

A BURNING MODEL FOR FIVE EMULSION EXPLOSIVES AND SOME APPLICATIONS

**En brinnmodell för fem emulsionssprängämnen
samt några tillämpningar**

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FÖRORD

I arbetet med att förstå sprängämnens verkan i berg har utvecklingen av en brinnmodell en viktig roll. Modellen beskriver det fysikaliska förloppet bakom detonationsfronten i en laddning. Tidigare arbeten med att bestämma parametrar för en sådan modell för ett typsprängämne har nu kompletterats med undersökningar av sprängämnen med olika halt av mikrosfärer och vatteninnehåll. Genom en serie experiment och jämförelser med teoretiska beräkningar har visats hur den varierande sammansättningen påverkar sprängämnets detonationshastighet och känslighet. Man har också visat att brinnmodellen kan användas för att förutsäga detonationsförloppet i stålrör, dvs. inneslutnings inverkan är möjlig att beräkna.

Resultaten är mycket lovande då de visar att modellerna efter kalibrering mot experimentresultat bör kunna användas för att hantera sprängningstekniska frågeställningar av stort praktiskt intresse, som effekten av frikoppling, vattenfyllda hål, olika initieringsteknik etc. Projektet är därmed en viktig del i det pågående arbetet med att vidareutveckla sprängämnen och laddningsteknik för ett effektivt och väl kontrollerat sprängningsresultat i olika tillämpningar.

Fortsatta undersökningar pågår nu för att med brinnmodellen och tryckmätningar i fulladdade spränghål i berg göra det möjligt att i givet berg välja sprängämne och håldiameter så att arbetsförmågan optimeras.

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En brinnmodell för fem emulsionssprängämnen och några tillämpningar

Utvidgad sammanfattning

Försöksserie

Sex rena AN-baserade emulsionssprängämnen har testats i plaströr med olika diameter. Laddningarna har alltså haft en relativt mjuk inneslutning och varit så gott som friliggande. Mätning av detonationshastighet (VOD, velocity of detonation), detonationsfrontens krökning och kritisk diameter har utförts. Med kritisk diameter menas den minsta diameter i vilken en stationär detonation är möjlig. Huvudsyftet med försöken var att förbättra vår förståelse av hur halten av mikrosfärer och vattenhalten i matrisen påverkar detonationen. Alla sprängämnena har varit syrebalanserade, dvs. förhållandet mellan AN och bränsle (olja samt emulgeringsmedel) har varit konstant, ca. 16,6 ggr.

De sex sprängämnena har haft följande sammansättning:

Beteckning	k1a	k1b	k1c	k1f	k1g'	k1g''
Vattenhalt i matris, %	14,8	14,9	14,5	16,2	17,8	17,2
Andel mikrosfärer, %	3,1	1,9	4,8	3,1	1,9	4,8
Densitet, kg/m ³	1165	1250	1090	1185	1240	1085

Försöksresultaten har använts till att bestämma materialdata som i detalj beskriver den hastighet med vilken sprängämnets energi omsätts till spränggaserna med högt tryck och hög temperatur. Dessa data är huvudsakligen parametrarna i en s.k. brinnekvation med två termer, en som beskriver hur reaktionen initieras och en som beskriver hur förbränningen fortskrider. En brinnmodell innehåller utöver brinnekvationen tillståndsekvationer och materialdata för det oreagerade sprängämnet och spränggaserna, vilka tas fram med fristående s.k. Hugoniotförsök eller termokemiska beräkningar, samt blandningsregler för de två faserna.

Analys av försöksresultat

Sprängämnenas brinnegenskaper, dvs. parametrarna i brinnekvationen, har bestämts genom att jämföra beräkningsresultat med försöksresultat i form av hur VOD och

detonationsfrontens krökning varierar med laddningens diameter ϕ . Parametervärdena har ändrats systematiskt tills överensstämmelse nåtts. Detta var möjligt för alla sprängämnen utom k1f.

Av nio ingående parametrar har fem varit viktiga. En intressant observation är att VOD-data främst påverkar tryckexponenten i brinnekvationens förbränningsterm. Den beror nästan linjärt av lutningen i ett diagram där VOD plottas som funktion av $1/\phi$. De övriga parametrarna påverkas inte nämnvärt. För att bestämma dessa är data över detonationsfrontens krökning på laddningens centrumaxel, R_0 , nödvändiga.

Att ta fram krökningsdata är betydligt mer arbetskrävande än att mäta VOD. Därför har åtskilliga försök gjorts att hitta enklare sätt, bl.a. genom ansatsen att diameters inverkan på krökningen på axeln, storlekseffekten, kan ersättas av krökningens variation längs fronten för en enda laddningsdiameter. Om detta vore sant så skulle 8~10 krökningsförsök kunna ersättas av ett enda. Det är det tyvärr inte för våra sprängämnen.

En annan förenklande ansats som prövats är att R_0 skulle kunna beräknas med kännedom om den kritiska diametern ϕ_{crit} och ett generellt samband $\phi/R_0 = \alpha + \beta \cdot \phi_{crit}/\phi$ där α och β har givna värden. Inte heller detta är sant för våra sprängämnen. Konsekvensen av detta är, tyvärr, att man måste mäta detonationsfrontens krökning som funktion av laddningsdiameteren för att bestämma brinnekvationens parametrar.

Däremot har vi funnit att om vi och plottar $1/R_0$ som funktion av ϕ_{crit}/ϕ så faller våra data snällt på en rät linje. Om detta gäller även för andra sprängämnen kan det reducera antalet krökningsradieförsök som behöver göras. Analysen visar också att om vi ur diagrammet bestämmer detonationsfrontens krökningsradie R_{0min} när laddningsdiameteren närmar sig den kritiska och sedan plottar R_{0min}/R_0 som funktion av ϕ_{crit}/ϕ kommer lutningen att bero enbart av matrisens vattenhalt, inte av mikroballedhalten.

Slutsatser av försök och beräkningar

Med en kalibrerad brinnmodell för ett sprängämne kan man i detalj beräkna hur en detonation initieras och fortskrider samt hur förloppet påverkas av geometrin, t.ex. borrhålsdiameter, och inneslutningens styvhet.

Beräkningarna visar för alla fem sprängämnen att detonationszonens tjocklek inte är liten i förhållande till laddningsdiameter, något som den per definition är i en ideal

detonation. Den varierar t.ex. mellan 3,7 och 5,8 mm på axeln i en friliggande ϕ 60 mm laddning. Dessa värden stämmer rätt väl med den krökta frontens uppmätta eftersläpning på laddningens yta. Den icke-ideala detonationen karakteriseras av att detonationen påverkas av faktorer som håldiameter, inneslutningens styvhet etc.

Vid detonationszonens slut är reaktionen ännu inte fullständig. För våra sprängämnen, i vilka syregivaren AN och bränslet är rätt intimt blandade, ligger omsättningsgraden där inom intervallet 68~99% (för en laddningsdiameter mellan 40 och 80 mm). Om t.ex. prillad ANFO med kornstorleken någon mm eller aluminiumkorn blandas in för att förstärka emulsionen förväntas såväl zonens längd som mängden oreagerat sprängämne vid zonens slut öka avsevärt.

Följande slutsatser har dragits av analysen av försöksresultaten och tillämpningsberäkningarna beträffande VOD-värdena för en stationär detonation:

- VOD-värdet i en mycket tjock cylinderladdning beror främst på halten mikrosfärer, eller vilket i vårt fall är samma sak, på densiteten. Om ett känsligt sprängämne definieras som ett där den kritiska diametern är liten och VOD inte ändras så snabbt med laddningsdiametern, så beror känsligheten mer på halten mikrosfärer än på vattenhalten.
- För tre av sprängämnena har VOD-värdena vid stålörnsinneslutning, ϕ 19 mm, beräknats. Överensstämmelsen med mätvärdena är god. De beräknade värdena ligger 1,2, 2,1 och 4,9% för högt. För sprängämne k1a ligger t.ex. mätvärdet på 5460 m/s och det beräknade värdet på 5520 m/s.
- Såväl VOD-värdet som detonationsfrontens krökning påverkas starkt av inneslutningen. Ju stelare inneslutning desto högre VOD-värde och desto plattare detonationsfront. Mätt VOD-värde för en laddning av sprängämne k1a i ϕ 19 mm plaströr är t.ex. i medel 4470 m/s. För en oändligt tjock laddning, vilket har samma effekt som en helt stel inneslutning, ger extrapolerade mätvärden 6030 m/s och termokemiska beräkningar 6180 m/s.

Några tillämpningar av brinnmodellen

Initieringen till full, stationär detonation har också studerats genom att räkna på förloppet för emulsion k1a i ett ϕ 32 mm borrhål i berg, kol eller granit. I beräkningarna har initieringen gjorts antingen med bara en sprängkapsel med aluminiumhylsa eller

med en sådan sprängkapsel plus en liten primer om 27 gram. Det visar sig att:

- I granit blir initieringen mycket snabb när en primer används. VOD-värdet överskrider först det stationära värdet 5600 m/s som nås efter någon håldiameters avstånd längs axeln. Om en sprängkapsel men ingen primer används startar detonationen med ett VOD-värde under 2000 m/s och värdet 5600 m/s nås först efter ca 3 håldiametrar. Skillnaden i borrhålstryck och därmed brytförmåga blir avsevärd och användningen av en primer skulle t.ex. kunna ge en mätbart bättre indrift vid tunneldrivning.
- I kol liknar initieringsförloppet med primer det utan primer i granit fast det stationära VOD-värdet är något lägre, 5200 m/s. Utan primer klarar inte sprängkapseln att initiera sprängämnet till en stationär detonation. Det blir ett detonationsavbrott trots att laddningsdiametern, ϕ 32 mm, är nästan dubbelt så stor som den kritiska laddningsdiametern för en helt friliggande laddning vilken är 18~19 mm!

Beräkningarna förutsäger följaktligen att initieringsprocessen påverkas kraftigt av både berg och primer. Dessa förutsägelser bör verifieras i försök.

För alla fem sprängämnen med kalibrerade brinnmodeller har tryckförloppet på borrhålsväggen vid en stationär detonation i ett ϕ 40 mm borrhål i granit respektive kol beräknats. Det transienta tryckförloppet uppvisar, trots att somliga påstår detta, inget kvasistatiskt jämviktstryck men väl en platta vars nivå vi kallar 'kvasistabilt' borrhålstryck. Likaledes har beräknats hur det expansionsarbete som spränggaserna uträttar förändras med spränggasernas expansion samt hur detta fördelas på stötvågs- och kastenergi. Fördelningen bestäms av det kvasistabila borrhålstrycket. Det visar sig att:

- I granit varierar det kvasistabila borrhålstrycket mellan 3,8 GPa (sprängämne k1g") och 5,1 GPa (sprängämne k1b). I kol varierar det mellan 2,4 GPa (sprängämne k1g") och 2,9 GPa (sprängämne k1a). Dvs. både trycknivån och rangordningen mellan sprängämnena beror av berget!
- Det sprängämne av de fem som uträttar mest gasexpansionsarbete i granit är emulsion k1b med 2,63 MJ/kg, beräknat vid gasernas expansion till 5 ggr borrhålsvolymen. Samma sprängämne uträttar minst gasexpansionsarbete i kol, 1,97 MJ/kg. Det sprängämne som uträttar minst gasexpansionsarbete i granit är k1g" med 2,27 MJ/kg. De som uträttar mest arbete i kol är k1g' och k1a med 2,32 MJ/kg. Vid

den givna expansionen har alltså det svagaste sprängämnet i graniten uträttat nästan lika mycket arbete som det starkaste i kolet!

- Från energianvändningssynpunkt är k1a det effektivaste sprängämnet både i kol och granit med 81 eller 83% av den tillgängliga kemiska energin omsatt till gasexpansionsarbete. Sprängämne k1b som har en verkningsgrad på 83% i granit ger bara 62% i kol. För de andra sprängämnena ligger verkningsgraden inom 76~83%. Vissa sprängämnen kan alltså uppvisa radikalt olika verkningsgrad i olika bergarter medan andra påverkas mycket litet!
- Gasexpansionsarbetets fördelning på stötvågs- och kastenergi kan variera kraftigt. För t.ex. sprängämne k1a i kol fördelas gasexpansionsarbetet 2,32 MJ/kg på 0,54 MJ/kg i stötvågsenergi och 1,78 MJ/kg i kastenergi. För sprängämne k1g' i kol, som uträttar samma gasexpansionsarbete, blir fördelningen 0,87 MJ/kg respektive 1,46 MJ/kg. Då många hävdar att styckefallet är hårt knutet till stötvågsenergin och framkastet i salvan till kastenergin så bör skillnaden i sprängningsresultat mellan k1a och k1g' kunna observeras relativt lätt.

Beräkningarna visar följaktligen att både det expansionsarbete som spränggaserna uträttar och deras fördelning på stötvågs- och kastenergi beror kraftigt av sprängämnets koppling till berget. Likaledes torde dessa storheter påverkas av håldiametern!

Vidare användning av brinnmodeller

Om sambanden mellan sprängämnets komposition, t.ex. mikrosfär- och vattenhalterna å ena sidan samt brinnmodellen och dess ingående materialparametrar å andra sidan kan klarläggas med någorlunda säkerhet för emulsionsrecept som används i fält, så öppnas möjligheterna att skraddarsy ett sprängämne för varje tillämpning.

Kalibrerade brinnmodeller kan också användas för att beräkna effekten av andra praktiskt intressanta problem såsom:

- effekten av frikoppling på detonationen; oavsett om spalten är fylld med luft eller vatten,
- effekten av initieringspunkt; toppen eller botten av borrhålet samt sidoinitiering,
- effekten av upptändningen; primerns form, förekomst av luftficka i botten eller lös sprängkapsel,

- beräkning av hur LHM-cellen och dess utformning påverkar de tryck-tidförlopp som registreras samt
- olika former av detonationsstörningar.

Brinnmodellerna kommer förhoppningsvis att kunna ge riktiga, verifierbara förutsägelser både om dessa och om andra praktiskt intressanta sprängningsförlopp. Det finns nu goda förutsättningar för detta.

Nyckelord: Emulsionssprängämne, brinnmodell, brinnekvation, tillståndsekvation, DYNA2D, simulering, kalibrering, detonationshastighet, VOD, detonationsfront, krökningsradie, kritisk laddningsdiameter, expansionsarbete, stötvågsenergi, kastenergi.

SUMMARY

Totally six emulsion explosives with cylindrical charges have been tested, mostly in PVC pipes. Measuring quantities are the steady-state VOD values, the detonation front curvatures and the critical charge diameters. The main goals of the tests are to improve our understanding the influences of the microballoon and water contents on the explosives' performance and to provide experimental data for calibrating the burning rate parameters.

The Ignition and Growth model with a two-term burning rate function was used to describe the non-ideality of the emulsion explosives. The burning rate parameters of five emulsion explosives have been calibrated against the 2D cylindrical tests. Using the calibrated burning models, the actual non-ideal performance of the emulsion explosives, e.g. the VOD value and other detonation parameters as functions of charge diameter, initiation conditions and the confinement can easily be predicted.

The concept of the 'quasi-stable' borehole pressure has been introduced by analyzing the pressure–volume relations from computations of actual detonations of charges in blastholes. The blast energy partitioning, i.e. the shock energy and the heave, can be analyzed accordingly.

The main conclusions based on the analyses of the test results and the application computations are summarized as follows:

- The VOD value at infinite diameter of an emulsion explosive is mainly a function of the microballoon content or the density of the explosive. The sensitivity of the explosive is determined more by the microballoon content than by the water content. By sensitivity in this case is meant a combination of a small critical diameter and a VOD value which is relatively unaffected by the diameter. Both the microballoon content and the water content affect the detonation front curvature.
- The VOD values of three explosives in iron pipes have been successfully predicted using the calibrated burning models. This implies that the burning models obtained from the well-controlled laboratory tests are able to predict the detonation processes in production blasts.

- The steady-state VOD value and the detonation front are severely affected by the confining material. The denser the confining material is, the higher the VOD and the flatter the detonation front will be.
- The primer and the confinement control the initiation run-up process.
- The ‘quasi stable’ borehole pressure can be determined by analyzing the pressure history in the explosive–rock blast system. Its value depends both on the explosive and the rock to blast. The expansion work, the shock and heave energies are functions of the borehole pressure.

Key words: emulsion explosive, burning model, burning rate function, equation of state, DYNA2D, simulation, calibration, velocity of detonation (VOD), detonation front, curvature radius, critical charge diameter, expansion work, shock energy and heave.

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A Burning Model for Five Emulsion Explosives and Some Applications

1. INTRODUCTION

There are increasing demands for numerical modelling of non-ideal detonations of commercial explosives (Leiper & Plessis 1987, Kennedy & Jones 1993, Dussell 1997, Abermathy et al. 1998). Commercial explosives react rather slowly, compared to ideal high explosives. The slower reaction results in a thicker detonation zone, a more curved detonation front and a larger critical charge diameter. By changing charge diameter, for example, the reaction process of the explosive is interfered with so that the velocity of detonation (VOD) along the charge axis and the curvature of the detonation front are changed. Therefore, the relations of the measured VOD values and the curvature radii of the detonation fronts vs. charge diameters, together with the critical diameter, represent the practical detonation characteristics of a commercial explosive. A correctly built numerical model must be able to reproduce these quantities.

Our calibrated burning model describes non-ideal detonations of commercial (or non-ideal) explosives. The main part of the model consists of a set of parameters that describe the burning kinetics in detail. The parameters are those of the equations of state of the reactive flow and those of a phenomenological burning rate function. The reactive flow is that of a mechanic mixture of the inert emulsion and its reaction products, which are modelled by two JWL (Jones-Wilkins-Lee) equations of state. The burning rate parameters are calibrated against the VOD values and the curvature radii of the detonation fronts (vs. charge diameter) from the cylindrical tests, within the frame work of the *Ignition and Growth* model implemented in the hydrodynamic code DYNA2D (Lee & Tarver 1980).

Totally six emulsion explosives with different water and microballoon contents have been tested. The main goals are to improve our understanding the influences of the microballoon and water contents on the explosives' performance and to provide experimental data for calibrating the burning rate parameters. Stationary VOD values and the detonation front curvatures have been measured. The results show clearly the non-ideality of the emulsion explosives. The VOD values and the curvature radii of the detonation fronts are functions of charge diameter, microballoon and water contents. The critical charge diameters for the six explosives have also been measured.

The burning rate parameters of five emulsion explosives have been calibrated. The calibrated burning model can be used to model the actual performance of the emulsion explosives. Detonation parameters such as the steady-state VOD value and the CJ pressure are not input parameters but calculated results. Their values are truly predicted and are functions of charge diameter, confining material and initiation conditions. Thus the performance of the non-ideal explosives can be readily seen in the variation of the VOD value and other detonation parameters with charge diameter, initiation conditions and the confinement. The partitioning of energy between the shock energy and the heave in a production blast can also be predicted using such a burning model.

In this report, we have illustrated the following three applications of the burning models:

- (1) The charge diameter effect on the performance of an emulsion explosive in different blast media;
- (2) The initiation run-up or run-down processes of different explosives in different rocks; and
- (3) Partitioning of the blast energy: the shock energy and the heave.

The calculations show that the burning rate model is very useful in solving engineering problems. For example, the charge diameter effects on the VOD values for different confining media can easily be calculated using the burning model. The study provides a tool to study many practical problems, such as the detonation of a decoupled charge in rock blasting, where different media (air or water) may exist in the borehole. The study on the initiation run-up or run-down process shows the functions of the primer and the confining material in the initiation of explosive charges. The analyses of the different forms of energies in a blast (the shock energy and the heave) provide a useful tool for the overall matching of an explosive to the rock to blast, which is crucial for utilizing the explosive energy efficiently. The correct solution of many engineering problems can be considerably improved by using burning models.

2. NON-IDEAL EXPLOSIVES AND BURNING MODELS

In order to understand the need for using burning models for non-ideal explosives, the concepts of non-ideality of an explosive and of burning models are first discussed briefly.

2.1 Non-ideal Explosives

Non-ideal explosive is an engineering term. An ideal explosive has a detonation zone which is thin compared to all other dimensions and the chemical reaction is similarly fast. A non-ideal explosive detonates at a lower reaction rate and has a relatively thicker detonation zone (Abernathy 1998, Dussell 1997). For a finite cylindrical charge of a non-ideal explosive, the detonation is severely affected by the charge diameter and the confinement. Most of the industrial or commercial explosives, for example ANFO and emulsion explosives are in this sense non-ideal ones. The detonation of an ideal high explosive is relatively independent of the charge diameter and the confining material. Most molecular and compound explosives used by the military, for example, TNT and PBX-9404, are ideal ones.

The ideality of an explosive is however a relative term. All explosives can be made to detonate more or less non-ideally, depending on the detonation conditions (Fickett 1979). An ideal detonation might be achieved if the explosive could be fired at the infinite diameter or with a rigid confinement, which would eliminate the side effect completely during detonation. This so called 1D detonation has the highest VOD value and the maximum total released chemical energy. Both are completely determined by the original density of the explosive and its chemical composition. Such conditions can never be achieved in practice. An ideal explosive normally detonates under conditions close to the ideal or 1D detonation, but it is not an ideal detonation. As long as the side effect exists, the detonation is two- or three-dimensional.

Ideal high explosives have higher VOD values and thinner detonation zones, while the non-ideal explosives have lower VOD values and thicker detonation zones. For example, the military explosive LX-04 at a density of $1,86 \text{ g/cm}^3$ detonates with a VOD of $8,49 \text{ km/s}$ and has a detonation zone of $0,3\sim 0,4 \text{ mm}$. Composition B at a density of $1,67 \text{ g/cm}^3$ detonates with a VOD of $7,87 \text{ km/s}$ and has a detonation zone of $0,3 \text{ mm}$.

(Fickett 1997, Souers 1998). The two most commonly used commercial explosives, HANFO and emulsion explosive, detonate with speeds from 3 to 6 km/s, and the detonation zones can be from 3 to 10 mm thick (Kennedy 1996, Souers 1998). Although the difference between a non-ideal explosive and an ideal explosive is rather large, there is no absolute dividing line between them.

The emulsion explosives discussed in this report are non-ideal explosives. The steady-state cylinder experiments show that both VOD value and the detonation front curvature are affected by the charge diameter. These diameter-dependent results are used in the calibrations of the burning rate parameters.

2.2 Burning Models of Non-ideal Detonations

The conventional theories of ideal detonation, for example the CJ theory and the ZND (Zeldovich-von Neumann-Döring) theory, can not be used to simulate the non-ideality of a commercial explosive. They describe a plane detonation wave of an instantaneous reaction (CJ theory) and of a finite reaction zone (ZND theory). The JWL-detonation model (programmed-burning model) implemented in the hydro-dynamic code DYNA2D (Hallquist 1990) is based on the CJ theory. In this model, fully reacted products are obtained instantaneously. These are modelled by a JWL equation of state. With a constant input VOD value and CJ pressure, the model simulates an idealized detonation, under conditions where the JWL parameters have been calibrated (e.g. by cylinder tests).

In order to simulate the non-ideality of commercial explosives, the reactive flow and the chemical kinetics of the burning process must be included. The Ignition and Growth burning model is the one, which describes both the reactive flow and the chemical kinetics. Although the model was initially built to study the sensitivity of ideal high explosives (Lee & Tarver 1980), it essentially simulates the non-idealities of explosives. The model contains equations of state for the reactive flow of the mechanical mixture of the unreacted (inert) explosive and the fully reacted products under the assumed conditions of pressure and temperature equilibrium between the two phases. The gradual transition from the inert explosive to blast fumes is described by a three-term reaction rate function. This model has been implemented in the hydro-dynamic code DYNA2D (Lee & Tarver 1980). The physics of the interaction between the reactive flow and the

confinements can be simulated by the code without extra effort. This is a great advantage, both in building the burning model and using it in solving engineering problems. In both cases, we can concentrate on defining the explosive, not other materials. Therefore, we decided to use this model together with the code DYNA2D as a tool to build our own burning rate parameter determination system.

Other burning models, like ICI's small divergent model (Kirby & Leiper 1985) and the model by Lee (1990) have been used to model non-ideal explosives. The later one is based on the DSD (detonation shock dynamics) theory (Bdzil 1989). With the ICI's burning model, it is rather complicated to calibrate all the burning parameters. First, the so-called CPeX program (standing for Commercial Performance of eXplosives) is used to model a 1D detonation with experimentally determined lateral divergent flow (Kennedy 1995). Then the parameters have to be calibrated by use of a 2D program like DYNA2D against 'rate-stick' or cylindrical charge tests.

Our experimental results show that there does not exist a single relation between the normal detonation velocity and the local front curvature, which is a key assumption in the DSD theory. Kennedy also found that the DSD theory is not valid for heavily non-ideal explosive HANFO (Kennedy 1998). Therefore the calibration method used by Lee (1990) is not appropriate for our analysis.

We have previously proved that it is possible to use the DYNA2D code and the implemented Ignition and Growth model to model one of our tested emulsion explosives k1a (Deng et al. 1995). This model is relatively simple compared with ICI's small divergent model. Here we are using the same method for four other emulsion explosives with different microballoon and water contents.

In principle, there are no major differences among the above three non-ideal burning models. All three models consist of a mechanical description of the reactive flow and a reaction rate law of different forms. The accuracy of the models depends on the experiments, from which the parameters of EOS (equation of state) of all materials involved and those of the burning rate laws are obtained. In practice however the quality of the predictions may differ. Our long range purpose with this study is to develop simple methods to calibrate the burning rate parameters and to demonstrate the usefulness of burning rate models to solve engineering problem.

3. CALIBRATION OF BURNING RATE PARAMETERS USING DYNA2D

In the following sections, we will discuss the calibration method, the governing equations for the reactive flow and the reaction rate function. Then the results of the calibrated parameters in the burning rate function are presented. Finally, the results are discussed. The technical details are given in Appendices.

3.1 Two Dimensional Steady-state Experiments

The accuracy of a burning model depends very much on the experiments, from which the burning rate parameters and other material parameters are obtained. The measured quantities should be representative and give enough information on the reaction process.

An emulsion explosive is basically a mixture of an aqueous solution of inorganic oxidizer salts, such as ammonium nitrate (AN), with fuel oil. A thin oil film surrounding the oxidizer droplets makes the explosive water resistant (water-in-oil). The sensitivity of the explosive is controlled by adding a certain amount of e.g. small microballoons into the mixture. The chemical properties of the constituents basically determine properties such as crystallisation temperature or fudge point (oxidizer salts), rheology (fuel) and droplet size deformation tolerance and shelf life (emulsifier). The requirement of oxygen balance determines the oxidizer/fuel ratio. For a given physical system there thus remain two main factors that regulate the explosives' performance, the water content of the matrix and the microballoon volume mixed in. The effects of these two factors on the detonation properties of a simple and oxygen balanced straight AN emulsion are investigated here.

We have tested six emulsion explosives. Their compositions and densities are shown in Table 2-1. Their positions in the water and microballoon contents plane are shown in Figure 3-1.

According to the microballoon content or the density of the explosive, the three following explosive groups can be identified:

1. Emulsions k1b and k1g' contain nearly 2 percent (by weight) of microballoons and have the densities of 1,25 and 1,24 g/cm³ respectively. This is the group with highest density. A slightly higher contents of microballoons and water yield a slightly lower density for k1g'.

Table 2-1: Percentages of contents and densities of all tested emulsion explosives:

explosive	AN*(%)	EM*(%)	7514oil (%)	water(%)	MB*(%)	$\frac{AN}{EM + 7514}$	ρ_0 (g/cm ³)
k1a	77,49	0,748	3,926	14,76	3,075	16,58	1,165
k1b	78,46	0,757	3,975	14,94	1,868	16,58	1,250
k1c	76,09	0,734	3,855	14,49	4,831	16,58	1,090
k1f**	76,15	0,732	3,855	16,19	3,075	16,60	1,184
k1g'	75,78	0,729	3,836	17,76	1,90	16,60	1,240
k1g''	73,54	0,707	3,723	17,23	4,80	16,60	1,086

*: AN = Ammonium Nitrate; EM = Anfomul S6 emulsifier from Croda Oleochemicals; MB = B23/500 microballoons from 3M; 7514oil: ES 75-14 mineral oil from Mobil Oil.

