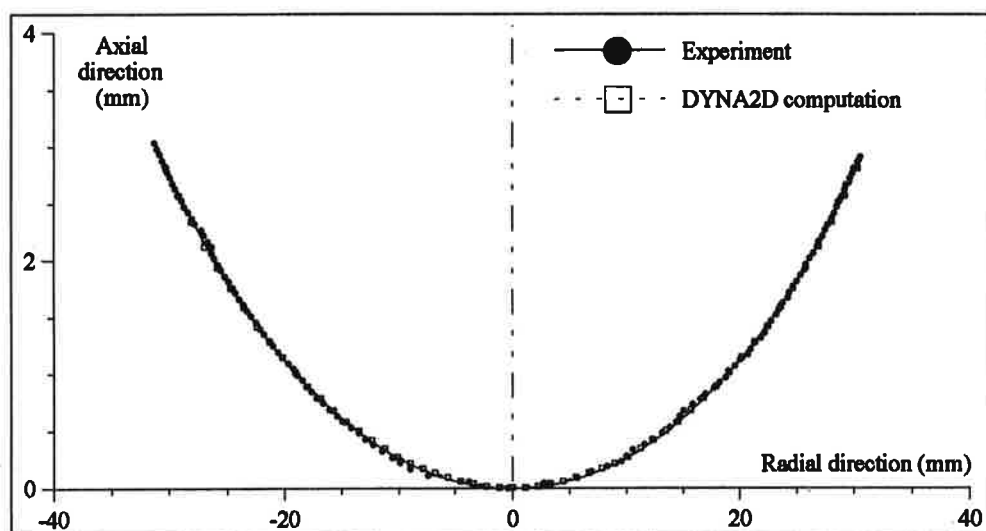




DETERMINATION OF BURNING RATE PARAMETERS FOR AN EMULSION EXPLOSIVE

Junhua Deng
Shulin Nie
Li Chen

STIFTELSEN SVENSK BERGTEKNISK FORSKNING
SWEDISH ROCK ENGINEERING RESEARCH
SveBeFo Report 17

**DETERMINATION OF BURNING
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SveBeFo

FÖRORD

SveBeFo:s forskningsprogram spänner över bergbyggandets olika stadier, från undermarksplanering och förundersökningar till berguttag, förstärkning, tätning och långtidsbeständighet hos anläggningar i drift. Forskningen bedrivs till stor del med externa forskare vid högskolor och företag, medan specialområdet sprängningsteknik och sprängämnesforskning huvudsakligen genomförs med egna forskare, anställda vid SveBeFo.

Inom detoniken ("detonationsfysiken") är en huvuduppgift att öka kunskaperna om sprängämnens verkningsätt med målet att bättre utnyttja den tillgängliga energin i samband med bergbrytning. Forskningen innefattar både teoriutveckling och experiment för att verifiera uppställda samband mellan olika faktorer under detonationen. Dessa data sammanfattas i en sk brinnmodell för sprängämnet.

I brinnmodellen ingår tillståndsekvationer med materialdata för sprängämnet och de resulterande spränggaserna samt en brinnekvation, som beskriver omsättningen i reaktionszonen bakom detonationsfronten. Denna rapport redovisar hur materialparametrarna i brinnekvationen bestämts. Detta har gjorts genom att välja den parameteruppsättning som ger bäst överensstämmelse mellan en uppsättning sprängförsök med cylindriska laddningar och en numerisk simulering av dem. Jämförelsevärden har varit hastighet och krökningsradie hos detonationsfronten som funktion av laddningsdiametern. En sammanfattande rapport som beskriver hur hela brinnmodellen tagits fram är under utarbetande.

En referensgrupp bestående av representanter för Nitro Nobel, Kimit och FOA har följt och givit värdefulla synpunkter på forskningsarbetet, som påbörjade inom ramen för SveDeFo:s tidigare ramprogram 1990 - 93 med Algot Persson som projektledare.

Stockholm i april 95

Tomas Franzén

SAMMANFATTNING

Förbrännings- eller brinnprocessen i reaktionszonen bakom detonationsfronten i ett emulsionssprängämne har modellerats med en initierings- och tillvästekvation med två termer vilken implementerats i beräkningsprogrammet DYNA2D. Parametrarna i denna brinnekvation har bestämts genom en jämförelse av beräkningsresultat med försök där detonationsfrontens krökning och hastighet i en cylindrisk laddning bestämts som funktion av laddningsdiametern.

Tillstånden i det oreagerade emulsionssprängämnet och hos spränggaserna har beskrivits med tillståndsekvationer av Jones-Wilkins-Lee eller JWL-typ. Sprängämnesdata härstammar från en experimentell bestämning av sprängämnesmatrisens stöt-Hugoniot. Spränggasvärdena har beräknats med termokemisk programvara.

DYNA2D-beräkningarna visar att det är möjligt att simulera brinnprocessen i emulsionssprängämnet med denna ekvation. Både detonationshastigheten och detonationsfrontens krökning kan beräknas med god noggrannhet. Antalet materialparametrar i brinnekvationen är egentligen åtta men två eller tre av dem dominerar.

Två parameteruppsättningar ger bra resultat för detta emulsionssprängämne. Den ena ger en bättre beskrivning av detonationshastigheten när den plottas som funktion av inversa laddningsdiametern, den andra en bättre beskrivning av detonationsfrontens krökningsradie som funktion av laddningsdiametern.

Begynnelsevärdet för spränggasernas inre energi, E_0 i JWL-ekvationen, påverkar resultat rätt så mycket. När värdet sätts ner från teoretiskt beräknade 0,030 till 0,028 Mbar·cm³/cm³ (2,8 GJ/m³) erhålls en tredje uppsättning brinnekvationparametrar som ger en mycket god beskrivning av både detonationshastigheten och detonationsfrontens krökningsradie. Därför är parametrarna i JWL-ekvationerna också viktiga för resultaten och borde verifieras nog experimentellt.

Nyckelord: emulsionssprängämne, brinnmodell, brinnekvation, tillståndsekvation, DYNA2D, numerisk simulering, kalibrering, detonationshastighet, krökning hos detonationsfront.

SUMMARY

The burning process of an emulsion explosive has been simulated by the two-term ignition and growth model implemented in the hydrodynamic code DYNA2D. The parameters in the burning rate function are calibrated by the detonation velocities and the curvature radii of detonation fronts at different charge diameters which were measured earlier by two dimensional steady-state experiments. The states in the unreacted emulsion and in the reaction products are described by two JWL (Jones-Wilkins-Lee) equations of state.

Computations show that it is possible to use the two-term ignition and growth model to simulate the burning process of the emulsion explosive. Both detonation velocities and detonation front curvatures can be predicted. The number of the adjustable parameters in the burning rate function is originally eight, but a preliminary analysis shows that only two or three are truly free.

Two burning rate functions are found suitable for the emulsion explosive. One gives a better prediction of the detonation velocity as a function of inverse charge diameter, the other a better prediction of the curvature radius of detonation front at the charge axis as a function of charge diameter.

The initial internal energy (E_0) in the JWL equation of state for the reaction products is found to be very important for the calibration. Therefore, the parameters for JWL equation of state for both unreacted emulsion and reaction products should be carefully verified by experiments.

Key words: emulsion explosive, burning model, burning rate function, equation of state, DYNA2D, simulation, calibration, detonation velocity, detonation front curvature.

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Determination of Burning Rate Parameters for an Emulsion Explosive

1. INTRODUCTION

To model the burning process of emulsion explosives is an integral part of our research program on commercial explosives /1/. We have been working on this program since 1990. Great efforts have been made to develop a burning rate function for an emulsion explosive.

It is very complicated to describe the burning process of an emulsion explosive, since it contains multiple components in different phases. However, in a simple approach, this burning process may be regarded to consist of two stages. The first stage is the formation of the hot spots by the shock compression. When a shock wave propagates through the unreacted explosive, the microballoons are severely compressed by the high pressure, which results in very high temperature in the microballoons (hot spots) and the surrounding matrix starts burning. The second stage is the growth of the burning hot spots. This releases more chemical energy from the explosive and accelerates the burning process. The second process takes longer time and depends on such conditions as the confinement and the charge diameter. Experiments show that the larger the diameter of the charge and the stronger the confinement are, the faster the burning process will be.

There are many burning rate functions in the literature /2-7/. For example, the ignition and growth model was proposed by Lee and Tarver /2-4/ for military explosives based on TATB (Triamino-trinitrobenzene). The reaction zone of the detonation is simulated by the gradual transition of the unreacted explosive into reaction products. The burning products behind the detonation front are described as the mixture of two materials: the unreacted explosive and the reaction products, to which two JWL equations of state are applied. In the mixing of the two materials it is assumed that the pressure and temperature at any moment are in equilibrium, and that their volumes are additive. The transition is controlled by a burning rate function, which depends on the pressure and the degree of compression.

We believe that this two-terms phenomenological ignition and growth model is a suitable starting point for emulsion explosives. First, the two terms should be sufficient to simulate the phenomenon of the two stages of the burning process. Secondly, the number of parameters in the burning rate function is relatively small. Finally, the model has already been implemented in the hydrodynamic code DYNA2D.

By using this burning model and the DYNA2D code, it is possible to separate the hydrodynamics and the chemical burning process. This simplifies our research program into three parts: (1) determination of the JWL parameters for the unreacted explosive, (2) determination of the JWL parameters for the reaction products and (3) determination of the parameters in the burning rate function. This report focuses on the determination of the parameters in the two-term ignition and growth burning rate function. A flow diagram of all three parts of this work is shown in Figure 1.

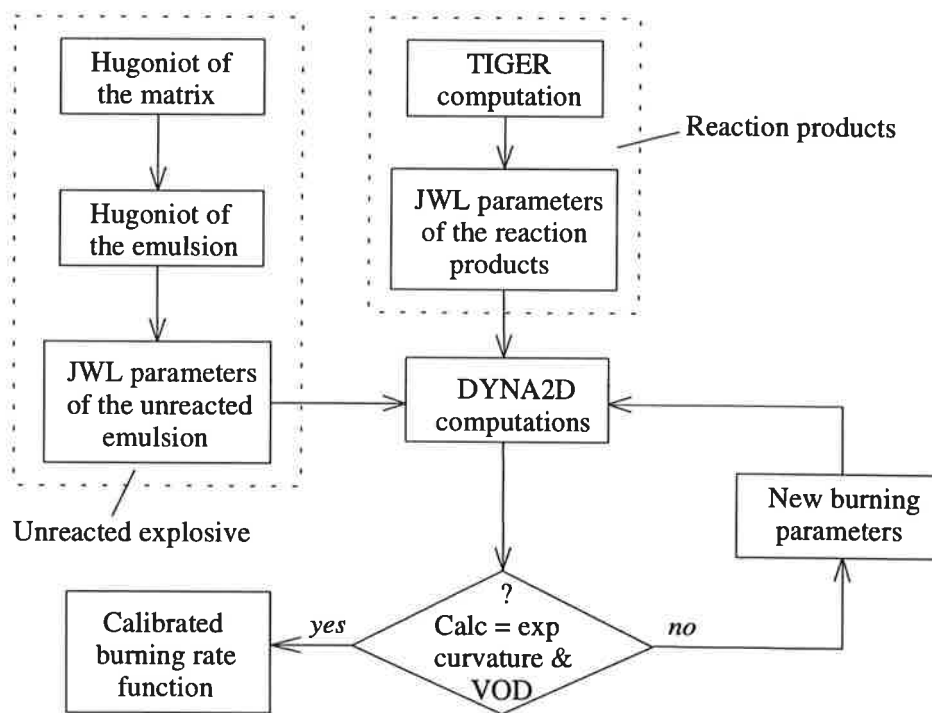


Figure 1: Flow diagram for the burn model determination of emulsion explosive K1.

The JWL parameters of the unreacted emulsion were determined both experimentally and computationally. First, the Hugoniot of the emulsion matrix was determined by experiments and DYNA2D computations /8/. Then the Hugoniot of the explosive was calculated by the method proposed by Voskoboinikov /9/. After that, the isentrope of the explosive was calculated and the JWL parameters were determined by fitting the isentrope into the JWL form. The details of the computation are reported in Appendix 1.

The JWL parameters for the reaction products were calculated by fitting the expansion isentrope of the reaction products which was calculated by the thermo chemical code TIGER. The results are reported in Appendix 2.

The emulsion explosive studied is a research explosive named emulsion K1. It consists of an AN-based matrix and microballoons. Detail compositions have been reported in /8 and 10/.

The data used for the calibration are the VOD (velocity of detonation) values and the radii of the detonation front in different charge diameters. They were obtained from two dimensional steady-state detonation experiments with cylindrical charges /11/. The VOD values from the experiments show a nearly linear relationship with the inverse charge diameter. The detonation fronts recorded clearly indicate the side effects from the charge boundaries. We believe that the experiments contain enough information of the chemical burning kinetics of the explosive. The parameters based on these experiments should properly simulate the burning process of the explosive.

2. EXPERIMENTS AND DYNA2D COMPUTATIONS

2.1 Two Dimensional Steady-State Experiments

Two types of experiments were carried out by Nyberg et al [11]: measuring the detonation velocities and detonation front curvatures at different charge diameters. Totally 17 test shots were fired to determine VOD vs charge diameter. In 8 of them the detonation front curvature was measured simultaneously. The critical diameter of the explosive was determined as about 12 mm. All experiments were carried out in cylindrical PMMA (Plexiglass) tubes with thicknesses from 2 to 5.7 mm.

The VOD values were measured by 5 optical fibres inserted in the PMMA tubes. In order to have a stable detonation velocity, the ratio of charge length to diameter was from 10 to 18. The VOD value for each test was calculated by averaging the VOD values over the four time intervals. Figure 2 shows a good linear relation between VOD and the inverse charge diameter.

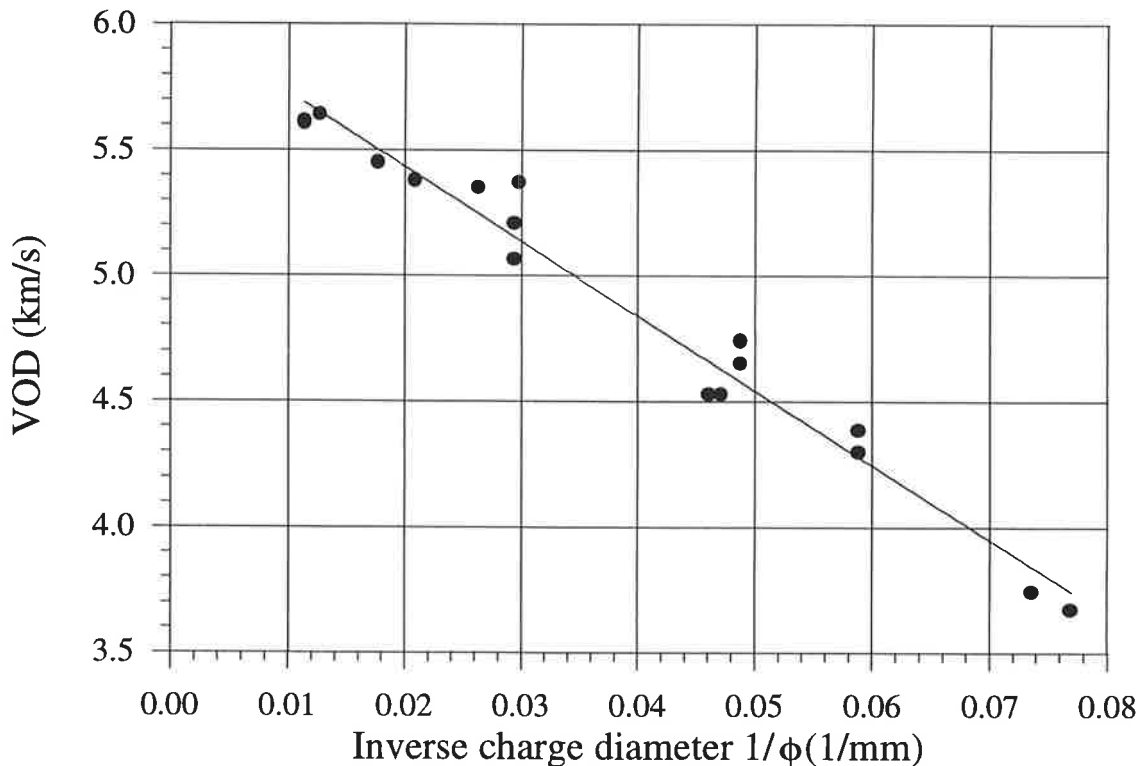


Figure 2: The relationship between VOD and the inverse charge diameter from the 17 experiments with emulsion K1 ($\phi = 13 \sim 80$ mm)

The detonation front curvatures were recorded with a high speed streak camera. The recorded negatives in the time-position space were digitised and then transformed into position-position space under the condition of a constant detonation velocity for each test. The curvature of the detonation front was fitted to an ellipse $r = \sqrt{az^2 + bz + c}$, where r and z are the radial and axial coordinates respectively, a , b and c are the fitting constants. The radius of the curvature is a function of r (or z) and can be calculated by the following equation:

$$R(r) = \frac{(1 + r'^2)^{3/2}}{r''} \quad (1)$$

where $r' = dr / dz$ and $r'' = d^2r / dz^2$ are the first and second derivatives of the curvature function. The value used for calibration is the radius at the charge axis $R^0 = R(r = 0)$. We believe that the radius at the charge centre is more important than that near the charge boundary. Figure 3 shows an example of the experimental detonation front and the radius calculated by equation 1. Relative coordinates are used in the axial direction. Note that the enlarged scale of the z -axis gives a smaller apparent curvature at the origin than at the flanks. This figure shows that the experimental detonation front is described well by the elliptical function.

The relationship between the radius at the charge axis and the charge diameter is shown in Figure 4.

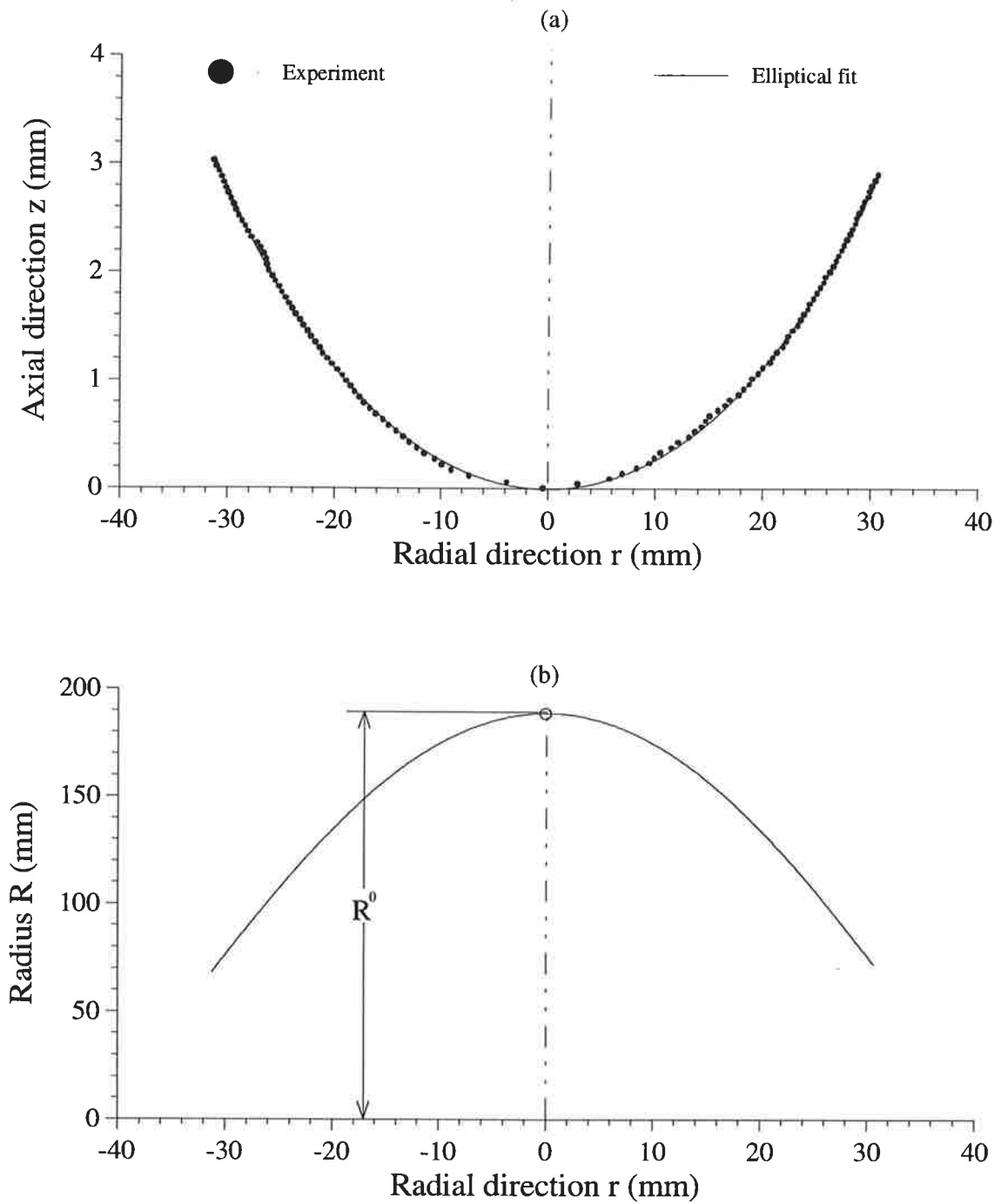


Figure 3: An example of an experimental detonation front and the radius ($\phi = 78.6$ mm, VOD = 5.64 km/s).

(a) detonation front and its elliptical fit;

(b) the radius as a function of the radial position calculated by Equation 1. $R^0 = 188.7$ mm is the value at the charge axis and is used for calibration.

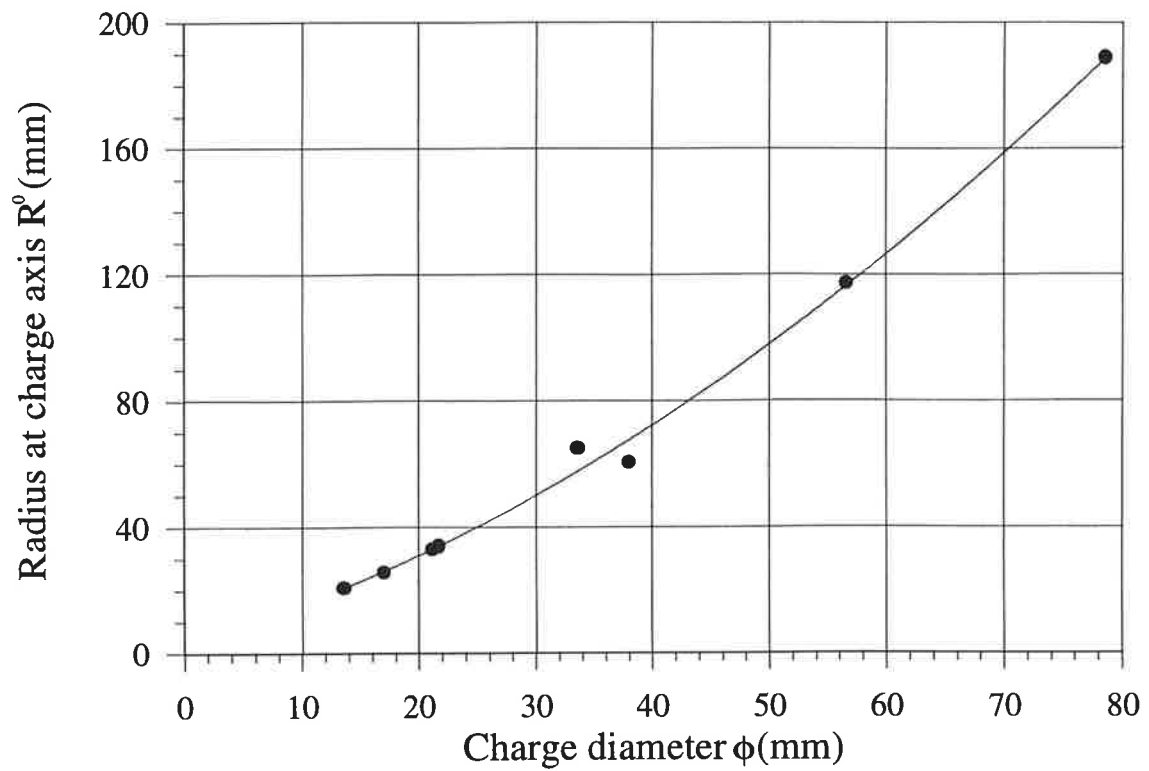


Figure 4: The relationship between the radius of the detonation front curvature at the charge axis and the charge diameter from 8 experiments with emulsion K1 ($\phi = 13.6 \sim 78.6$ mm).

2.2 DYNA2D Computation Set-up

The DYNA2D set-up for the computations is shown in Figure 5. In order to simplify the computations, two material regions were used for the PMMA tube. After a certain computation time, the first part (PMMA1 in Figure 5) is deleted so that the computation can be carried out smoothly to the end. Otherwise, the computation will be very slow or stop because of the large deformation in the first part of the PMMA tube. Axially symmetric geometry is used in the computation.

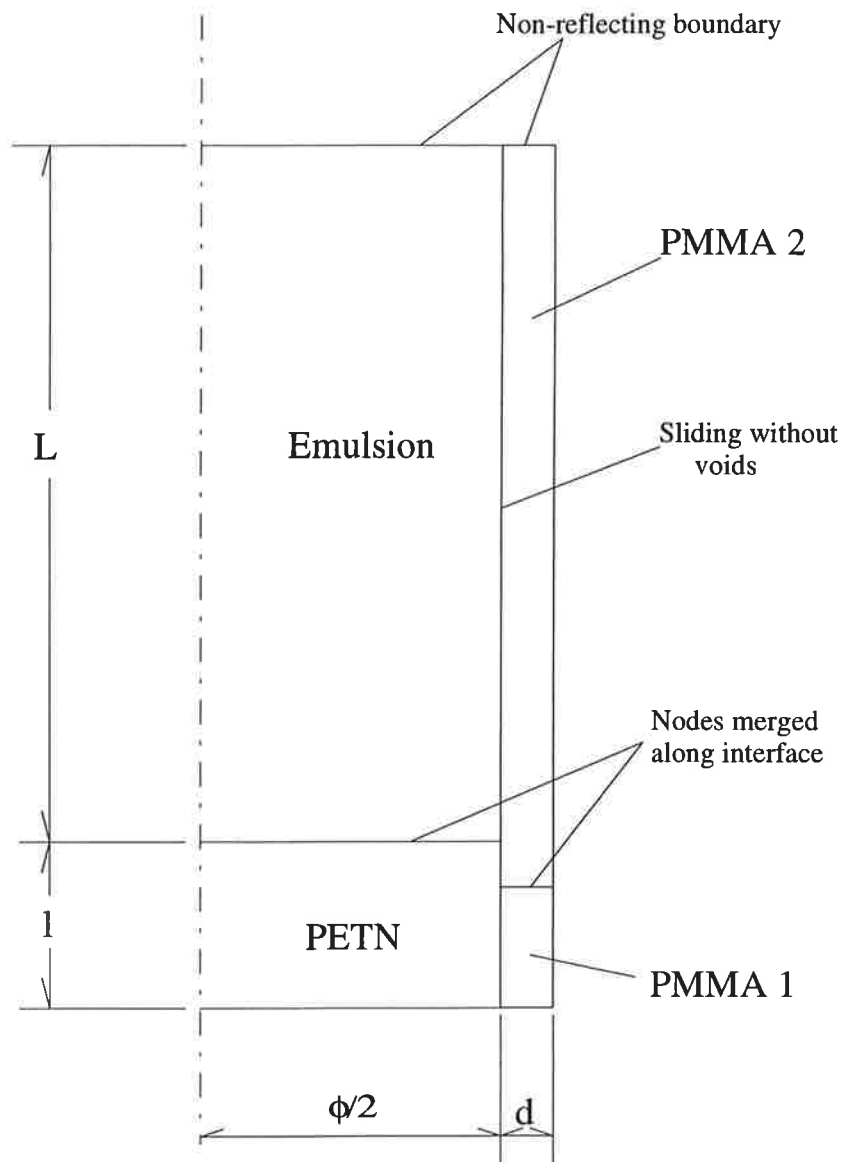


Figure 5: DYNA2D computation set-up.

Totally 8 computational set-ups were used for the simulation of each parameter set. The dimensions of the computation set-ups are shown in Table 1. The cell sizes range from about 1 to 2 elements per millimetre. This is sufficient for commercial explosives, according to Kennedy [12].

Table 1: Dimensions for DYNA2D computation set-ups (see also Figure 5):

No.	Charge diameter: ϕ (mm)	Thickness of the PMMA tube: d (mm)	Length of the charge: L (mm)	Length of the donor: l (mm)	Cell size in the emulsion explosive (mm×mm)
1	13.6	1.2	97.1	14.6	0.486×0.486
2	17.0	1.5	100.0	10.0	0.50×0.50
3	21.2	1.9	121.1	10.1	0.505×0.505
4	21.7	2.4	124.0	10.3	0.517×0.517
5	33.6	3.2	123.2	10.6	0.56×0.56
6	38.0	3.2	130.6	11.9	0.594×0.594
7	56.6	3.2	176.9	17.7	0.884×0.884
8	78.6	5.7	238.1	15.0	1.12×1.12

In the early stages of our computations, models with coarser cells were used (with element size of 2 mm) for the diameter of $\phi = 80$ mm. The results turned out to differ about 5% in VOD values compared with the results obtained using the finer cells. The qualitative conclusions drawn using coarser cells were still valid for the later computations. Errors become much smaller however when the finer cells were used.

The computation starts with the initiation of the PETN (Pentaerythritol Tetranitrate), for which a standard JWL equation of state is used (see Appendix 3). A strong shock is generated for initiation of the emulsion explosive. In our computations, larger PETN donors were used than in the experiments. We thus believe that they are sufficient to initiate the emulsion explosive. With this set-up, we are not testing the initial (or shock to detonation) property of the emulsion explosive. We assume that all measurements from the experiments were obtained from steady detonations, i.e. that both VOD values and the curvature radii of the detonation fronts are independent of time.

The JWL equation of state for both unreacted emulsion explosive and reaction products in the ignition and growth model is in the following form [2]:

$$p = A \cdot e^{-R_1 V} + B \cdot e^{-R_2 V} + \frac{\omega C_v T}{V} \quad (2)$$

where: p — the pressure in Mbar*;

V — specific volume of unreacted explosive and reaction products in cm^3/cm^3 ;

T — temperature in $^\circ\text{K}$;

C_v — specific heat in $\text{Mbars}/^\circ\text{K}$;

A, B, ω, R_1 and R_2 — constants.

The parameters were calculated from experiments or TIGER computations and are listed in Table 2. The details of the computations and the results are described in Appendices 1 and 2 in this report. An example of a DYNA2D computation is presented in Appendix 3.

Table 2: JWL parameters for the unreacted emulsion explosive and its reaction products.

JWL parameter	Unit	Unreacted explosive	Reaction products
A	Mbar	4269.3	4.4423
B	Mbar	-0.0601	0.1547
R_1	—	22.628	6.1054
R_2	—	1.7907	2.2733
ω	—	3.0908	0.9353
Specific heat C_v	Mbar/ $^\circ\text{K}$	1.0885×10^{-5}	1.55567×10^{-5}
Initial internal energy E_0	Mbar cm^3/cm^3 **	—	0.0320

*: 1 Mbar = 100 GPa.

** : 1 Mbar cm^3/cm^3 = 100 GJ/ m^3 .

2.3 Analysis of DYNA2D Results

DYNA2D does not produce the VOD value and the curvature of the detonation front directly. They must be calculated separately from the coordinates and the particle velocity (or pressure) histories of nodes.

2.3.1 VOD analysis

The detonation velocity can be calculated in a similar way as in the experiments. The particle history for a given node can be easily obtained from the ORION (the post-processor of the DYNA2D) data base. The shock arrival time can be defined by setting a certain level of particle velocity in axial direction (300 m/s in our case). Then from the displacement curve of the node, the current position can be calculated (see Figure 6).

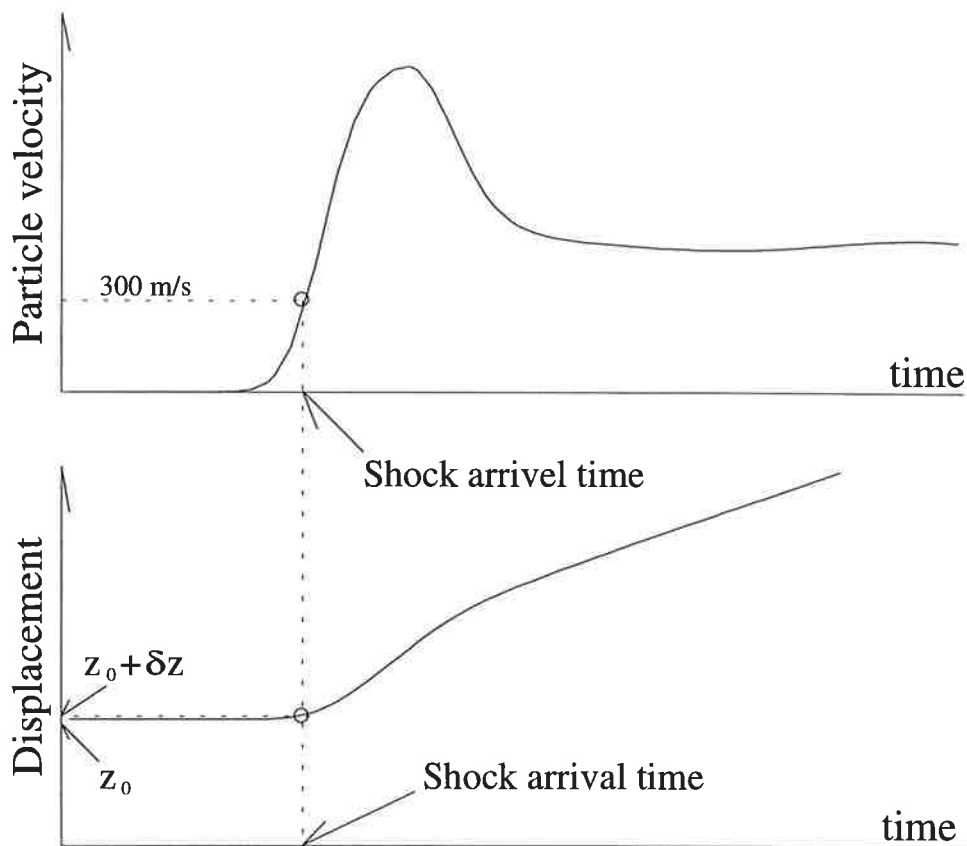


Figure 6: Determination of shock arrival time and the displacement of a given node. z_0 is the original position, δz is the small displacement when the shock arrives.

Five nodes along the charge axis were chosen and the shock travel history was plotted in the time-position space. The detonation velocity is determined by the slope of the line, which is obtained by the least square fit to the arrival times of the five nodes. Figure 7 shows a regression line for the shock arrival time versus position. The high value of the correlation coefficient shows the high stability of the detonation velocity.

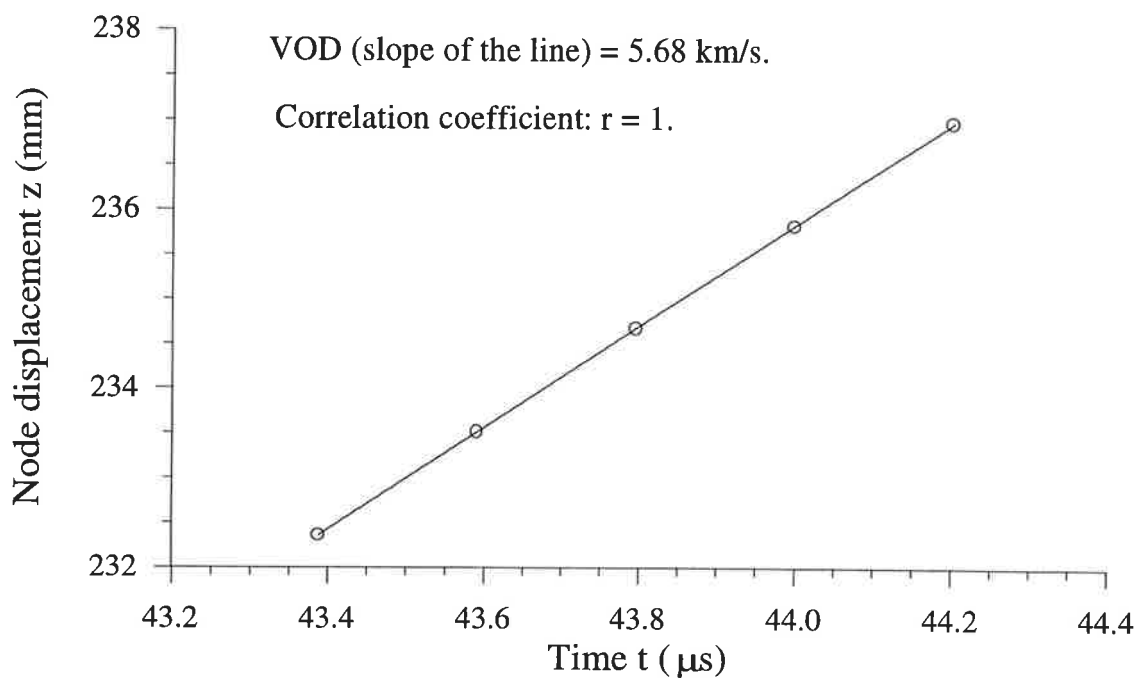


Figure 7: An example of determination of detonation velocity from DYNA2D computation ($\phi = 78.6$ mm).

2.3.2 Analysis of detonation front curvatures

The detonation front curvatures are analysed in a similar way. The nodes used for the curvature determinations lie on a radial line. First the shock arrival times for these nodes can be calculated in the same way as we did with the VOD analysis. Assuming a constant axial detonation velocity for all nodes, their relative positions can be calculated by the following equations:

$$\left. \begin{aligned} z &= z_0 + \text{VOD}_{\text{com}} \times \delta t + \delta z \\ r &= r_0 + \delta r \end{aligned} \right\} \quad (3)$$

where: z_0 — the original z-coordinate of the node;

VOD_{com} — the computed detonation of velocity;

δt — the relative time difference of the node;

δz — small displacement in axial direction when shock arrives;

r_0 — the original r-coordinate of the node;

δr — the small displacement in radial direction when shock arrives.

These points, then, were fitted to an ellipse as we did to the experimental detonation fronts. The curvature radius is calculated by equation 1. Figure 8 shows an example of a computed detonation front and the curvature radius as a function of the radial position. Relative coordinates are used in the axial direction.

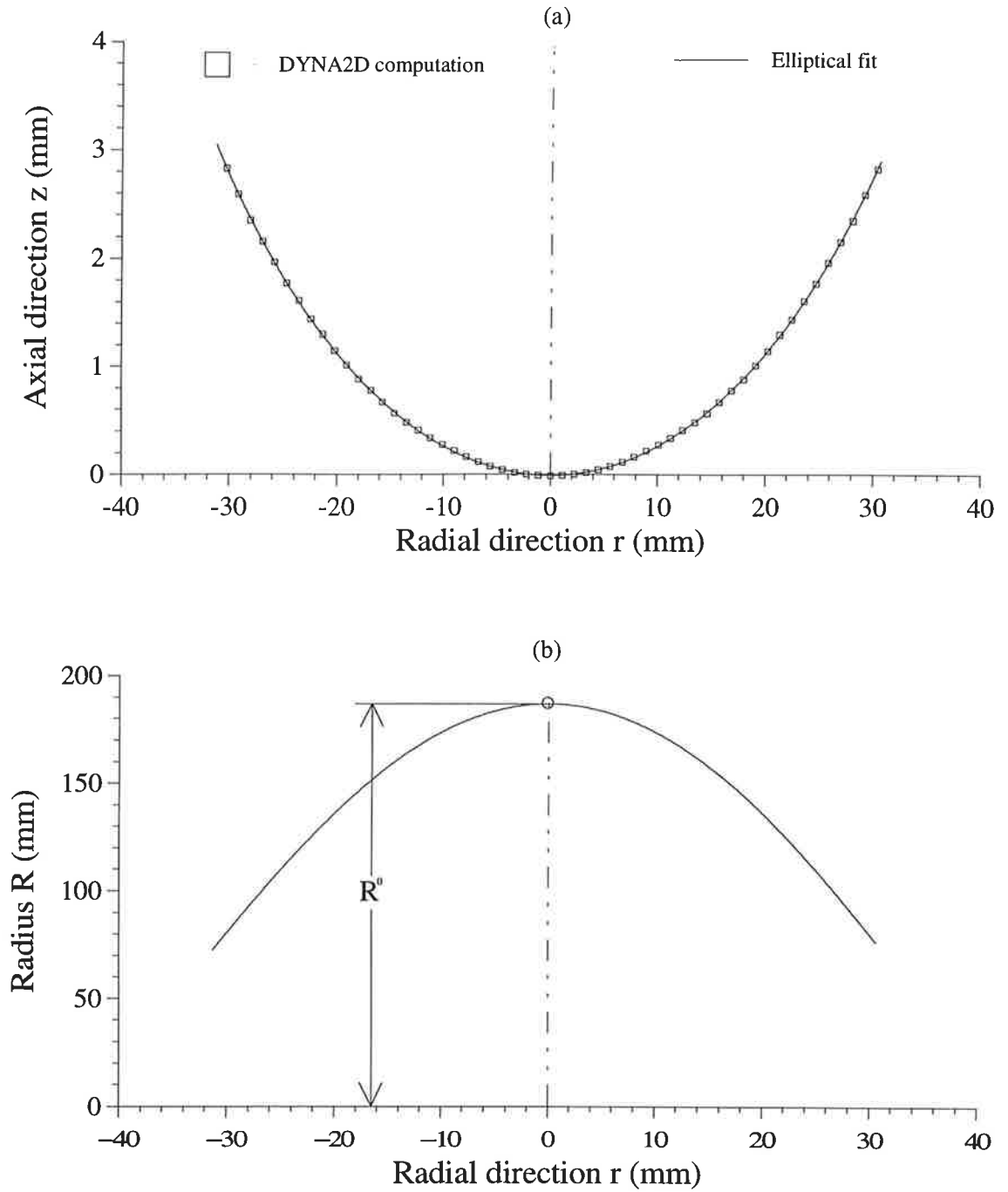


Figure 8: An example of a calculated detonation front and the radius ($\phi = 78.6$ mm, $VOD = 5.64$ km/s).