** : The burning parameters of this explosive have not been determined.

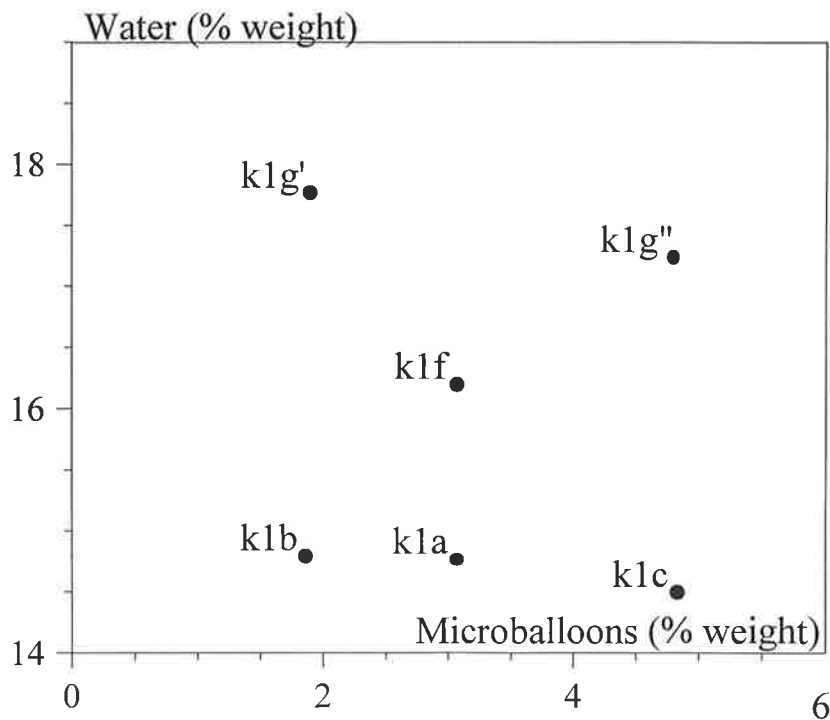


Figure 3-1: Microballoon and water contents of the tested explosives.

2. Emulsions k1a and k1f contain about 3% (weight) of microballoons and have densities of 1,165 and 1,184 g/cm³ respectively. For unknown reasons, the density of k1f emulsion is higher than k1a emulsion, although emulsion k1f contains the same amount of microballoons as emulsion k1a and more water.
3. Emulsions k1c and k1g” contain 4,8% (weight) of microballoons and have densities of 1,090 and 1,086 g/cm³ respectively. This is the lowest density group.

We have measured the steady-state VOD values and the detonation front curvatures. All experiments were carried out with cylindrical charges or the so-called ‘rate-stick’ configuration. PMMA (plexiglass) was used as the confining material for tests of emulsion k1a, and PVC (polyvinyl chloride), for tests of the other emulsions. The steady-state VOD values were measured with a continuous resistance probe. At the beginning of the research, the optical fibre method was also used, mostly for k1a emulsion. The critical diameters for all explosives were estimated by averaging the minimum diameter of successful detonations and the maximum diameter of detonation failures. The detonation front curvatures were measured by a streak-camera recording the breakout at the end of charges. All tests were made using cylindrical tubes with the ratios of charge length to diameter varying from 20 to 6, for diameters (inner) from 13 to 96 mm. We believe that the recorded VOD values and detonation front curvatures have stabilized. The experimental setup is shown in Figure 3-2. Two examples of recordings are shown in Figures 3-3 and 3-4.

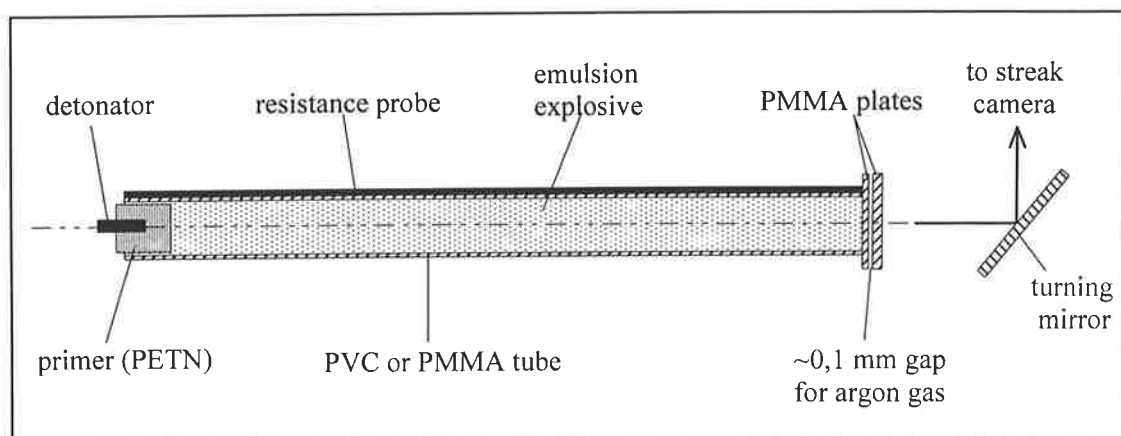


Figure 3-2: The experimental setup for measuring steady-state VOD value and detonation front curvature.

The following linear relation between VOD values and the inverse charge diameter was used for the calibration (Figure 3-5):

$$D(\phi) = a - b/\phi \quad (3-1a)$$

where ϕ is the (inner) charge diameter in mm, a and b are fitting constants. Using two dimensionless variables D/D_0 and ϕ/ϕ_{crit} , we obtain a normalized form of the relation:

$$\frac{D}{D_0} = 1 - k \left(\frac{\phi_{crit}}{\phi} \right), \quad (3-1b)$$

where $D_0 = a$ is the VOD of a charge with infinite diameter, ϕ_{crit} is the critical charge diameter and k is a fitting constant. See Appendix 1 for the detailed analyses.

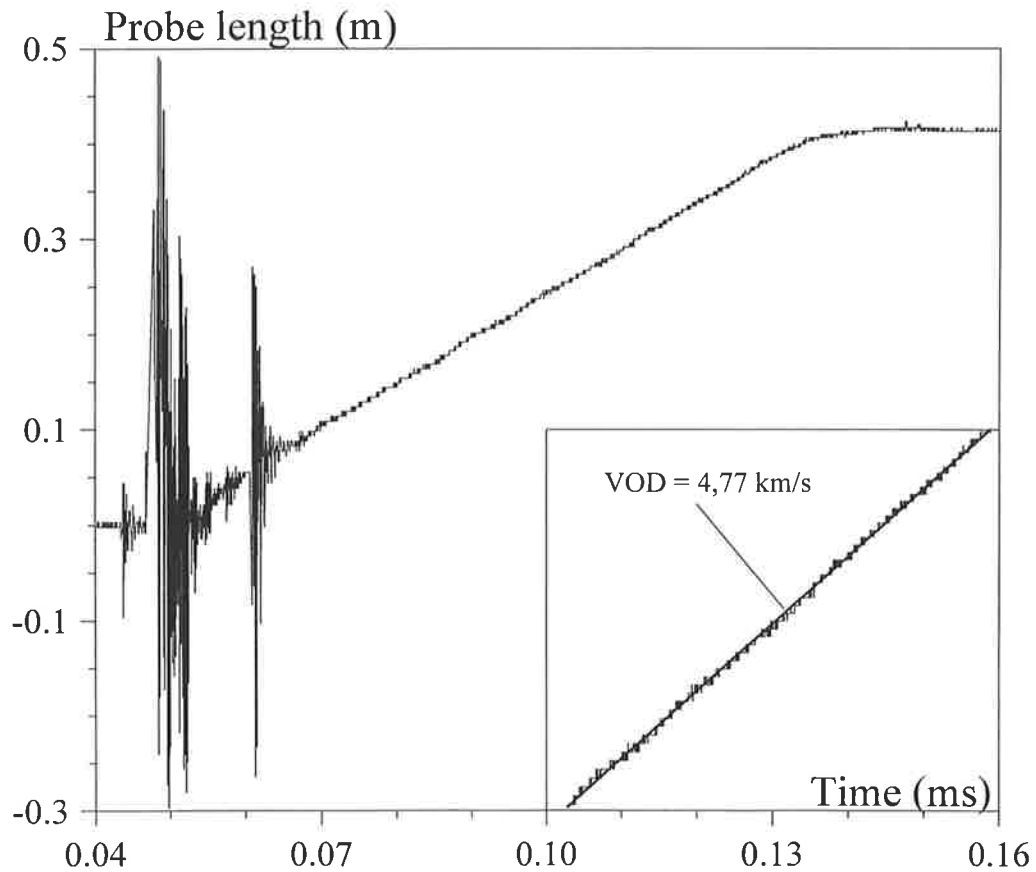


Figure 3-3: An example of a VOD recording. The VOD value is the slope of a linear fit to about 50% of the data near the charge end (klg' emulsion, $\phi = 33,6$ mm).



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Figure 3-4a: An example of recorded detonation front (k1g' emulsion, $\phi = 67,6$ mm and VOD = 5,71 km/s).

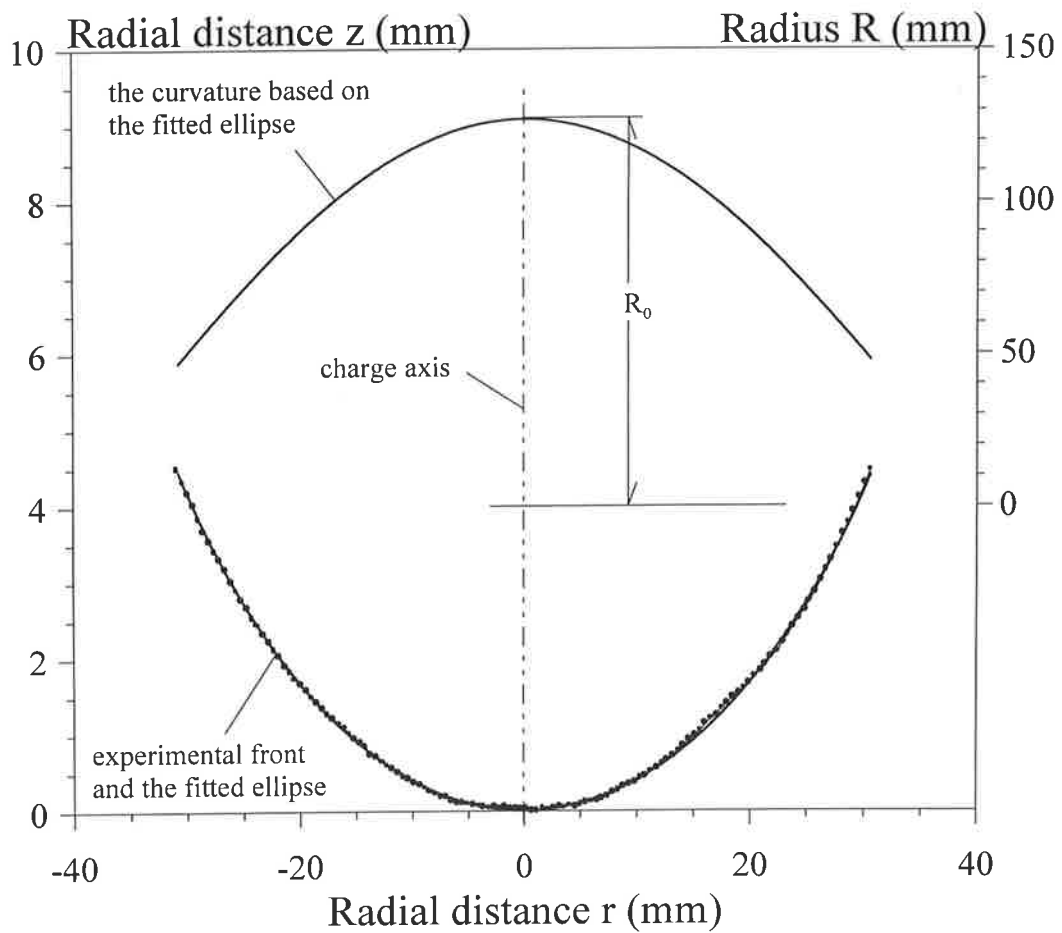


Figure 3-4b: An example of an ellipse fitted to the detonation front (the same test as in Figure 3-4a. The radius at the charge axis $R_0 = 171$ mm).

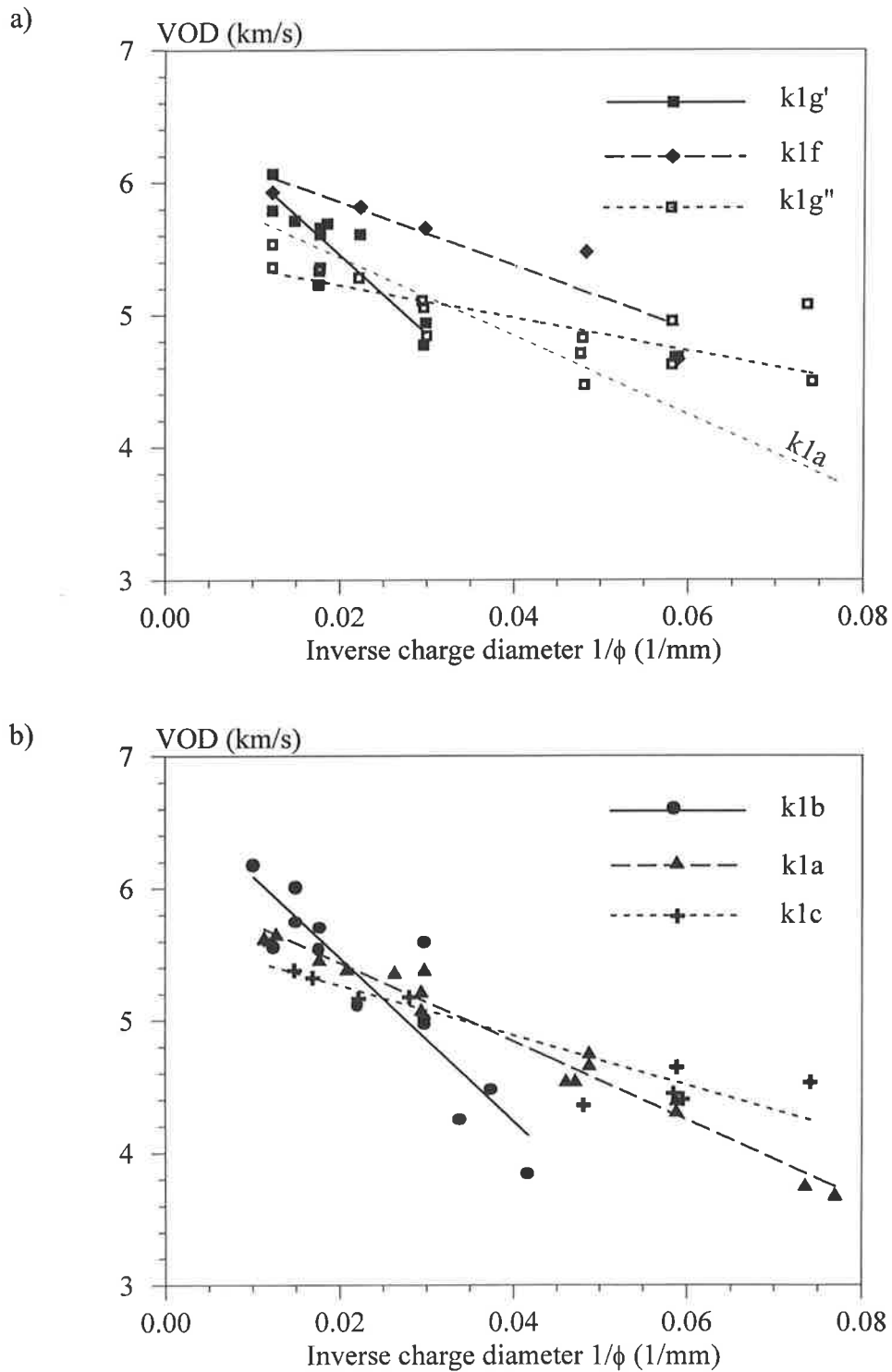


Figure 3-5: Diameter-effect curves (1): VOD vs. inverse charge diameter.

a) High water content emulsion explosives: $k1g'$, $k1f$ and $k1g''$.

b) Low water content emulsion explosives: $k1b$, $k1a$ and $k1c$.

For two of the six tested explosives k1c and k1g”, a non-linear relation may be more reasonable, but considering the scatter in the VOD values, the above linear relations are considered to be sufficiently accurate.

Ellipses were fitted to the measured detonation fronts and the curvatures at the charge axis (R_0) were used for the subsequent calibrations (Figure 3-4b). A polynomial function of the second degree was found best to describe the relation between the curvature at charge axis R_0 and the charge diameter ϕ (Figure 3-6):

$$R_0(\phi) = c_0 + c_1\phi + c_2\phi^2, \quad (3-2a)$$

where c_i are fitting constants. In the subsequent analyses, a more convenient way of plotting the curvature radius as a function of the charge diameter was found:

$$\frac{R_{0\min}}{R_0} = \xi + \zeta \frac{\phi_{crit}}{\phi} = (1 - \zeta) + \zeta \frac{\phi_{crit}}{\phi}, \quad (3-2b)$$

Here $R_{0\min}$ is the minimum curvature radius of a stable detonation front in a charge of near critical diameter ϕ_{crit} , ζ and $\xi (= 1 - \zeta)$ are fitting constants (see Appendix 1).

Equations 3-1 and 3-2 represent the diameter effects of the explosives. The first ones of each relation have been used in the calibration procedure. The detailed analyses of the experimental results (see Appendix 1) show that the microballoons are a very important ingredient in the emulsion explosives. The microballoon content controls the density, which in turn controls the VOD value at infinite diameter. The sensitivity of an explosive, which is represented by the slope in the VOD vs. inverse charge diameter plane and the critical charge diameter, is determined more by the microballoon content than by the water content.

The detailed analyses also show that both the microballoon content and the water content affect the detonation front curvature but in different ways. The microballoon content affects the absolute curvature radius of the detonation front more than the water content does. The critical diameter and the minimum curvature radius of the detonation front (the radius corresponding to the critical charge diameter) also change significantly with the microballoon content. The water content affects the scaled curvature radius (radius/charge diameter) more than the microballoon content does. It does not influence the critical diameter and the minimum curvature radius significantly however.

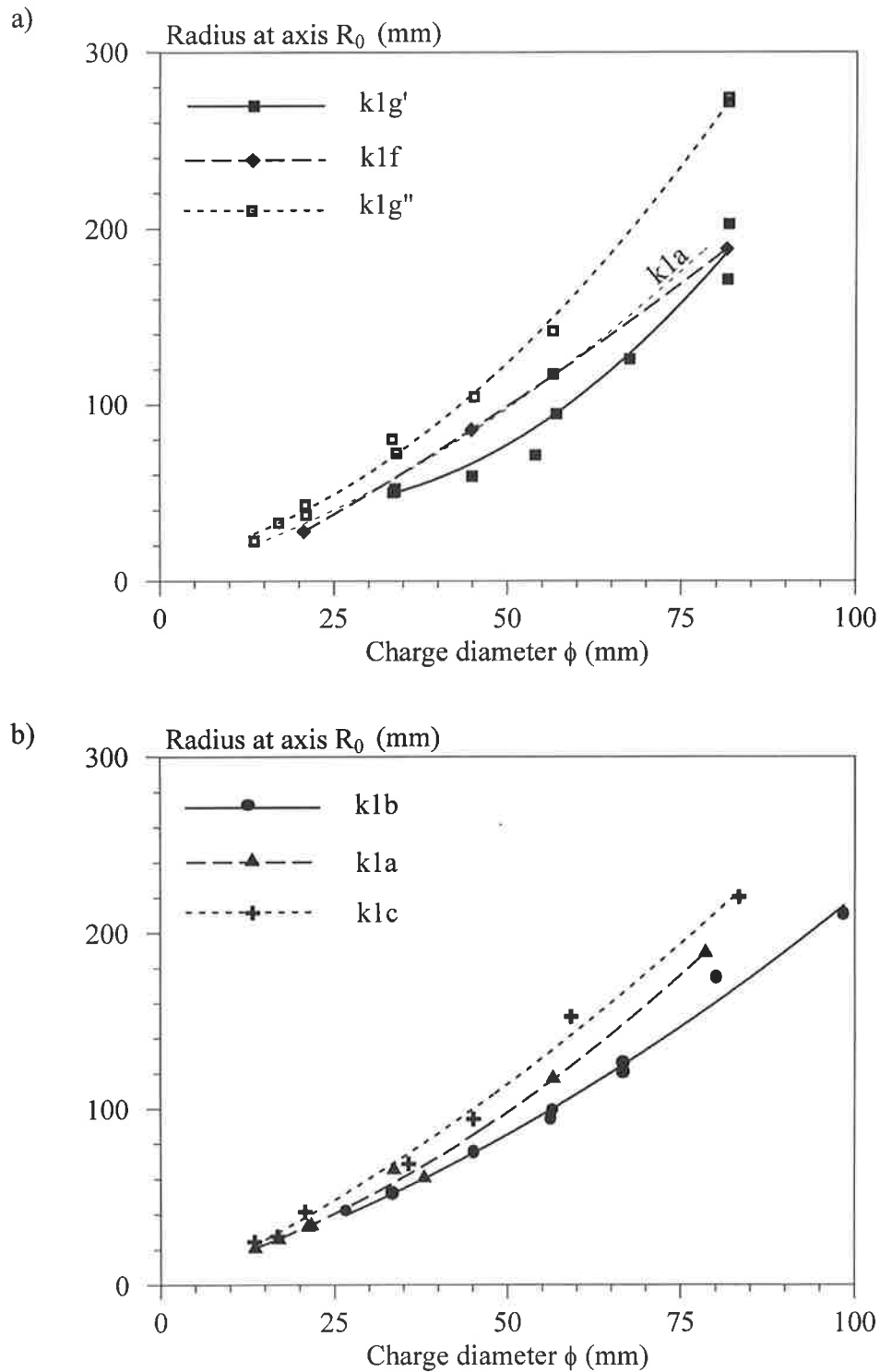


Figure 3-6: Diameter-effect curves (2): detonation front curvature vs. charge diameter.

a) High water content emulsion explosives: $k1g'$, $k1f$ and $k1g''$.

b) Low water content emulsion explosives: $k1b$, $k1a$ and $k1c$.

According to conventional detonation theories, the total released explosive energy is proportional to the square of the VOD value and it depends on the chemical composition of the explosive, the initial density, the charge diameter and the confinement. The detonation front curvature is the result of the interaction between the reaction products and the confinement. Therefore the relations of measured VOD values and the detonation front curvatures vs. charge diameters represent the detonation characteristics of commercial explosives. The numerical model calibrated against these quantities can be used to simulate the non-ideal performance of commercial explosives under other conditions.

3.2 Equations of State for the Reactive Flows

The original Ignition and Growth model in DYNA2D uses JWL equations of state for both the unreacted emulsion and the fully reacted products in the following form (Murphy 1995):

$$P = Ae^{-R_1V} + Be^{-R_2V} + \omega C_v \frac{T}{V}, \quad (3-3)$$

where P is the pressure, $V = \rho_0/\rho$ is the relative volume, where ρ_0 and ρ are the initial and the current densities of the explosive, T is the absolute temperature, ω is the Grüneisen coefficient, and A , B , R_1 and R_2 are fitting constants. The heat capacity C_v is the value corresponding $P = 0$ at $V = 1$ and $T = 298^\circ\text{K}$.

The Hugoniot of the inert emulsions are determined by measuring shock transmission processes in the matrices and then calibrated by DYNA2D computation. The Hugoniot are then used to generate the isentrope curves of the inert emulsions and the JWL parameters are obtained by recasting these curves into the JWL form. The isentropic expansion curves of the fully reacted explosive products are obtained by the thermochemical code Cheetah (Fried 1996). The details of the parameter determinations and all parameters of the five emulsion explosives are reported in Appendix 2.

The reactive flow is defined by the mixture of the two components: the unreacted emulsion, for which the relative extent of reaction λ in kg/kg = 0, and the fully reacted products, for which $\lambda = 1$. The pressure and temperature in the two components are

assumed to be in equilibrium and their relative volumes to be additive.

The transition from the unreacted emulsion to the reaction products is defined by a burning rate function. We use the following two-term Ignition and Growth burning rate function to describe the burning process of our emulsion explosives:

$$\frac{d\lambda}{dt} = ig(1 - \beta\lambda)^2 (\mu_e - \mu_c)^4 + gr(1 - \lambda)^{2/3} \lambda^{2/9} P^y. \quad (3-4)$$

Here λ is the reaction extent, t is the time, $\mu_e = \rho_e/\rho_0 - 1$ is the relative compression of the explosive, ρ_e/ρ_0 is the ratio of the current density to the initial density of the explosive and μ_c is the critical relative compression. The burning parameters ig , gr , β and y are calibration constants. The reaction starts when the relative compression μ_e exceeds the critical value μ_c . In order to get a smoother transition from the ignition phase (the ig -term) to the growth phase (the gr -term), a new parameter β was introduced into the ignition term (Deng et al. 1995), where β is greater than 1. The ignition phase terminates when $\beta\lambda = 1$ (or $\lambda_{mxig} = 1/\beta$, compared with the original burning rate function). This could also be expressed by mathematical step functions.

3.3 Calibration Method

After obtaining all parameters of the equations of state for both the unreacted emulsion and the fully reacted products, the DYNA2D computation models are set up so that the burning rate parameters can be calibrated against the steady-state cylinder experiments, i.e. the VOD values and detonation front curvatures. The flow diagram of the calibration system is illustrated in Figure 3-7.

The original three-term Ignition and Growth burning rate function models phenomenologically the three stages of the burning process: the ignition of hot spots by shock compression in the ig -term, the slow growth of reaction from these isolated hot spots in the gr -term and the rapid completion of the reaction as the hot spots coalesce in the 2nd gr -term or the completion term (Lee & Tarver 1980). It is difficult to calibrate this type of the burning model, since to date very little is known about the details of the detonation process in the micro scale. All parameters are free until we clearly know their physical meanings. Although some burning parameters may be set a priori assuming certain forms

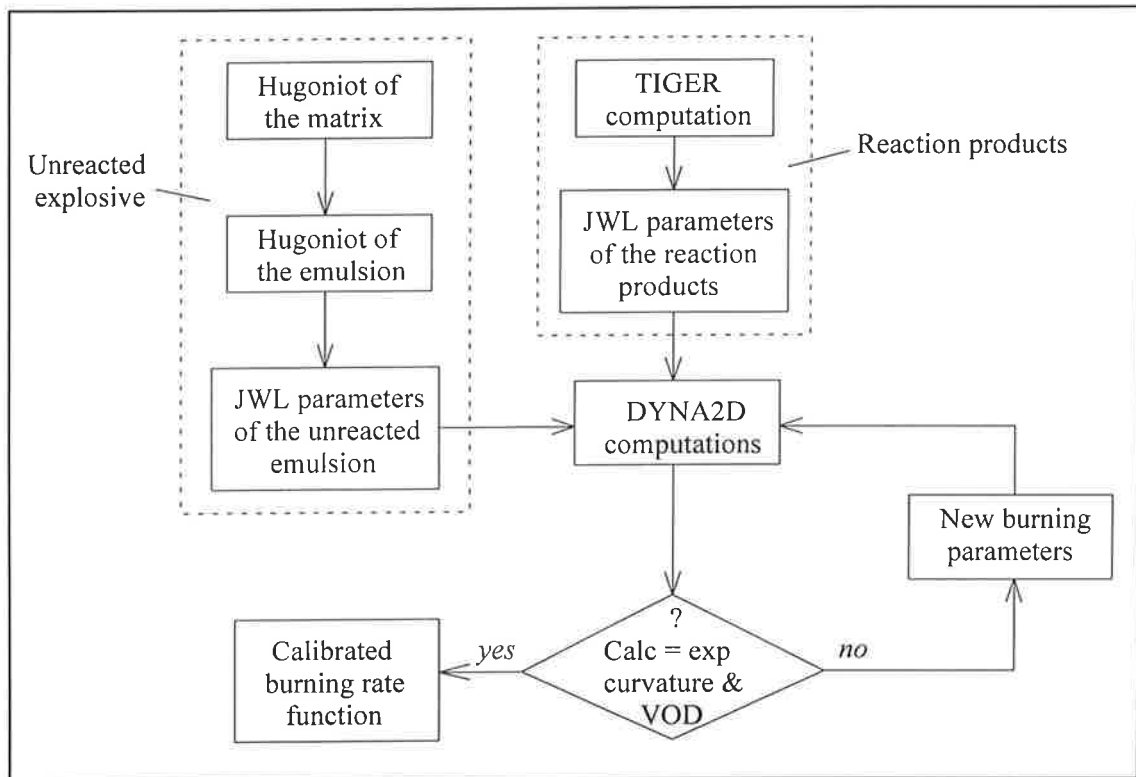


Figure 3-7: The flow diagram for the burn parameter determination.

of burning geometry of the hot spots, most of the parameters will be determined by comparing computations with experiments (Lee & Tarver 1980). The calibration method is usually unsystematic.