(a) detonation front and its elliptical fit;

(b) the radius as a function of the radial position calculated by equation 1. R^0 is the value at the charge axis and is used for calibration.

2.3.3 Calibration criteria

The experimental data used for calibration are the detonation velocities and the curvature radii of the detonation fronts at different charge diameters. It is very difficult to link these data to the burning rate parameters.

According to non-ideal detonation theories, the detonation velocity is proportional to the total energy released from the explosive. It depends on the chemical composition of the explosive, density, the charge geometry and the confinement.

The detonation front curvatures show the influence of the side rarefaction from the charge boundary. This is the result of the interaction between the reaction products and the boundary material. It is understandable that the curvature radius of a detonation front gives more details of the burning process. Therefore, a burning model should be able to predict this phenomenon.

The "best" parameters for the burning rate function are determined by minimising the following quantity:

$$Q = \sum_{i=1}^8 \left(\frac{\text{VOD}_{\text{com},i} - \text{VOD}_{\text{exp},i}}{\text{VOD}_{\text{exp},i}} \right)^2 + \sum_{i=1}^8 \left(\frac{R_{\text{com},i}^0 - R_{\text{exp},i}^0}{R_{\text{exp},i}^0} \right)^2 \quad (4)$$

where $\text{VOD}_{\text{com},i}$ and $R_{\text{com},i}^0$ are the VOD values and the curvature radii of detonation fronts at different charge diameters calculated by the DYNA2D. $\text{VOD}_{\text{exp},i}$ and $R_{\text{exp},i}^0$ are those from experiments. Eight is the number of experiments. The radii used for the calibration are the values at the charge axes.

The exact critical diameter is not easily obtained from experiments. Usually rather big ranges are given for commercial explosives. On the other hand, this value has somehow been taken into account when the VOD values at different charge diameters are calibrated, since the smallest charge diameter is rather close to the critical one. Therefore, we think this value is less important than the VOD values and the curvature radii at different charge diameters. We will use this value only for the final check. If the difference between experiments and computations is sufficiently small, the burning rate function is accepted.

3. BURNING RATE FUNCTION

The original three-term burning rate function given by Lee and Tarver /3/ describes the burning process in great details. The simplified two-term model is sufficient though for some military high explosives /4, 13/. Because of the slower reaction, the two-term burning rate function should be sufficient to begin with for the emulsion explosive K1.

3.1 Two-term Burning Rate Function

The two-term burning rate function can be expressed as /2, 3, 4, 13 and 14/:

$$\frac{\partial \lambda}{\partial t} = f(1 - \lambda)^{\alpha_1} (\mu_e - \mu_c)^{\beta_1} + g(1 - \lambda)^{\alpha_2} \lambda^{\alpha_3} p^{\beta_2}, \quad (5)$$

where: λ — the relative amount of explosive which has reacted;

μ_e — the relative compression of the explosive: $\mu_e = \rho_e / \rho_0 - 1$, ρ_e / ρ_0 is the ratio of the current density to the initial density of the explosive, in g/cm³;

μ_c — the critical relative compression;

p — pressure in Mbars;

$f, g, \alpha_1, \alpha_2, \alpha_3, \beta_1$ and β_2 — constants.

There are totally 8 free adjustable parameters in this burning rate function. In practice, only two or three of them are used as adjustable parameters. The others are set to constants. For example, Murphy /13/ used the following burning rate function for some high explosives:

$$\frac{\partial \lambda}{\partial t} = f(1 - \lambda)^{2/9} (\mu_e - \mu_c)^{4.0} + g(1 - \lambda)^{2/9} \lambda^{2/3} p^{\beta_2}, \quad (6)$$

where $\mu_c = 0.01$ and $\beta_2 = 2.0$ for PBX-9404 etc. and $\mu_c = 0$ and $\beta_2 = 3.0$ for LX-17 etc. The parameters were determined by experiments. For example, β_2 was determined by the so called pop-plot of the explosive, which was obtained from wedge tests. Shock to detonation transition experiments could provide sufficient information for the determination of the compression exponent β_1 and the compression threshold μ_c in the ignition term. Therefore, only the values of two parameters f and g need to be

determined perhaps by the VOD and detonation front experiments. This would make the calibration much simpler.

Leiper and Kennedy used the following burning rate function to simulate emulsion explosives /14/:

$$\frac{\partial \lambda}{\partial t} = f\phi(\lambda - \lambda_h)(\lambda - \lambda_h)^{2/9}(\rho_e / \rho_0)^{\beta_1} + g(1 - \lambda)^{2/3}\lambda^{\alpha_3}p^{\beta_2}p_s \quad (7)$$

where ρ_0 and ρ_e are the initial and current densities of the explosive in g/cm³, λ_h is the mass fraction of hot-spot phase and it is equal to the initial void volume of the explosive, p_s is the initial shock pressure and $\phi(\lambda - \lambda_h)$ is a unitary step function. In this burning rate function, there are five adjustable parameters, if the pressure exponent β_2 is treated as an adjustable parameter. The advantage of this function is that it may be possible to predict the density effect, since λ_h is a function of the initial voidage of the emulsion explosive.

We have carried out the Gap Test to determine the critical pressure for a successful detonation of the emulsion explosive K1. The corresponding value determined is $p_c = 0.045$ Mbar or $\mu_c = 0.26$ /10/. However, the physical meaning of these values is different from those represented here in the burning rate function. In the burning rate function, the critical relative compression means the least compression for the explosive to *start burning*, while the parameter obtained from our experiment is the critical compression for a *successful detonation*. The critical pressure for the burning start should be much lower than that for a successful detonation. Therefore we can only conclude from the Gap Test that the critical relative compression in the burning rate function is less than 0.26.

The computation would be too complicated and time consuming, if all 8 parameters in equation 5 were taken into account. It is necessary to use available references and assumptions to define some parameters in the burning rate function before the detailed calibrations.

First, the compression exponent β_1 and pressure exponent β_2 and the critical relative compression μ_c were determined preliminary. Then, the exponents, α_1 , α_2 and α_3 were roughly tested by both VOD values and radii of the detonation fronts at different charge diameters. Finally, the model was verified by focusing on the three remaining parameters:

the two linear coefficients f and g and the critical relative compression μ_c . The final burning rate function will contain only three adjustable parameters, f , g and μ_c .

3.2 Preliminary Determination of Some Burning Rate Parameters

3.2.1 The pressure exponent β_2

A very important burning parameter in the burning rate equation 5 is the pressure exponent β_2 . Usually this parameter is determined by the so called pot-plot of the explosive which can be obtained from wedge tests [5, 13]. The value of this parameter varies from 1.0 to 3.0, implying different growth sensitivities to pressure. We set $\beta_2 = 2$, since the emulsion explosives are less sensitive than some military explosives (where $\beta_2 \approx 3.0$) but more sensitive than most propellants (where $\beta_2 \approx 1.0$).

3.2.2 The compression exponent β_1

This is also an experimentally determined parameter. It is believed that the ignition of the explosive (the ignition of the hot spots) is dependent of shock pressure. For some solid high explosives, $\beta_1 = 4.0$ is used. This shows that the amount of explosive ignited by shock is proportional to the compression to the fourth power or to the pressure squared. We have no experiments concerning such a property of the explosive and the only way to estimate this parameter is to determine it numerically. We have tested β_1 from 1.0 to 5.0. Higher values result in higher detonation velocities. Further more, higher value of this parameter makes the computations too sensitive to the switch (more discussion in section 3.2.4) in the burning rate function, especially for the VOD values. From a numerical point of view, we set $\beta_1 = 2$ to start with. In other words, we assume that the amount of the explosive ignited by the shock is linearly proportional to the pressure.

3.2.3 The critical relative compression μ_c

This is also a parameter which should be determined experimentally. As discussed before, the results from our Gap Tests can not be used directly. Thus we have to determine this value numerically. We have made many computations, mainly by checking the VOD values at different charge diameters. The μ_c value was found to lie between 0.08 to 0.1. Since this value is not so important for large diameters, we used $\mu_c = 0.09$ for rough computations. After we located the ranges of the two linear coefficients f and g , we

changed the μ_c value according to the results of computations so that the best fit between experiments and computations is obtained.

3.2.4 The switch in the burning rate function

There are three switches in the three-term ignition and growth model in DYNA2D /2, 3/. For the two-term burning model, only one is left: λ_{mixig} . The meaning of this parameter is that at this state of the reaction, the ignition phase will be switched off. Our computations show that there is a VOD jump when we increase the parameter g for a certain value of f . In some cases, it was difficult to find proper parameters which give the same VOD values as the experiments.

The reason for this phenomenon seems obvious. When the reacted fraction λ reaches a certain value, for example 0.5 as we used in DYNA2D computations, the ignition term is switched off. Curve 1 in Figure 9 shows the dramatic burning rate drop of the ignition term. If this happens before the second term reaches a sufficient high value, it will cause a sudden decrease of the burning rate (see curve 1 in Figure 10).

To solve this problem, we think that it is better to add a constant to the first term. We employ $(1-2\lambda)^{2/9}$ to replace $(1-\lambda)^{2/9}$. The first term is totally switched off when $\lambda = 0.5$. This "switch" is more smooth than the original one, since the ignition term is switched off gradually (see curves 2 in Figures 9 and 10). In this way, it becomes easier to use the model for our calibration.

The physical meaning of the original ignition term is that the ignition of hot spots is proportional to the amount of unreacted explosive $(1-\lambda)$. Numerically speaking, the replacement of $(1-\lambda)$ by $(1-2\lambda)$ does not affect the final results much. The difference between these two cases can be adjusted by the exponent β_1 . When we decrease β_1 , the difference between the two forms will be smaller.

The physical meaning of the new ignition term is that the ignition is proportional to the material difference between the unreacted explosive $(1-\lambda)$ and the reaction products λ , i.e. $(1-\lambda)-\lambda = 1-2\lambda$. With this factor implemented, the first term is always switched off when 50% of the emulsion explosive has reacted.

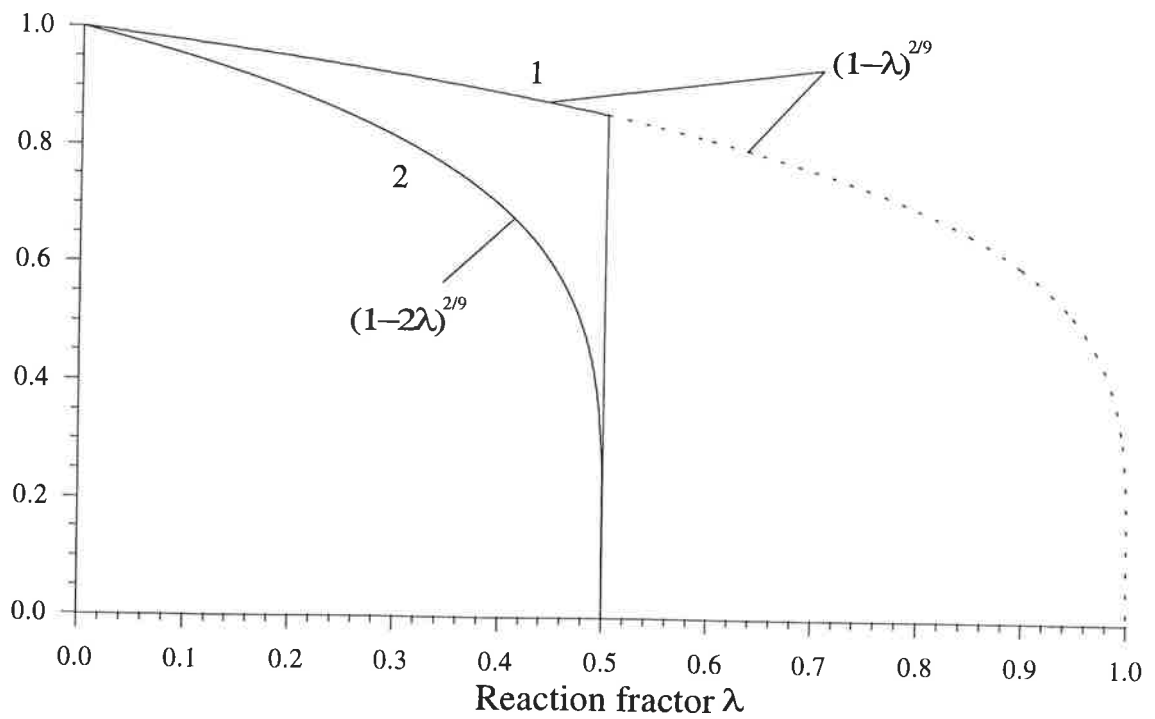


Figure 9: Comparison between the two ignition terms: $(1-\lambda)^{2/9}$ and $(1-2\lambda)^{2/9}$.

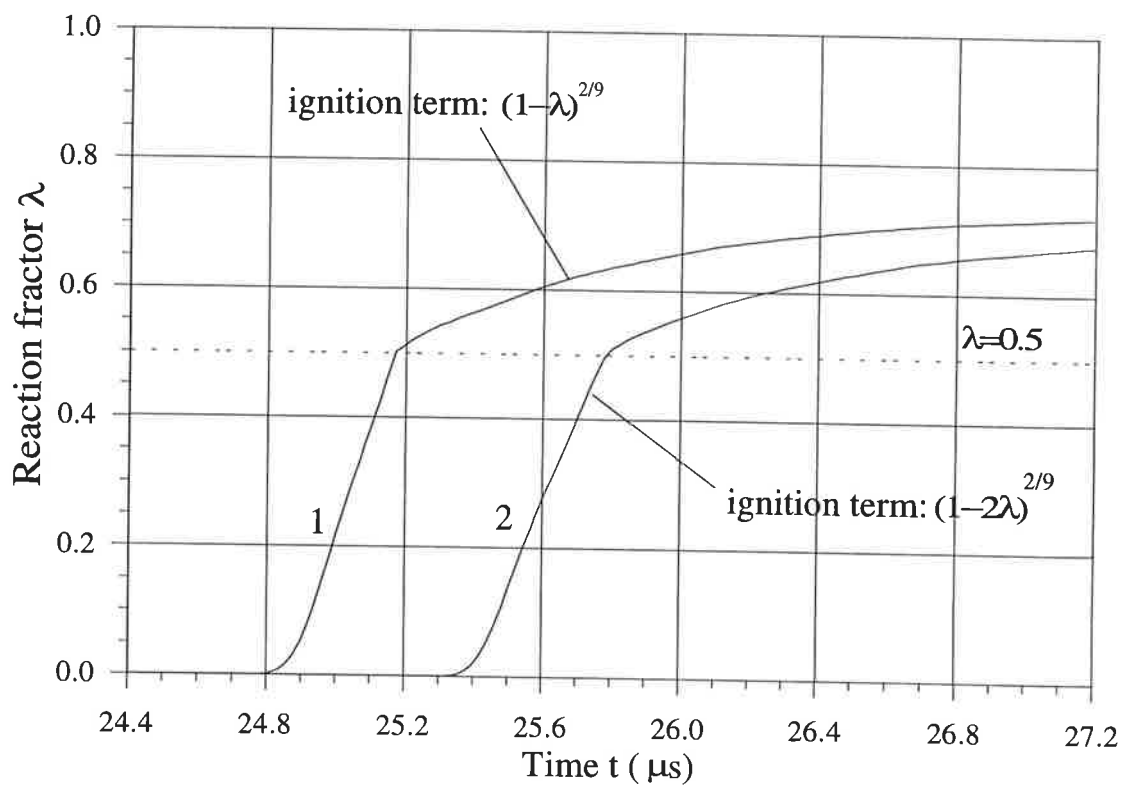


Figure 10: Comparison of reaction histories for the two ignition terms: $(1-\lambda)^{2/9}$ and $(1-2\lambda)^{2/9}$.

3.3 First Optimisation of Burning Rate Parameters

Mainly we have tested two burning rate functions. The first one is based on Murphy's growth term $(1-\lambda)^{2/9}\lambda^{\alpha_3}$ with $\alpha_3 = 2/3$ (see equations 5 and 6). For this function, however, we found that the parameter $\alpha_3 = 1.0$ gives much better fits between experiments and computations for the emulsion explosive. The second one is based on Leiper and Kennedy's growth term $(1-\lambda)^{2/3}\lambda^{\alpha_3}$ (see equations 5 and 7). The exponent $\alpha_3 = 2/9$ gives the best fits between experiments and computations for our emulsion explosive.

3.3.1 Computations with growth term $(1-\lambda)^{2/9}\lambda^{\alpha_3}$

We started with the following burning rate function:

$$\frac{\partial \lambda}{\partial t} = f(1-2\lambda)^{2/9}(\mu_e - \mu_c)^2 + g(1-\lambda)^{2/9}\lambda^{\alpha_3}p^2 \quad (8)$$

First we tested the growth term exponent α_3 , by checking the VOD values and radii at the largest and the smallest diameters. We found that $\alpha_3 = 1$ gave the best fit between the experiments and the computations. At the same time, we also found that the ignition exponent $\alpha_1 = 1/9$ gave better fits than $\alpha_1 = 2/9$, especially for the small diameters.

Then we used the other three parameters (f , g and μ_c) to adjust the computations to experiments. By minimising the quantity Q value in the equation 4, the best parameters of the burning rate function were found as in the following function:

$$\frac{\partial \lambda}{\partial t} = 5(1-2\lambda)^{1/9}(\mu_e - 0.09)^2 + 180(1-\lambda)^{2/9}\lambda p^2 \quad (9)$$

The comparisons of the computed VOD values and the radii of the detonation fronts with the experimental results are shown in Figures 11 and 12. The average VOD difference between experiments and computations is 2.3%, while the radius difference is 9.0%. Figures 13 shows the comparison of the computed detonation front with the experimental one at diameters of $\phi = 78.6$ mm (the biggest one). The results show that with equation 9, both the VOD values and the curvature radii are fitted well for smaller diameters, but not for the large diameters. See Appendix 4 for more examples of equation 9 with different values of f , g and μ_c .

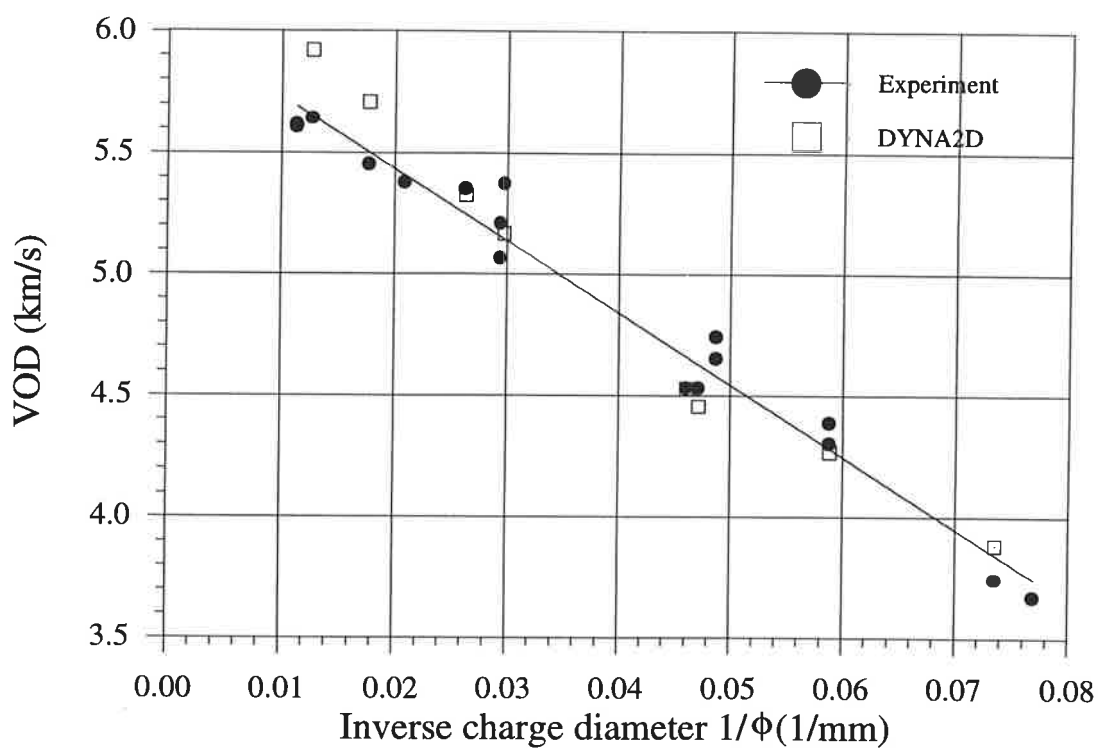


Figure 11: Comparison of VOD values computed by the burning rate equation 9 with the experiments.