Lee and Tarver (1980) used a series of experiments with embedded manganin gauges (wedge tests) to calibrate their burning parameters. The recorded shock trajectories and pressure and particle velocity histories were used to compare with the DYNA2D calculated ones. Baker et al. (1995) applied a nonlinear optimization method to the calibration of inert explosives and reacted products equations of state and the burning rate functions. The one-dimensional small-scale wedge test has proved to be a good method to study the initiation properties of ideal high explosives.

The charge diameter dependence of the non-ideal explosives is truly a two- or three-dimensional problem however. The wedge tests provide little information on the non-ideality of a commercial explosive (Kennedy 1995). We thus believe that the two-

dimensional steady-state cylinder tests are more representative for non-ideal explosives than wedge tests. This is fortunate because it is more complicated and expensive to conduct the wedge tests for emulsion explosives.

The quantities used for the calibration are the VOD values and the curvature radii of the detonation fronts at the charge axis. The calculated VOD values have been evaluated by the shock trajectories over six nodes along the charge axis, while the radii of the calculated fronts are evaluated by the shock trajectories over ten nodes along a radial line normal to the charge axis. Ellipses have been fitted to the curvatures of the detonation fronts (Deng et al. 1995) just as we have done to the experimental detonation fronts. The calculated VOD values and detonation front radii have been compared with those from experiments and the best parameters for the burning rate function have been determined by minimising the following quantity:

$$Q = \sum_{i=1}^n \left[\left(\frac{VOD_{com,i} - VOD_i}{VOD_i} \right)^2 + \left(\frac{R_{0com,i} - R_{0i}}{R_{0i}} \right)^2 \right]. \quad (3-5)$$

Here $VOD_{com,i}$ and $R_{0com,i}$ are the calculated VOD values and the detonation front radii at the charge axis for the different charge diameters. VOD_i and R_{0i} are the corresponding quantities on the lines fitted to the experimental data (see Equations 3-1 and 3-2 and Figures 3-5 and 3-6). n is the number of the DYNA2D computation set-ups.

The critical diameter was important for determining the critical relative compression μ_c for the first emulsion k1a (Deng et al. 1995). In this study, this value has not been used in the calibration however and the critical relative compression μ_c was only roughly estimated from the critical diameters for the remaining emulsion explosives.

The details of the calibration of the burning rate parameters are given in Appendix 3. The procedure was to manually search the parameter space over a coarse mesh before concentrating on narrower interesting intervals. Each step was evaluated manually. This made the calibration relatively difficult and time consuming.

3.4 Calibrated Burning Rate Parameters

The calibrated burning rate parameters in Equation 3-4 are summarised in Table 3-1. Together with the EOS parameters of the unreacted explosives and the reaction products (see Table A2-4), the burning processes of these five emulsion explosives can be simulated completely.

Table 3-1: The calibrated burning rate parameters for five emulsion explosives:

Emulsion	ig	gr	y	β	(μ_c)	$\lambda_{mxi} (=1/\beta)$
k1a	18	190	1,92	1,5	0,08	0,6667
k1b	60	90	2,20	1,2	0,08	0,8333
k1c	18	120	1,80	1,0	0,05	1,0
k1g'	20	220	2,10	2,5	0,09	0,40
k1g''	37	150	1,79	1,2	0,05	0,8333

The comparisons of DYNA2D computations with the above parameters and the experiments are shown in Figures A3-10 through A3-14 in the Appendix 3. The average VOD difference between computations and experiments is 0,28 km/s, while the average radius difference is 7,5 mm. This corresponds to only 4,6% and 6,6% respectively. For most explosives, the computed VOD values for large diameters are higher than the experimental ones, probably because of the larger elements used. For example, for the 80 mm diameter charges, elements of 0,8×0,8 mm were used, which usually gave higher VOD values. It was impossible to use smaller elements for the computations for the large diameters using our computers.

We have found that the pressure exponent y in the burning rate function 3-4 depends on the slope b in the experimental relation $D(1/\phi)$ (Equation 3-1). Figure 3-8 shows a linear relation between the two variables. Using this relation, the pressure exponent for a new emulsion explosive can probably be estimated relatively accurately before the actual calibration of the burning rate parameters takes place. This, according to our experience, will save much time during the calibration. It is our intention to see if this relationship holds for new emulsion explosives that we are going to test.

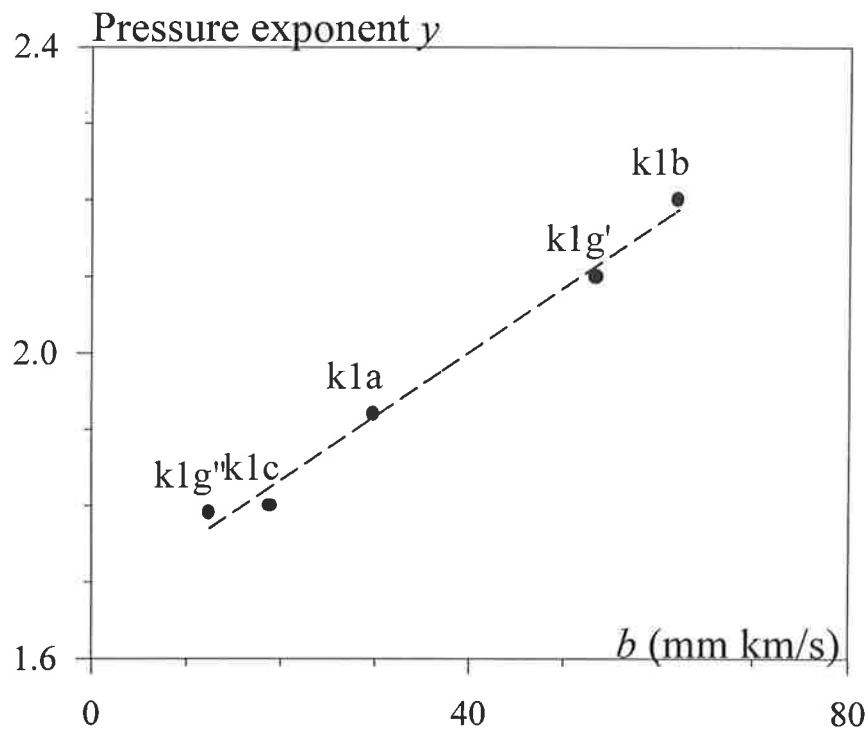


Figure 3-8 The pressure exponent γ in the burning rate function as a function of the slope b in the experimental function $D(1/\phi)$.

3.5 Discussion of the Burning Models

1. Effects of steel confinement

It is important to know how well the burning models work under other detonation conditions, when e.g. the charge geometry, the confining material and the way of initiation are different. Although the models were calibrated for the 2D steady-state cylinder tests in PMMA or PVC tubes, the effects of other confinements should be predictable.

We have tested the burning models for three explosives in 2D steady-state cylinder tests in steel tubes. The tests were conducted by Kimit AB (Stenberg 1995). The charges were confined in steel tubes of 19 mm inner diameter and 3 mm in thickness. Only steady-state VOD values were measured. The same geometry was used for the

DYNA2D computations. The confining material is modelled by an elasto-plastic hydrodynamic material model and the Grüneisen equation of state (Murphy 1995). The emulsion explosives are modelled by the Ignition and Growth model with the calibrated burning parameters in Table 3-1.

The comparison of VOD values from the tests and DYNA2D computations is shown in Table 3-2. The agreement between experiments and computations is relatively good. The computed VOD values for all three emulsions are higher than those from experiments. From an engineering point of view, a maximum of 5% difference between experiment and computation is acceptable.

Table 3-2: Comparison of experimental and computed VOD values from the cylindrical charge tests in steel tubes ($\phi = 19$ mm):

Explosive	k1a	k1b	k1c
VOD from experiment (km/s)	5,458	5,629	5,446
VOD by computation (km/s)	5,521	5,904	5,558
difference (%)	+1,15	+4,89	+2,06

The above results support that the burning models could be used to model a detonation confined by any medium. Charge size and confining material will of course affect the detonation process. We show some predictive computations with our burning models in the following chapter, where, the explosives are fired in different rock types, in water or without confinement.

2. Simulating 1D detonations with the burning models

The one-dimensional detonation is a basic limiting case for the burning models. Although a 1D detonation is not feasible in practice, it is rather easy to calculate with the DYNA2D code. The thermo-dynamic code Cheetah also calculates the 1D detonations. The extrapolated VOD values at infinite diameter and the 1D VOD values from DYNA2D and Cheetah codes are shown in Table 3-3. They are all linearly related to the explosive density (see also Appendices 1 and 2).

Table 3-3: Comparisons of 1D VOD values by different methods

Explosive	k1a	k1b	k1c	k1g'	k1g''
Explosive density (g/cm ³)	1,165	1,250	1,090	1,240	1,086
Experiment (extrapolated)	6,028	6,710	5,640	6,530	5,470
Computation by DYNA2D	6,070	6,545	5,845	6,463	5,795
Computation by Cheetah	6,179	6,622	5,844	6,515	5,774

The results show that, in general, the agreement between extrapolated experimental VOD values and the calculated ones is good. For explosives with higher densities, for example, explosives k1b and k1g', the agreement is better than those with lower densities, for example, explosives k1c and k1g''. The linearly extrapolated VOD values for the lower density explosives k1c and k1g'' are higher than that they would be, if we had used either a non-linear relation between the VOD and inverse charge diameter, or a linear curve fit to the experimental data for only large diameters. For example, if only experiments greater than 30 mm in diameter are used for the extrapolation, the extrapolated VOD values for explosives k1c and k1g'' become 5,77 km/s and 5,79 km/s respectively, which is somewhat closer to the calculated 1D values.

The 1D computation model can also be used to check the JWL EOS parameters used by the DYNA2D code. The DYNA2D outputs, for instance, the isentropic relations for the reacted products, should be identical or at least very close to the inputs, since the JWL EOS parameters for the reaction products are obtained by the Cheetah calculations, which represent the 1D detonations (see Appendix 2 for details).

Since the 1D model is simple and it takes short time to run, we used this set-up for preliminary calibration of the burning rate parameters. The 2D set-ups (the finite diameter set-ups) were used for the detailed calibrations (see Appendix 3).

3. Detonation zone length

Detonation zone is the area between the shock front surface and the sonic surface. This is the area where conditions are subsonic and in which the different parts can influence each other. Behind the sonic surface, the material flow is supersonic.

It is difficult to measure the detonation zone length, especially for non-ideal explosives such as emulsion explosives (Kirby & Leiper 1985). The concept is however very important in the study of the detonation properties of an explosive. Using the burning models, the detonation zone can be studied relatively easily. In the following, we have examined the 1D detonation zone length (the CJ set-up) and the zone length on the charge axis for the charges with finite diameters.

For 1D set-ups, it is rather easy to locate the sonic point by examining the following condition (Johansson & Persson 1970)

$$D = C + U_p, \quad (3-6)$$

where D is the detonation velocity, C , the local sound velocity, and U_p , the particle velocity. Since the DYNA2D code does not give the sound velocity as an output, it is calculated by the following equation:

$$C = \sqrt{-\frac{V}{\rho} \left(\frac{dP}{dV} \right)}, \quad (3-7)$$

where P is the pressure, $V = \rho_0 / \rho$ is the relative volume, where ρ_0 and ρ are the initial and the current densities of the explosive. From the sonic point, the detonation zone length can be calculated (see Appendix 4).

For the charges with finite diameters, it is more difficult to define the sonic point, since the pressure trajectories oscillate. The oscillations are probably caused by the coarse elements used and the charge boundary effects. For example, elements of 0,8×0,8 mm were used for the charges of 80 mm diameter. It is not possible to use finer elements with this version of the DYNA2D code.

These oscillating pressure curves sometimes display two sonic points. This is a spurious numerical phenomenon, not a physical one. We use the last one as the sonic point, since the first one usually yields an incredibly thin detonation zone. The sonic point is then determined by Equation 3-7. The detonation zone lengths estimated for the finite diameter charges are thus relatively inaccurate (see Appendix 4).

The calculated detonation zone lengths are different for the different charge diameters. Figure 3-9 shows the detonation zone length versus the inverse charge diameter. For the

1D case, there is a unique detonation zone length everywhere. For the finite diameter cases, the zone length is a function of the distance from the charge axis and the zone lengths shown in the figure are those on the charge axes. The figure shows that the detonation zone lengths generally decrease with decreasing charge diameter.

Based on 56 curvature measurements for 26 explosives, Souers (1997) has presented simplified expressions for the average detonation zone length $\langle x_e \rangle$. The simplest one is that it is approximately equal to the edge lag of the detonation front on the charge surface L_0 , or $\langle x_e \rangle \approx L_0$. The other is a functional relation between VOD size effect and detonation zone length, which reads as follows:

$$\frac{D}{D_0} = 1 - \frac{\langle x_e \rangle}{\sigma r_0}, \quad (3-8)$$

where r_0 is the charge radius and D/D_0 is the ratio of the VOD value of the charge to the VOD value for infinite diameter. For an unconfined charge, σ is a function of the variables $\langle x_e \rangle$ and r_0 (Souers 1997). Later Souers and Garza (1998) proposed another formula to calculate variable σ through the concept of the average angle of the detonation front $\langle \Theta \rangle$:

$$\sigma = \frac{1}{\cos\langle \Theta \rangle \sin\langle \Theta \rangle}, \quad (3-9)$$

where $\langle \Theta \rangle$ is the average angle between the direction normal to the detonation front and the charge axis at the average radius $\langle r \rangle = r_0 / \sqrt{2}$. Combining Equations 3-8 and 3-9, the average detonation zone length can be expressed in the following:

$$\langle x_e \rangle = \frac{r_0(1 - D/D_0)}{\cos\langle \Theta \rangle \sin\langle \Theta \rangle}. \quad (3-10)$$

Figure 3-9 also shows the average detonation zone lengths for k1a using the relations $\langle x_e \rangle \approx L_0$ and Equation 3-10.

The results show that the average detonation zone length is measured better by the edge lag L_0 than that by Equation 3-10. The interesting thing is that the edge lag method was found only “approximately true” (Souers & Garza 1998). The new proposed ratio of the variables $\langle x_e \rangle$ and L_0 equals to 2.3 ± 1.6 instead of 1. Thus considerably longer detonation zone lengths can be expected. The detonation zone lengths estimated by

Equation 3-10 are considerably longer than our values and show no overall influence of the charge size. This discrepancy demonstrates the necessity of a detailed description of the detonation process.

The concepts of detonation zone and reaction zone are different. The reaction zone of a detonation ends on the surface where the chemical reaction is complete. For an ideal or 1D detonation, the chemical reaction is complete at the sonic surface, while for the non-ideal detonation, the reaction is not necessarily complete there. For non-ideal explosives, therefore, the reaction zone of a detonation is usually longer than the detonation zone (See Appendix 4).

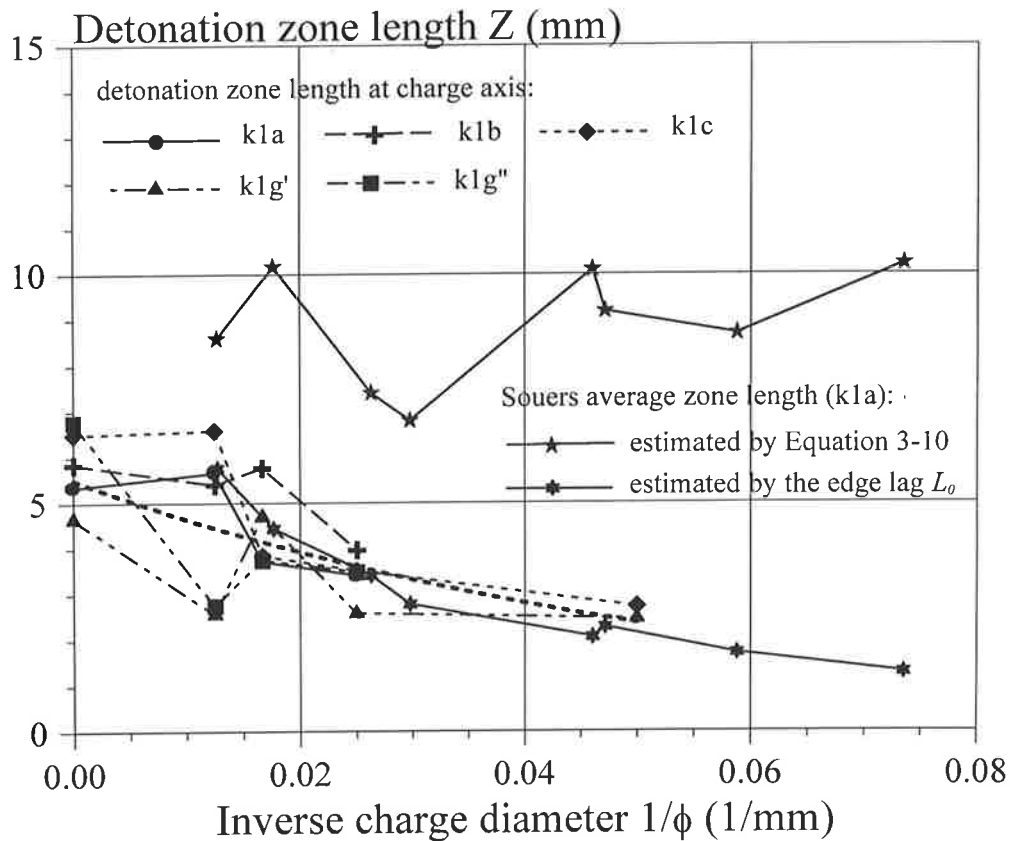


Figure 3-9: Relation of detonation zone length and inverse charge diameter.

4. APPLICATIONS OF THE BURNING MODEL

All engineering uses of commercial explosives have a general goal: to make full use of the explosive energy. It is not always the case that the energy from a detonation can be utilized in blasting. Both the total energy and the way by which the energy is released are important. It is generally difficult to study such problems in detail without a burning model. We illustrate some applications of our burning models in the following sections. Further application studies of the model are planned for the future.

4.1 Effects of Charge Diameter on Detonations for Different Confinements

In production, commercial explosives are used in different rocks, sometimes, even in water and air. It is well recognised that a commercial explosive can perform radically differently, depending on charge geometry and in what medium the charge is fired. An explosive can detonate well in one confining material, may detonate badly in other confining material or it may even fail. Many engineering problems are related to these aspects of non-ideality of commercial explosives. With the help of a burning model, the actual performance of an explosive can be simulated with, hopefully, a sufficient accuracy.

The explosive we use for the simulation below is k1a emulsion. The explosive contains 3,1% of microballoons and has a density of 1,165 g/cm³. The extrapolated experimental VOD value at infinite diameter is 6,03 km/s and the CJ VOD value by Cheetah code is 6,18 km/s. The difference is only 2,5%.

With the calibrated burning parameters (see Table 3-1), we simulate the detonation of the explosive in granite, coal, water and air (i.e. without confinement) for a constant charge diameter of 40 mm. The computation setups are shown in Figure 4-1. A 50 gram PETN primer is used to initiate the main charge. The primer is simulated by the following JWL equation of state:

$$P = A(1 - \frac{\omega}{R_1 V})e^{-R_1 V} + B(1 - \frac{\omega}{R_2 V})e^{-R_2 V} + \frac{\omega E}{V}, \quad (4-1)$$

where P is the pressure, V is the relative volume, E is the internal energy, ω is the Grüneisen coefficient and A , B , R_1 and R_2 are fitting constants. The JWL parameters for the PETN explosive are listed in Table 4-1.

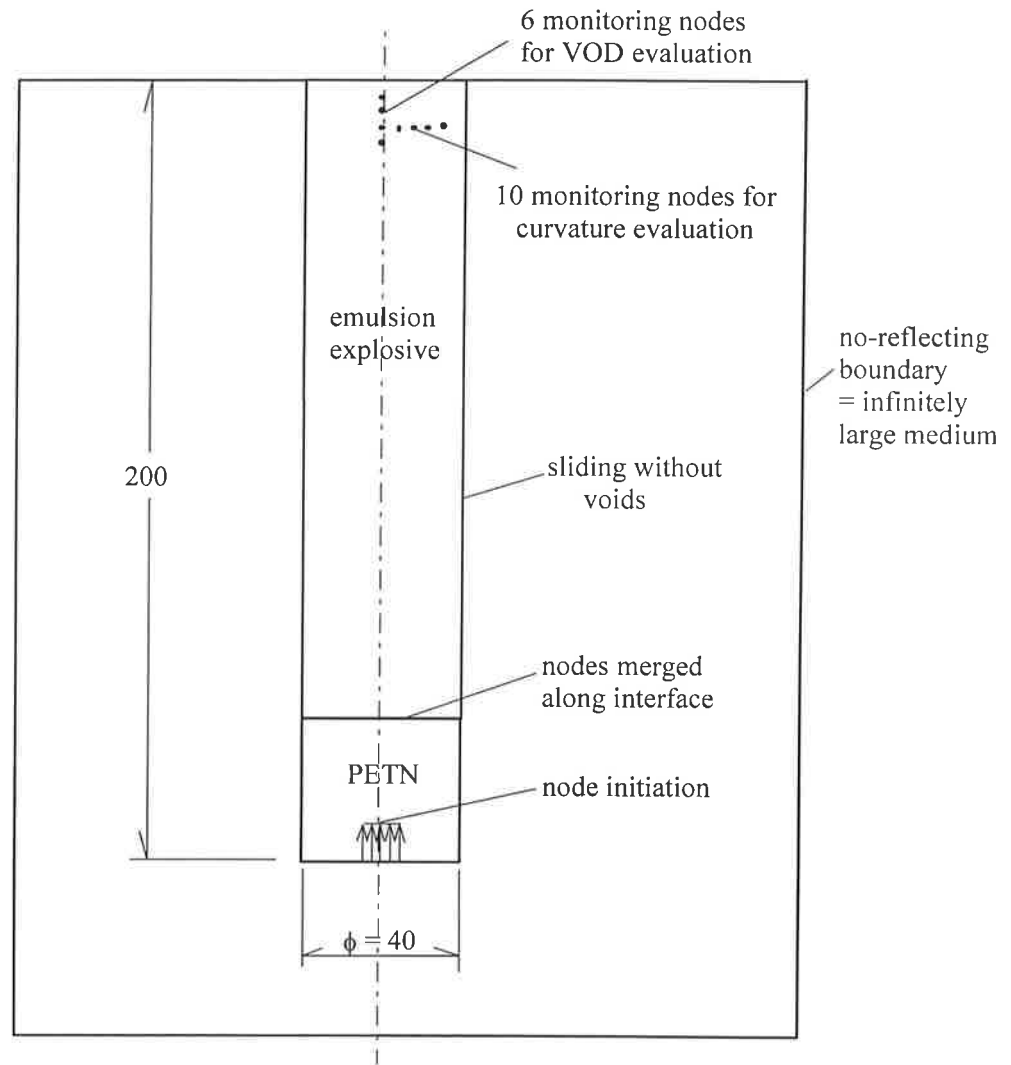


Figure 4-1: Computation setup for simulating the charge diameter effects on the detonations of different confinements.

Table 4-1: JWL EOS parameters for the donor explosive PETN (Murphy 1995):

variable and unit	parameter	variable and unit	parameter
density ρ_0 , g/cm ³	1,77	A , Mbar	6,170
CJ pressure, Mbar	0,335	B , Mbar	1,693
VOD, km/s	8,30	R_1	4,4
initial internal energy E_0 , Mbar cm ³ /cm ³	0,101	R_2	1,2
		ω	0,25

The Elasto-plastic Material Model is used for the granite and coal and the so-called Null Material Model is used for the water. The following Grüneisen equation of state is used for all the three materials (Hallquist 1990):

$$P = \frac{\rho_0 C_0^2 \mu [1 + (1 - \gamma_0/2)\mu]}{\left[1 - (S_1 - 1)\mu - S_2 \frac{\mu^2}{\mu + 1} - S_3 \frac{\mu^3}{(\mu + 1)^2}\right]^2} + (\gamma_0 + a\mu)E. \quad (4-2)$$

Here P is the pressure, $\mu = 1/V - 1$ is the relative compression, where V is the relative volume, E is the internal energy, ρ_0 is the initial material density and γ_0 and a are the Grüneisen coefficients. Constants C_0 and S_i ($i = 1, 2, 3$) are the coefficients of the following material shock Hugoniot relation:

$$U_s = C_0 + S_1 U_p + S_2 U_p^2 + S_3 U_p^3, \quad (4-3)$$

where U_s and U_p are the shock and particle velocities respectively. All parameters for the three confining materials are listed in Table 4-2 (Butcher & Stevens 1975, March 1980, Murphy 1995).

Table 4-2: Parameters for the confining materials:

Variable and unit	granite	coal	water
Parameters of the Grüneisen equation of state			
density ρ_0 , g/cm ³	2,627	1,26	1,0
C , cm/ μ s	0,37	0,175	0,148
S_1	1,136	2,5	2,56
S_2	0	0	-1,986
S_3	0	0	0,2268
Grüneisen γ_0	2,0	0,7	0,5
a	0,5	0,5	0
Parameters of the elasto-plastic hydrodynamic material model			
Shear modulus, Mbar	0,2826	0,0256	—
Yield stress, Mbar	0,005	0,00125	—

The confinement effects on the steady-state detonation can be seen clearly in Figure 4-2. The expansion contours of the reaction products show that the granite keeps a higher pressure in the charge, which results in a faster detonation and a flatter detonation front. The detonation zone structures of the two detonations show also the importance of the confining materials. The stronger confining material will cause a thinner detonation zone. For example, the detonation zone for the granite case is about 4 mm, while for the unconfined case, it is longer than 8 mm. The evaluated VOD values and the detonation front radii are listed in Table 4-3.

Table 4-3: Effects of confining material on VOD values and radii at charge axis ($\phi = 40$ mm):

Confining material	granite	coal	water	no confinement
VOD (km/s)	5,70	5,53	5,42	5,0
R_0 (mm)	110,2	71,6	60,2	50,5

Using the approximate linear relation found between the VOD and the inverse charge diameter, the diameter effects can be illustrated by Figure 4-3. For the charge of diameter 40 mm, the VOD value increases from 5 km/s for the no confinement case to 5,7 km/s for the granite confinement case. The line for the no confinement case represents the lower bound of different confining materials, while the horizontal line for the 1D case represents the upper bound. All possible VOD values fall in the area between the two lines.

The detonation front curvature depends on the confining material. The radius at charge axis increases from 50,5 mm for the no confinement case to 110,2 mm for the granite confinement case. Figure 4-4 shows all detonation fronts for the four confinement cases.

The confining material also affects the critical charge diameter. It will decrease when a denser confining material is used. This was tested by a charge with a coning of 1:7 in different confining materials. The preliminary results showed that the critical charge diameter increases from less than 8 mm for the granite confinement to more than 15 mm for the unconfined charge. The critical diameter for an unconfined charge is important for blasts with a large degree of decoupling. The choice of a charge diameter too close to its critical value might cause problems.

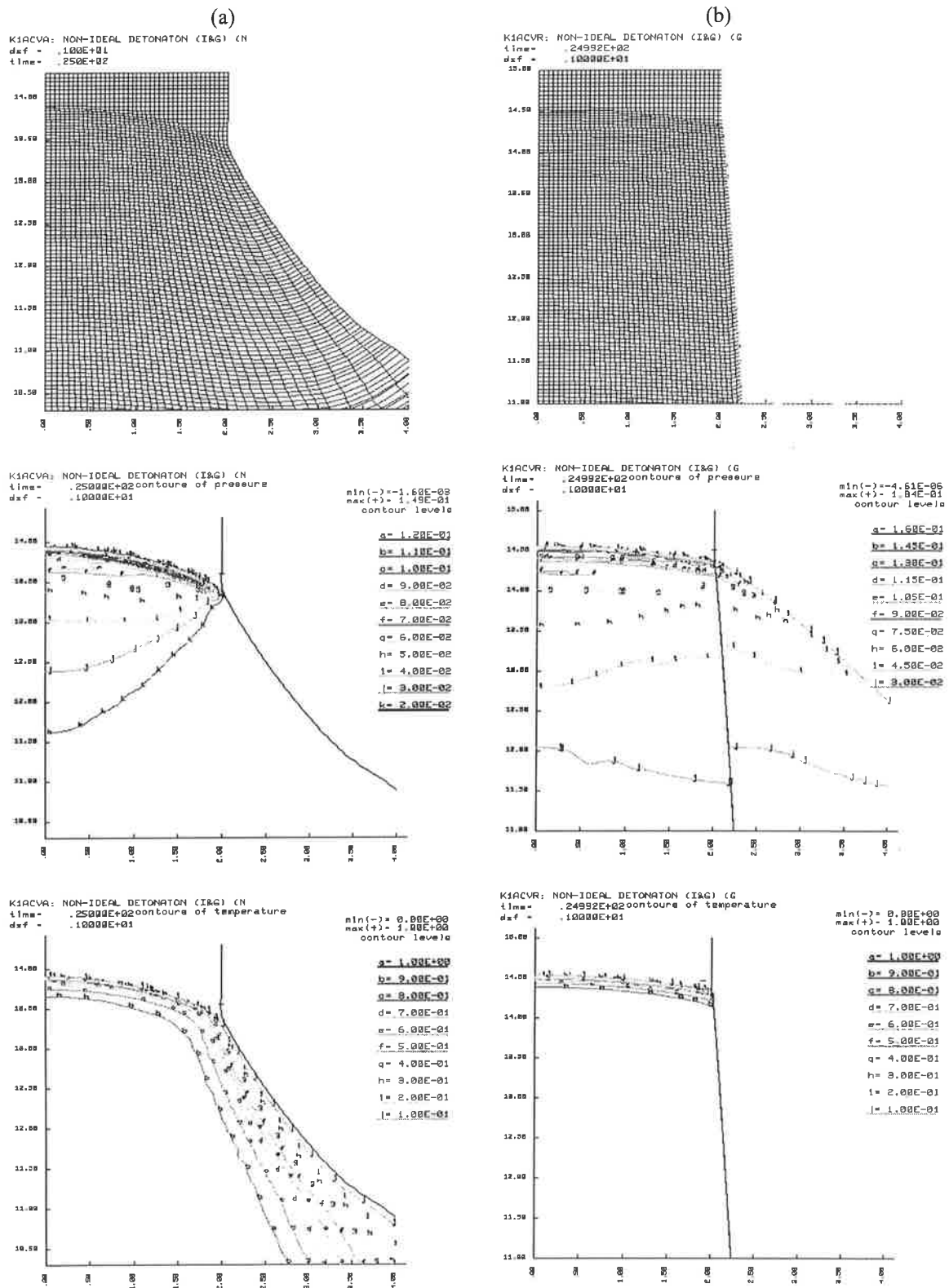


Figure 4-2: The confinement influences on the steady-state detonations: (a) no confining material (vacuum) and (b) granite confinement. Emulsion k1a and $\phi = 40$ mm.

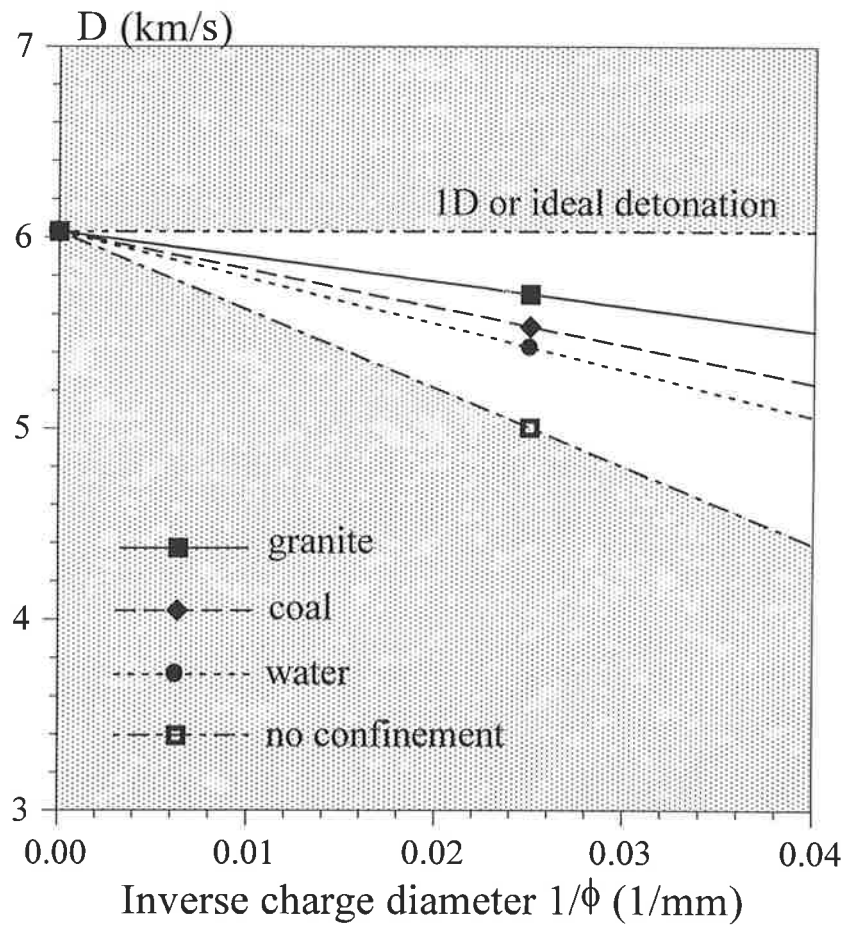


Figure 4-3: Effects of charge diameter on VOD for different confining materials.

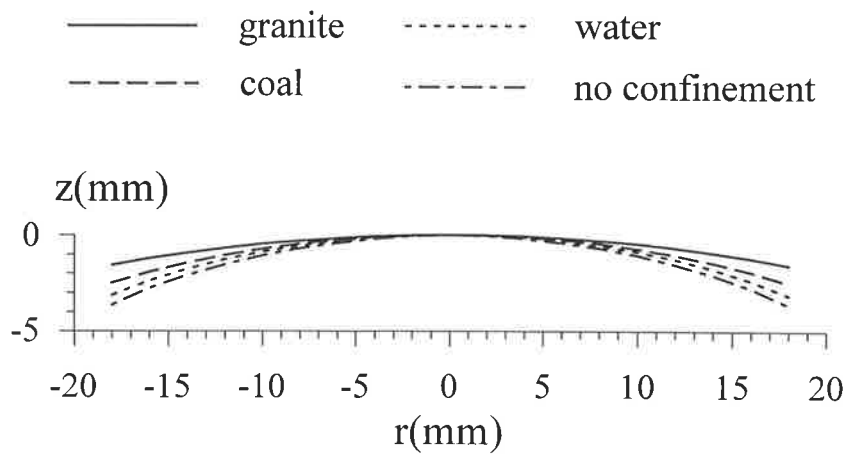


Figure 4-4: Effects of confining material on detonation front curvature.

To know the performance of an explosive in different blast media has a great engineering importance. For example, decoupled charges are often used in different blast techniques. According to the above results, the performance of the charge depends very much on the confining material. For a decoupled charge, the material directly surrounding the charge becomes the confinement. Therefore, the performance of the explosive depends on the degree of the decoupling and the material in the annulus between the charge cylinder and the rock. For a large degree of the decoupling with an air annulus, the charge will perform in the same way as the no confinement case unless the channel effect comes into play. If the borehole is filled with water, the water becomes the confining material and the explosive will perform differently.

4.2 Importance of Primer on Detonation Run-Up (Initiation) Process

The sensitivity of a commercial explosive depends also on the conditions under which the explosive is fired. A typical engineering problem is the explosive sensitivity to the primer under different conditions, namely, the charge diameter and different confining materials. Here, we will concentrate on the effect of a primer on the detonation run-up process. Run-up distances of 7~10 blasthole diameters have e.g. been measured for emulsion explosives in field tests (Neill & Torrance 1988).

A borehole diameter of 32 mm is filled with k1a emulsion (see Appendix 2 for a detailed description of the explosive). Two initiation setups are employed: (a) a standard detonator is used to initiate the main charge directly and (b) a 27 g and 20 mm high PBXN3 primer is used to initiate the main charge. For comparison purpose, two types of rocks, granite and coal, are chosen as the blast media or the confining materials. The setups for the computations are shown in Figure 4-5. Totally we have four combinations of different initiation methods and confining materials (Table 4-4).

The detonation starts with a detonator, for which only the base chamber is simulated. The base charge, which is enclosed in an aluminium shell, is simulated by 0,5 gram of Comp B with a JWL model (see Equation 4-1). When only a detonator is used, the main charge will be initiated, if the shock produced by the detonator is strong enough. When the primer is used, the primer is first initiated by the detonator. Then the main charge will be initiated by the shock produced by the primer. For the primer, the Ignition and Growth model is used, so that the shock initiation process can be simulated more closely.

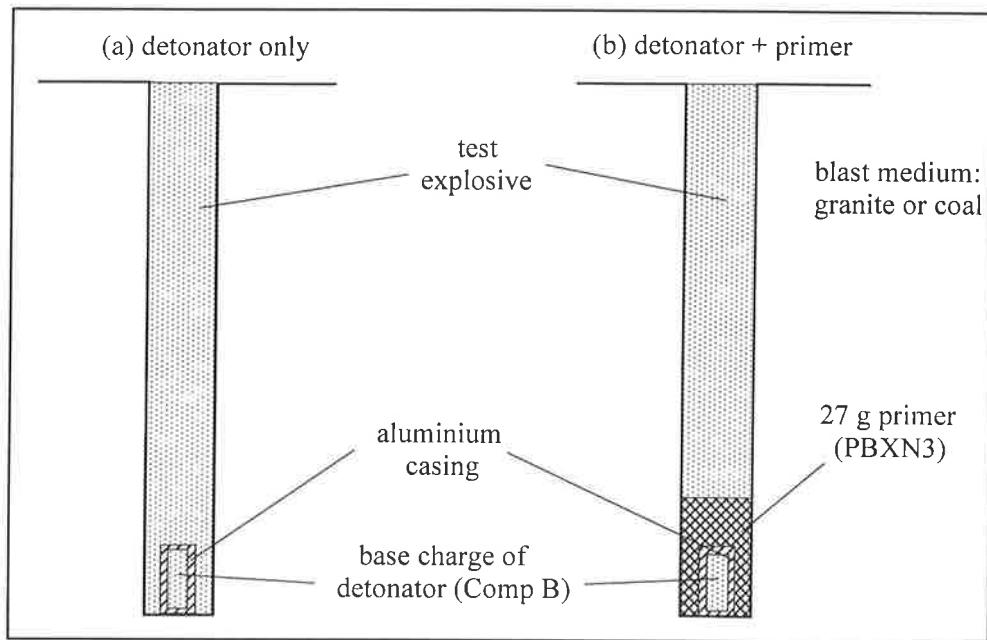


Figure 4-5: Computation setups for modelling the detonation run-up processes.

Table 4-4: Four computation cases of combinations of initiation setups and rock types:

Case no.	1	2	3	4
initiation method	detonator only	detonator + primer	detonator only	detonator + primer
rock type	granite	granite	coal	coal

The Grüneisen equation of state (see Equation 4-2) is used to describe the dynamic response of the shell. The same model is used for the granite and coal (for the parameters of the two materials see Table 4-2). The parameters for the aluminium shell are listed in Table 4-5 (Murphy 1995).

Parameters for the detonator base charge Comp B are listed in Table 4-6 (Murphy 1995).

For the primer explosive PBXN3, the following three-term burning rate function is used (Murphy 1995):

$$\frac{d\lambda}{dt} = ig(1-\lambda)^{2/3}(\mu_e - \mu_c)^x + gr1(1-\lambda)^{2/3}\lambda^{2/3}P^y + gr2(1-\lambda)^{1/3}\lambda P^z. \quad (4-4)$$

Here λ is the reaction extent (the fraction of the explosive that has reacted, kg/kg), t is

Table 4-5: Grüneisen EOS parameters for the aluminium:

Variable and unit	parameter	Variable and unit	parameter
Density ρ_0 , g/cm ³	2,77	C_0 , cm/ μ s	0,52
Shear modulus, Mbar	0,276	S_1	1,4
Yield stress, Mbar	0,0029	Grüneisen γ_0	2,0

Table 4-6: Parameters of the JWL EOS for the Comp B:

Variable and unit	parameter	Variable and unit	parameter
Density ρ_0 , g/cm ³	1,717	A , Mbar	5,242
CJ pressure, Mbar	0,295	B , Mbar	0,07678
VOD, km/s	7,98	R_1	4,2
Initial internal energy E_0 , Mbar cm ³ /cm ³	0,085	R_2	1,1
		ω	0,25

Table 4-7: Parameters of the Ignition and Growth model for the PBXN3:

Parameters for equation of state and material model			Burning rate parameters	
Variable and unit	unreacted	products	variable	parameter
density ρ_0 , g/cm ³	1,693		ig	$4,0 \times 10^8$
A , Mbar	152,7	8,364	a	0
B , Mbar	-0,5175	0,1298	x	7,0
R_1	9,5	4,620	$gr1$	11,75
R_2	0,95	1,250	y	1,0
ω	0,97594	0,420	$gr2$	10750
C_v , bar/°K	29,51	10,0	z	3,0
E_0 , Mbarcm ³ /cm ³		0,08	λ_{mxig}	0,04
Shear modulus, Mbar	0,0423		λ_{mxgr}	0,5
Yield stress, Mbar	0,002		λ_{mngr}	0

the time, P is the pressure and $\mu_e = \rho_e/\rho_0 - 1$ is the relative compression of the explosive, ρ_e/ρ_0 is the ratio of the current density to the initial density of the explosive. The parameters of the equation of state of the explosive and other burning rate parameters are listed in Table 4-7. The term λ_{mxig} determines when the ignition term is switched off, λ_{mxgr} when the first growth term is switched off and λ_{mngr} when the second growth term is switched on (Murphy 1995).

Figures 4-6 and 4-7 show the detonation run-up processes for the different cases. In the granite, when only a detonator is used, the detonation is underdriven (case 1). The detonation stabilizes after three diameter run-up. When a primer is used (case 2), the detonation becomes an overdriven one. The detonation stabilizes after a short run-down process. The steady-state detonation velocity in the granite is 5,6 km/s. The pressure contours in Figure 4-7 show that it takes longer time, when only the detonator is used, to reach the fully detonation state. Whenever the steady state is reached, the two detonations become identical.

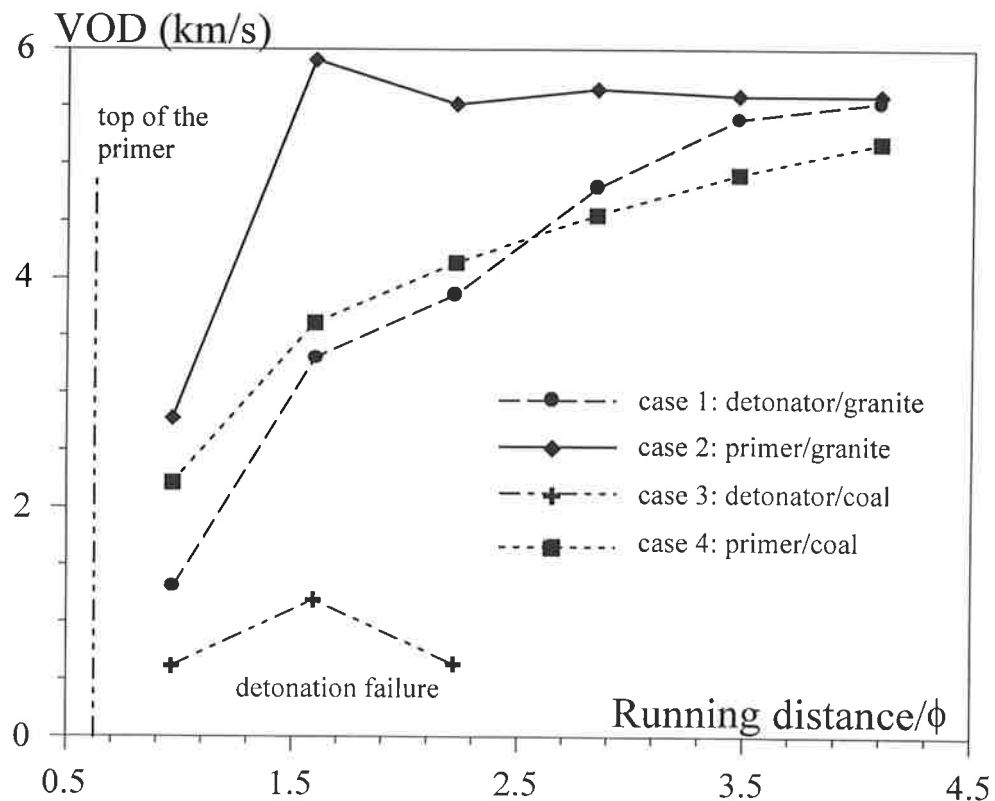


Figure 4-6: Effects of primer on detonation run-up process (1): the VOD vs. the running distance.

In the coal, the charge fails to detonate when only a detonator is used (case 3). When a primer is used (case 4), the detonation is underdriven and stabilizes after a run-up distance of 3~4 times diameter. The steady-state VOD value in coal is 5,2 km/s.

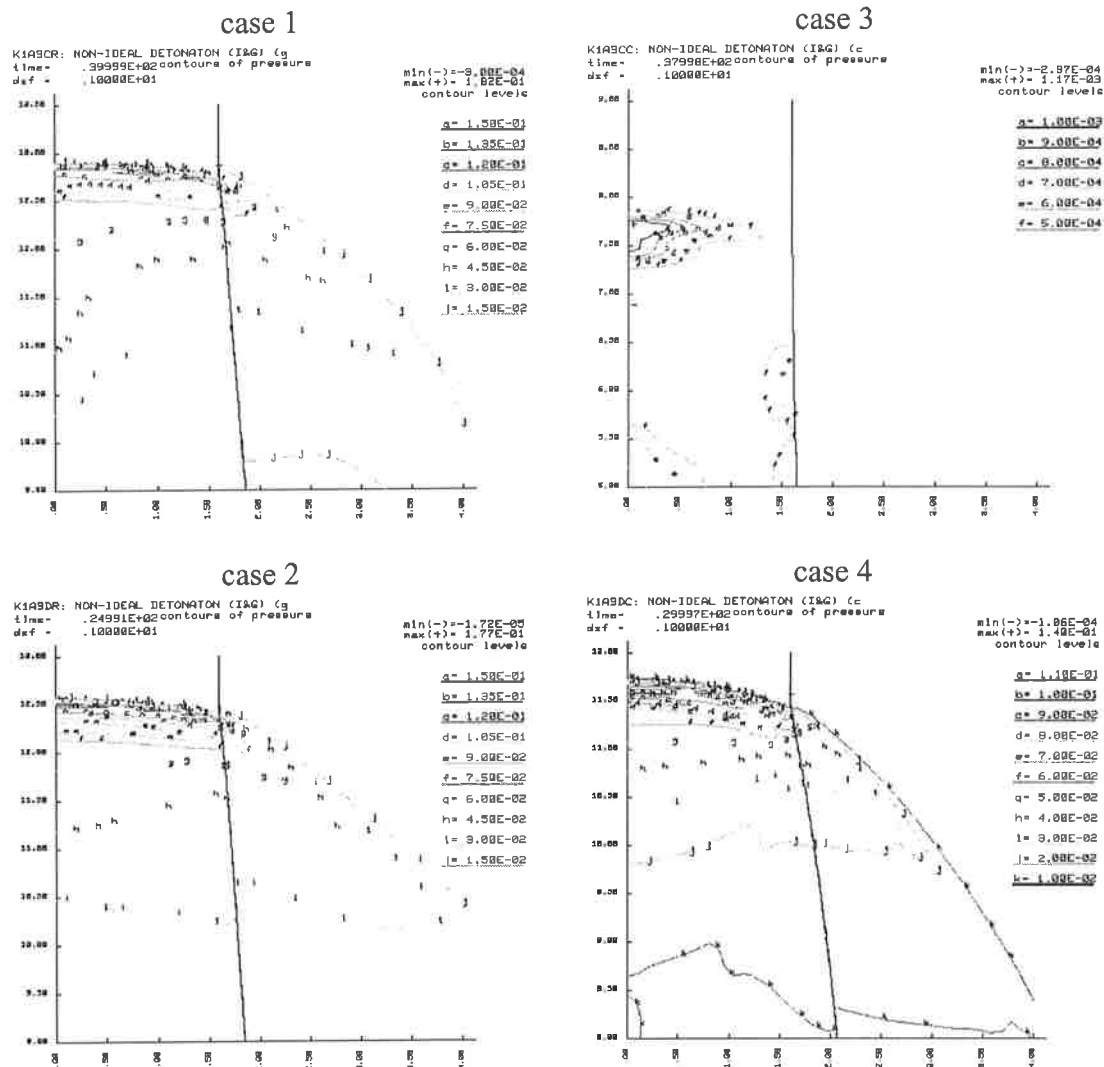


Figure 4-7: Effects of primer on detonation run-up process (2): the pressure contours.

The above results show clearly the functions of the primer and the confining material. The primer can change an initiation process from run-up to run-down. Even when the detonator itself, as in granite, is capable of initiating a stable detonation, the use of a primer raises the breakage capacity or energy utilisation considerably in the interval of 1,5~3,5 times charge diameter. Converted to tunnel driving with ϕ 45~64 mm holes, a

potential extra advance of $2\phi \approx 100$ mm per round would probably more than compensate for the cost of the primers, see also Kennedy (1997).

Confinement during initiation is very important. In a very soft rock like coal, initiation by detonator alone causes detonation failure in a charge whose diameter (ϕ 32 mm) is about twice as large as the critical value for an unconfined charge ($\phi_{crit} \geq 12,5$ mm in PMMA or $\phi_{crit} \approx 18 \sim 19$ mm in air). This is in direct contrast to the simplistic expectation that ϕ 32 mm would be on the safe side for a cap sensitive explosive when the critical diameter $\phi_{crit} \approx 18 \sim 19$ mm in coal. It is easily conceivable that initiation would become even more difficult with an air pocket at the bottom of the hole or if the detonator is misaligned.

A word of caution is necessary though because initiation is a transient process and our burning models have been obtained from a steady-state process, the 'rate-stick' with a constant VOD. Even if the results above are reasonable, the predictions ought to be verified by the experiments so that the predictive capability of our burning model is validated for transient processes.

4.3 Blast Energy Partitioning: Shock Wave Energy and the Heave Energy

With help of the burning model, it is possible to calculate the total energy transferred from a cylindrical charge to the surrounding rock or other media. For blast engineering, it is important to study different energy components, say the shock wave energy and the heave energy, since they are considered to play different roles in crushing losses, crack development, fragmentation and the throw. Brinkman (1990) used lined boreholes to stop the gases from penetrating into the rock, thereby separating shock and gas expansion work. He found fragment size to be governed by shock and break out to be governed by gas penetration. In order to give a basis for a discussion of the work capacity of emulsion explosives, the energy partitioning for our five formulas in coal (soft rock) and granite (hard rock) will be attempted here.

The total explosive work done on the surroundings can be calculated by integrating the isentrope curve from the CJ volume i.e. V_{CJ} to a specified larger volume V_1 as follows (Persson et al. 1992):

$$W = \int_{V_{CJ}}^{V_1} P dV - \frac{1}{2} u_p^2, \quad (4-5)$$

where P is the pressure, V is the relative volume of the products and u_p is the particle velocity at the CJ state.

With a programmed burning model or a thermal chemical code like Tiger, the state path followed in P - V space is the same, independent of the confining medium. Thus such a calculation is only valid for the ideal detonation case or the specific case when the burning parameters have been calibrated. By the non-ideal burning model, the P - V state path is a function of the explosive, the confining material and the initiation conditions. All blast conditions contribute to the final results.

In order to separate the shock and heave energies, Brinkman like many others makes use of the so called the 'equilibrium state' within the borehole. This state is determined by the intersection of the static linear elastic expansion line of a point on the wall of an infinitely long (2D) pressurized borehole with the expansion isentrope for the blast fumes. Its construction defies many basic facts, e.g:

1. There exists no equilibrium in the dynamic process of blasting.
2. The dynamic P - V states of a point on the borehole wall do not describe a straight line from the origin.
3. For a fully charged hole, the wall would fail by crushing or cracking long before the 'equilibrium' pressure is reached.

Since we have determined the non-ideal burning model for the detonation of the charge in a borehole, we can calculate the pressure history of the reaction products, which is a function of the explosive properties, the charge diameter and the properties of the confining rock. See example of a pressure curve in Figure 4-8. Here the pressure peak of 16,6 GPa represents the so called von Neumann pressure at the detonation front and the CJ pressure is 8,59 GPa.

We have found that there is a special region on these pressure curves when the curve stabilizes temporarily. We call this pressure the 'quasi stable' borehole pressure. This is the point in time at which the shock wave effects inside the borehole have ceased to be important. We believe that this pressure level represents the borehole pressure better than the 'equilibrium' one and use it to divide the total energy into shock compression and heave expansion energies.

The estimated 'quasi stable' borehole pressure values for a charge of 40 mm diameter are listed in Table 4-8. The results show that the 'quasi stable' borehole pressure depends very much on the confining material. For example, the average borehole pressure is 2,65 GPa in coal and 4,37 GPa in granite. For the coal, a larger expansion of the borehole wall can be expected at the 'quasi stable' state, which results in a lower borehole pressure. For the granite, it is more difficult to 'push' the borehole wall and the 'quasi stable' borehole pressure becomes much higher.

After the borehole pressure is determined, the total explosive energy can be separated into two parts: the shock energy and the heave energy. The method used here is illustrated in Figure 4-9. The total explosive energy to the surrounding rocks is represented by the area SODC. The position of point D ($V = 5,0$) is the cut-off, where the expanding gases cease to do useful work, by expansion to the atmosphere. The sonic point is determined by the method in section 3.5 (see also Appendix 4). Therefore, the shock energy is the area SORB and the heave energy is the area BRDC.

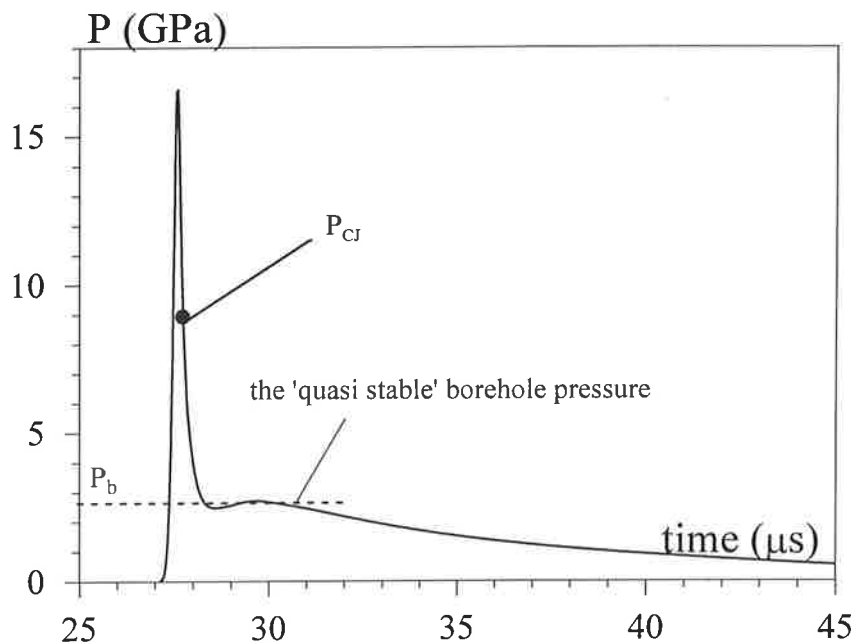


Figure 4-8: Determination of the 'quasi stable' borehole pressure or the borehole pressure (klb emulsion in coal, $\phi = 40$ mm and the estimated borehole pressure $P_b = 2,68$ GPa).