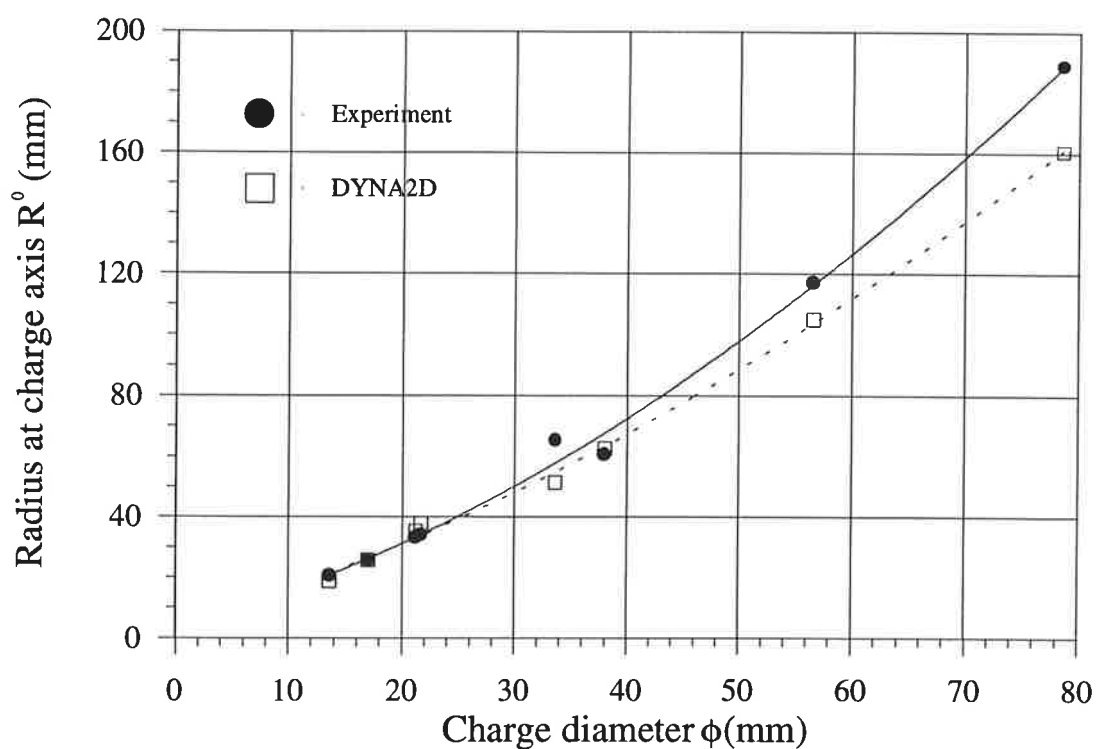


Figure 12: Comparison of the curvature radii computed by the burning rate equation 9 with the experiments.

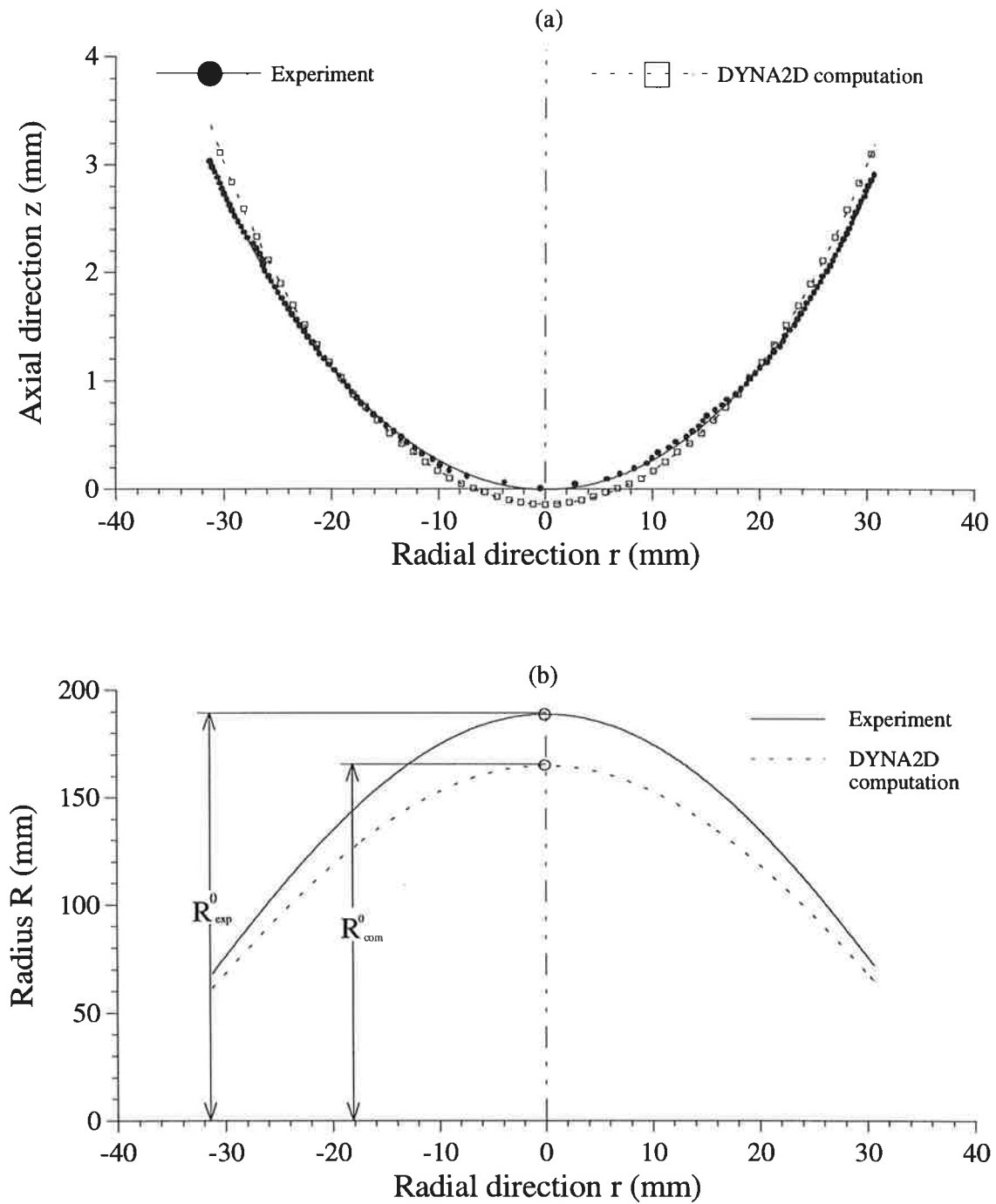


Figure 13: Comparisons of detonation front and curvature radius at charge axis between experiment and computation with equation 9 for diameter $\phi = 78.6$ mm.

(a) comparison of the detonation front;

(b) comparison of the curvature radius: $R_{exp}^0 = 188.7$ mm; $R_{com}^0 = 160.7$ mm
($VOD_{exp} = 5.64$ km/s; $VOD_{com} = 5.92$ km/s).

3.3.2 Computations with growth term $(1 - \lambda)^{2/3} \lambda^{\alpha_3}$

Another alternative for the growth term is to have higher value of α_2 as in Leiper and Kennedy's formula (see equations 5 and 7). We started with the following burning rate function:

$$\frac{\partial \lambda}{\partial t} = f(1 - 2\lambda)^{2/9} (\mu_e - \mu_c)^2 + g(1 - \lambda)^{2/3} \lambda^{\alpha_3} p^2 \quad (10)$$

Surprisingly, this type of burning function gives much better fit of the curvature radii between experiments and computations when $\alpha_3 = 2/9$ is used. With this formula we found very soon that the following function gives best fit for both VOD values and curvature radii between experiments and computations:

$$\frac{\partial \lambda}{\partial t} = 4.5(1 - 2\lambda)^{2/9} (\mu_e - 0.09)^2 + 270(1 - \lambda)^{2/3} \lambda^{2/9} p^2 \quad (11)$$

Comparisons between experiments and computations are shown in Figures 14 and 15. The computed VOD values are now higher than the experimental ones by an average of 160 m/s, varying from 30 to 310 m/s. Figure 15 shows a very good fit of curvature radius between the computations and the experiments. The average difference between the experiments and the computations is only 3.8%. Figure 16 shows an example of the good fit between the computed curvature radius at charge axis and the experimental one for the diameter $\phi = 78.6$ mm (the biggest diameter). See Appendix 4 for more examples of equation 11 with different values of f , g and μ_c .

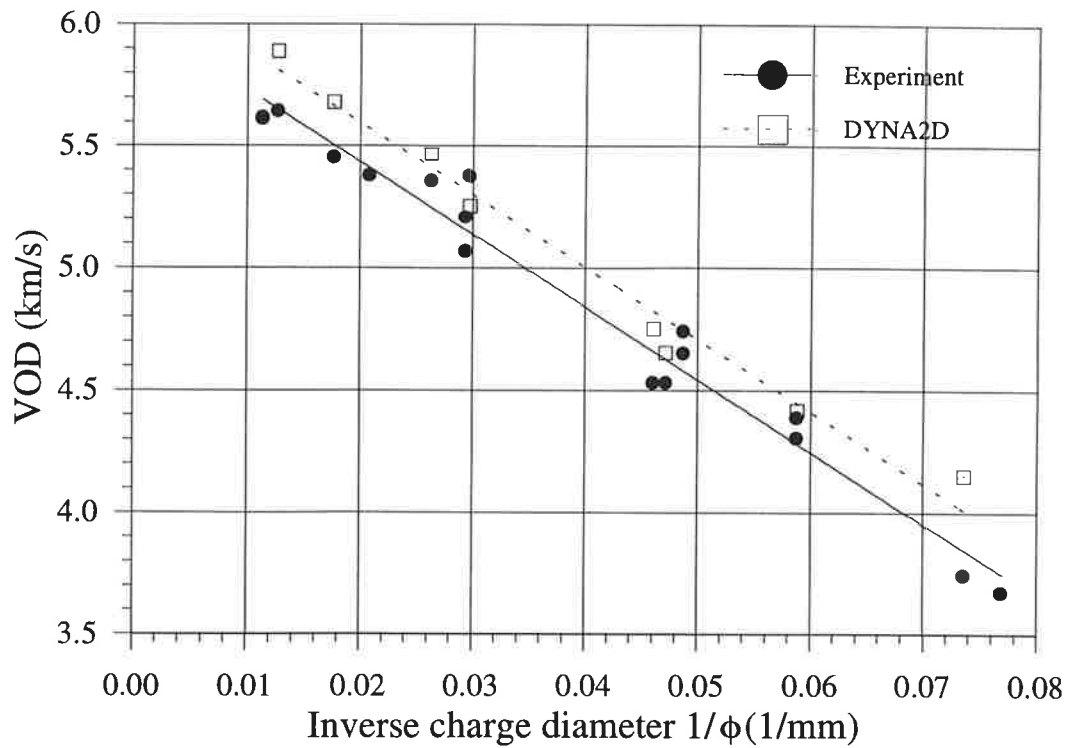


Figure 14: Comparison of VOD values computed by the burning rate equation 11 with the experiments.

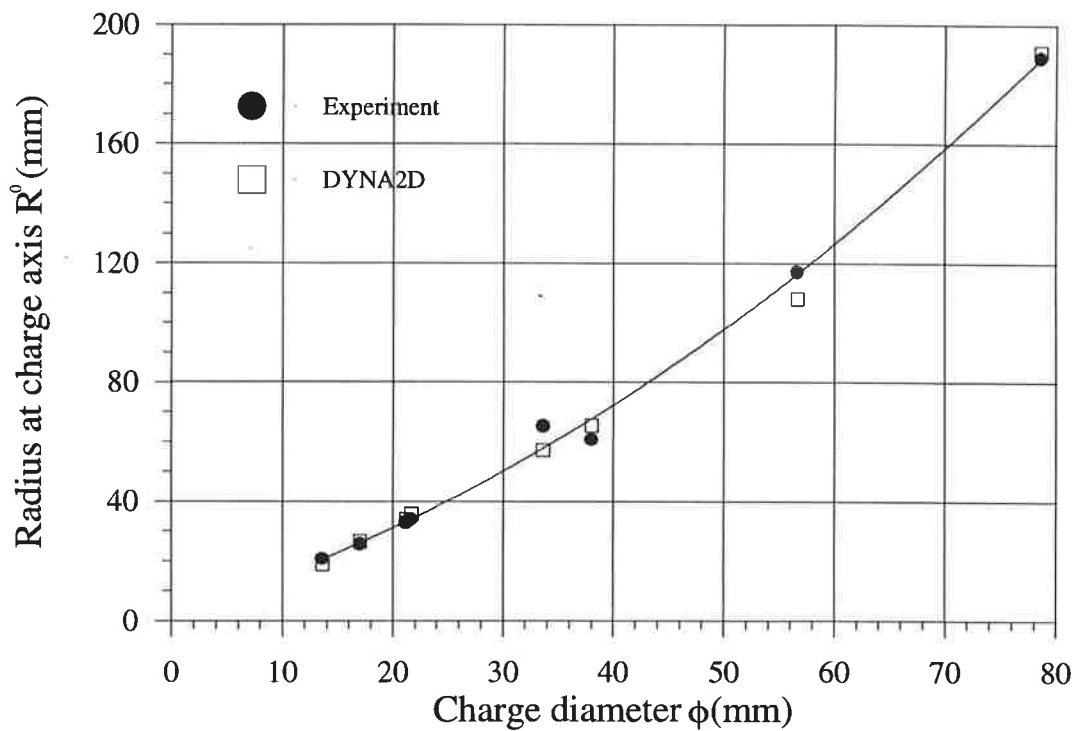


Figure 15: Comparison of the curvature radii computed by the burning rate equation 11 with the experiments.

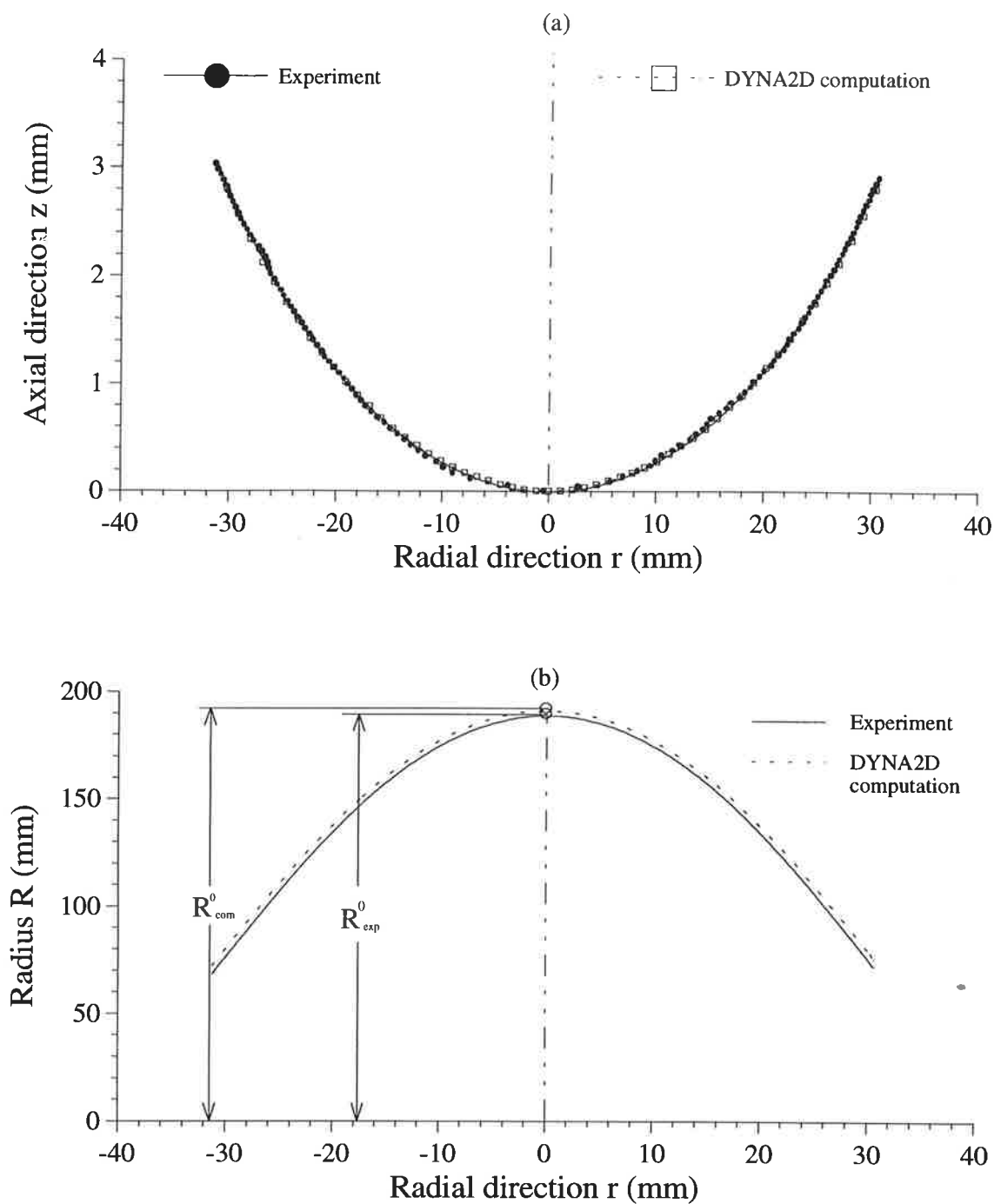


Figure 16: Comparisons of detonation front and radius at charge axis between experiment and computation with equation 11 for diameter $\phi = 78.6$ mm.

(a) comparison of the detonation front;

(b) comparison of the curvature radius: $R_{exp}^0 = 188.7$ mm; $R_{com}^0 = 191$ mm
($VOD_{exp} = 5.64$ km/s; $VOD_{com} = 5.89$ km/s).

3.3.3 The critical diameter

Up till this point, the critical diameter has not been used in our calibration. We think that this value is related to the first term, especially to the critical relative compression μ_c . Computations showed that if a higher μ_c value was used, the computed critical diameter became smaller.

For the burning rate function in equation 9, the computations give a critical diameter of about 12 mm, which is very close to the experimental one. For the burning rate function in equation 11, the critical diameter is about 10 mm, which is smaller than that from experiments. From the fit to VOD values (see Figures 11 and 14), we can see that a better fit with experiments at the smallest diameter gives a computed critical diameter which is closer to the experimental one. Therefore, we can conclude that if a burning model can simulate the VOD values at different diameters accurately, it will also simulate the critical diameter well.

3.4 Optimisation of Burning Rate Parameters with New Initial Internal Energy

All above calibrations were made with constant JWL parameters for both the unreacted emulsion explosive and the reaction products. The accuracy of the JWL parameters, especially those of the reaction products could be questioned because we have obtained them from the TIGER calculation. It is difficult to determine how much the JWL parameters affect the calibration, compared with the parameters in the burning rate function.

Often the JWL parameters for the reaction products are calibrated by the so-called cylinder expansion tests [15]. The detonation velocity and the initial internal energy E_0 are however usually overestimated by the TIGER code. For example, in our case, the detonation velocity from TIGER is 6.18 km/s, while the experimentally extrapolated value to the infinite diameter is 6.03 km/s.

If we allow the initial internal energy E_0 to decrease in our calibration, the results become better. For example, the following burning rate function with an initial internal energy for the reaction products of 0.028 Mbar cm³/cm³ (0.032 Mbar cm³/cm³ from TIGER code) gives best fits for both VOD values and curvature radii at different charge diameters:

$$\frac{\partial \lambda}{\partial t} = 5(1 - 2\lambda)^{2/9}(\mu_c - 0.09)^2 + 300(1 - \lambda)^{2/3}\lambda^{2/9}p^2 \quad (12)$$

The comparison between computations and experiments is shown in Figures 17 and 18. The average VOD difference between the experiments and the computations is about 1.3%, while the curvature radius difference is 4.1%. The comparison of curvature radius between the experiment and the computation for the largest diameter is shown in Figure 19. In this case we changed only the two linear coefficients f and g in equation 11 and the initial internal energy E_0 . See Appendix 4 for more computations with equation 12 using different initial internal energies for the reaction products of the emulsion explosive.

This result shows that the initial internal energy in the JWL equation of state for the emulsion explosive is very important for the calibration. We can further conclude that the JWL parameters for both the unreacted explosive and the reaction products are very important and should probably be carefully verified by experiments.