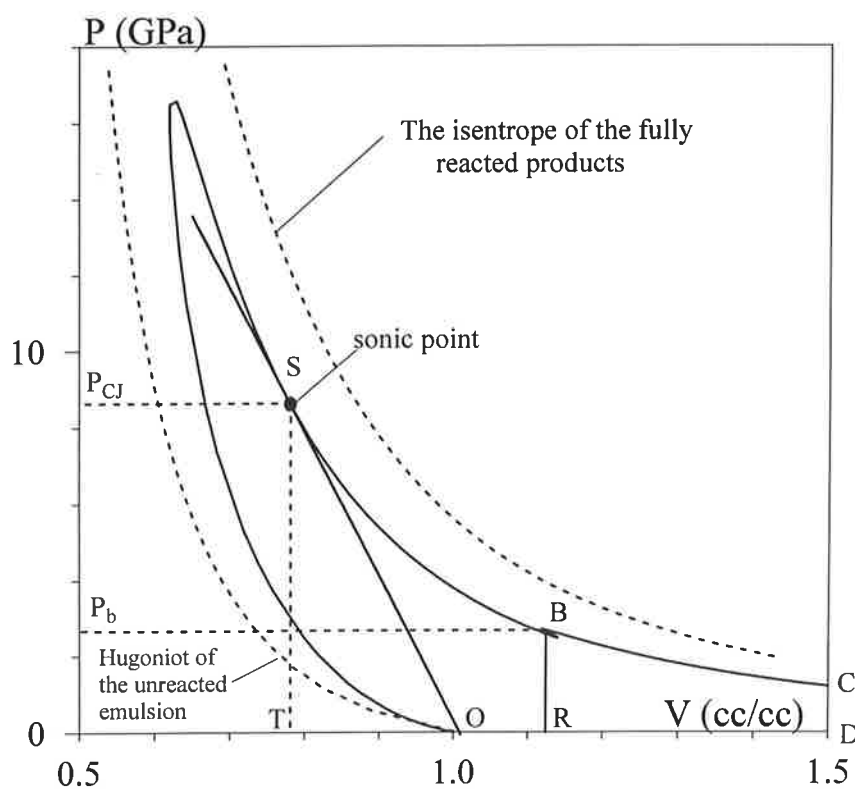


Figure 4-9: Determination of different energy components. S is the sonic point. The borehole pressure is represented by the 'quasi stable' borehole pressure at B. The gas expansion work is then represented by the area SODC, which is the sum of the shock energy of the area SORB and the heave energy of area BRDC (klb emulsion in coal, $P_{CJ} = 8,59$ GPa and $P_b = 2,68$ GPa).

The point S represents the specific internal energy of blast fumes at the CJ-state. The fumes move with the CJ velocity and thus have kinetic energy. On the other hand they do a work to maintain the CJ-state, which is nearly twice the kinetic energy. The triangle STO represents this work minus the kinetic energy (not the kinetic energy itself) and is consequently not available for expansion work on the surrounding rock.

We have calculated the shock and heave energies for a charge of 40 mm diameter. The rocks are again coal and granite. The total energy of the reaction products for the five emulsion explosives in the two rocks are shown in Figure 4-10. The estimated borehole pressures and different energy components at a volume expansion of the gases to five times the initial volume of the explosive are listed in Table 4-8. The results show that the expansion work and the different energy components strongly depend on the confining material.

Table 4-8: Estimated borehole pressures and different energy components:

explosive	E ₀ * MJ/kg	P _b ** GPa	shock energy, E _s		heave energy, E _h		gas expansion work, E _{tot}		E _{tot} /E ₀
			MJ/kg	GJ/m ³	MJ/kg	GJ/m ³	MJ/kg	GJ/m ³	
Soft rock: coal									
k1a	3,35	2,92	0,538	0,626	1,782	2,076	2,320	2,702	0,81
k1b	3,95	2,68	0,510	0,638	1,456	1,820	1,967	2,458	0,62
k1c	3,33	2,70	0,530	0,578	1,775	1,934	2,305	2,513	0,76
k1g'	3,65	2,58	0,865	1,072	1,457	1,807	2,322	2,880	0,79
k1g''	3,15	2,38	0,726	0,789	1,475	1,602	2,201	2,390	0,76
Hard rock: granite									
k1a	3,35	4,50	0,346	0,403	2,046	2,384	2,046	2,384	0,83
k1b	3,95	5,10	0,273	0,341	2,352	2,941	2,352	2,941	0,83
k1c	3,33	4,10	0,291	0,317	2,091	2,279	2,091	2,279	0,78
k1g'	3,65	4,35	0,567	0,704	1,866	2,314	1,866	2,314	0,83
k1g''	3,15	3,80	0,318	0,345	1,956	2,125	1,956	2,125	0,78

*: E_0 : the chemical energy content of the explosive (see Table A2-4 in Appendix 2).

** : P_b : the 'quasi stable' borehole pressure.

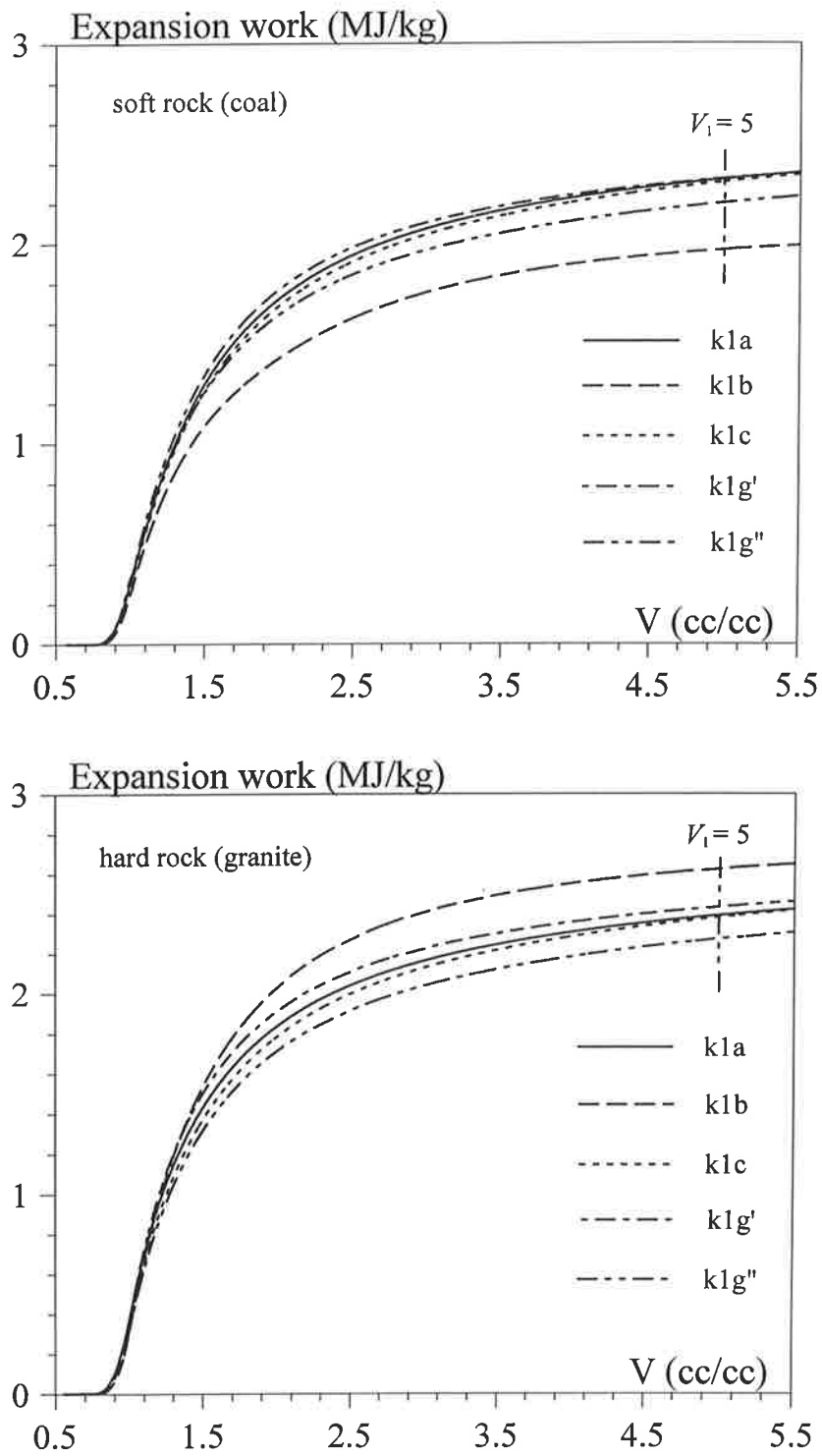


Figure 4-10: Expansion work of the reaction products for different emulsion explosives in soft rock (coal) and hard rock (granite).

The expansion work is larger for the hard rock than for the soft rock. For example, the average expansion work increases from 2,22 MJ/kg for the coal confinement to 2,42 MJ/kg for the granite. For the granite confinement, the expansion work increases with explosive density, while in coal no such relation between the expansion work and the explosive density is found. This relation is shown in Figure 4-11. Note that for unknown reasons, the expansion work for the k1b emulsion differs very much for the two rocks. A back check of the parameter values of the burning rate equation shows that the values for k1b emulsion differ somewhat from the others. See Table 3-1.

In terms of efficient energy use, i.e. the ratio of gas expansion work to available chemical energy, the picture looks different, see Table 4-8. In coal the percentage of energy used lies in the relatively narrow range 76-81%, except for k1b where it is 62%. Emulsion k1a is in this sense the most efficient explosive. In granite k1a is again the most efficient explosive at 83%, closely followed by k1b and k1g'. The range is 78-83%.

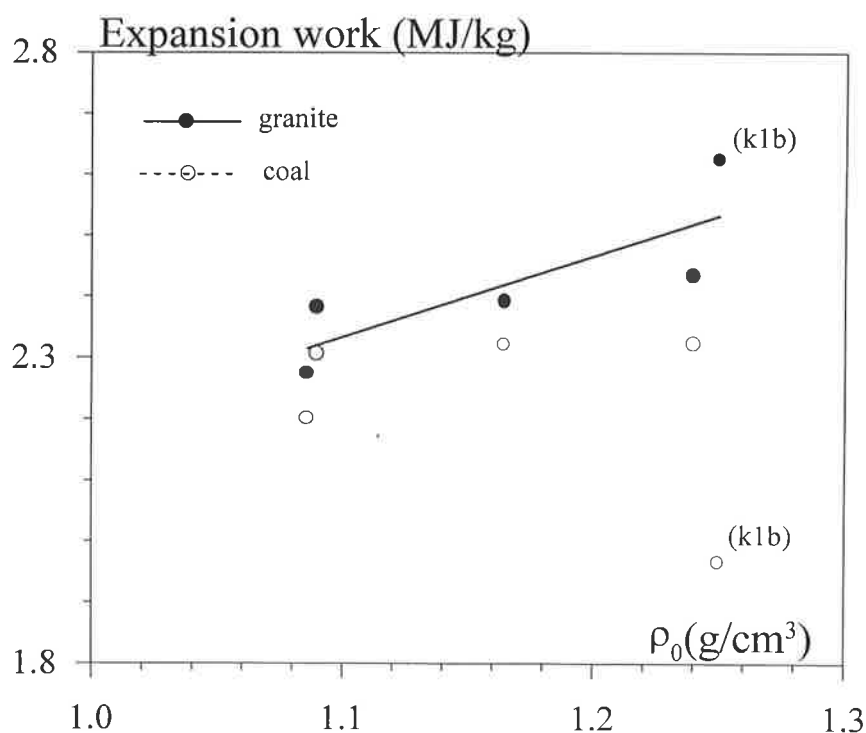


Figure 4-11: The relation between the expansion work and the explosive density in soft rock (coal) and hard rock (granite).

The gas expansion work from the explosives consists of the two components: the shock energy and the heave energy, which are functions of the borehole pressure. Figure 4-12 shows the relations between different energy components and the borehole pressure in the two rocks.

For the soft rock, the shock energy decreases with the borehole pressure, while for the hard rock, the shock energy is almost constant with the borehole pressure. The heave energy increases with the borehole pressure for both soft and hard rocks. For the soft rock, the heave energy is roughly 2 times of the shock energy, while for the hard rock, the heave energy is about 4 times of the shock energy. The borehole pressure controls the differences of the different components of the energies.

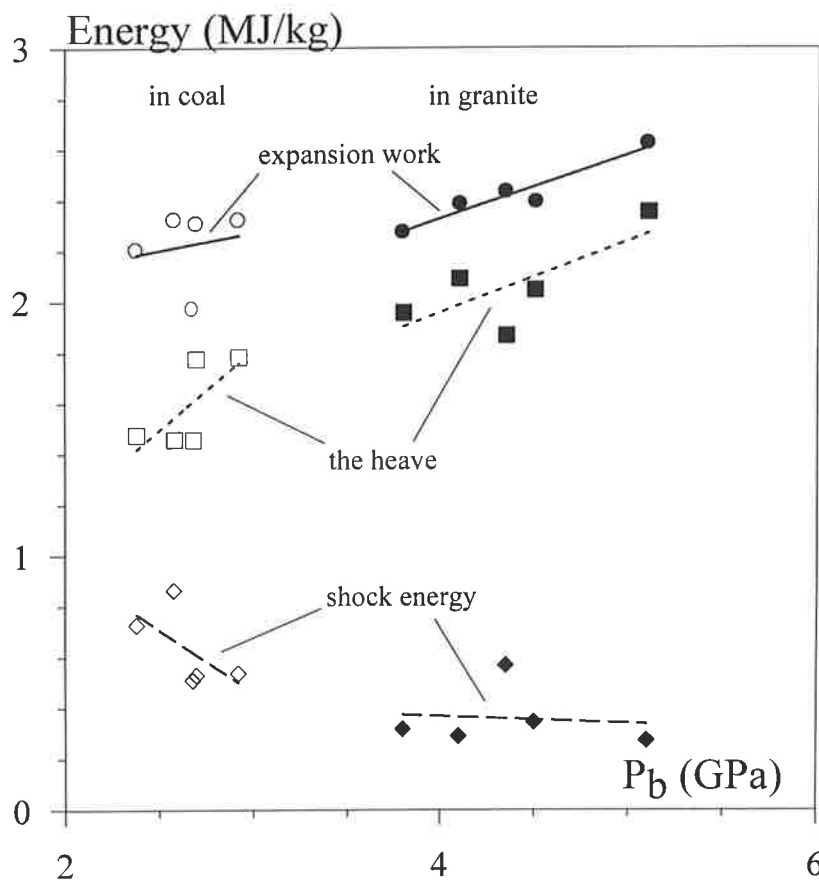


Figure 4-12: The relation between the energy components and the borehole pressure in soft rock (coal) and hard rock (granite).

The analyses above could be a helpful tool for a blasting engineer when choosing the 'right' explosive for a specific rock. For example, the k1a emulsion gives the maximum heave energy in the coal, 1,78MJ/kg, while k1b emulsion gives the maximum heave energy in the granite, 2,35MJ/kg. If the throw is important for the blast, one should thus choose k1a emulsion for the coal and k1b for the granite, since they give maximum heave energies for the corresponding rocks. The high water content emulsion k1g' gives maximum shock energy both for the granite and the coal, 0,57 and 0,87MJ/kg, respectively, which probably means that more crushing of the borehole walls and a better fragmentation can be expected. The energy analyses thus make it possible to 'match' a given rock with a specific explosive.

Other matching methods, which are used in shock wave and blasting problems, are impedance matching and wave velocity matching. In the impedance match method only the impedance of the explosive ($\rho_e D$) and that of the rock to blast are compared. In the explosive-rock system, the impedance of the explosive is no longer a constant however, since the VOD is a function of charge diameter, rock type and the initiation conditions. The impedance match concept may say something about the initial contact between blast fumes and rock but doesn't follow the rest of the process when the blast fumes do work on the surrounding medium.

Kristiansen et al. (1990) is one example. They plot the average mean particle size k_{50} from blasting tests versus the impedance ratio rock/explosive based on the expectation that the (shock) wave energy transferred is maximum when this ratio is one. They get the logical result that k_{50} has a minimum there. When the ratio is smaller, the results for low gas volume and high gas volume explosives differ quite substantially. With the energy analysis approach using our burning model we can hopefully explain these and other observations better.

5. DISCUSSIONS

Although differences between experiments and computations by the calibrated burning rate parameters are small, some problems remain in calibrating the burning rate parameters and in utilizing the burning model to solve engineering problems.

1. Simplification of calibration method

Some computational instabilities and the difficulties associated with determination of the parameters of the reactive flow have made the calibration difficult. The manual calibration method we used in calibrating the burning rate parameters is cumbersome and time consuming.

Our burning rate calibration system is based on the 2D cylindrical tests with the emphasis on the charge diameter and the confinement dependence of the detonation of the commercial explosives. The experimental observations are the steady-state VOD value, the curvature radius of the detonation front and the critical charge diameter. The cost function 3-3 can only be used during the final period of the calibration, when narrow intervals of the burning rate parameters have been determined. Extremely long time was consumed during the preliminary calibration. An important reason is that the computations become unstable when some corner elements are severely distorted and some unsuitable burning rate parameters are used.

The cost function 3-3 implies an equal importance of the steady-state VOD value and the curvature radius of the detonation front in determining the burning rate parameters. Our experience shows however that the curvature radius is more important than the VOD value. The experiments show that the VOD value and the curvature radius of the detonation front are not truly independent of each other. By studying the relation between the two variables, both experimentally and computationally, it might be possible to build a cost function, which correctly represents the functions of the two variables in determining the burning rate parameters of an explosive.

It is always problematic to determine the relevant intervals for the burning rate parameters when the burning physics are unknown. Matters could be improved by parametrical investigation of the relationship between the burning rate parameters with the physical or chemical properties of the explosive. Unfortunately little work has been done in this area.

2. *Computation errors caused by the finite element sizes*

For 2D modelling, the charge has to be long enough to obtain a stabilized VOD and curvature radius. Thus the minimum element size for the computation is limited by the charge size and the capacity of the computer.

We used uniform meshes with element sizes from $0,2 \times 0,2$ to $0,8 \times 0,8$ mm for charge diameters from 20 to 80 mm. This has proven enough to obtain stabilized VOD values and curvature radii. The charge with 80 mm diameter, where $0,8 \times 0,8$ mm elements were used, is the worst case. For most computations, the VOD values and the curvature radius of the detonation fronts stabilize within the given mesh limits. In some cases, they did not stabilize within the narrow intervals for the burning rate parameters. The reason is probably that the element size was too large and/or that the burning rate parameters were not properly chosen.

We have tested that smaller elements such as $0,5 \times 0,5$ mm will improve the computation stability for the charge of 80 mm diameter, but to use them throughout is beyond the capacity of our computer.

To resolve the detonation zone is another requirement for the element size. For example, the detonation zone lengths for the emulsion explosives studied here are from 4~6 mm for the charge diameter 80 mm. A minimum uniform element size of $0,8 \times 0,8$ mm can be used with our computer. Therefore, only 5~7 elements along the detonation zone, which is too coarse to resolve the detonation zone or to have a stabilized result for small changes of the burning rate parameters. For smaller charge diameters, smaller elements can be used. For the 1D setup, much smaller elements ($0,02 \times 0,02$ mm) are used for the calibration.

According to Kennedy (1995), about 20 elements along the detonation zone are needed to resolve the detonation zone completely. For the detailed analyses of the detonation zone, therefore, a more powerful computer (and code version) is required.

A large number of the elements takes a long time to compute and more easily causes the computations unstable. Therefore, the 1D setup is still useful for the calibration even when a more powerful computer is available. The simple 1D setup takes a very short time to run. We have used 1D setup during the preliminary stage of the calibration, which would otherwise take much more time.

3. Simplification of the 2D measurements

The quality of the calibration also depends on experiments. The measuring error is always added to the final calibration results and deteriorates the predictive ability of the burning models. Our initial ambition was to use non specialized methods available to the industry at reasonable cost. There are a number of such methods to measure the steady state VOD value.

To measure the detonation front is however relatively difficult. Our experience is that it takes at least twice the time to measure a detonation front than to measure the VOD. In order to measure the detonation front, a high-speed camera, a blasting chamber to confine the explosion and a well-trained camera operator have been necessary. Therefore, it is important to find new method to simplify the front measurements, so that the test can be easily done with sufficient accuracy.

4. Suggestions for further studies

Our application computations show that it is promising to use the burning model in solving many engineering problems. Many more engineering problems can be studied using this burning model. For example,

- The effect of charge decoupling
- The effect of water around decoupled charges
- Top vs. bottom initiation of blast holes
- The effect of imperfect initiation and primer form
- The effects of air decks and other stem plugs
- The effects of sheared blast holes, etc.

It is our ambition to study some of the problems in greater detail.

A drawback of our burning model is presently that the burning rate parameters have been obtained from a steady-state process, the 'rate-stick' with a constant VOD and a steady-state detonation front. Therefore, it is necessary to verify the model for transient

processes, e.g. shock to detonation or the initiation process, so that it can be used to model such processes with greater confidence.

We are also about to measure the borehole pressure in granite and other rocks in field with different degrees of coupling (Nie 1999). Our burning model can be verified by comparing the experiments with DYNA2D computations. This study can also be used as a part of the calibration process so that some of the burning parameters can be adjusted according to the field tests, in the case that the experiments and computations differ too much. By doing this, the predictive ability of the burning model can be improved.

6. CONCLUSIONS

Based on the above analyses of the test results and the application computations using the burning models, the following conclusions can be drawn:

1. The microballoons are a very important ingredient. Their content controls the density of an emulsion explosive, which in turn controls the VOD value at infinite diameter. The sensitivity of an explosive, which is represented by the slope in the VOD vs. inverse charge diameter plane and the critical charge diameter, is determined more by the microballoons content than by the water content. Both the microballoon content and the water content affect the detonation front curvature.
2. The calibrated burning models simulate the detonation process well. Agreement between the experiments and the computations is generally very good. The VOD values of three explosives in steel pipes have been successfully predicted using the calibrated burning rate parameters. This implies that the burning models obtained from the well-controlled laboratory tests are able to predict the detonation processes in other conditions, such as production blasts, where the charge size, confining media and other detonation conditions are quite different.
3. The extrapolated experimental VOD values at infinite diameter are in very good agreement with those obtained by the ideal detonation code Tiger and by the 1D DYNA2D computations. This supports the statements that the 1D detonation is the “ideal” one for any explosive and that all explosives detonate more or less non-ideally, since absolute 1D condition can not be achieved in reality. The 1D detonation can be used in the calibration of the burning rate parameters and it has proven very useful.
4. The burning model has proven to be a good tool for studying the detonation structure. The detonation zone length can be easily calculated. It depends on the charge diameter, the explosives properties and the confining material. The CJ and/or the parameters at sonic state, like the pressure and the compression can also be calculated.
5. The confinement dependence of the detonation can easily be predicted using the burning models. Our calculations for $\phi = 40$ mm charge show that both the steady-

state VOD value and the detonation front are severely affected by the confining material. The denser the confining material is, the higher the VOD and the flatter the detonation front will be. The steady-state VOD values for the free charge of a given size and the 1D detonation are the lower and upper bounds for the VOD of that charge.

6. The burning models simulate the initiation run-up process well. The calculations with different initiation conditions and different rocks show that both the primer and the confinement affect the initiation run-up process. Under a certain confinement, a primer can change a run-up process to a run-down one. When only a detonator is used, a weak confinement can lead to detonation failure.
7. The burning model is a good tool to study energy partitioning in rock blast. The 'quasi stable' borehole pressure can be easily determined by analyzing the pressure history in the explosive – rock system. Our calculations show that the 'quasi stable' borehole pressure depends both on the explosive and the rock to blast. The expansion work, the shock and heave energies are functions of the borehole pressure.

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Appendix 1: Two Dimensional Steady-state Experiments

The performance of commercial explosives depends severely on the confining material and the charge diameter. By changing charge diameter, for example, the reaction process in the explosive is interfered with so that the velocity of detonation (VOD) along charge axis and the detonation front curvature are changed. Therefore, the measured VOD and the detonation front curvature, together with the critical diameter, represent a set of detonation characteristics of a commercial explosive.

In order to test the effects of the microballoon and water contents on the performance of emulsion explosives, six straight AN based explosives with different compositions were tested. The test results substantiate that the microballoon content is very important for the explosives' performance. The interpolated VOD value at infinite diameter, the diameter effect and the critical charge diameter all change significantly. This can be important in the practical use of such explosives.

A1.1 Explosives Description

An emulsion explosive is basically a mixture of an aqueous solution of inorganic oxidizer salts, such as ammonium nitrate (AN), with fuel oil. A thin oil film surrounding the oxidizer droplets makes the explosive water resistant (water-in-oil). The sensitivity of the explosive is controlled by adding a certain amount of e.g. small microballoons into the mixture. The chemical properties of the constituents basically determine properties such as crystallisation temperature or fudge point (oxidizer salts), rheology (fuel) and droplet size deformation tolerance and shelf life (emulsifier). The requirement of oxygen balance determines the oxidizer/fuel ratio. For a given physical system there thus remain two main factors that regulate the explosives' performance, the water content of the matrix and the microballoons volume mixed in. The effects of these two factors on the detonation properties of a simple and oxygen balanced straight AN emulsion are investigated here.

The compositions and densities of the six emulsion explosives investigated here are listed in Table A1-1. Their positions in the water and microballoon contents plane are shown in Figure A1-1. Kimit AB manufactured all explosives. All compositions were designed to be oxygen balanced, i.e. the ratio of the AN to EM + 7514 oil (AN:

Table A1-1: Percentages of contents and densities of all tested emulsion explosives:

explosive	AN*(%)	EM*(%)	7514oil (%)	water(%)	MB*(%)	$\frac{AN}{EM + 7514}$	ρ_0 (g/cm ³)
k1a	77,49	0,748	3,926	14,76	3,075	16,58	1,165
k1b	78,46	0,757	3,975	14,94	1,868	16,58	1,250
k1c	76,09	0,734	3,855	14,49	4,831	16,58	1,090
k1f	76,15	0,732	3,855	16,19	3,075	16,60	1,184
k1g'	75,78	0,729	3,836	17,76	1,90	16,60	1,240
k1g''	73,54	0,707	3,723	17,23	4,80	16,60	1,086

*: AN = Ammonium Nitrate; EM = Anfomul S6 emulsifier from Croda Oleochemicals; MB = B23/500 microballoons from 3M; 7514oil: ES 75-14 mineral oil from Mobil Oil.

Ammonium Nitrate; EM: Anfomul S6 emulsifier; 7514oil: ES 75-14 mineral oil) is kept approximately at 16,6 (Karlström 1996). According to the contents of microballoons or the densities of the explosives, the three following explosive groups can be identified:

1. Emulsions k1b and k1g' contain nearly 2 percent (weight) of microballoons and have densities of 1,25 and 1,24 g/cm³ respectively. This is the group with highest density. Slightly higher contents of microballoons and water yield a slightly lower density for k1g'.
2. Emulsions k1a and k1f contain about 3% (weight) of microballoons and have densities of 1,165 and 1,184 g/cm³ respectively. For unknown reasons, the density of k1f emulsion is higher than k1a emulsion, although emulsion k1f contains the same amount of microballoons as emulsion k1a and more water.
3. Emulsions k1c and k1g'' contain 4,8% (weight) of microballoons and have densities of 1,090 and 1,086 g/cm³ respectively. This is the lowest density group.

Assuming that only the oxidizer has gone into the solution and that other ingredients just form a mixture, the density of the explosive may be computed. By the volume consistency law $\sum v_i = v$, we obtain:

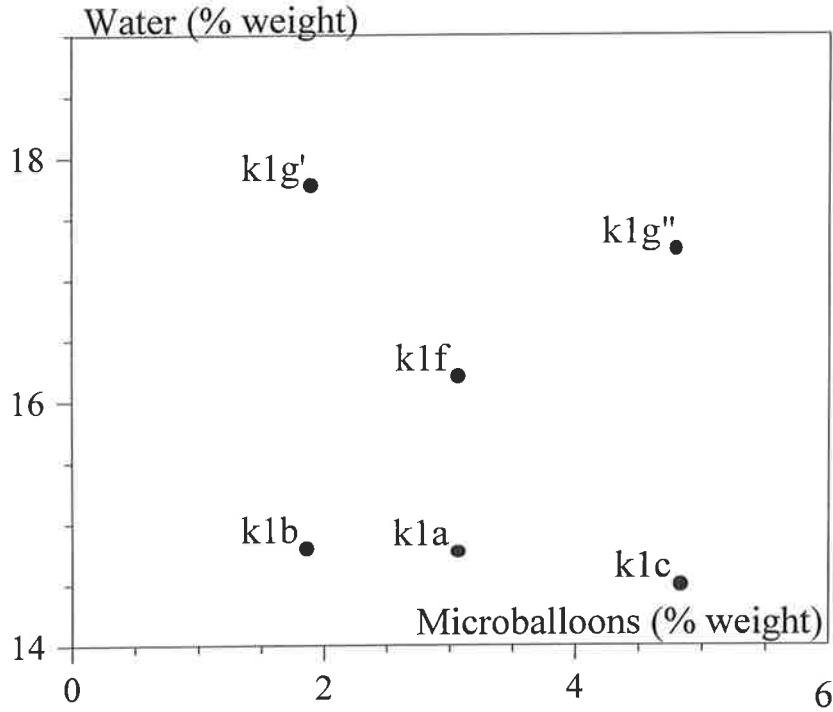


Figure A1-1: Microballoon and water contents of the tested explosives.

$$\sum \frac{m_i}{\rho_i} = \frac{m_{AN} + m_{H_2O}}{\rho_{AN}} + \frac{m_{em}}{\rho_{em}} + \frac{m_{oil}}{\rho_{oil}} + \frac{m_{MB}}{\rho_{MB}} = \frac{100}{\rho_{exp}}, \quad (A1-1)$$

where m_i are the weight percentage numbers of the different ingredients, ρ_i , their corresponding densities and ρ_{exp} , the explosive density. The first term is the oxidizer solution. The density of the solution ρ_{AN} depends on the relative weight factors of the two materials and how well they mix, which is a function of temperature (Wang 1996). Therefore, the density of an explosive is a function of the microballoon and the water contents. On the other hand, an emulsion explosive can be treated simply as a mixture of the matrix and the microballoons. Thus the first three terms in Equation A1-1 reduce to one. By using the volume consistency law, we obtain the following equation:

$$\frac{m_{matrix}}{\rho_{matrix}} + \frac{m_{MB}}{\rho_{MB}} = \frac{100}{\rho_{exp}}, \quad (A1-2)$$

where m_{matrix} and ρ_{matrix} are the weight percentage number and the density of the matrix

and the m_{MB} and ρ_{MB} are the relative weight factor and density of the microballoons. The first term is a function of the weight factors of all ingredients in the matrix, including water. For the explosives in this study, the ratio ranges from 69,2 to 71,2 with an average value of 70,1 cm³/g. Therefore, the density change caused by the water content is rather small and we can neglect it as a first approximation. Thus the density of an explosive can be calculated as follows:

$$\frac{100}{\rho_{exp}} = \frac{m_{MB}}{\rho_{MB}} + k \quad (A1-3)$$

Here $k = m_{matrix}/\rho_{matrix} \approx 70,1$ cm³/g is the average value of the six emulsion explosives. Knowing $\rho_{MB} = 0,23$ g/cm³, we obtain:

$$\rho_{exp} = \frac{1}{0,0435m_{MB} + 0,701} \quad (A1-4)$$

The comparison between the computed and measured densities is shown in Figure A1-2.

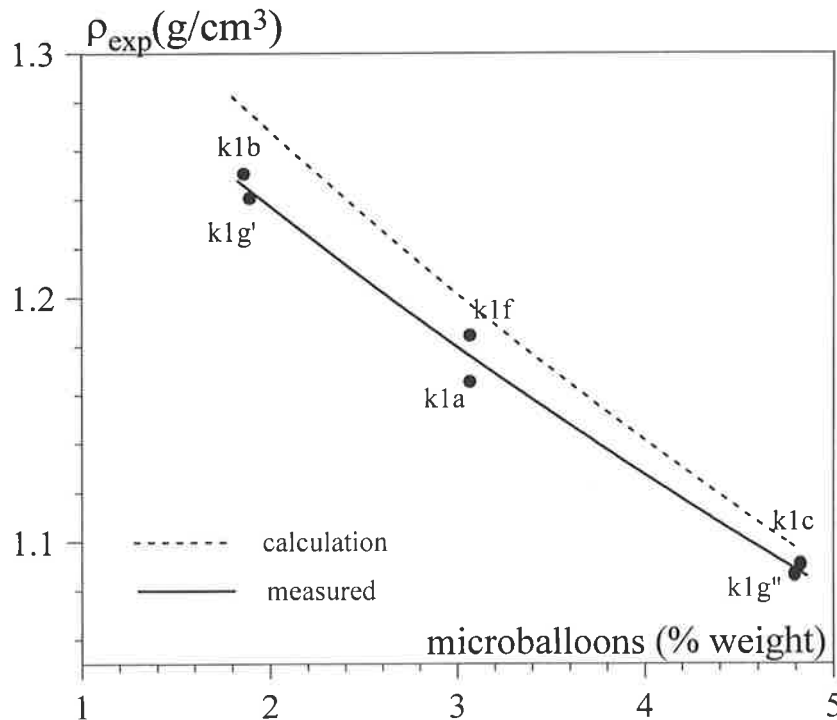


Figure A1-2: The relation between explosive density and the amount of microballoons.

The computed values are about 2% higher in average than the measured ones. One possible reason is that extra air is mixed in during the explosive manufacturing process. Note that in Equation A1-4, we have ignored the influence of the water content on the explosive density.

The property of an emulsion explosive is usually related to the explosive density. The density dependence can be interpreted as microballoon dependence through Equation A1-4.

A1.2 Two Dimensional Steady-state Experiments

1. Experiment set-up

All experiments were carried out with cylindrical charges (see Figure A1-3). PMMA (plexiglass) was used as the confining material for the tests on emulsion k1a and PVC (polyvinyl chloride), for the tests on the other emulsions. The steady-state VOD values were measured with a continuous resistance wire. At the beginning of tests, the optical fibre method was also used, mostly for k1a emulsion. The critical diameters for all explosives were estimated by averaging the minimum diameter of successful detonations and the maximum diameter of detonation failures. The detonation front curvatures were measured by a Cordin streak-camera recording the breakout at the end of charges. All rate stick tests were made using cylindrical tubes with the ratios of charge length to diameter varying from 20 to 6, for inner diameters from 13 to 96 mm. We believe that the recorded VOD values and detonation fronts were obtained from stable state detonations.

2. Detonation velocity as a function of inverse charge diameter

An example of the VOD measurement is shown in Figure A1-4. The strong signals at the beginning come from the primer initiation. The last part of the curve shows that the detonation velocity has stabilised near the end of the charge. Usually the data from the last 50% of a charge are used for the VOD evaluation. The VOD value is calculated as the slope of the linear curve fitted to the run time data.

A linear relation between the VOD value and the inverse charge diameter can be obtained from the test results by linear regression e.g.:

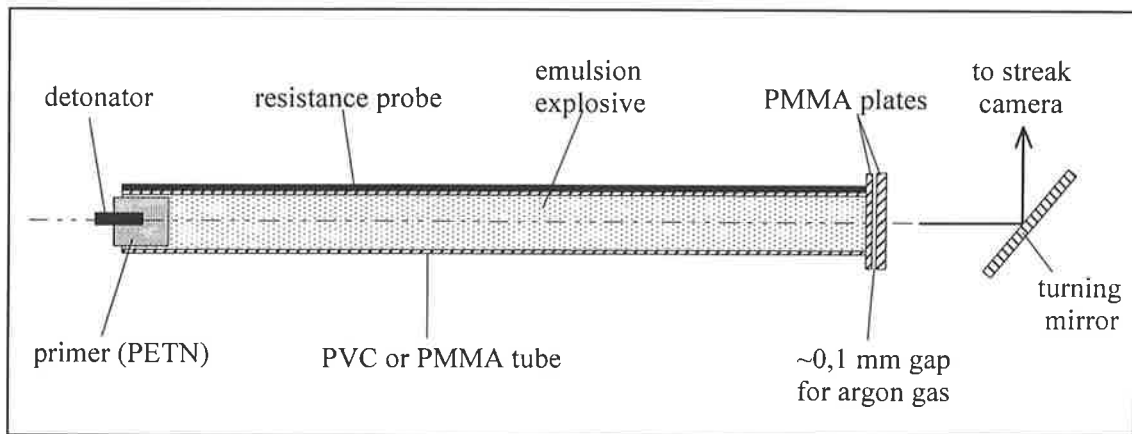


Figure A1-3: Experimental setup for the steady-state cylinder tests.

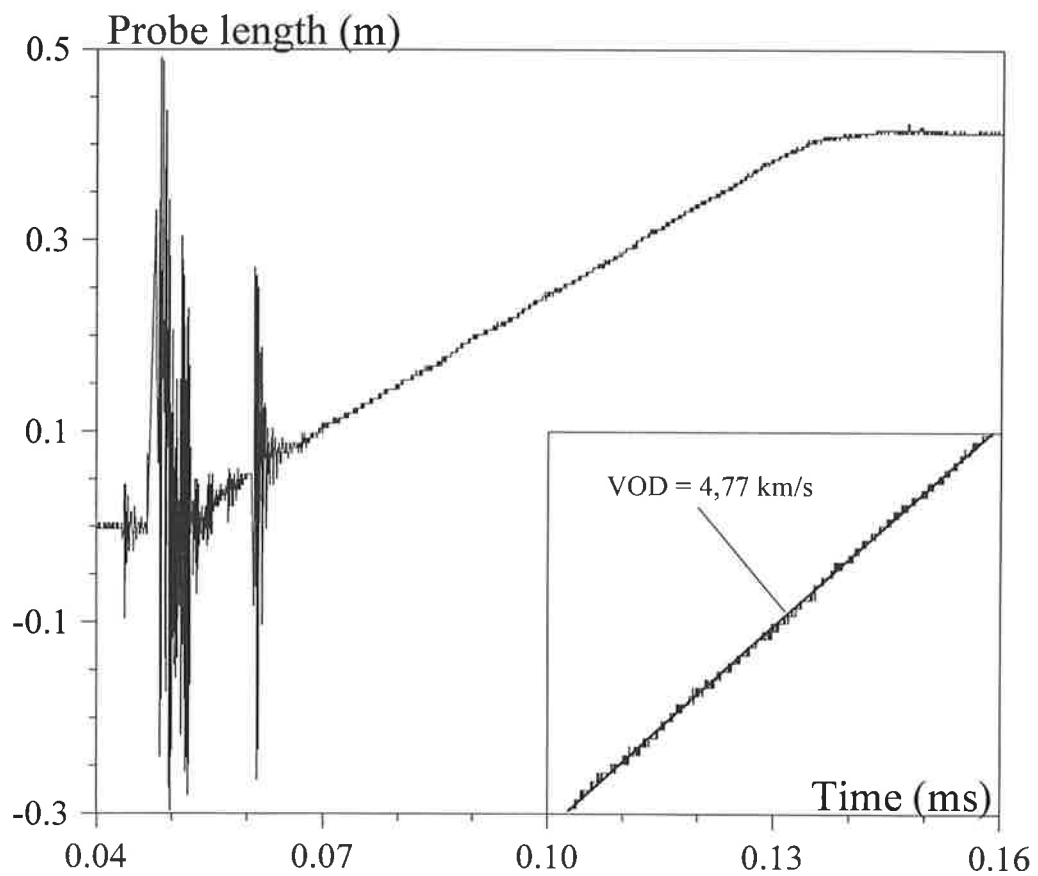


Figure A1-4: An example of the VOD evaluation (klg' emulsion, $\phi = 33,6$ mm and charge length $L_c = 0,4$ m).

$$D(\phi) = a - b/\phi, \quad (\text{A1-5})$$

where ϕ is the (inner) charge diameter in mm, and a and b are fitting constants. Let $\phi \rightarrow \infty$, we have $D(\infty) = D_0 = a$. Thus the constant a becomes the extrapolated VOD value at infinite diameter. Using two dimensionless variables D/D_0 and ϕ/ϕ_{crit} , we obtain the normalised form of the relation:

$$\frac{D}{D_0} = 1 - k \left(\frac{\phi_{crit}}{\phi} \right), \quad (\text{A1-6})$$

where $D_0 = a$ in km/s, $k = b/(a\phi_{crit})$ and ϕ_{crit} is the critical charge diameter.

The parameters in Equations A1-5 and A1-6, together with the critical diameters are listed in Table A1-2. The equations are shown in Figures A1-5 and A1-6. These parameters are valid only for the test actual conditions, namely, for the confinement of the PMMA tubes (for emulsion k1a) or PVC tubes (for the remaining emulsions).

Table A1-2: Parameters in Equations A1-5 and A1-6 and critical diameters:

explosive	ρ_0 (g/cm ³)	MB (%)	water(%)	a (km/s)	b (mm km/s)	k (mm)	ϕ_{crit} (mm)
k1a	1,165	3,075	14,76	6,03±0,12	29,72±2,71	0,3944	12,5
k1b	1,250	1,868	14,94	6,71±0,50	61,95±19,2	0,4395	21,0
k1c	1,090	4,831	14,49	5,64±0,29	18,87±6,43	0,2478	13,5
k1f	1,184	3,075	16,19	6,33±0,77	23,99±20,1	0,2229	17,0
k1g'	1,240	1,90	17,76	6,53±0,26	53,39±9,85	0,4287	21,0
k1g''	1,086	4,80	17,23	5,47±0,25	12,46±5,43	0,1686	13,5

The parameters in Table A1-2 represent two important properties: the maximum chemical energy and the sensitivity of a commercial explosive. The square of the VOD value at infinite diameter is proportional to the maximum chemical energy from the explosive and the other parameters represent somewhat the sensitivity of the explosive. For example, the smaller the slope of the $D(\phi)$ or the $D/D_0(\phi/\phi_{crit})$ curve is, the smaller the critical diameter of an explosive will be, and hence the more sensitive the explosive is. The two properties are functions of the microballoon and water contents.

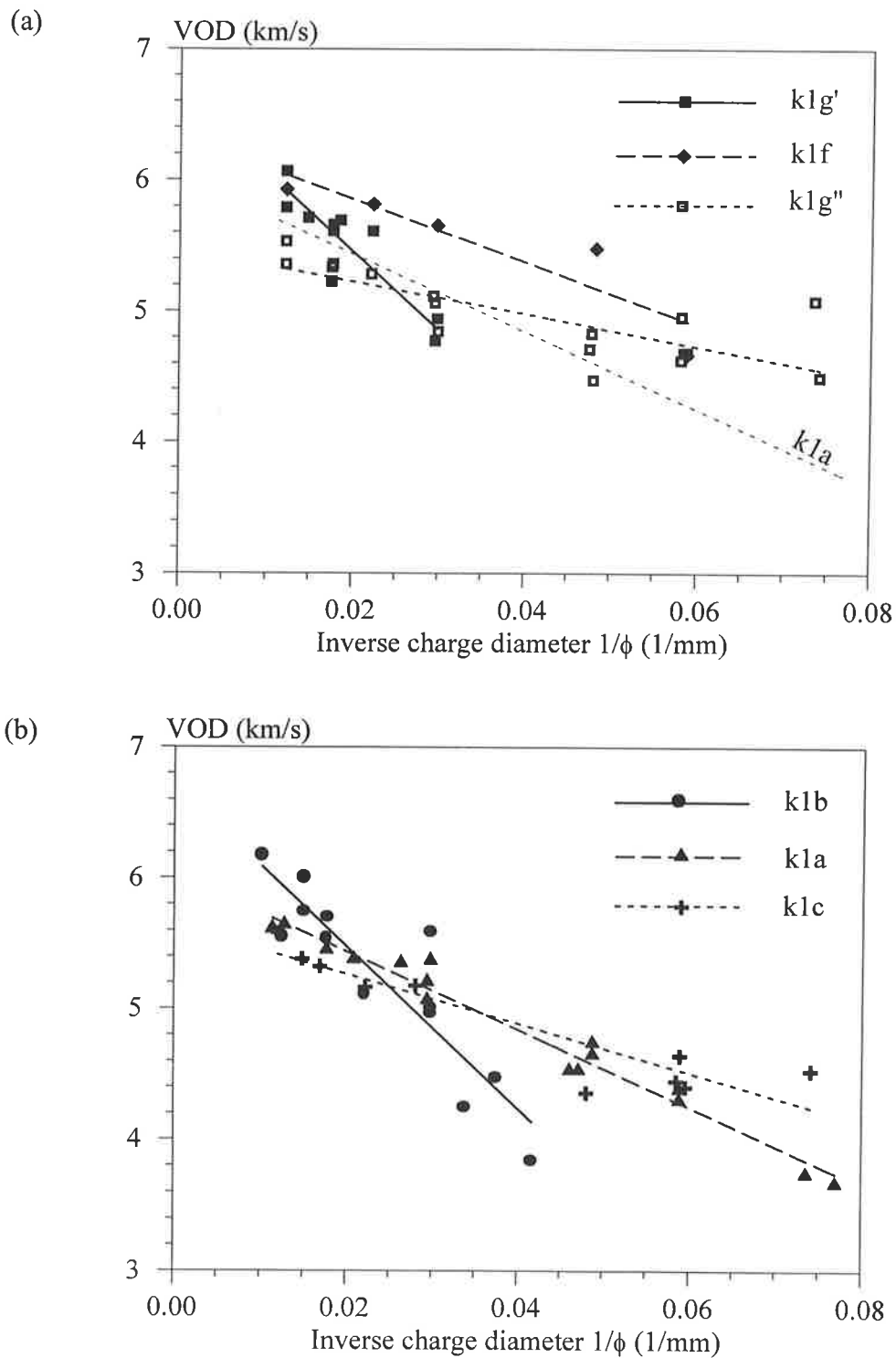


Figure A1-5: Diameter-effect curves (1): VOD vs. inverse charge diameter.

(a) High water content emulsion explosives: $k1g'$, $k1f$ and $k1g''$.

(b) Low water content emulsion explosives: $k1b$, $k1a$ and $k1c$.

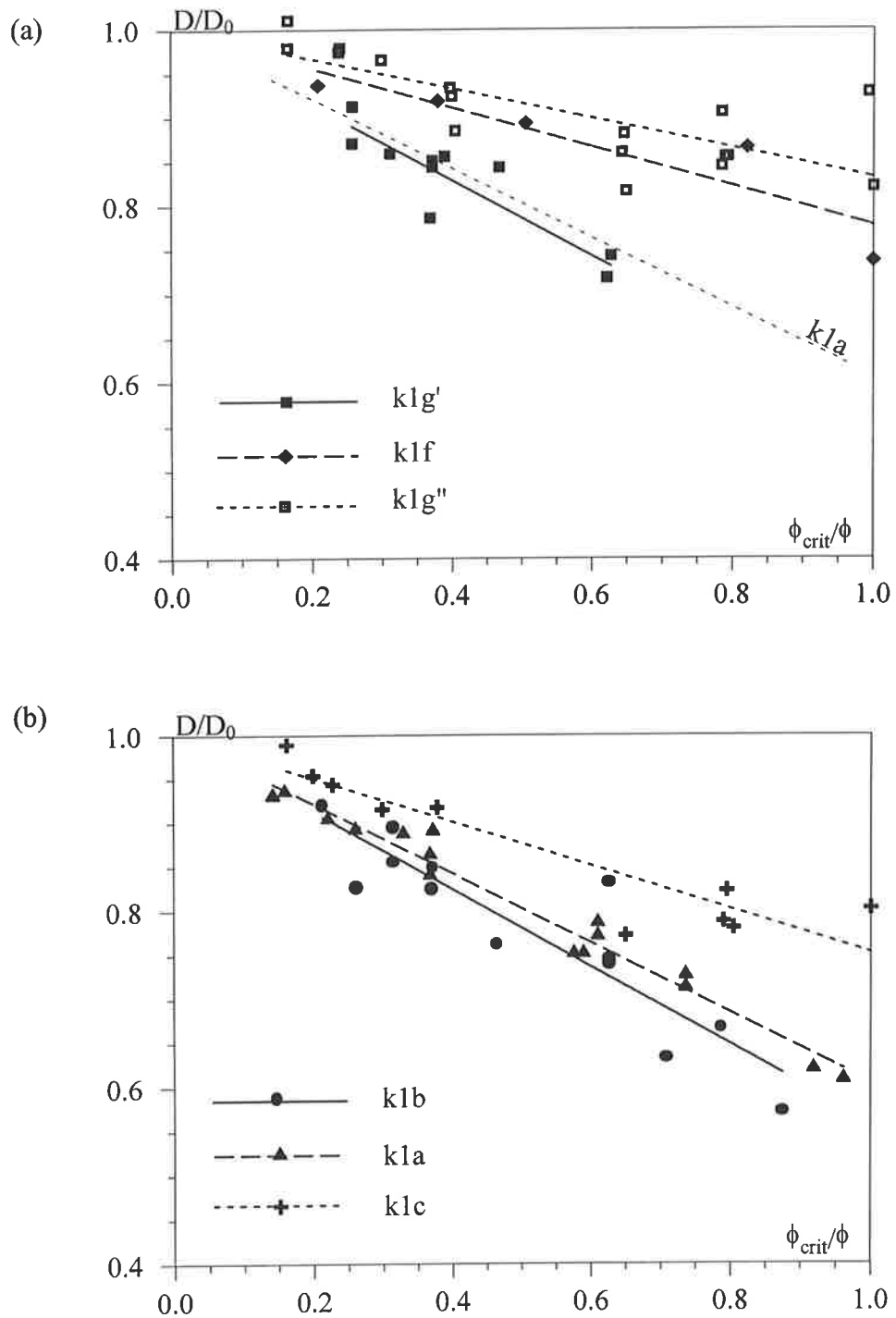


Figure A1-6: Diameter-effect curves (2): the relative VOD vs. scaled charge diameter.

(a) High water content emulsion explosives: $k1g'$, $k1f$ and $k1g''$.

(b) Low water content emulsion explosives: $k1b$, $k1a$ and $k1c$.

The relation between the extrapolated VOD value at infinite diameter D_0 and the microballoon content can be extracted from the relation between the VOD value and the explosive density. A linear relation between the VOD value at infinite diameter and the explosive density is found in the following:

$$D_0 = 6,88\rho_0 - 1,93, \quad (\text{A1-7})$$

where D_0 is the extrapolated experimental VOD value at infinite diameter in km/s and ρ_0 is the explosive density in g/cm³. Note that we have ignored the effect of the water content, since no significant relation between D_0 and the water content has been found. This relation shows that the VOD value at infinite diameter increases with the explosive density. Combining Equations A1-4 and A1-7, we obtain easily the VOD value D_0 as a function of the microballoons content $D_0(m_{MB})$ or we can directly fit the experimental data as follows:

$$D_0 = 7,3 - 0,3627m_{MB}, \quad (\text{A1-8})$$

where m_{MB} is the weight percentage number of the microballoons content. For the 1D case, therefore, the detonation velocity increases monotonically with the explosive density or decreases monotonously with the microballoon content. These conclusions are valid only when the explosive contains a certain amount microballoons. If an emulsion explosive contains too much or too little microballoons, it would not be an explosive any longer.

For the finite diameter cases, non-linear relations were found between the VOD values and the explosives densities or the microballoons content. The relations A1-7 and A1-8 and those for the finite diameter cases are shown in Figures A1-7 and A1-8. The results here are quite comparable with those obtained by Lee (1990).

Both parameters b and k in the functions $D(\phi)$ and $D/D_0(\phi_{crit}/\phi)$ (Equations A1-5 and A1-6) represent the explosives sensitivity. The parameter k is dimensionless and therefore is more representative than b . But this parameter contains information of the critical diameter and the VOD value at infinite diameter.

The slope of the $D/D_0(\phi_{crit}/\phi)$ function k represents the sensitivity of an explosive. An explosive with a larger value of k is less sensitive than an explosive with a smaller k value. We plot the inverse value of k as a function of the microballoons content in Figure A1-9.

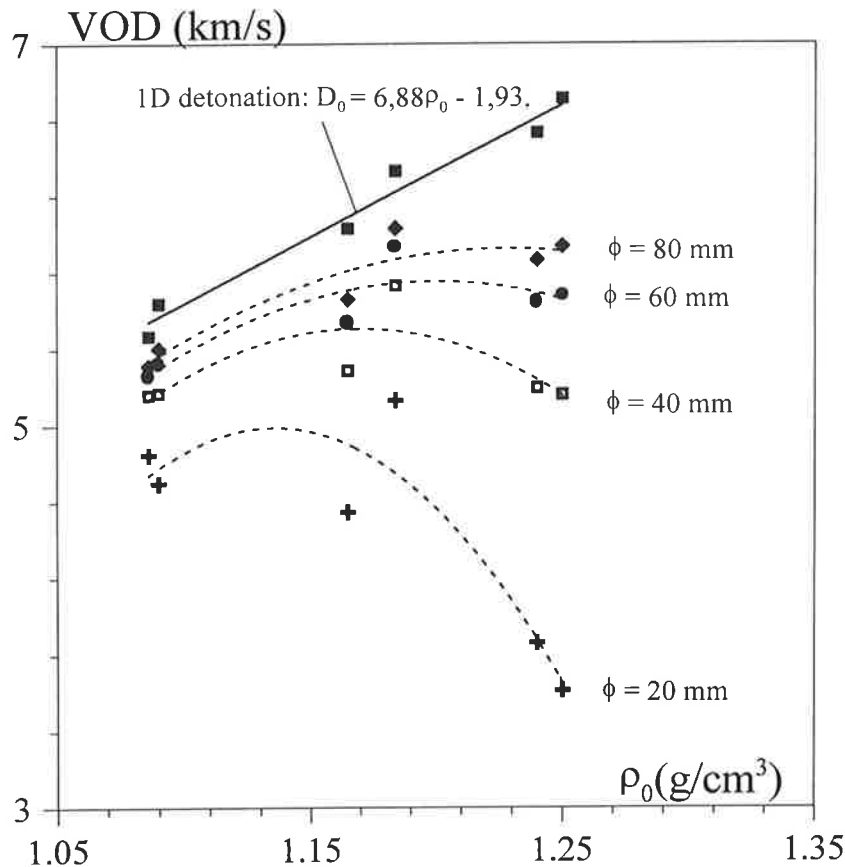


Figure A1-7: The relation of the VOD vs. the explosive density.

Here we find two lines for different water contents. This figure shows that the sensitivity of the emulsion explosives increases with both the microballoon and water contents. The critical diameter as function of the microballoons content will be discussed in next section, together with the minimum curvature radius.

It is worth noting though that in Figure A1-9, the vertical distance between the k1f and k1a points is the largest despite that the difference in water content is only about half of that between either k1g' and k1b or k1g'' and k1c, see Table A1-1. Like the density anomaly for k1a this point to an inconsistency in the data. There are two contributing factors. Firstly the k1a tests were made in PMMA pipes, and secondly the k1f value is based on much fewer points than the other values. See further below.

According to the discussion above, we can conclude that the microballoon content controls the density of an emulsion explosive, which in turn controls the VOD value at infinite diameter. Both the microballoon content and the water content have a significant influence on the explosive sensitivity.

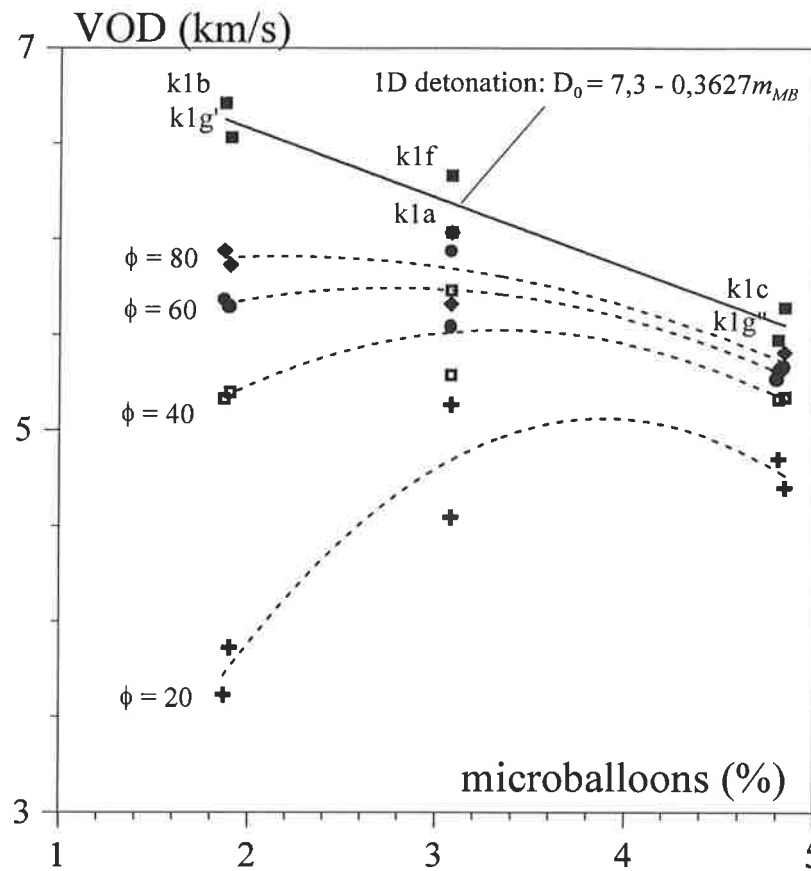


Figure A1-8: The relation of the VOD vs. the relative weight factor of the microballoons.