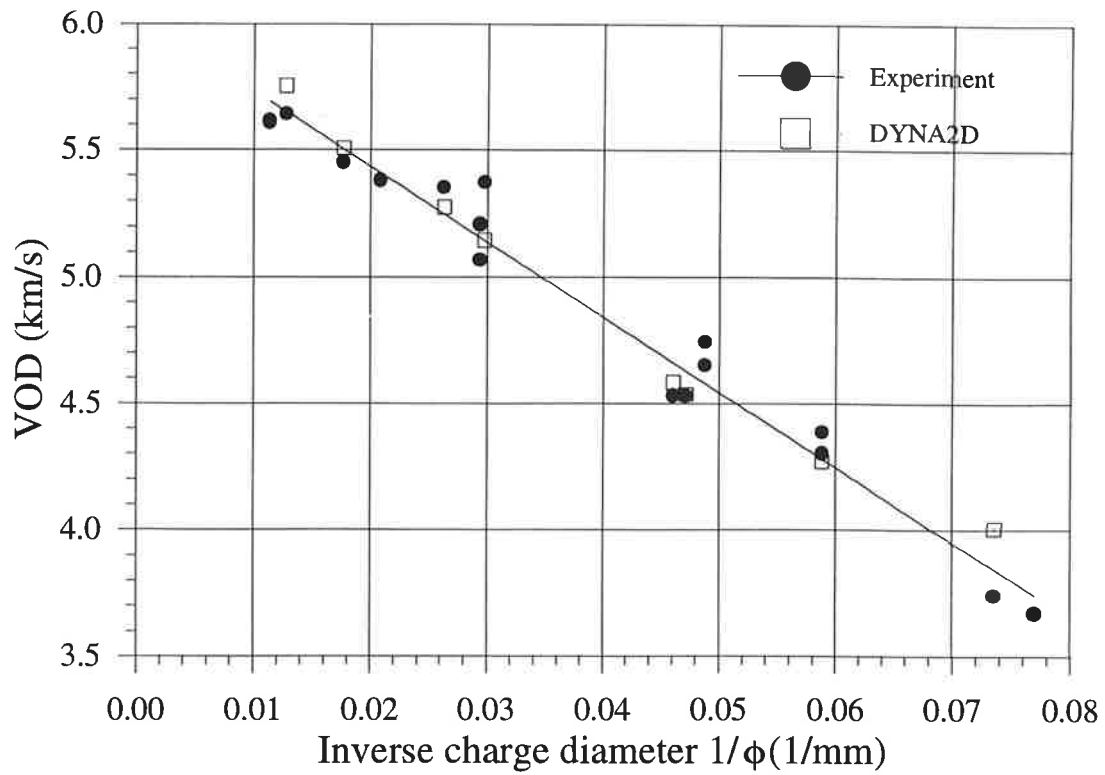


Figure 17: Comparison of VOD values computed by the burning rate equation 12 ($E_0 = 0.028 \text{ Mbar cm}^3/\text{cm}^3$) with the experiments.

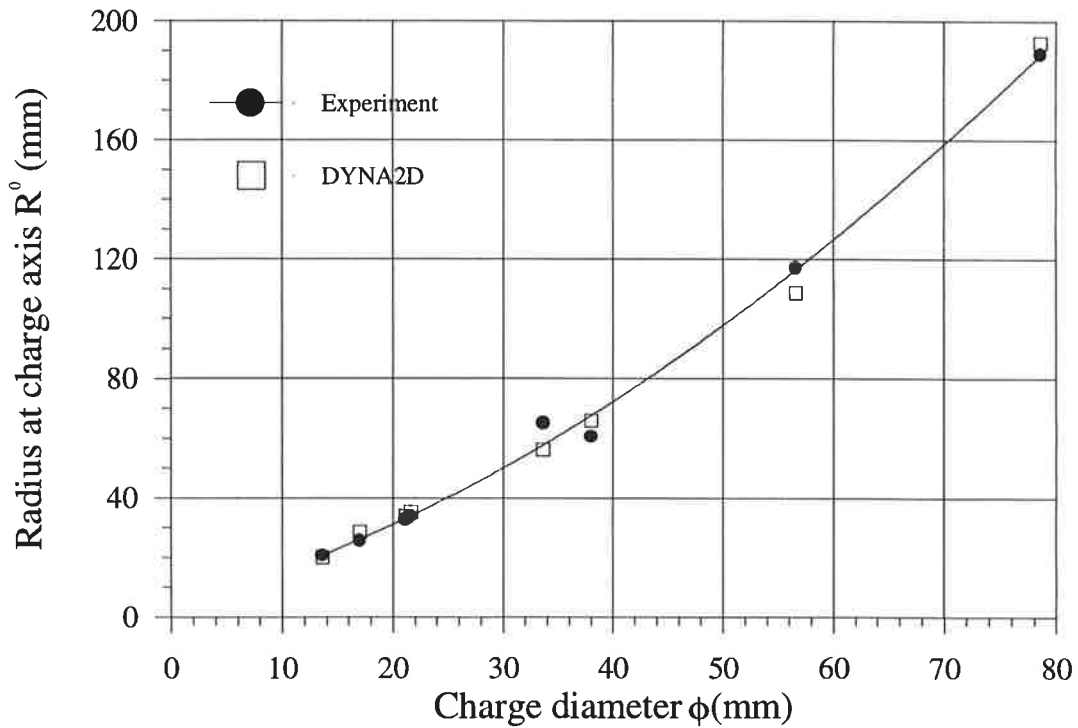


Figure 18: Comparison of the curvature radii computed by the burning rate equation 12 ($E_0 = 0.028 \text{ Mbar cm}^3/\text{cm}^3$) with the experiments.

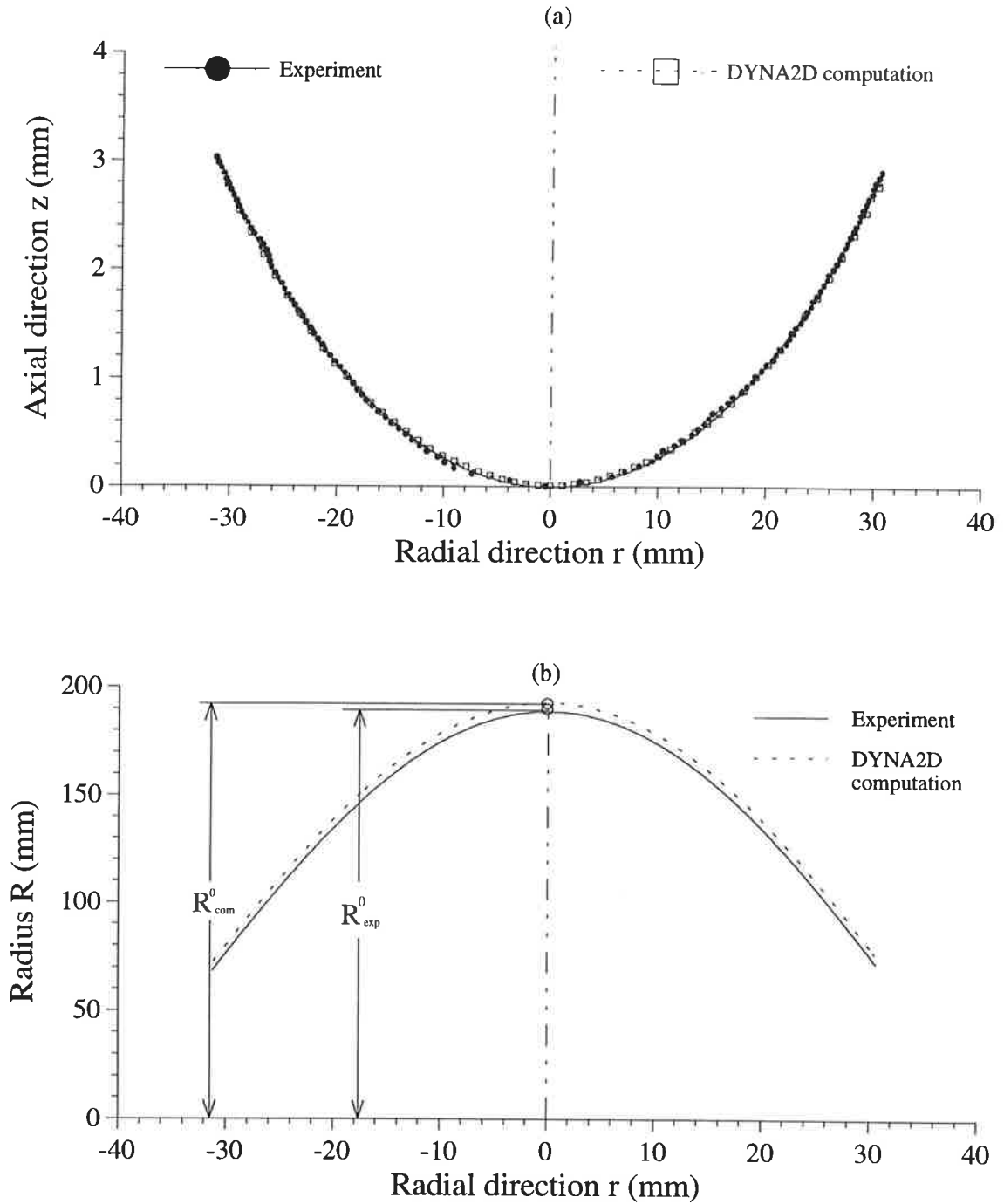


Figure 19: Comparisons of detonation front and radius at charge axis between experiment and computation with equation 12 for diameter $\phi = 78.6$ mm.

(a) comparison of the detonation front;

(b) comparison of the curvature radius: $R_{\text{exp}}^0 = 188.7$ mm; $R_{\text{com}}^0 = 192.7$ mm
($\text{VOD}_{\text{exp}} = 5.64$ km/s; $\text{VOD}_{\text{com}} = 5.75$ km/s).

4. DISCUSSION

The agreement between the computations and the experiments is good using burning rate equations 9 and 11, but in different aspects. The drawbacks with equation 9 is that the absolute differences between the computations and the experiments for the large diameters are large. For example, VOD and curvature radius differences between the computation and the experiment are 280 m/s and 28 mm for the charge diameter of 78.6 mm. With this burning rate equation, the computed curvature radius is always smaller than that from the experiments with the large diameter. This might indicate the wrong burning geometry, which is represented by the two exponents α_2 and α_3 in the growth term /4/.

Better fits of the curvature radii between the experiments and the computations than VOD fits were obtained by the burning rate equation 11. The drawback with this equation is the high computed VOD values at different charge diameters. For example, the maximum VOD difference can be as large as 8% for the small diameters. The perfect curvature radius agreement with experiments indicates that the model is better in terms of the burning geometry.

Although both burning rate functions were found suitable for the emulsion explosive, there are still some unsolved problems with this model. First, none of the two equations give the best fits for both VOD values and curvature radii at large diameters. It is generally believed to be much easier to achieve a good fit for the larger diameters than for the smaller diameters, because more stable results can be obtained both experimentally and computationally. The reason for the large discrepancy at large diameters is unknown to us.

Secondly, it is very difficult to make a systematical calibration based on the experiments we have made, especially for the ignition term. One would think that this term could be calibrated by experiments with smaller diameters. But this is not always true since the influence of the second term can not be separated from the first term.

We found also that the critical relative compression μ_c has little effect on the VOD value for the large diameters. This compression can be restricted within a rather small range by the critical diameter.

Finally, we have already proven the importance of the initial internal energy E_0 in the JWL equation of state for the reaction products. In fact, all the JWL parameters are important for the calibration. The problem with this is that we do not know whether the differences between the computations and the experiments are due to the burning rate parameters or due to the JWL parameters for both the unreacted explosive and the reaction products. What we can do to improve the calibration is to calibrate these JWL parameters as accurately as possible by experiments and ensure that their influences on the computations are negligible.

The model needs to be verified by more experiments, for example, experiments with different confinements and different amounts of microballoons. Such experiments are planned for the near future.

Further more, the model might not accurately predict unsteady detonations of the explosive, for example, the shock to detonation process, since the burning parameters have not been calibrated for such experiments. Such data could e.g. be obtained from experiments with embedded EMV or pressure gauges /16/.

5. CONCLUSIONS

1. It is possible to use the two-term ignition and growth model for our emulsion explosive. Both the VOD values and the curvature radii at different charge diameters can be simulated to an acceptable level of accuracy by the model.
2. The following burning rate function gives the best fit for VOD value versus charge diameter:

$$\frac{\partial \lambda}{\partial t} = 5(1 - 2\lambda)^{1/9} (\mu_e - 0.09)^2 + 180(1 - \lambda)^{2/9} \lambda p^2$$

The critical diameter determined by this function is about 12 mm, which is close to the experimental value.

3. The following burning rate function gives the best fit for front curvature radius versus charge diameter:

$$\frac{\partial \lambda}{\partial t} = 4.5(1 - 2\lambda)^{2/9} (\mu_e - 0.09)^2 + 270(1 - \lambda)^{2/3} \lambda^{2/9} p^2$$

The critical diameter determined by this function is about 10 mm, which is smaller than the experimental value.

4. When the initial internal energy E_0 is set to 0.028 Mbar cm³/cm³, the following burning rate function gives the best fit for both VOD value and curvature radius versus charge diameter:

$$\frac{\partial \lambda}{\partial t} = 5(1 - 2\lambda)^{2/9} (\mu_e - 0.09)^2 + 300(1 - \lambda)^{2/3} \lambda^{2/9} p^2$$

5. Calibrations show that the initial internal energy for the reaction products of the emulsion is very important for the calibration. This indicates that the accuracy of the JWL parameters for the unreacted emulsion, obtained from the Hugoniot of the matrix and mixing rules, and the reaction products, obtained with the TIGER calculation, should be verified independently by experiments.

6. Improvements to the model can be made in the following ways:

- Cylinder tests should be carried out for an accurate estimation of the JWL parameters for the reaction products;
- Shock to detonation experiments should be carried out for the determination of the compression threshold and the compression exponent. Then the ignition term can be given with a much greater confidence.

ACKNOWLEDGMENTS

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APPENDICES

Appendix 1: Equation of State of the Unreacted Emulsion Explosive

For the burning model used in this study, the properties of both unreacted explosive and reaction products are necessary. In this Appendix we will describe the method used to deduct the Equation-of-State parameters for the unreacted explosive. The method consists of two steps. First the Hugoniot of the emulsion matrix was determined experimentally. Then the Hugoniot of the emulsion explosive was calculated.

1. Hugoniot of the matrix

The impedance-matching method was employed for determination of the Hugoniot of the emulsion matrix /8/, and the Hugoniot determined is:

$$U_s = 2.26 + 1.554 \cdot U_p \quad (\text{A-1})$$

where: U_s — shock wave velocity in the matrix in km/s;

U_p — particle velocity in the matrix in km/s.

2. Hugoniot of the unreacted emulsion explosive

The emulsion explosive is a mixture of the matrix and the microballoons. Therefore it can be regarded as a "porous" matrix. For such a porous material, its Hugoniot may be calculated by the Voskoboinikov's method /9/. This method is based on the following two assumptions:

- 1) The microballoons in the matrix behave as an ideal gas.
- 2) A mechanical equilibrium exists between the matrix and the microballoons. That is, the pressure is the same in the matrix and in the microballoons.

The detail calculations are described in the following.

The Hugoniot of the matrix can be written in the form:

$$\frac{U_{sm}}{a_0} = \alpha_1 + \alpha_2 \cdot \frac{U_{pm}}{a_0} \quad (A-2)$$

where: U_{sm} — shock wave velocity in the matrix in km/s;

U_{pm} — particle velocity in the matrix in km/s;

a_0 — the sound velocity of the matrix. Here $a_0 \approx 2.26$ km/s was used.

The Hugoniot of the mixture of the matrix and the ideal gas is also a linear relation between the shock wave velocity and the particle velocity and can be written as:

$$\frac{U_{se}}{a_0} = \sigma + \xi \cdot \frac{U_{pe}}{a_0} \quad (A-3)$$

where: U_{se} — shock wave velocity in the emulsion explosive in km/s;

U_{pe} — particle velocity in the emulsion explosive in km/s.

Here σ and ξ are constants. Their values are determined by the initial density of the matrix, initial density of the emulsion explosive, constant α_1 and constant α_2 :

$$\sigma = \frac{\rho_{0m}}{\rho_{0e}} \cdot (B_1 + 1.141 \cdot B_3) \quad \xi = \frac{\rho_{0m}}{\rho_{0e}} \cdot (B_2 - 0.2958 \cdot B_3) \quad (A-4)$$

where: ρ_{0m} — the initial density of the matrix in g/cm³;

ρ_{0e} — the initial density of the emulsion explosive in g/cm³;

B_1 , B_2 and B_3 — constants which can be calculated by the following equations:

$$\begin{aligned} B_1 &= \frac{\alpha_1}{(\beta \cdot \alpha_2 + 1)^{1.5}} & B_2 &= \frac{\alpha_2}{\beta \cdot \alpha_2 + 1} \\ B_3 &= -\frac{\alpha_1^2}{2 \cdot (\beta \cdot \alpha_2 + 1)^2} & \beta &= \frac{2}{\gamma + 1} \cdot \left(\frac{\rho_{0m}}{\rho_{0e}} - 1 \right) \end{aligned} \quad (A-5)$$

where: γ — the ratio of specific heats of the ideal gas.

Comparing equations A-1 and A-2, we have $\alpha_1 = 2.26/a_0 = 1.0$ and $\alpha_2 = 1.554$. The densities of the matrix and the emulsion explosive are $\rho_{0m} = 1.38$ g/cm³ respective $\rho_{0e} = 1.165$ g/cm³. The value for γ is taken as 1.40 for an ideal gas. By equations A-4 and A-5, the values achieved are $\sigma = 0.7912$ and $\xi = 1.5033$. Therefore, the Hugoniot of the unreacted emulsion explosive is:

$$U_{se} = \sigma \cdot a_0 + \xi \cdot U_{pe} = 1.788 + 1.503 \cdot U_{pe} \quad (\text{km/s}) \quad (A-6)$$

3. JWL parameters for the unreacted emulsion explosive

In the DYNA2D code, the JWL equation of state is used for unreacted explosive. Therefore we have to express the equation of state of the unreacted explosive in the JWL form. This has been performed in two calculations.

First the isentrope of the unreacted explosive between the initial state and the Von Neumann pressure was calculated based on the Hugoniot of the explosive. The Von Neumann pressure was taken as twice the C-J pressure which was calculated by the TIGER code, see Appendix 2.

Then the isentrope was fitted to the JWL equation. The curve fitting was carried out by a computer program ANPASS, which was made by Henrik Almström at FOA.

In the following, the deduction of the isentrope will be outlined and the final JWL equation for the unreacted explosive will be presented.

Since the Hugoniot of the explosive K1 is known (equation A-6) and the Grüneisen gamma is assumed to be 1.5, the equation of state of the explosive can be expressed in the Grüneisen form /2/:

$$p = \frac{\rho_0 C^2 \mu \left[1 + \left(1 - \frac{\gamma_0}{2}\right) \mu - \frac{a}{2} \mu^2 \right]}{\left[1 - (S_1 - 1) \mu - S_2 \frac{\mu^2}{1 + \mu} - S_3 \frac{\mu^3}{(1 + \mu)^2} \right]^2} + (\gamma_0 + a\mu)E \quad (\text{A-7})$$

where: $\mu = v_0/v - 1$;

E = internal energy in Mbar cm^3/cm^3 ;

γ_0 = Grüneisen gamma;

p = pressure in Mbar;

V = specific volume.

Other constants for our explosive are: $a = S_2 = S_3 = 0$ and $S_1 = 1.503$. Thus the Grüneisen equation of state (Equation A-7) can be transformed into:

$$\begin{aligned}
 p &= \frac{\rho_0 C^2 \left(\frac{v_0}{v} - 1 \right) \left[1 + \left(1 - \frac{\gamma_0}{2} \right) \left(\frac{v_0}{v} - 1 \right) \right]}{\left[1 - (S_1 - 1) \left(\frac{v_0}{v} - 1 \right) \right]^2} + \gamma_0 E \\
 &= \frac{\rho_0 C^2 (v_0 - v) \left[v + \left(1 - \frac{\gamma_0}{2} \right) (v_0 - v) \right]}{\left[v - (S_1 - 1)(v_0 - v) \right]^2} + \gamma_0 E
 \end{aligned} \tag{A-8}$$

Assign:

$$\begin{aligned}
 F(v) &= \frac{\rho_0 C^2 (v_0 - v) \left[v + \left(1 - \frac{\gamma_0}{2} \right) (v_0 - v) \right]}{\left[v - (S_1 - 1)(v_0 - v) \right]^2} \\
 &= \frac{-\frac{\gamma_0}{2} v^2 + (\gamma_0 - 1)v_0 v + \left(1 - \frac{\gamma_0}{2} \right) v_0^2}{\left[S_1 v + (1 - S_1)v_0 \right]^2}
 \end{aligned}$$

Equation A-8 can be further written into:

$$E = E[p(s, v), v] = \frac{p - F(v)}{\gamma_0} \tag{A-9}$$

where: s = entropy.