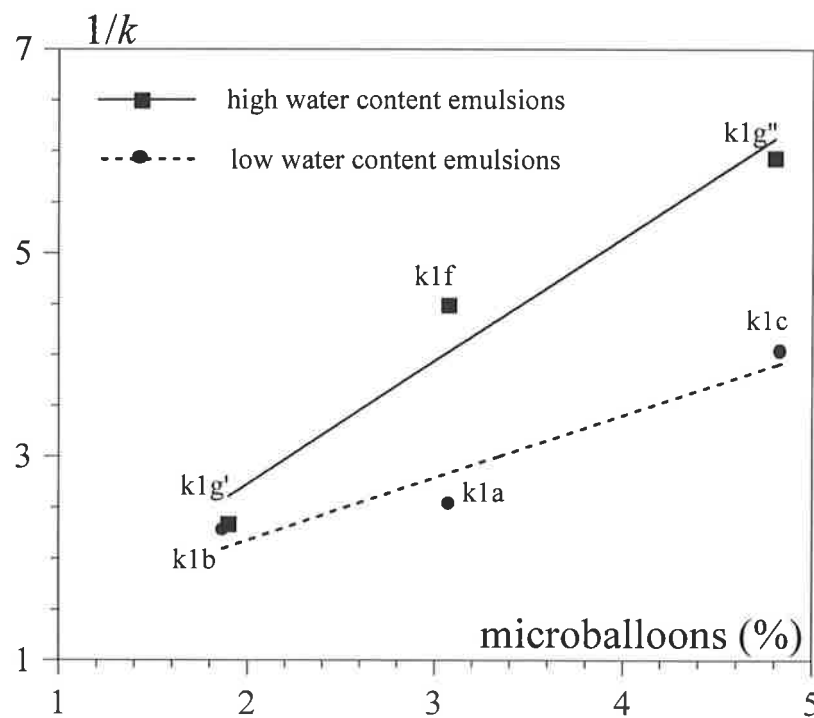


Figure A1-9: The relation of the slope of the function $D/D_0 (\phi_{crit}/\phi)$ and the amount of microballoons.

3. Detonation front curvature as a function of charge diameter

The detonation fronts were recorded with a Cordin model 116 high-speed streak camera. The recorded negatives in the time-position space were scanned with a resolution of 0,1 mm. A MathCad program was made to analyse the scanned BMP files and to transform the curve front location on the negative into position-position space under the condition of a constant detonation velocity. An example of the negative and the curve front evaluated by the MathCad program is shown in Figure A1-10.

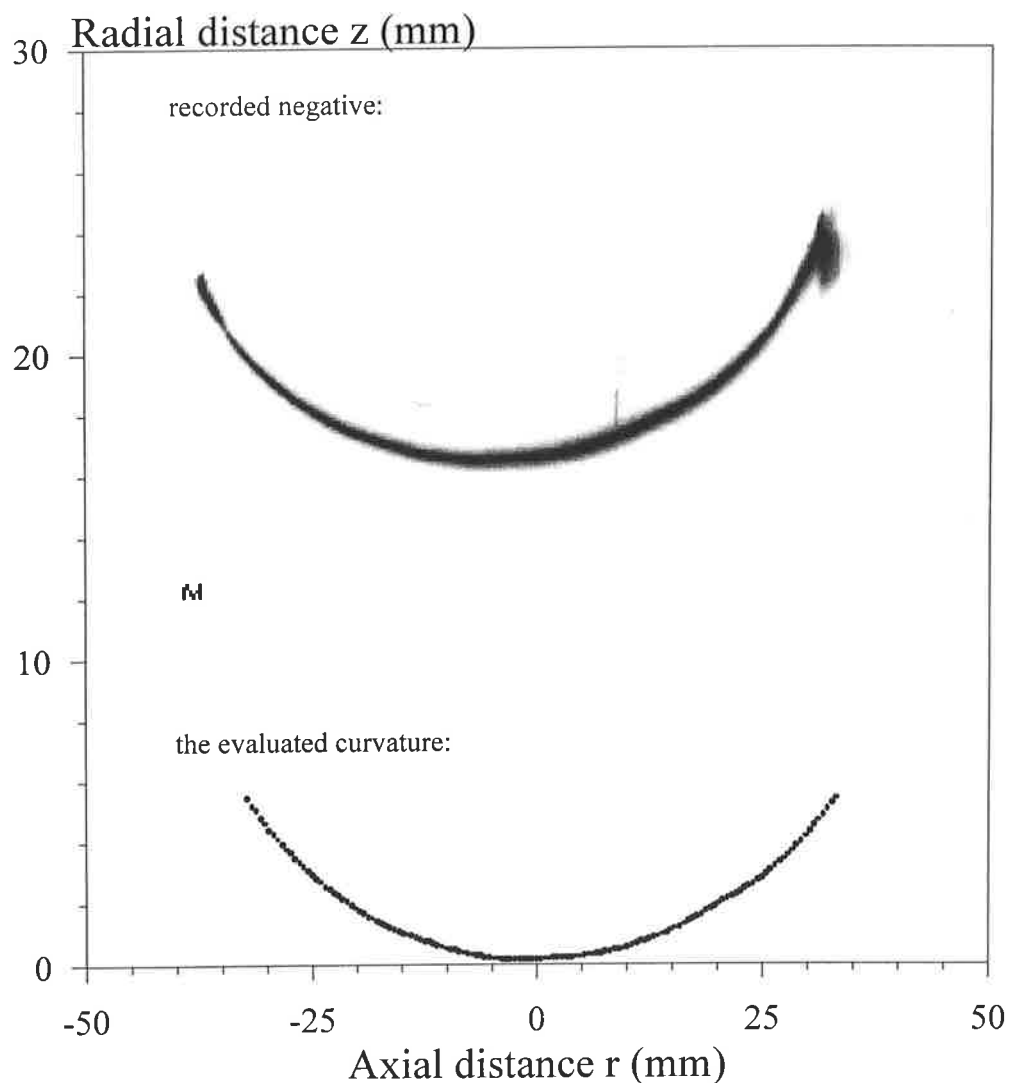


Figure A1-10: An example of a recorded negative and the evaluated front curvature (k1g' emulsion, $\phi = 67,6$ mm).

Circles, ellipses and Bessel functions were fitted to the curvatures of the detonation fronts. Both ellipses and Bessel functions are good, while the circle function fits are not so good. Bessel functions give slightly better fits than the ellipses do. Considering the relatively simpler function form, we decided to use the ellipses for the curvature fitting. About 90% of the data closest to the charge centre were used.

The curve function used for data fitting is in the following form (Deng et al. 1995):

$$r = \sqrt{az^2 + bz + c} \quad (\text{A1-9})$$

where r and z are the radial and axial coordinates respectively, a , b and c are the fitting constants. The curvature radius of the front is a function of r (or z) and can be calculated by the following equation:

$$R(r) = \frac{(1 + r'^2)^{3/2}}{r''} \quad (\text{A1-10})$$

where $r' = dr / dz$ and $r'' = d^2r / dz^2$ are the first and second derivatives of the curve function. The value used for calibration is the radius at the charge axis $R_0 = R(r = 0)$. Figure A1-11 shows an example of the elliptical data fitting and the radius calculated by Equation A1-10.

A non-linear relation between the radius at the charge axis R_0 and the charge diameter ϕ can be fitted to our data. Using the scaled charge diameter ϕ / ϕ_{crit} , we find that the following relation fits our test results best:

$$\frac{1}{R_0} = a + b \frac{\phi_{crit}}{\phi} \quad (\text{A1-11})$$

The constants a and b are listed in Table A1-3. The fitted relations are shown in Figure A1-12. Note that this equation is not valid for the infinite diameter, since the right side of the equation tends to the constant a instead of zero. Equation A1-11 is only valid for the finite diameter case, which includes all practical use of the explosives.

The parameter b as a function of the microballoon content is shown in Figure A1-13. There is no significant dependence of the parameter b on the water content. This means that the absolute value of the curvature radius is affected more by the microballoon content than by the water content.

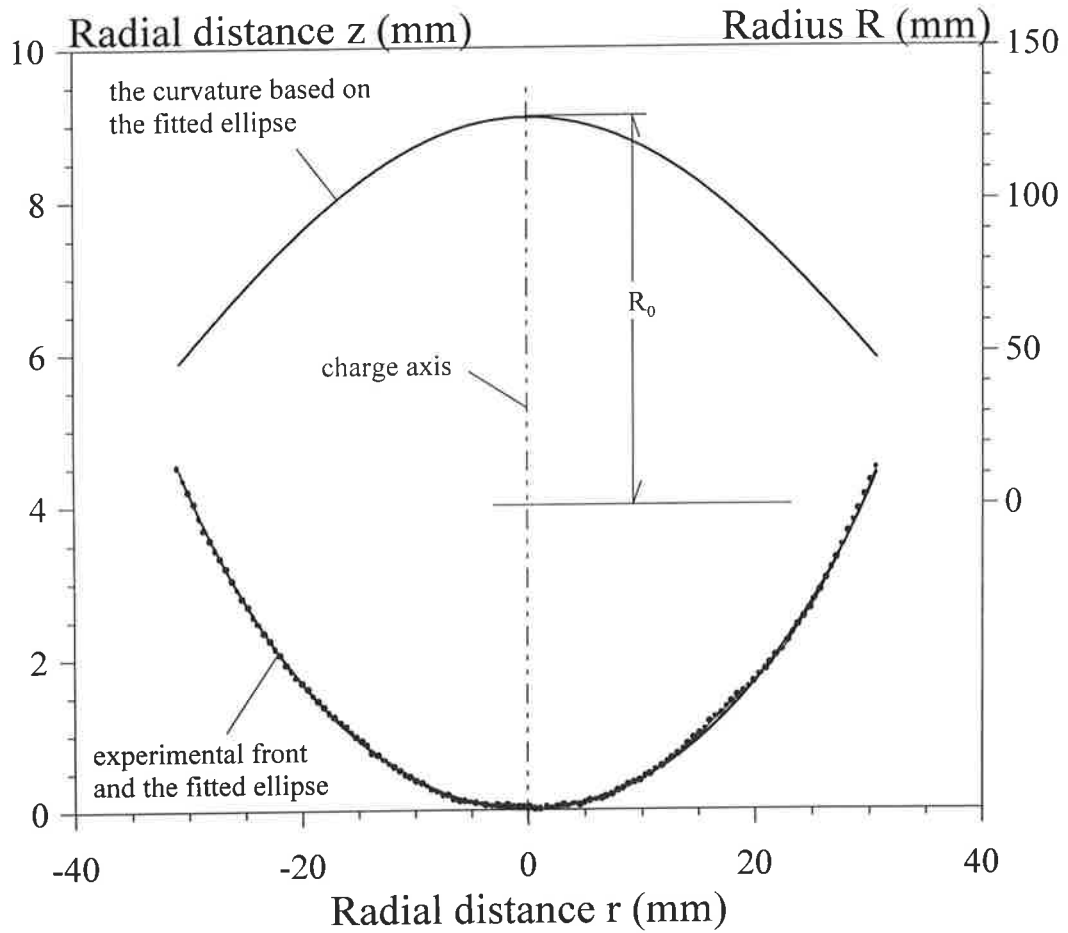


Figure A1-11: The elliptical fit to a curve front and the calculated radius (k1g' emulsion, $\phi = 67,6$ mm and the curvature radius at the charge axis $R_0 = 127$ mm).

Table A1-3: Parameters in Equation A1-11:

explosive	$\rho_0(\text{g/cm}^3)$	MB (%)	water(%)	a (1/mm)	b (1/mm)	ϕ_{crit} (mm)
k1a	1,165	3,075	14,76	$-0,0041 \pm 0,0022$	$0,0579 \pm 0,0040$	12,5
k1b	1,250	1,868	14,94	$-0,0027 \pm 0,0008$	$0,0347 \pm 0,0017$	21,0
k1c	1,090	4,831	14,49	$-0,0031 \pm 0,0035$	$0,0455 \pm 0,0061$	13,5
k1f	1,184	3,075	16,19	$-0,0062 \pm 0,0255$	$0,0507 \pm 0,0475$	17,0
k1g'	1,240	1,90	17,76	$-0,0038 \pm 0,0039$	$0,0386 \pm 0,0086$	21,0
k1g''	1,086	4,80	17,23	$-0,0047 \pm 0,0024$	$0,0468 \pm 0,0044$	13,5

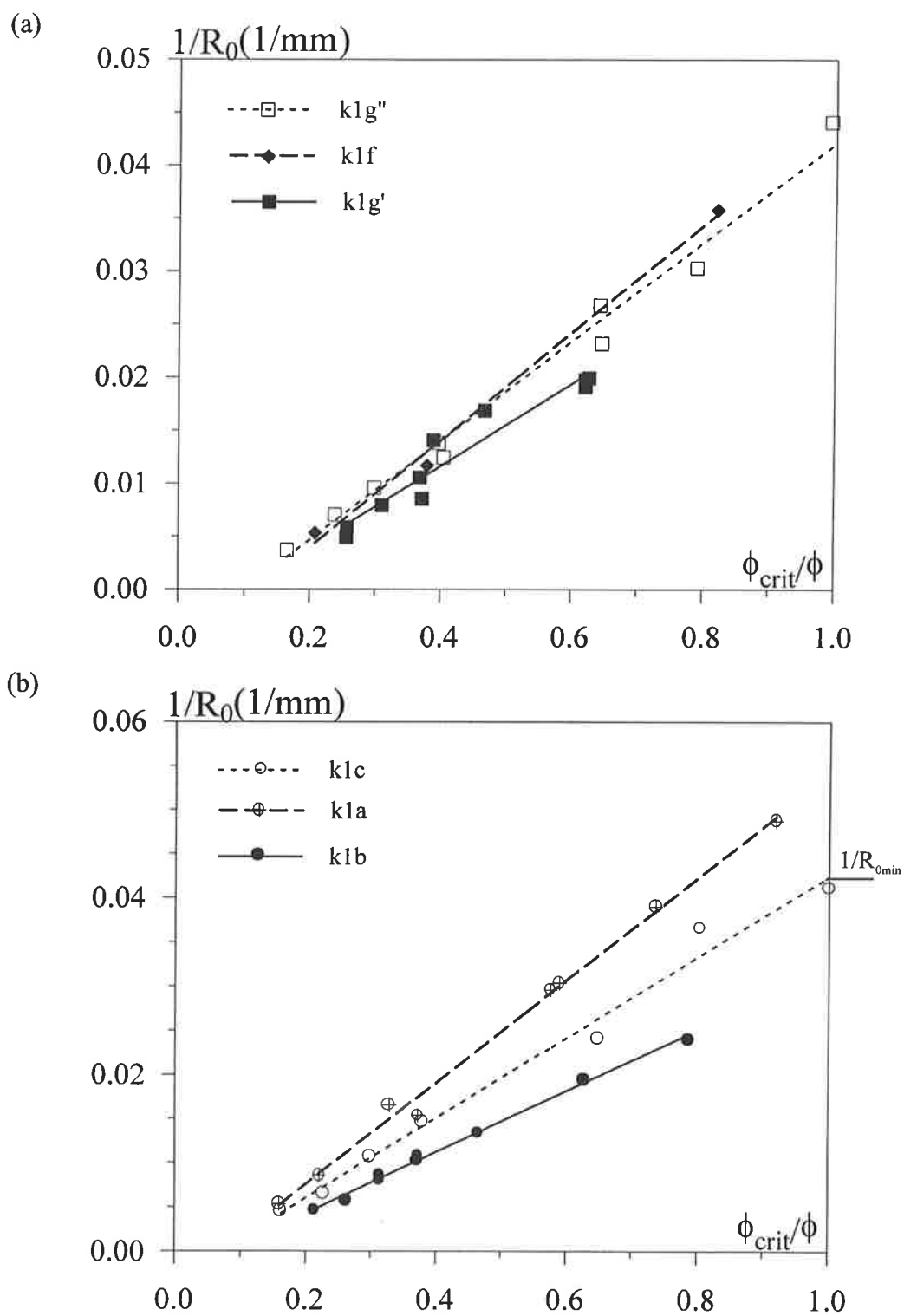


Figure A1-12: Diameter-effect curves (3): detonation front radius vs. charge diameter.

(a) High water content emulsion explosives: $k1g'$, $k1f$ and $k1g''$.

(b) Low water content emulsion explosives: $k1b$, $k1a$ and $k1c$.

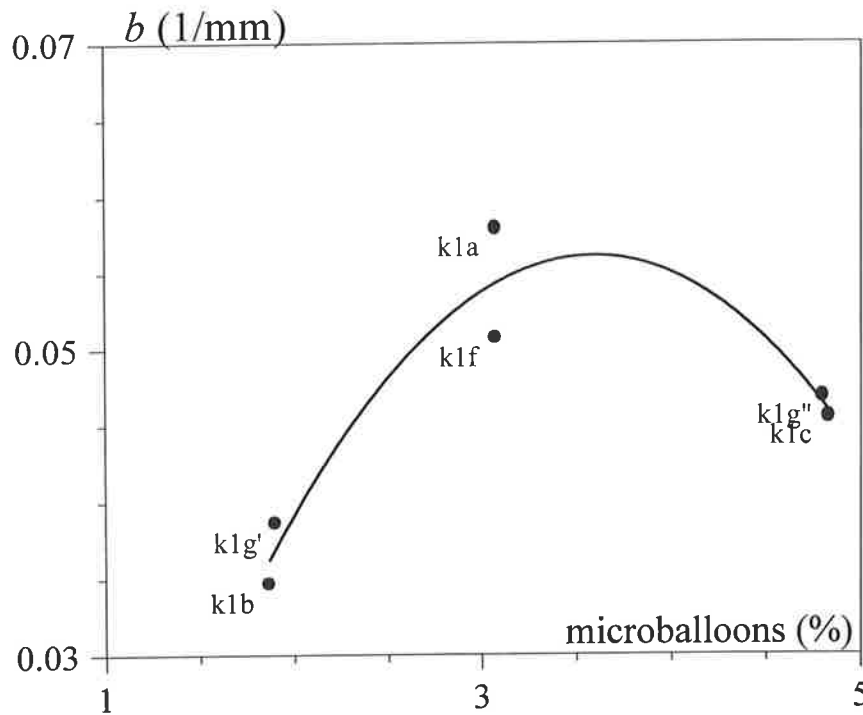


Figure A1-13: The slope of the function $1/R_0$, b , as a function of the microballoon content.

Figure A1-13 shows also that there exists a range of the microballoon content, within which the maximum values of the curvature radii can be obtained. Again the relative position of the pair $k1a$ and $k1f$ is inconsistent with the other data pairs for which a higher water content corresponds to a higher value of b .

When the charge diameter approaches to its critical value, i.e. when $\phi_{crit}/\phi \rightarrow 1$, R_0 approaches a minimum value R_{0min} given by:

$$\frac{1}{R_{0min}} = a + b. \quad (A1-12)$$

Therefore, the intercept of the curve of Equation A1-11 with the line $\phi_{crit}/\phi = 1$ has a physical meaning, namely the inverse of the minimum curvature radius $1/R_{0min}$. R_{0min} is a geometrical parameter of the detonation front. It can not be measured experimentally, since the detonation is unstable when $\phi = \phi_{crit}$. Like the critical diameter, R_{0min} is also a measure of the explosive sensitivity. Equation A1-11 thus can be further simplified by

introducing this parameter as follows:

$$\frac{R_{0\min}}{R_0} = \zeta + \zeta \frac{\phi_{crit}}{\phi} = (1 - \zeta) + \zeta \frac{\phi_{crit}}{\phi}, \quad (\text{A1-13})$$

where

$$\zeta = \frac{b}{a + b}. \quad (\text{A1-14})$$

Here ζ is a dimensionless parameter. It is listed in Table A1-4, together with the minimum radius $R_{0\min}$. Like Equation A1-11, Equation A1-13 is not valid near the origin.

Equation A1-13 is showed in Figure A1-14. All experimental fitted curves have a common point (1, 1) with different slopes. By making the relation dimensionless, the microballoons influence has been eliminated somewhat and the parameter ζ turns out to be a function mainly of the water content. This is shown in Figure A1-15. Therefore, the scaled curvature radius is affected more by the water content than by the microballoon content, whose influence is contained in $R_{0\min}$, the physical basis for this, if any, is not clear.

Table A1-4: Parameters in Equation A1-13:

Explosive	$\rho_0(\text{g/cm}^3)$	MB (%)	water(%)	ζ	$R_{0\min}$ (mm)
k1a	1,165	3,075	14,76	1,075±0,004	18,58
k1b	1,250	1,868	14,94	1,085±0,002	31,28
k1c	1,090	4,831	14,49	1,074±0,006	23,62
k1f	1,184	3,075	16,19	1,140±0,048	22,50
k1g'	1,240	1,90	17,76	1,109±0,009	28,73
k1g''	1,086	4,80	17,23	1,112±0,004	23,77

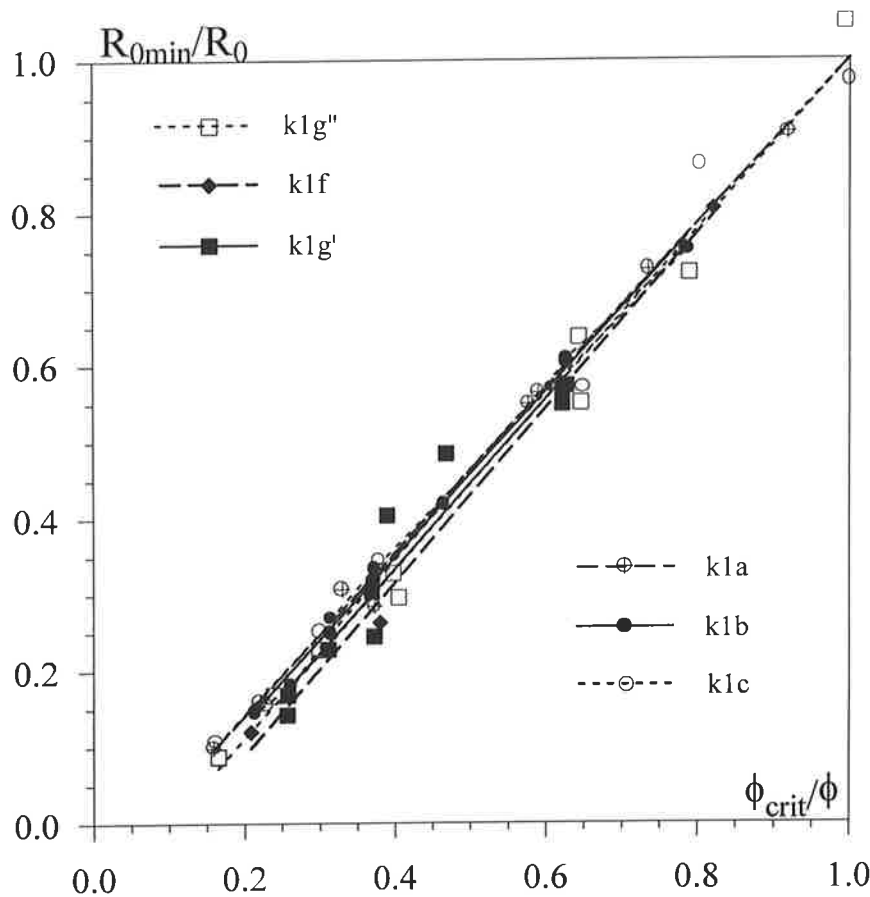


Figure A1-14: The relation between the two dimensionless variables R_{0min}/R_0 and ϕ_{crit}/ϕ of all tested emulsion explosives.

The other two measures of explosives sensitivity, the critical diameter ϕ_{crit} and the minimum curvature radius R_{0min} show little overall dependence on the water content. Figure A1-16 shows the inverse critical diameter $1/\phi_{crit}$ and the inverse minimum curvature radius $1/R_{0min}$ as functions of the microballoon content. Again the pair k1a and k1f is anomalous since the two other pairs, k1b and k1g', and k1c and k1g'' show practically no dependence. One expects $1/\phi_{crit}$ to increase if the k1a tests had been made in the denser PVC instead of in PMMA. The same should be true for $1/R_{0min}$. Unfortunately this accentuates the inconsistency in the data. Despite these, the results imply that the microballoons are important for the sensitivity of an emulsion explosive.

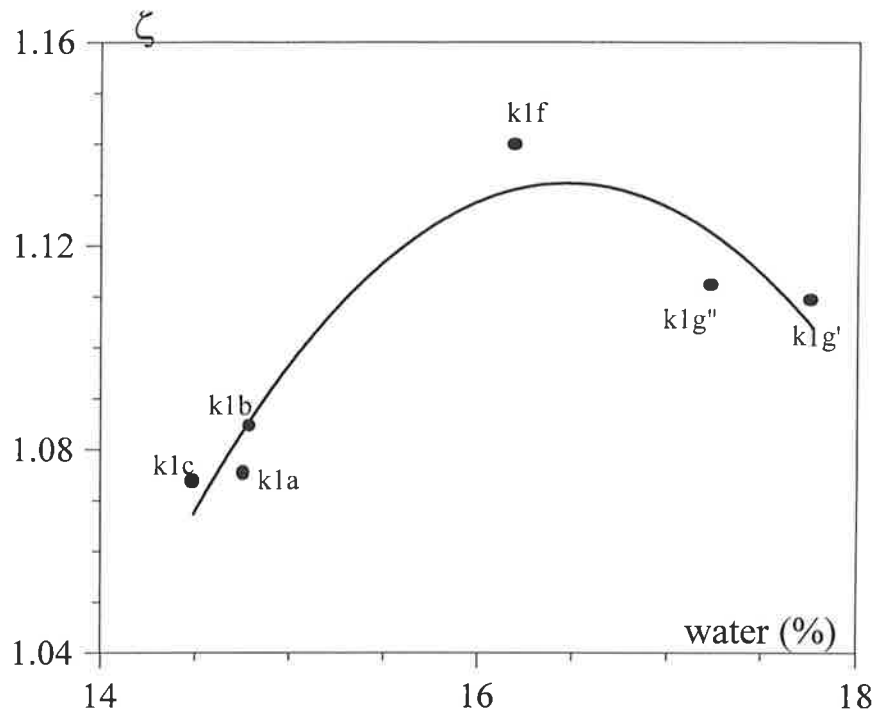


Figure A1-15: The slope of the function $R_{0\min}/R_0$, ζ , as a function of the water content.

Based on the above discussion, the following conclusions can be drawn:

1. Both the microballoon content and the water content affect the detonation front curvature. There are combined effects of the two components on the detonation front curvature.
2. The microballoon content affects the absolute curvature radius of the detonation front more than water content does. The critical diameter and the minimum curvature radius of the detonation front also change significantly with the microballoon content.
3. The water content affects the scaled detonation curvature radius more than microballoon content does. It does not influence the critical diameter and the minimum curvature radius of the detonation front radius significantly.

A complete statistical analysis of the dependence of VOD and R_0 on the variables ϕ , the microballoon and water contents can be made but it requires that the influence of the PMMA on the k1a data be compensated first. This can be done once the burning model parameters have been determined.