The isentrope can be derived accordingly, since at the isentrope we have:

$$ds = 0$$

$$\text{or} \quad dE/dv = -p \tag{A-10}$$

while dE/dv can be obtained from Equation A-9:

$$\frac{dE}{dv} = \frac{1}{\gamma_0} \frac{dp}{dv} - \frac{1}{\gamma_0} \frac{dF}{dv} \tag{A-11}$$

Equating A-10 and A-11, the equation for dp/dv can be obtained:

$$\frac{dp}{dv} + \gamma_0 p = \frac{dF}{dv} = f(v)$$

where:

$$f(v) = \rho_0 C^2 \cdot \left\{ \frac{-\gamma_0 v + (\gamma_0 - 1)v_0}{[S_1 v + (1 - S_1)v_0]^2} - \frac{2S_1 \left[-\frac{\gamma_0}{2} v^2 + (\gamma_0 - 1)v_0 v + \left(1 - \frac{\gamma_0}{2}\right)v_0^2 \right]}{[S_1 v + (1 - S_1)v_0]^3} \right\}$$

$$= \frac{C^2(S_1 - \gamma_0)v + C^2(\gamma_0 - 1 - S_1)v_0}{[S_1 v + (1 - S_1)v_0]^3} = \frac{a_1 v + a_2}{[S_1 v + (1 - S_1)v_0]^3},$$

$$a_1 = C^2(S_1 - \gamma_0)$$

$$a_2 = C^2(\gamma_0 - 1 - S_1)v_0$$

Finally the differential equation for the isentrope is:

$$\frac{dp}{dv} + \gamma_0 p = \frac{a_1 v + a_2}{[S_1 v + (1 - S_1)v_0]^3}$$

And the solution of this equation is:

$$p = k(v)e^{-\gamma_0 v}$$

$$\text{where: } k(v) = \int \frac{a_1 v + a_2}{[S_1 v + (1 - S_1)v_0]^3} e^{\gamma_0 v} dv + c$$

c = integration constant.

For the explosive K1, we have $\rho_0 = 1.165 \text{ g/cm}^3$, $C = 0.1788 \text{ cm}/\mu\text{s}$, $S = 1.503$ and $\gamma_0 = 1.5$. Then: $a_1 = 9.59 \cdot 10^{-5}$, $a_2 = -0.02752$ and

$$k(v) = \int \frac{9.59 \cdot 10^{-5} \cdot v - 0.02752}{(1.503v - 0.431)^3} \cdot e^{\gamma_0 v} dv + c$$

$$= \frac{9.109 \cdot 10^{-3} \cdot e^{1.5v}}{(1.5v - 0.431)^2} + \frac{9.067 \cdot 10^{-3} \cdot e^{1.5v}}{1.5v - 0.431} + c.$$

The value of the constant c is determined by the boundary condition: $p = 0$ at $v = v_0$, which implies: $k(v) = 0$ when $v = v_0$, or $c = 0.0834$. Therefore, the isentrope of the emulsion explosive K1 can be described by:

$$p = \left[\frac{9.109 \cdot 10^{-3} \cdot e^{1.5v}}{(1.5v - 0.431)^2} + \frac{9.067 \cdot 10^{-3} \cdot e^{1.5v}}{1.5v - 0.431} + 0.0834 \right] e^{-1.5v} \quad (\text{A-12})$$

Where the units are Mbar for p and cm^3/g for v .

After this, the isentrope in equation A-12 is fitted with the JWL form and the resulted JWL equation of state is:

$$p = 4269.3 \cdot \left(1 - \frac{3.0908}{22.628V}\right) \cdot e^{-22.628V} - 0.0601 \cdot \left(1 - \frac{3.0908}{1.7907V}\right) \cdot e^{-1.7907V} + \frac{3.0908E}{V}$$

Here $V = v/v_0$.

4. Estimation of the "Heat Capacity" of the emulsion explosive

The heat capacity is a parameter required by DYNA2D as a constant. This value is difficult to get experimentally, and it is a function of temperature. Here we calculate the value from the initial state on the isentrope: $p_0 = 0$ Mbar, $V_0 = 1 \text{ cm}^3/\text{cm}^3$ and $T_0 = 298^\circ\text{K}$. Then by the JWL equation /2/ (equation 2), we calculate the heat capacity of the unreacted emulsion $C_{vr} = 1.0886 \times 10^{-5}$ Mbar/ $^\circ\text{K}$.

Appendix 2: Equation of State of the Reaction Products

1. JWL parameters for the reaction products

Since the JWL equation of state is also used in DYNA2D code to describe the reaction products, the JWL parameters are necessary even for the reaction products. The deduction of these parameters have been done in two steps.

First, the reaction products and their isentropic expansion from the CJ-state were calculated by the thermodynamic code TIGER using the BKWR equation of state. The calculated CJ-state is shown below:

Detonation velocity = 6,18 km/s

Particle velocity at CJ state = 1,52 km/s

CJ pressure = 0.1085 Mbar

Specific volume at CJ state = 0.7544 cm^3/cm^3

Temperature at CJ state = 1919 °K

Then the calculated isentrope for the reaction products was again fitted in the JWL form by the program ANPASS and the JWL equation of state is:

$$p = 4.4423 \cdot \left(1 - \frac{0.9353}{6.1045V}\right) \cdot e^{-6.1045V} + 0.1547 \cdot \left(1 - \frac{0.9353}{2.2733V}\right) \cdot e^{-2.2733V} + \frac{0.9353E}{V}$$

Here $V = v/v_0$.

2. The initial internal energy of the reaction products

There are many ways to estimate the initial internal energy E_0 of an explosive. Here we calculate this value for the reaction products of the emulsion explosive by a TIGER computation.

From the TIGER computation, we got the following results:

- (1) the standard energy of explosive: $e_0 = -0.075578 \text{ Mbar cm}^3/\text{cm}^3$;
- (2) the energy after expansion to 10 times initial volume: $e_{10} = -0.107533 \text{ Mbar cm}^3/\text{cm}^3$.

Therefore, the initial internal energy of the reaction products of the emulsion explosive can be estimated as follows:

$$E_0 = e_{10} - e_0 = -0.031954 \text{ Mbar cm}^3/\text{cm}^3.$$

The value we used for DYNA2D computations is $0.032 \text{ Mbar cm}^3/\text{cm}^3$.

3. Estimation of the "Heat Capacity" of the reaction products

Heat capacity for the reaction products is calculated at the C-J point. From the TIGER computation, the C-J state is: $p_{cj} = 0.1085 \text{ Mbar}$, $V_{cj} = 0.7544 \text{ cm}^3/\text{cm}^3$, and $T_{cj} = 1919^\circ\text{K}$. Then by the JWL equation (equation 2), we calculated the heat capacity of the reaction product as $C_{vp} = 1.55567 \times 10^{-5} \text{ Mbar}/^\circ\text{K}$.

Appendix 3: A DYNA2D Computation Example

DYNA2D computations are demonstrated by the following example.

1. Geometry of the computational set up (see Figure 5 and Table 1)

(1) Charge and donor diameter: $\phi = 33.6$ mm; (2) Charge length: $L = 123.2$ mm ($L/\phi = 3.7$); (3) The thickness of the PMMA pipe: 3.2 mm and (4) The donor length: $l = 10.6$ mm.

Square cells are used and the cell size is about 0.56 mm×mm.

2. Material models

(1) The tested emulsion explosive

Two JWL equations of state are used, one for the unreacted emulsion explosive (see Appendix 1) and the other for the reaction products (see Appendix 2). The parameters are listed in Table 2.

The following burning rate function is used for the computation (Equation 11):

$$\frac{\partial \lambda}{\partial t} = 4.5(1 - 2\lambda)^{2/9} (\mu_e - 0.09)^2 + 270(1 - \lambda)^{2/3} \lambda^{2/9} p^2.$$

(2) The donor explosive PETN

The following JWL equation of state is used for the PETN explosive:

$$p = A(1 - \frac{\omega}{R_1 V})e^{-R_1 V} + B(1 - \frac{\omega}{R_2 V})e^{-R_2 V} + \frac{\omega E}{V} \quad (A-13)$$

where: p — the pressure in Mbar;

V — specific volume of unreacted emulsion and reaction products;

E — internal energy in Mbar cm³/cm³;

A , B , ω , R_1 , and R_2 — constants.

The values of these parameters are as follows /16/:

$$A = 6.253 \text{ Mbar}; \quad B = 0.2329 \text{ Mbar}; \quad C = 0.0778 \text{ Mbar};$$

$$R_1 = 5.25; \quad R_2 = 1.6; \quad \omega = 0.28.$$

$$E_0 = 0.0856 \text{ Mbar cm}^3/\text{cm}^3.$$

Besides the JWL equation, the other properties of the PETN are:

$$\text{the initial density } \rho_0 = 1.5 \text{ g/cm}^3,$$

$$\text{VOD} = 0.745 \text{ cm}/\mu\text{s} \text{ and}$$

$$\text{CJ pressure } p_{cj} = 0.22 \text{ Mbar}.$$

(3) The PMMA tube

The following Grüneisen equation of state is used for the PMMA tube /2/:

$$p = \frac{\rho_0 C^2 \mu \left[1 + \left(1 - \frac{\gamma_0}{2}\right) \mu - \frac{a}{2} \mu^2 \right]}{\left[1 - (S_1 - 1) \mu - S_2 \frac{\mu^2}{1 + \mu} - S_3 \frac{\mu^3}{(1 + \mu)^2} \right]^2} + (\gamma_0 + a\mu)E \quad (\text{A-14})$$

where: p — the pressure in Mbar;

μ — the relative compression: $\mu = \rho/\rho_0 - 1$, ρ/ρ_0 is the ratio of current density to the initial density, in g/cm^3 ;

E — internal energy in $\text{Mbar cm}^3/\text{cm}^3$;

C , S_1 , S_2 and S_3 — the coefficients of the shock Hugoniot of the PMMA.

The values of these parameter are as follows:

$$\rho_0 = 1.185 \text{ g/cm}^3, \quad C = 0.2572 \text{ cm}/\mu\text{s}, \quad S_1 = 1.536, \quad a = S_2 = S_3 = 0,$$

$$\gamma_0 = 0.97.$$

3. *Computation results*

Figures A-1 through A-4 show the computation set-up and the detonation front at different times. Figures A-5 and A-6 show the VOD value (5.248 km/s) and the computed detonation front (the radius at the charge axis $R^0 = 57.0 \text{ mm}$).

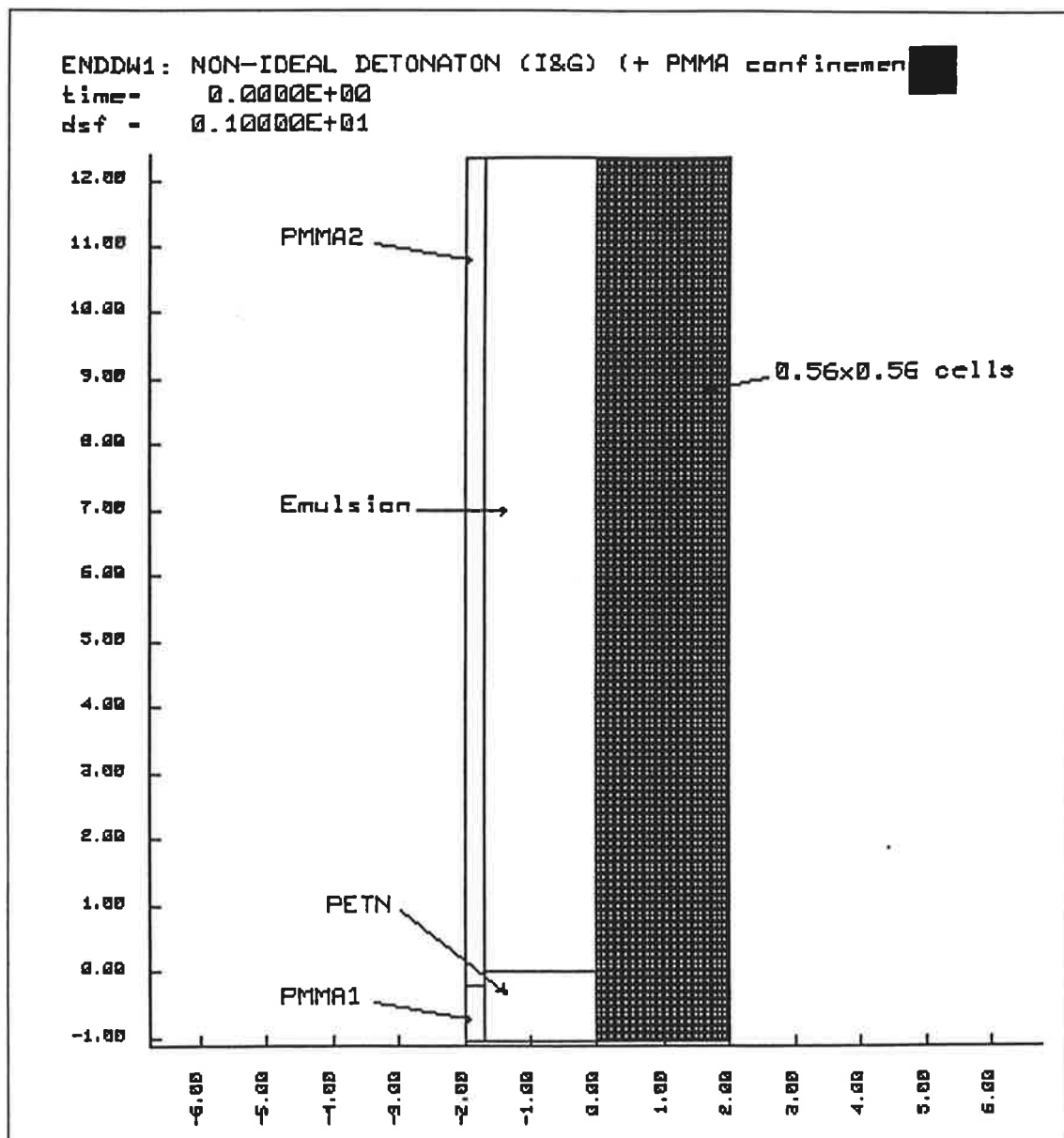
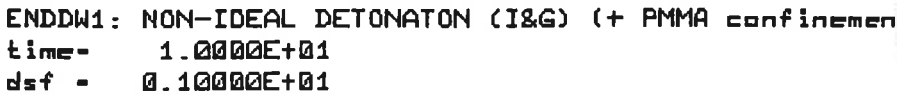


Figure A-1: The original computation set-up for $\phi = 33.6$ mm. Two material regions are used for the purpose of a better computational control. A sliding line is used between the explosives and PMMAs.



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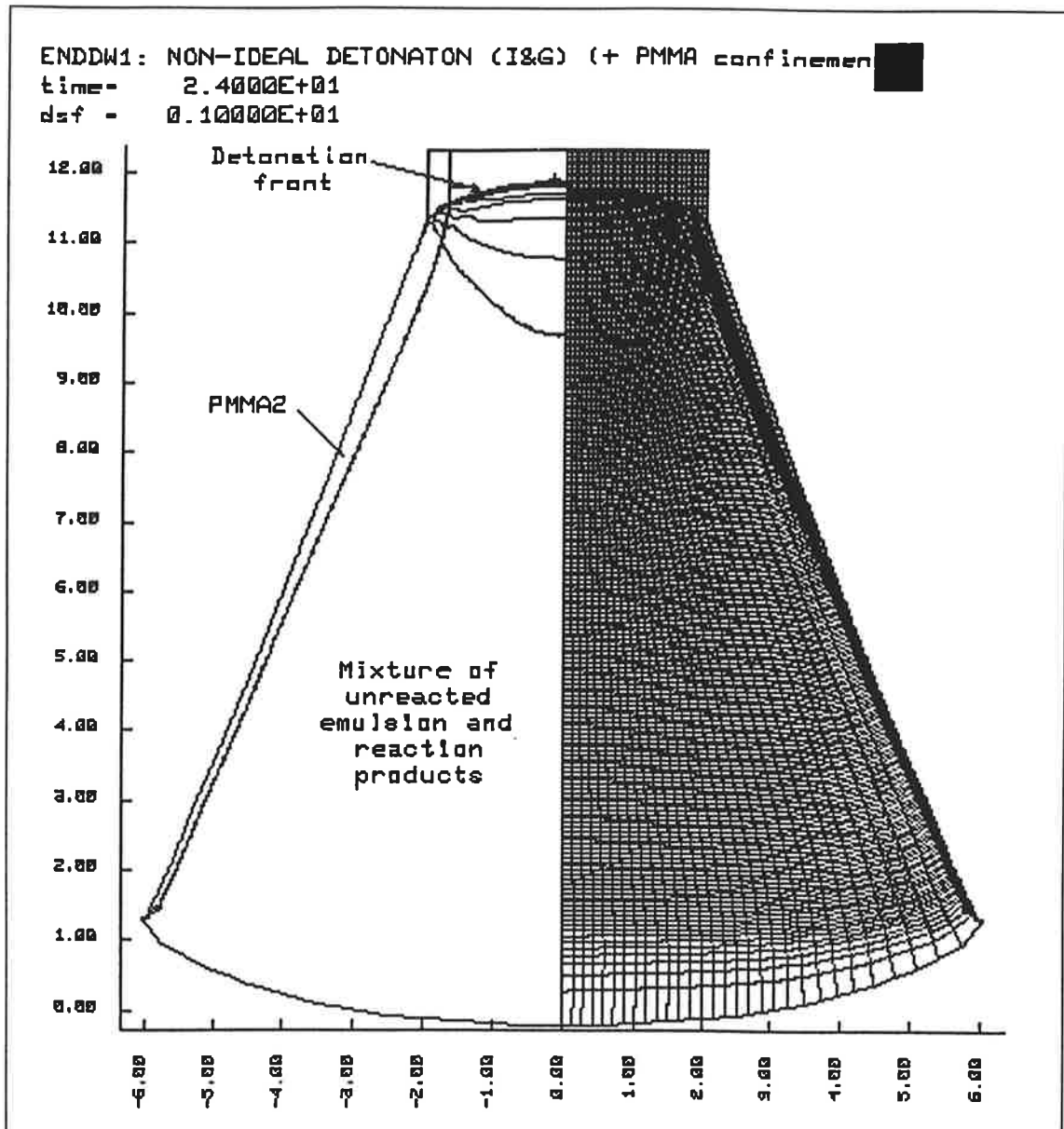


Figure A-3: The cells after $t = 24 \mu\text{s}$ of computation time. From the figure, we can see the steady detonation front and the expansion of the mixture of the unreacted explosive and the reaction products. The donor explosive PETN and the PMMA1 were deleted at $15 \mu\text{s}$.

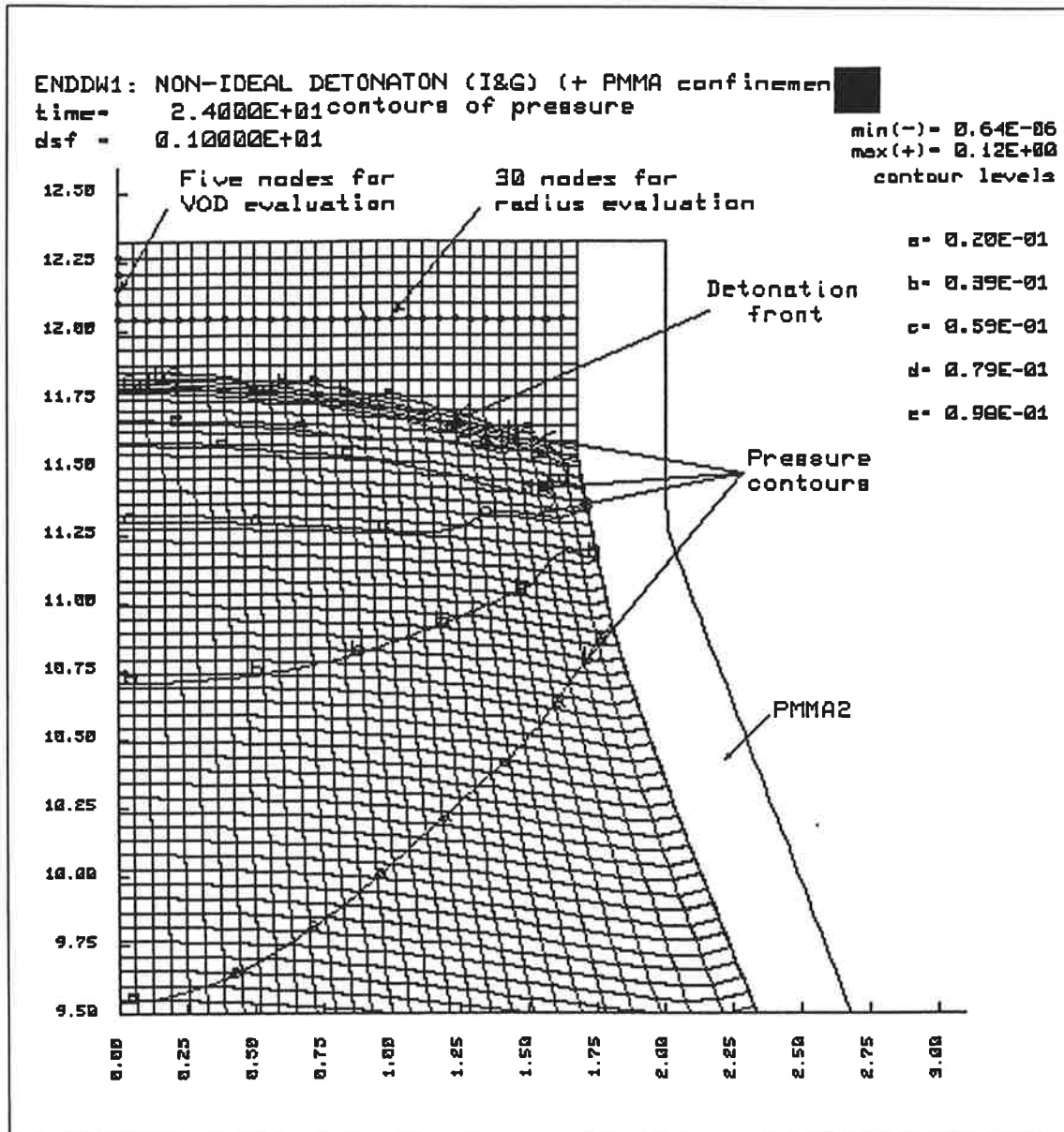


Figure A-4: The details of the detonation front ($t = 24 \mu\text{s}$). Five nodes were used for the VOD analysis and 30 nodes for the radius analysis.

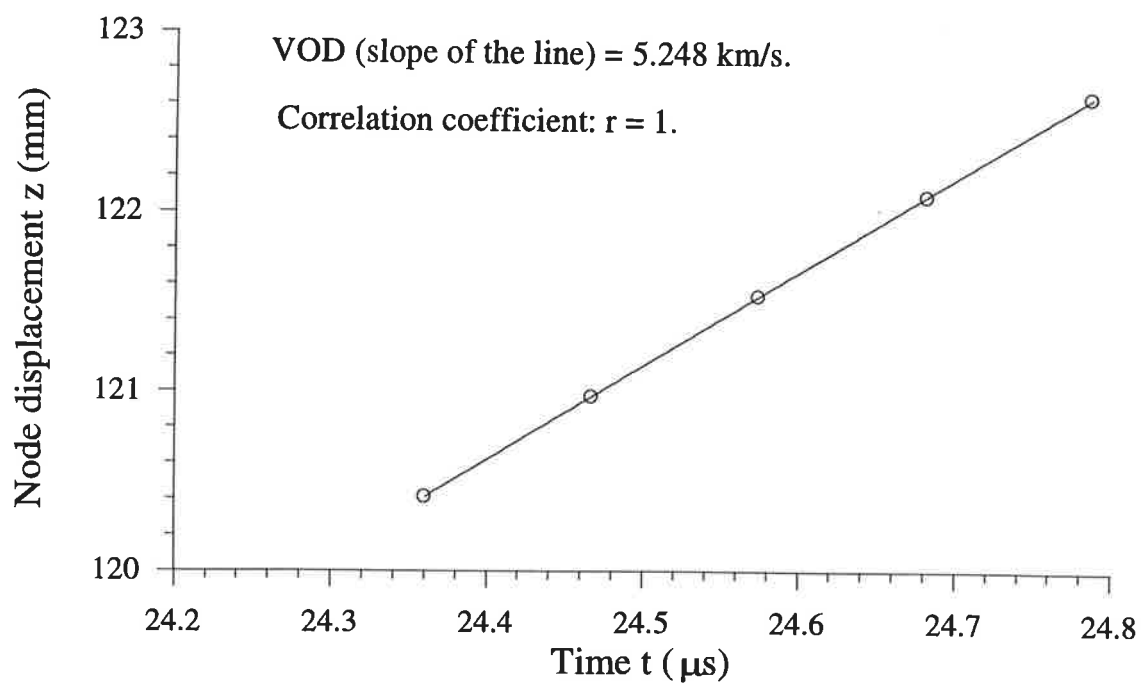


Figure A-5: Detonation velocity of the computation example ($\phi = 33.6$ mm, $\text{VOD}_{\text{exp}} = 5.37$ km/s).

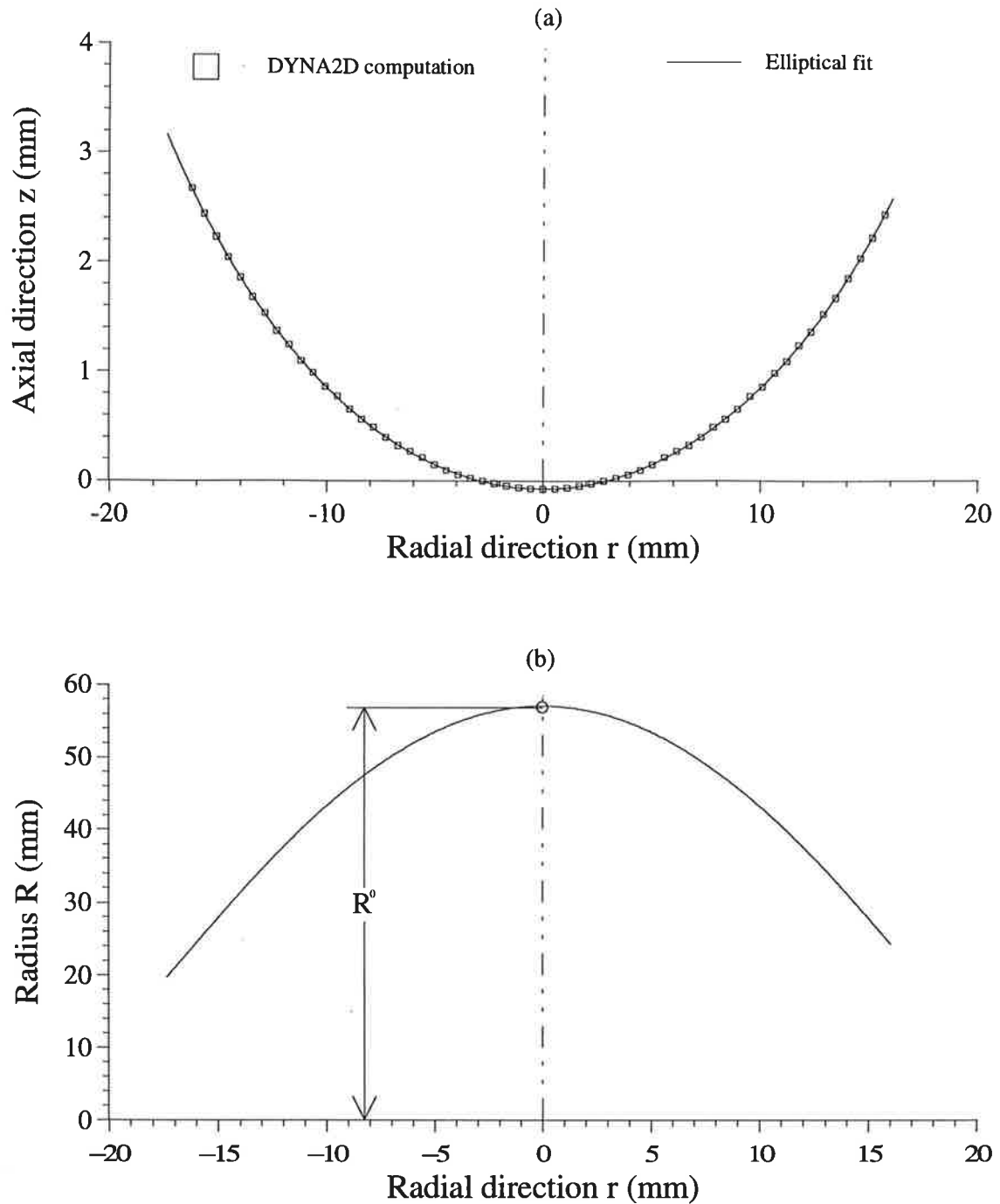


Figure A-6 The computed detonation front and the curvature radius ($\phi = 33.6$ mm, $R_{\text{exp}}^0 = 57.7$ mm).

(a) detonation front and its elliptical fit (relative coordinates were used in the axial direction);

(b) the curvature radius as a function of the radial position, $R_{\text{com}}^0 = 57.0$ mm.

Appendix 4: Computations with Different Burning Rate Functions

1. Computations with the growth term $(1 - \lambda)^{2/9} \lambda$

The following burning function is used for the computations with different values of f , g and μ_c :

$$\frac{\partial \lambda}{\partial t} = f(1 - 2\lambda)^{1/9} (\mu_e - \mu_c)^2 + g(1 - \lambda)^{2/9} \lambda p^2 \quad (\text{A-15})$$

Some parameter combinations used are listed in Table A-1. The results are shown in Figures A-7 and A-8 compared with the experiments.

Table A-1: Computations with equation A-15 using different burning rate parameters.

No.	Burning rate parameters			Figure	Fit with experiments		
					$\frac{1}{8} \sum_{i=1}^8 \frac{ \text{VOD}_{\text{com}i} - \text{VOD}_{\text{exp}i} }{\text{VOD}_{\text{exp}i}}$	$\frac{1}{8} \sum_{i=1}^8 \frac{ \text{R}_{\text{com}i}^0 - \text{R}_{\text{exp}i}^0 }{\text{R}_{\text{exp}i}^0}$	Q* value
	f	g	μ_c		%	%	
78	5.0	180	0.09	A-7a	2.29	9.01	0.0825
79	4.0	180	0.09	A-7b	5.93	10.4	0.150
7A	5.0	160	0.09	—	2.34	11.5	0.1313
7B	4.5	160	0.09	—	3.72	12.4	0.1663
7C	4.8	160	0.09	—	2.71	11.8	0.1403
7D	4.8	150	0.09	—	2.73	11.8	0.1410
7E	4.7	150	0.09	—	3.22	12.0	0.1497
7F	4.8	150	0.095	—	2.90	12.0	0.1516
7G	4.0	120	0.09	A-8a	8.30	12.0	0.2429
7H	4.0	120	0.085	—	7.30	12.1	0.2199
7L	5.52	165	0.09	A-8b	3.0	10.8	0.1178
7M	4.99	140	0.09	—	1.98	12.6	0.1641

*: See equation 4 on page 15.

From these figures we can see that all computations have too high VOD values for large diameters but too low for small diameters. That is, the computational VOD lines have steeper slopes than the experimental one. The radius curves lie below the experimental one and have flatter slopes, which results in bad fits for the large diameters.

The values of f and g are very important for the computations. The larger these values are, the higher the VOD values will be. Parameter f is more important for the smaller diameters. This value will give different slope in VOD-inverse charge diameter relation under a certain value of g (see Figures A-7a and b). Parameter g is more important for the large diameters. The only alternative to lower VOD value at large diameters is to use smaller g value. However, this will result in too low VOD values for the small diameters (see Figure A-8a). Therefore the suitable combination of the two parameters seems to be a relative high f value and a low g value, as in the computation number 7L (Figure A-8b).

It is very difficult to check the importance of the relative critical compression μ_c because of its dependence of other two parameters. What we know from these computations is that this value influences more on the small diameters. Increasing the μ_c value will lower the VOD values for the smaller diameters, but not appreciably for the big diameters.

In order to minimise the number of the computations, we have made a non-linear optimisation analysis to the two linear coefficients by checking the Q values. First we assumed the Q value is a second order polynomial function of the two coefficients f and g , i.e.:

$$Q \approx \Phi(f, g) = k_0 + k_1 f + k_2 g + k_3 f^2 + k_4 fg + k_5 g^2$$

where k_i ($i = 0, 1, \dots, 5$) are the coefficients by fitting j ($j > 9$) sets of computations with different values of f and g to the above function. Then the Q value was minimised to find the solution of f and g . Unfortunately, the solutions of f and g were not convergent over a small range. Therefore, we have to judge the computations directly by comparing the Q values. From Table A-1, we see that computation number 78 has the smallest Q value. The burning parameters of the computation are presented in function 9 in section 3.3.1.

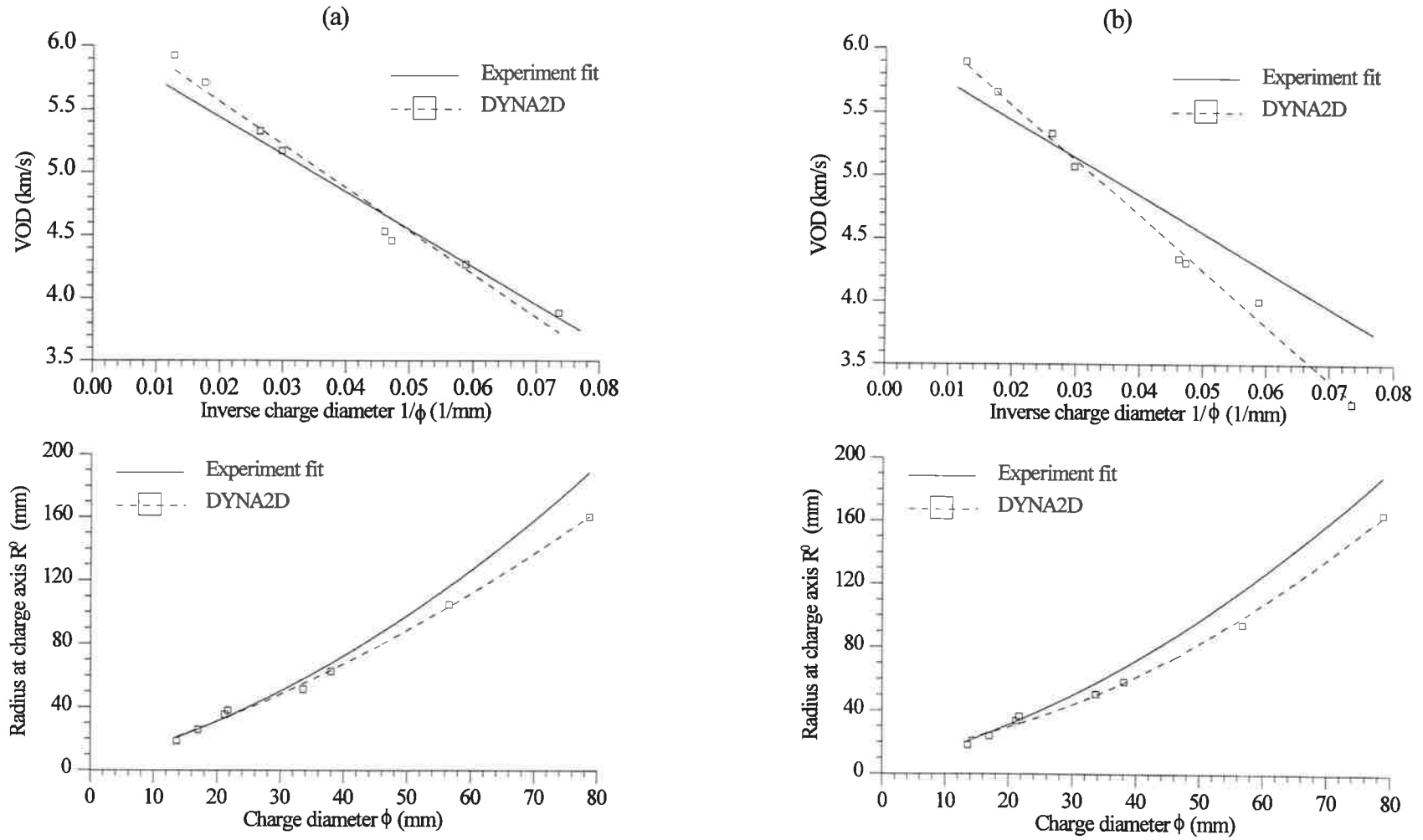


Figure A-7: Comparisons between experiments and computations with burning rate function A-15, using the following parameters:

(a) $f = 5.0$, $g = 180$ and $\mu_c = 0.09$ (No. 78); (b) $f = 4.0$, $g = 180$ and $\mu_c = 0.09$ (No. 79).

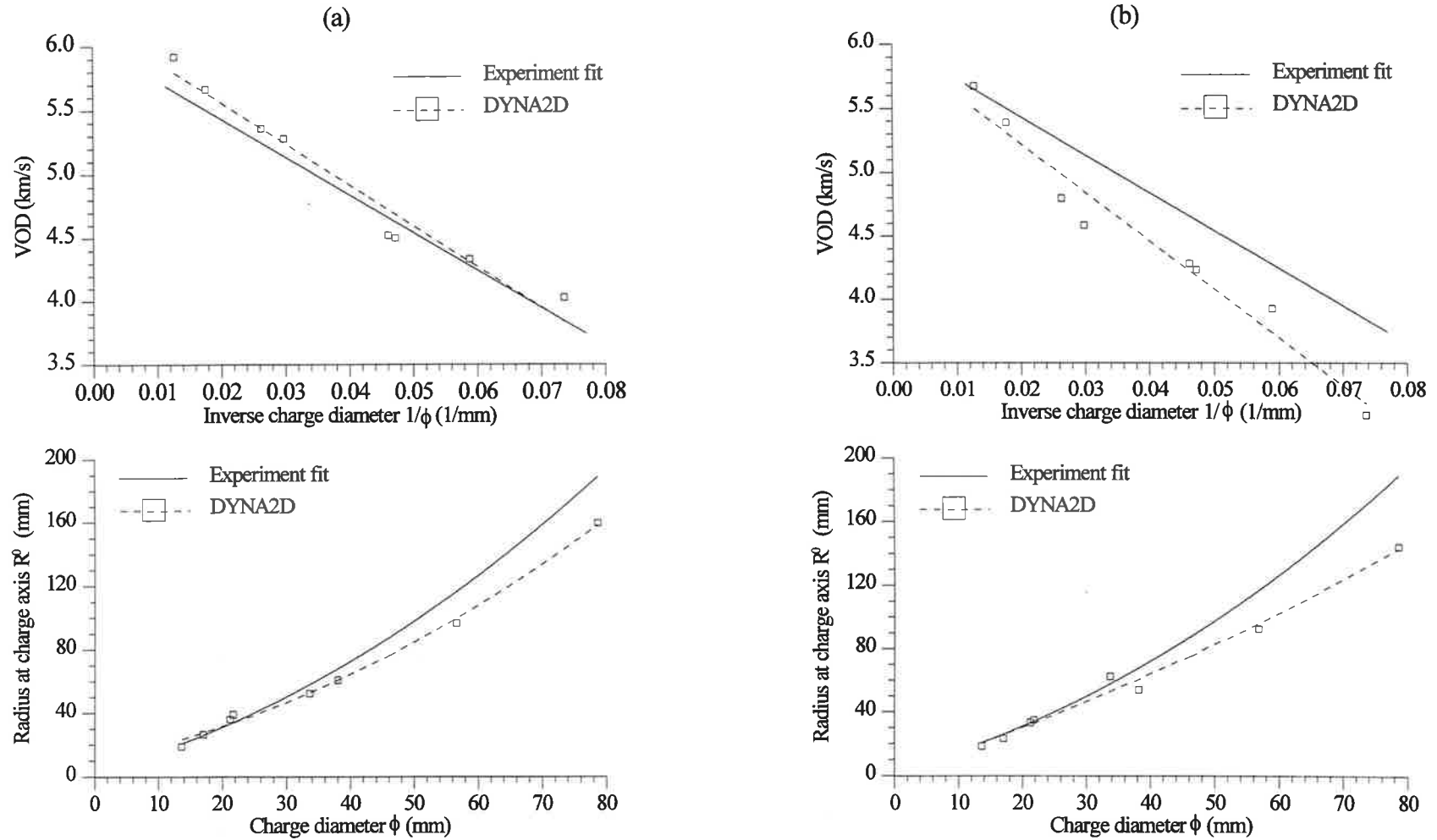


Figure A-8: Comparisons between experiments and computations with burning rate function A-15, using the following parameters:

(a) $f = 5.52$, $g = 165$ and $\mu_c = 0.09$ (No. 7L); (b) $f = 4.0$, $g = 120$ and $\mu_c = 0.09$ (No. 7G).

2. Computations with the growth term $(1-\lambda)^{2/3}\lambda^{2/9}$

Our computations showed that burning rate functions with a growth term of $(1-\lambda)^{2/3}\lambda^{2/9}$ gave better fits of curvature radius between experiments and computations. Here we present more examples with the following burning rate function:

$$\frac{\partial \lambda}{\partial t} = f(1-2\lambda)^{2/9}(\mu_e - \mu_c)^2 + g(1-\lambda)^{2/3}\lambda^{2/9}p^2 \quad (\text{A-16})$$

The three free parameters are the linear coefficients f and g and the critical relative compression μ_c . These parameters and the corresponding computation results are listed in Table A-2 and Figures A-9 and A-10.

Table A-2: Computations with equation A-16 using different burning rate parameters.

No.	Burning rate parameters			Figure	Fit with experiments		
					$\frac{1}{8} \sum_{i=1}^8 \frac{ VOD_{comi} - VOD_{expi} }{VOD_{expi}}$	$\frac{1}{8} \sum_{i=1}^8 \frac{ R_{comi}^0 - R_{expi}^0 }{R_{expi}^0}$	Q* value
	f	g	μ_c		%	%	
C1	4.5	270	0.09	A-9a	3.43	3.81	0.0299
D1	4.5	240	0.09	A-9b	2.11	6.10	0.0410
D2	4.0	240	0.09	A-10a	1.96	6.36	0.0448
D3	4.0	240	0.11	A-10b	1.44	7.09	0.0542

*: See equation 4 on page 15.

These figures show clearly the influences of the three parameters on the VOD values and the curvature radii at charge axes. For example, a 9% decrease in g results in a 1.5% of decrease in average VOD values, but for the curvature radii, rather large decreases for the larger diameters (see Figures A-9a and A-9b). A 9% decrease in the f value results in a small decrease in both VOD values and curvature radii at charge axes (see Figure A-9b and A-10a). Figure A-10b shows clearly the influence of the μ_c value on the computation: a 22% increase of μ_c value gives a large VOD decrease for small diameters, but hardly any for large diameters. The curvature radii at charge axes seem to be decreasing for all diameters.

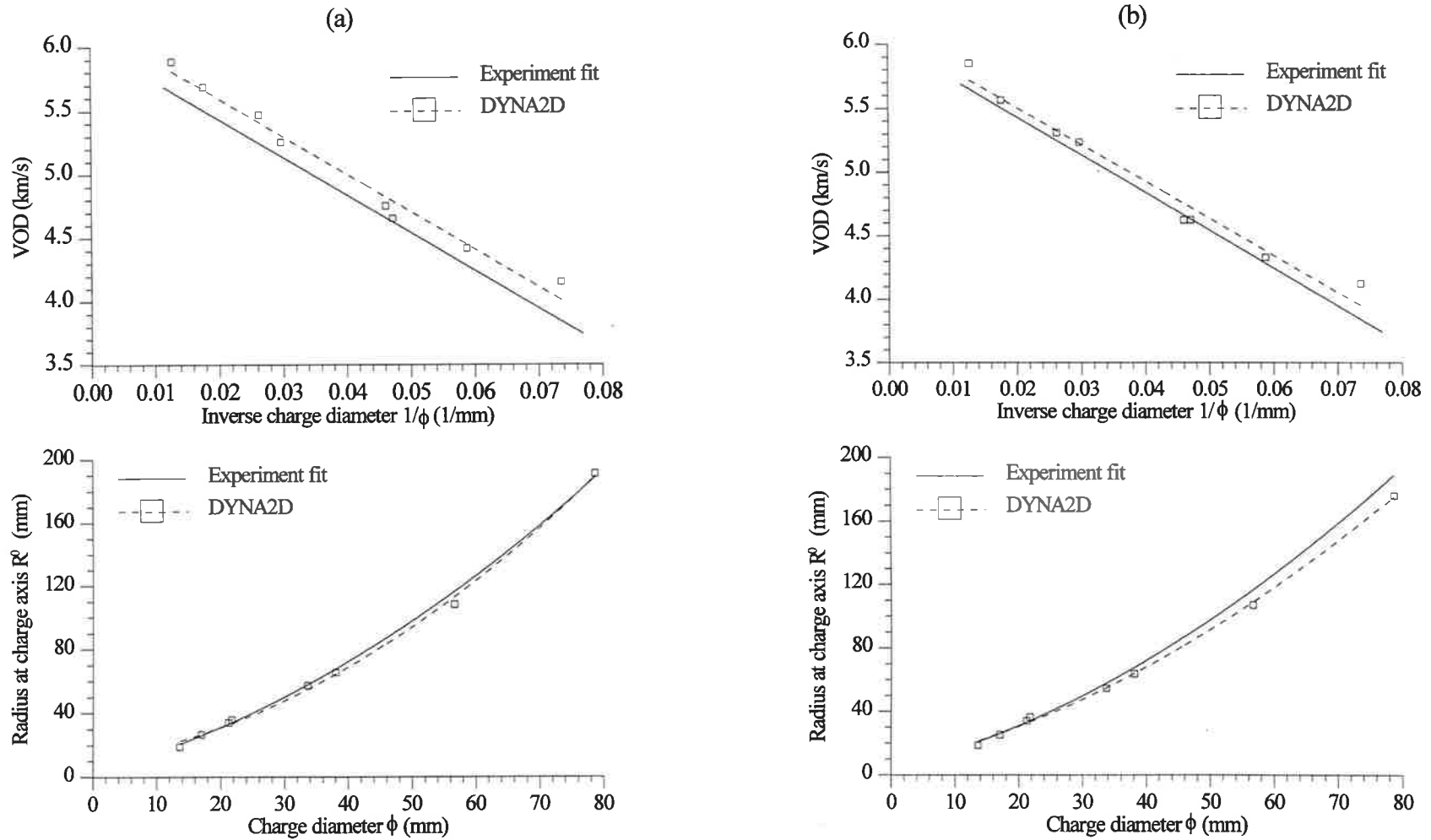


Figure A-9: Comparisons between experiments and computations with burning rate function A-16, using the following parameters:

(a) $f = 4.5$, $g = 270$ and $\mu_c = 0.09$ (No. C1); (b) $f = 4.5$, $g = 240$ and $\mu_c = 0.09$ (No. D1).

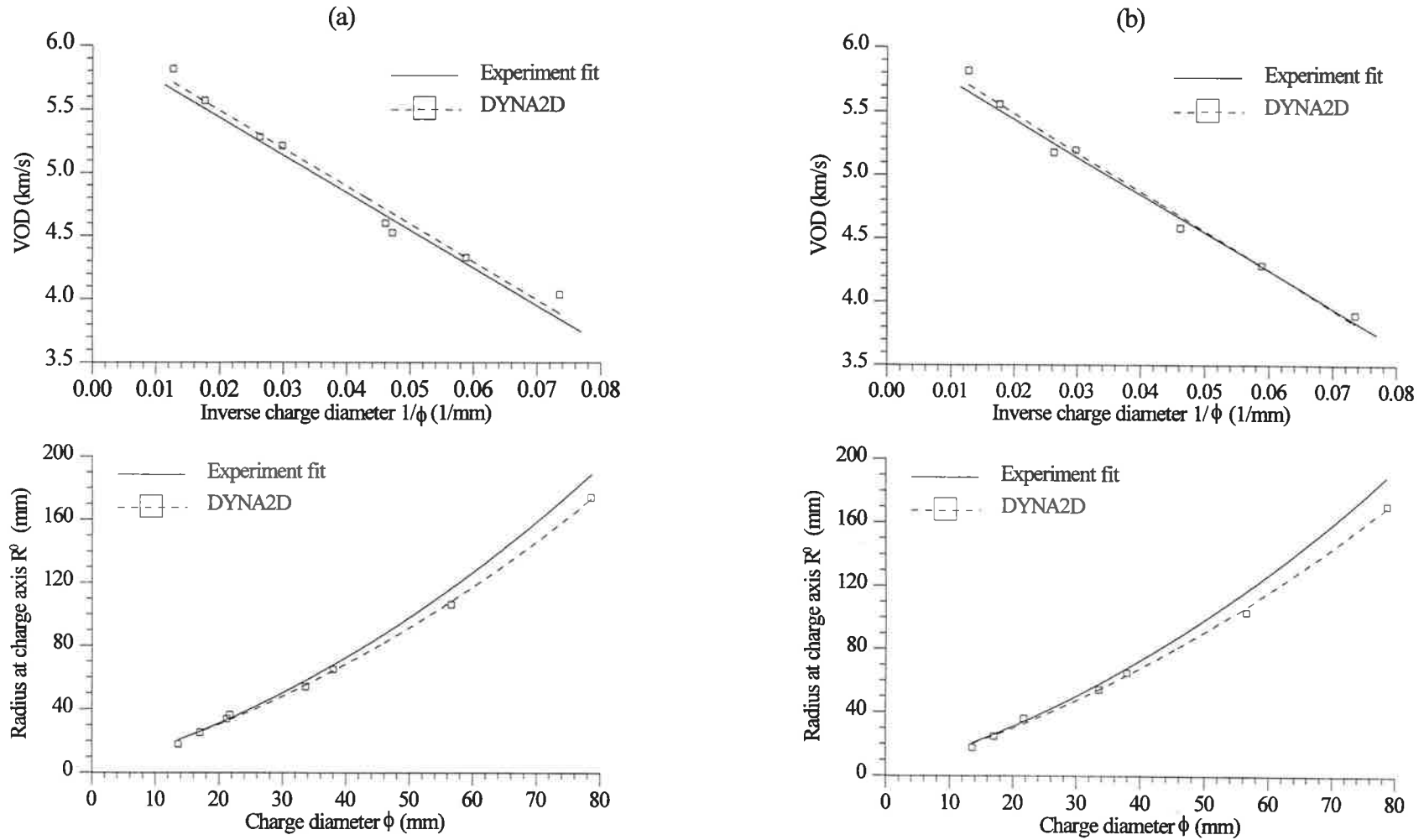


Figure A-10: Comparisons between experiments and computations with burning rate function A-16, using the following parameters:

(a) $f = 4.0$, $g = 240$ and $\mu_c = 0.09$ (No. D2); (b) $f = 4.0$, $g = 240$ and $\mu_c = 0.11$ (No. D3).

3. Computations with different initial internal energies and the growth term $(1-\lambda)^{2/3}\lambda^{2/9}$

In order to get better fits for both VOD values and curvature radii at charge axes with the burning rate function with the growth term $(1-\lambda)^{2/3}\lambda^{2/9}$, we used the initial internal energy E_0 in the JWL equation of state for the reaction products of the emulsion explosive as a free parameter. Here we used the burning rate function A-9 with a constant critical relative compression $\mu_c = 0.09$ as follows:

$$\frac{\partial \lambda}{\partial t} = f(1-2\lambda)^{2/9}(\mu_c - 0.09)^2 + g(1-\lambda)^{2/3}\lambda^{2/9}p^2 \quad (\text{A-17})$$

The three free parameters are the two linear coefficients f and g and the initial internal energy E_0 . These parameters and the corresponding computation results are listed in Table A-3 and Figures A-11 and A-12.

From the results shown in the following pages we can see that the VOD values are strongly influenced by the value of the initial internal energy E_0 . The lines in the VOD versus inverse diameter space are parallel to each other. The curvature radii is affected by the initial internal energy E_0 in a different way: lower internal energy gives smaller curvature radii for larger diameters. In order to get best fits for both the VOD values and curvature radii, we changed both the initial internal energy E_0 and the two burning rate parameters. We found that $E_0 = 0.028 \text{ Mbar cm}^3/\text{cm}^3$, $f = 5$ and $g = 300$ gave the best fits with experiments for both VOD values and curvature radii at the charge axes for different charge diameters (Figure A-12a).

Table A-3: Computations with equation A-17 using different parameters.

No.	Burning rate parameters		Initial internal energy E_0	Figure	Fit with experiments		
					$\frac{1}{8} \sum_{i=1}^8 \frac{ \text{VOD}_{\text{comi}} - \text{VOD}_{\text{expi}} }{\text{VOD}_{\text{expi}}}$	$\frac{1}{8} \sum_{i=1}^8 \frac{ R_{\text{comi}}^0 - R_{\text{expi}}^0 }{R_{\text{expi}}^0}$	Q* value
	f	g	Mbarcm ³ /cm ³		%	%	
C1	4.5	270	0.032	A-11a	3.43	3.81	0.0299
C4	4.5	270	0.030	A-11b	1.80	4.96	0.0303
CA	5.0	300	0.028	A-12a	1.31	4.08	0.0210
C3	5.0	300	0.0264	A-12b	2.56	4.93	0.0296

*: See equation 4 on page 15.

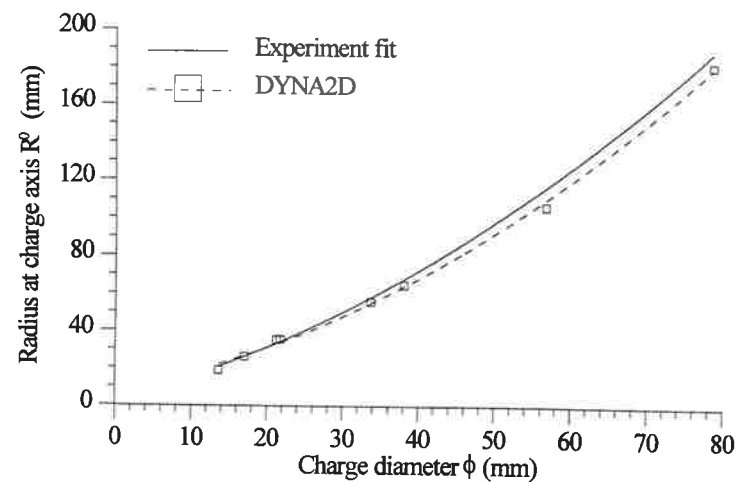
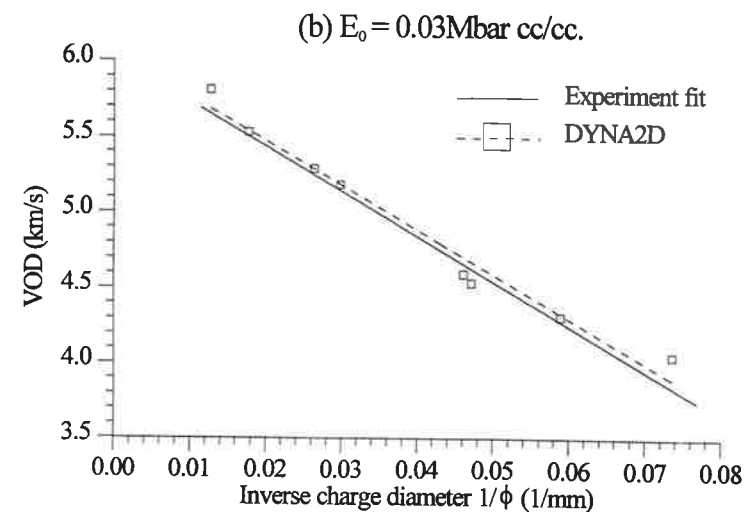
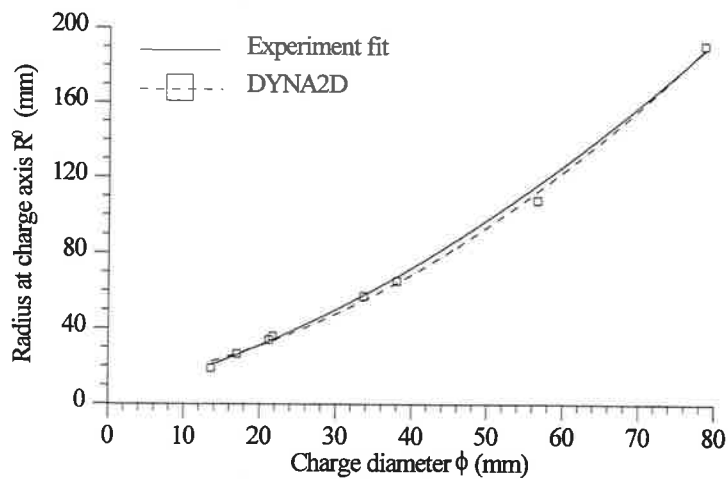
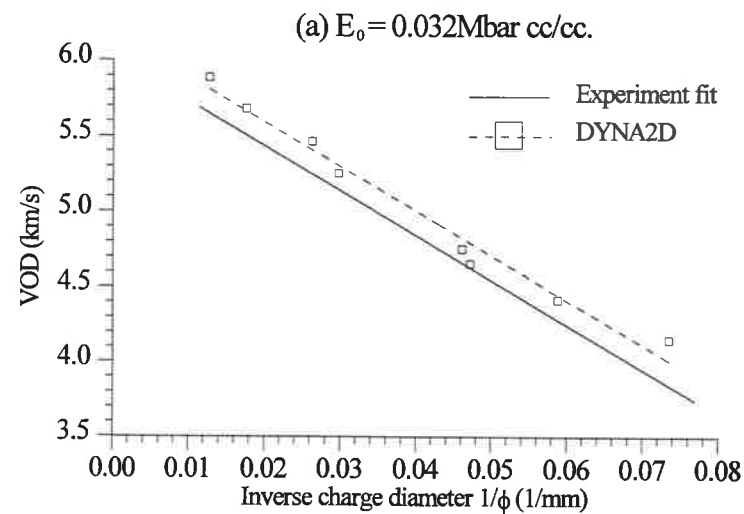


Figure A-11: Comparisons between experiments and computations with burning rate function A-17, using the following parameters:

(a) $f = 4.5$, $g = 270$ and $\mu_c = 0.09$ (No. C1); (b) $f = 4.5$, $g = 270$ and $\mu_c = 0.09$ (No. C4).

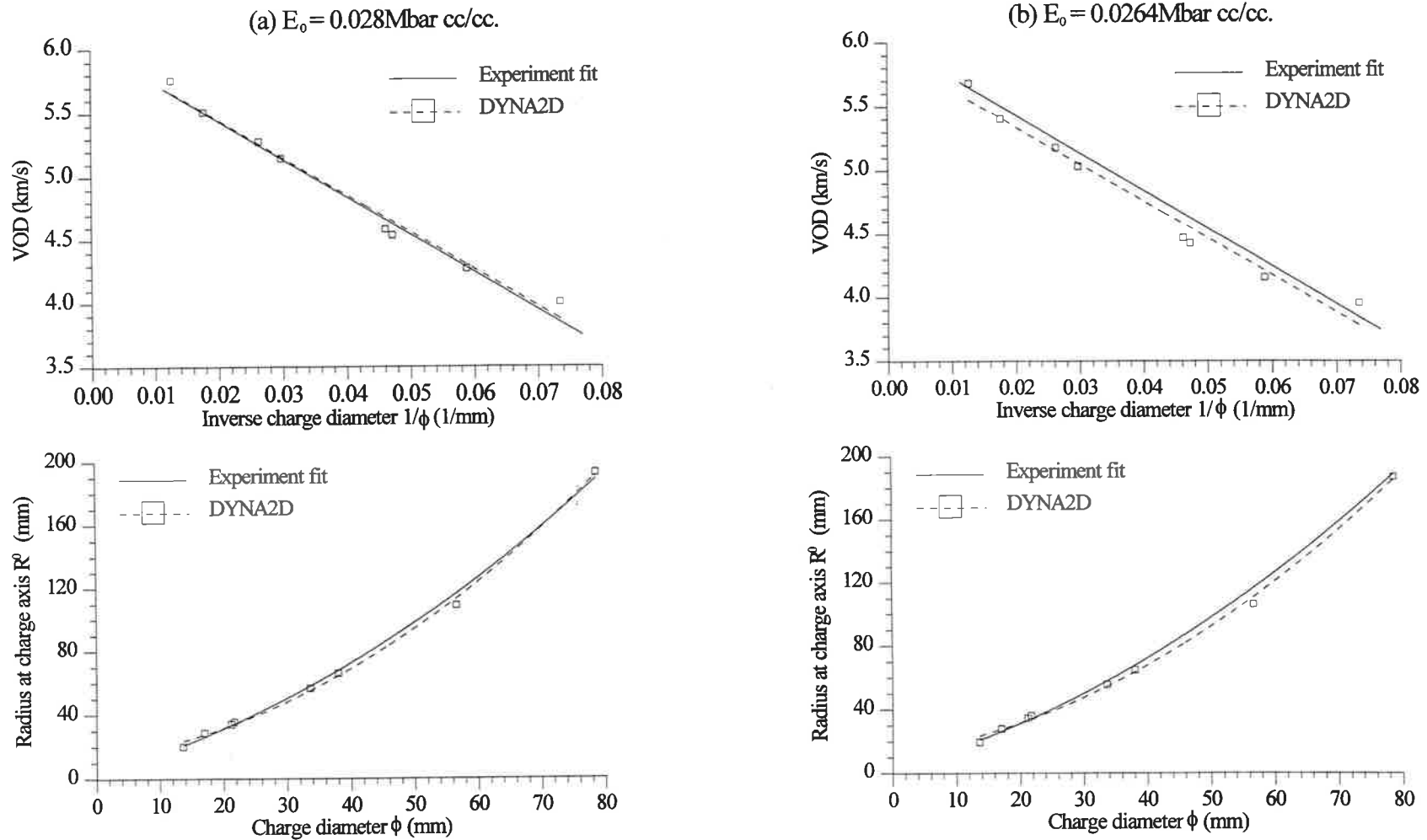


Figure A-12: Comparisons between experiments and computations with burning rate function A-17, using the following parameters:

(a) $f = 5.0$, $g = 300$ and $\mu_c = 0.09$ (No. CA); (b) $f = 5.0$, $g = 300$ and $\mu_c = 0.09$ (No. C3).