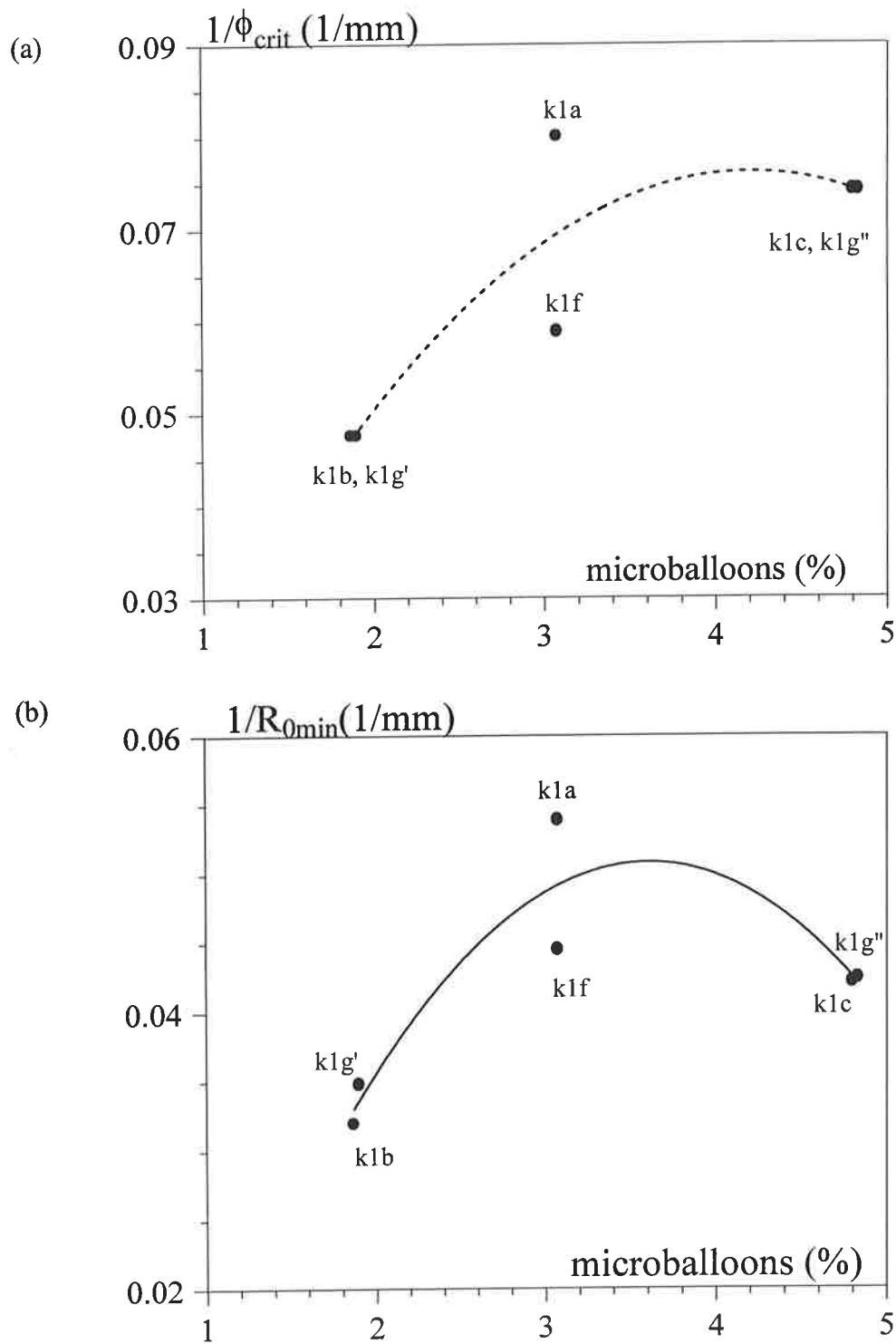


Figure A1-16: The inverse critical diameter $1/\phi_{crit}$ (a) and the inverse minimum curvature radius $1/R_{0min}$ (b), as functions of the microballoon content.

A1.3 Analyses of the Two Dimensional Steady-state Experiments

There are many ways to present the experimental results. A good presentation should have a simple mathematical form and the fitting coefficients should have clear physical meanings. This is important for studying the nature of the detonation processes of commercial explosives. In building a burning model, a good presentation of results will simplify both the experimental work and the calibration.

We have discussed the two dimensional steady-state experiments in section A1.2. Here we would like to discuss them in comparison with other theories.

1. Normal VOD as a function of the local curvature of the detonation front

According to the DSD theory (Bdzil et al. 1989), there exists a single-valued function between the normal VOD value and the local curvature $Dn(k)$. If it is true for the emulsion explosives, it would be unnecessary to do so many experiments of different charge diameters. We could rely on how R changes with r in Equation A1-10 for a single diameter instead. That would greatly simplify the calibration work.

Combining functions $D/D_0(\phi_{crit}/\phi)$ and $1/R_0(\phi_{crit}/\phi)$ in Equations A1-6 and A1-11 in section A1.2 and eliminating the variable ϕ_{crit}/ϕ , a linear function about the relative normal VOD and the inverse local radius (here the curvature radius at charge axis) $D/D_0(1/R_0)$ can be obtained. For the locus off the axes, the elliptical relation in section A1.2 can be used to calculate the relation of the normal VOD and the local radius. We have proven that the differences of using different functions, for example, the Bessel function, are negligible. Figure A1-17 is the result for the emulsion k1a. We can see from the figure that it is not possible to use one function $Dn(k)$ to cover all the individual lines.

The relations for remaining emulsion explosives are rather the same. From these results, we can conclude that there is no a single-valued function $Dn(k)$ existing for any of the emulsion explosives tested in this study. Hence the DSD theory is not suitable for our emulsion explosives. The result is the same as that which Kennedy (1998) obtained for HANFO (Heavy ANFO, a severely non-ideal explosive).

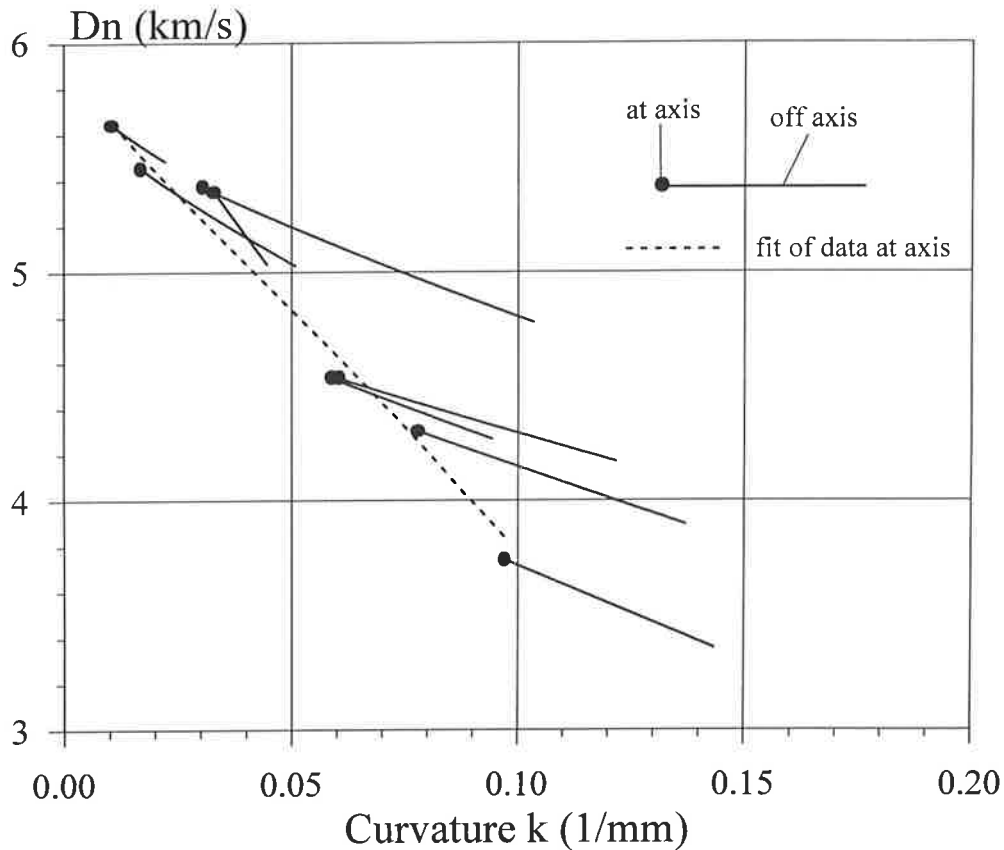


Figure A1-17: The normal VOD vs. the local front curvature (k1a emulsion).

2. Detonation front curvature as a function of charge diameter

The relationship between the radius of the detonation front and the charge diameter is a fundamental restriction in our calibration system. The present study shows that the curvature radius of the detonation front is more important than the VOD value in determination of the burning rate parameters.

In ICI's non-ideal detonation code CPeX (standing for Commercial Performance of eXplosives), the following empirical relationship between the curvature radius and charge diameter is required (Kennedy 1993):

$$\frac{\phi}{R_0} = \alpha + \beta \frac{\phi_{crit}}{\phi}, \quad (A1-15)$$

where R_0 is the curvature radius at the charge axis, ϕ is the charge diameter, ϕ_{crit} is the

critical charge diameter, α and β are the fitting constants. Kennedy (1995) gives $\alpha = 0,165$ and $\beta = 0,692$ for an emulsion explosive.

In order to be useful, the fitting constants α and β need to be relatively independent of say the microballoon and water contents. If this were true an equation like Equation A1-15 or A1-11 for that matter, could replace the relatively cumbersome detonation front measurements.

We have found however that the Equation A1-11 represents our test results better than Equation A1-15 and that a and b (or R_{0min} and ζ) are not universal constants but depend on microballoon and water content in the manner described in section A1.2.3 above. Figure A1-17 shows an example of the fitting lines of the two functions. The experimental results show a clear nonlinear relation between ϕ/R_0 and ϕ_{crit}/ϕ .

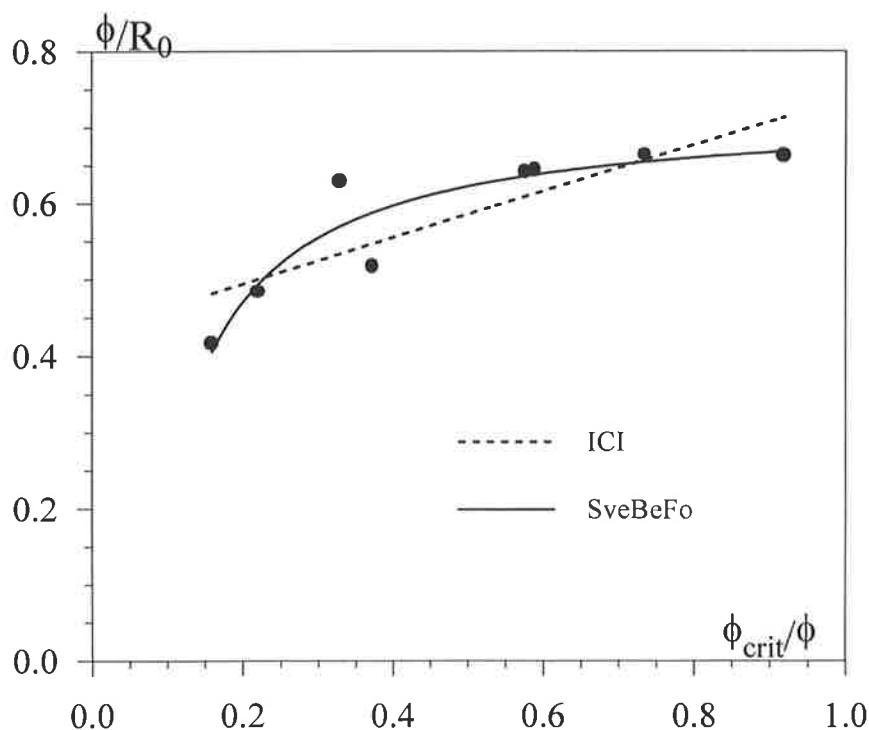


Figure A1-18: Fittings of the experimental data by the ICI's relation A1-15 and the relation suggested of this study Equation A1-11 (k1a emulsion).

Appendix 2: Determination of JWL Parameters of the Emulsion Explosives

In the Ignition and Growth model, the reactive flow is modelled by the mechanical mixture of the unreacted (inert) explosive and the fully reacted products under the assumed conditions of pressure and temperature equilibrium. The following form of the JWL equation of state is used, one each for the unreacted explosive and the reacted products (Murphy 1995):

$$P = Ae^{-R_1 V} + Be^{-R_2 V} + \omega C_v \frac{T}{V}, \quad (\text{A2-1})$$

where P is the pressure, $V = \rho_0/\rho$ is the relative volume, where ρ_0 and ρ are the initial and the current densities of the explosive, T is the absolute temperature, ω is the Grüneisen coefficient, C_v is the average heat capacity, and A , B , R_1 and R_2 are fitting constants. In the following, we will discuss the determinations of these parameters.

A2.1 Hugoniot of the Unreacted (inert) Explosives

The Hugoniot is the most important of the shock properties of the unreacted emulsion. In our study, the unreacted emulsion is treated as a porous material consisting of a liquid (the inert emulsion matrix) and an ideal gas (the air in the microballoons). First the Hugoniot of the emulsion matrix is obtained by comparing the shock arrival times with those from the DYNA2D computations. Then the Hugoniot of the unreacted emulsion is calculated as a porous material using a method suggested by Voskoboinikov et al. (1976).

1. Hugoniot of the inert emulsion matrices

Figure A2-1 shows the experimental setup of the shock transmission tests (Nyberg & Deng 1994). The PMMA (plexiglass) plates between the donor explosive and the tested matrix are used as the damping material. PVD-foils are used to record the shock arrival times at different positions. The foils are sensitive to the pressure and will give strong electric signals when a shock passes through them. A digital oscilloscope, LeCroy 9325, with a resolution of 2 ns/sample was used to record the electric signals. Figure A2-2 shows an example of recorded signals. It is very easy to determine the shock arrival times from these sharp signals.

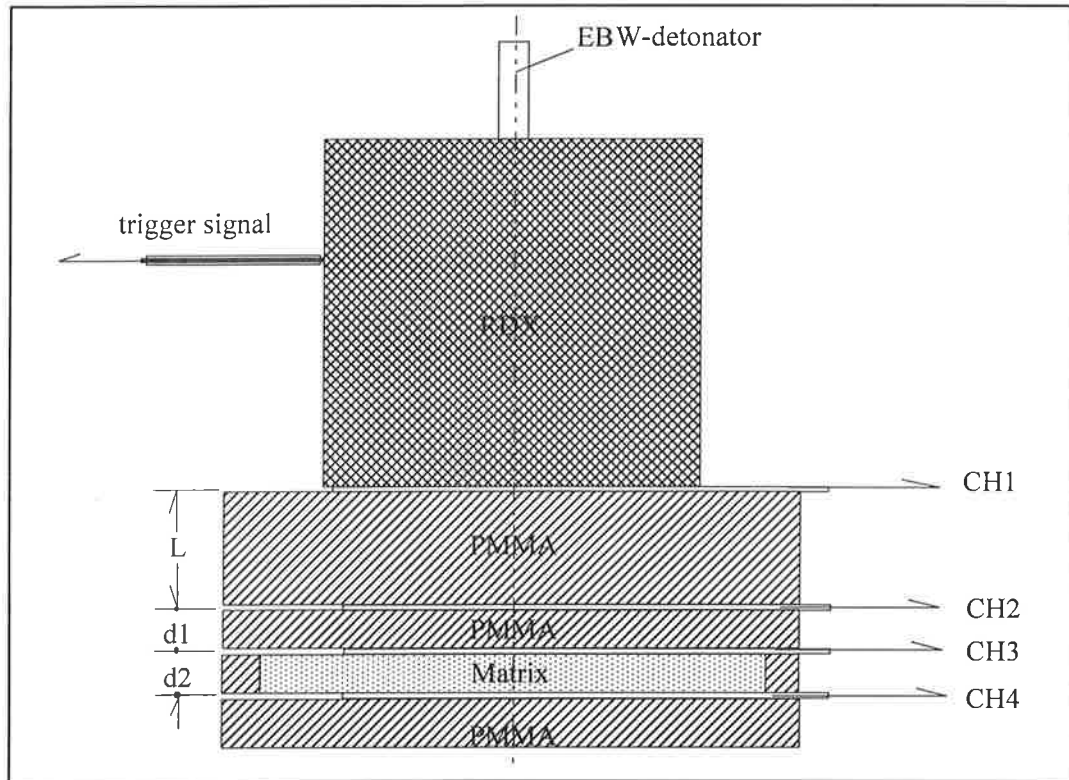


Figure A2-1: Experimental setup for measuring shock travelling times.

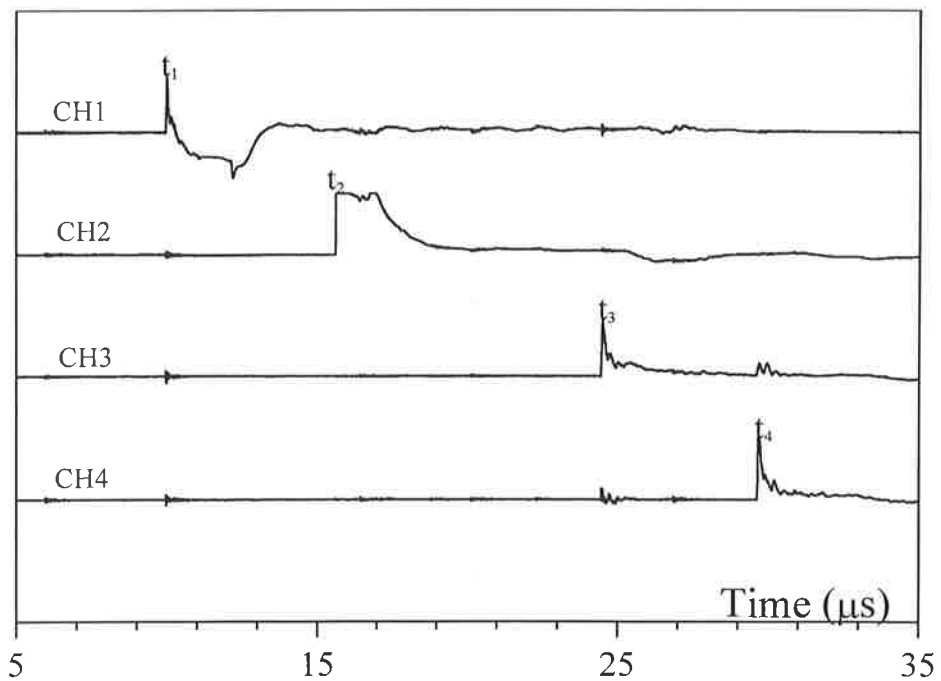


Figure A2-2: An example of recorded shock transmission through the four points.

The shock generated by the donor weakens with increasing thickness of the damping material. For a given donor, the shock arrival time at a certain point in the damping material is a function of the distance from the interface between the donor and the damping to the measuring surface. The accuracy of the experiments can be seen in Figure A2-3 in the relation of the arrival time vs. the damping distance, $x = L(+d_1)$ in Figure A2-1.

The same setup as the experimental one is used for the DYNA2D computations. The donor explosive PBXN-5 was simulated by a programmed-burning JWL model. The density of the explosive is $1,82 \text{ g/cm}^3$ and the VOD value is $8,697 \text{ km/s}$. The PMMA was simulated by the Grüneisen equation of state and the elastic-plastic hydrodynamic material model (Hallquist 1990). The accuracy of the numerical calculation can be seen in the comparison of the shock arrival times shown in Figure A2-4. In the following, we will describe the method for calibration of the Hugoniot coefficients of the matrices.

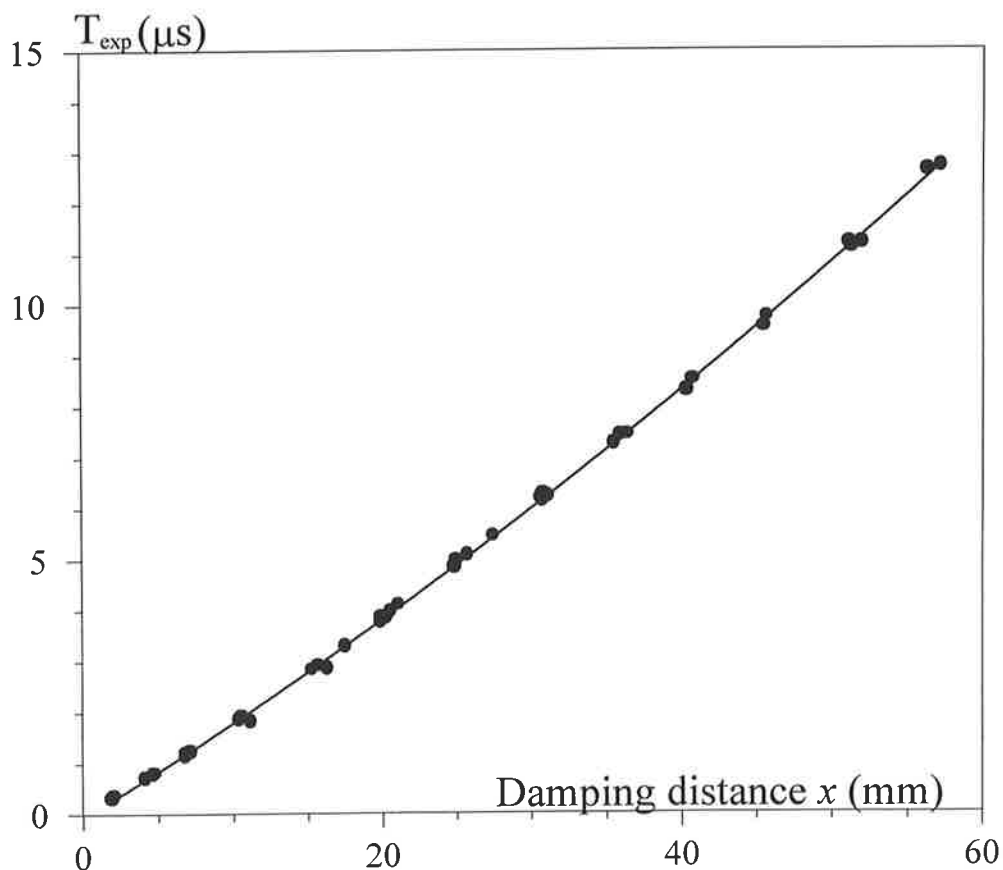


Figure A2-3: The relation of the shock arrival time to the damping distance.

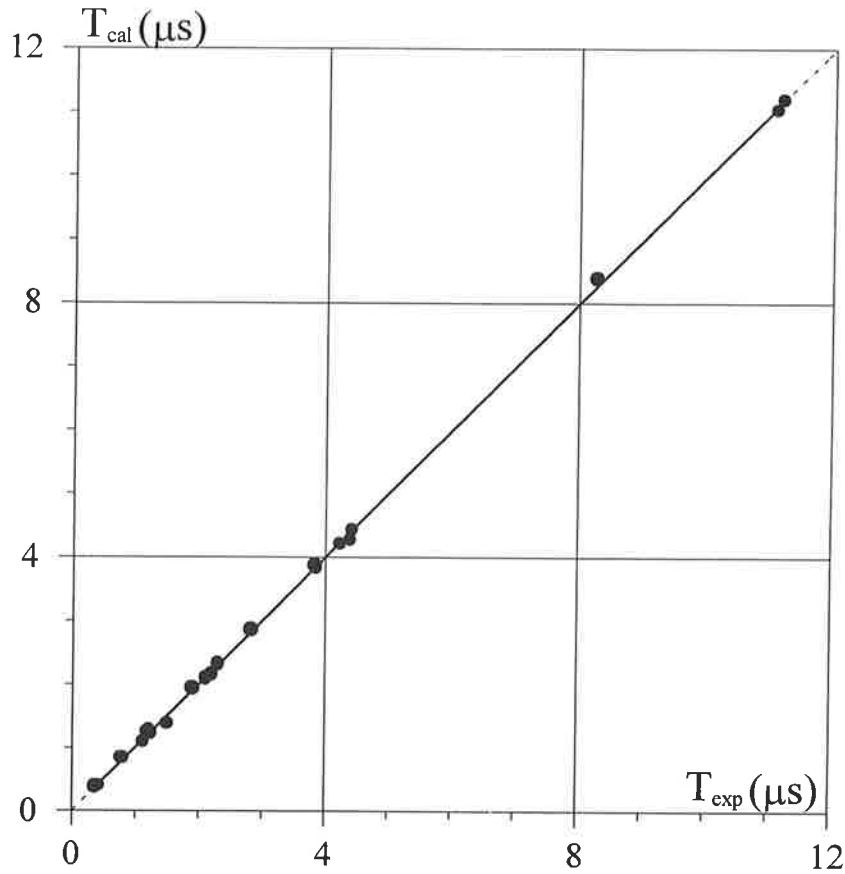


Figure A2-4: The comparison of the shock arrival times from the experiments and by the DYNA2D computations.

For the matrix, the experimental shock travelling time through the last two measuring surfaces is a function of the damping distance $x = L + d_1$ and the thickness of the matrix layer $d = d_2$, or $\delta T_{\text{exp}i} = f_{\text{exp}}(x_i, d_{2i})$, where $i = 1, 2, \dots, n$ (n is the total number of tests). The corresponding values of the DYNA2D computations can be written as $\delta T_{\text{cal}i} = f_{\text{cal}}(x_i, d_{2i}, a, b)$, here a and b are the two parameters of the simplified Grüneisen equation of state required by the DYNA2D code used for the matrix, c.f. Equation A2-6 below. We formulate the following function:

$$F(a, b) = \sum_{i=1}^n [f_{\text{exp}}(x_i, d_{2i}) - f_{\text{cal}}(x_i, d_{2i}, a, b)]^2. \quad (\text{A2-2})$$

The solution thus is to find values of (a, b) , which give a minimum of $F(a, b)$. Assume that the function $F(a, b)$ can be written as:

$$F(a,b) = F(a_0,b_0) + A_1(a-a_0) + A_2(b-b_0) + A_3(a-a_0)^2 + A_4(a-a_0)(b-b_0) + A_5(b-b_0)^2 + \dots$$

This can be simplified as:

$$F(a,b) \approx B_0 + B_1a + B_2b + B_3a^2 + B_4ab + B_5b^2. \quad (\text{A2-3})$$

We can run the DYNA2D code more than k times ($k \geq 5$) by choosing k sets of (a, b) values. Then those coefficients in Equation A2-3 can be determined by solving the following function:

$$\begin{bmatrix} 1 & a_1 & b_1 & a_1^2 & a_1b_1 & b_1^2 \\ 1 & a_2 & b_2 & a_2^2 & a_2b_2 & b_2^2 \\ \dots & & & & & \\ 1 & a_k & b_k & a_k^2 & a_kb_k & b_k^2 \end{bmatrix} \times \begin{bmatrix} B_0 \\ B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5 \end{bmatrix} = \begin{bmatrix} F(a_1,b_1) \\ F(a_2,b_2) \\ \dots \\ F(a_k,b_k) \end{bmatrix}. \quad (\text{A2-4})$$

Take the partial derivatives of the function A2-3 and set them to zero, we have:

$$\frac{\partial F}{\partial a} = B_1 + 2B_3a + B_4b = 0$$

and

$$\frac{\partial F}{\partial b} = B_2 + B_4a + 2B_5b = 0.$$

The solution to the above two equations gives an extreme of the function $F(a,b)$ in the neighbourhood of (a_0, b_0) . Since the coefficients B_i depend on the initial values of (a_0, b_0) , the computations may have to be carried out with a new starting point until the solution converges.

The following simplified Grüneisen equation of state is used to describe the inert emulsion matrices (Hallquist 1990), c.f. Equation 4-2 above:

$$P = \frac{\rho_0 C_0^2 \mu [1 + (1 - \gamma/2)\mu]}{[1 - (S_1 - 1)\mu]^2} + \gamma E. \quad (\text{A2-5})$$

Here ρ_0 is the initial density of the matrix, P is the pressure, $\mu = \rho/\rho_0 = v_0/v - 1$ is the

compression where $v_0 = 1/\rho_0$ and $v = 1/\rho$ are the specific volumes at the initial state and the current state, E is the internal energy, γ is the Grüneisen coefficient, C_0 and S_1 are the Hugoniot coefficients in the following relation:

$$U_s = C_0 + S_1 U_p. \quad (\text{A2-6})$$

Here U_s and U_p are the shock velocity and the particle velocity respectively. Since the Grüneisen coefficient γ has no significant influence on the physical process, it is accepted as a constant here.

For the case of the emulsion matrices, therefore, the two parameters to be calibrated are the Hugoniot coefficients C_0 and S_1 , corresponding to a and b in the Equation A2-2. Figure A2-5 shows an example of comparison of the shock travelling times through the matrix layer before and after calibration. The calibrated Hugoniot coefficients of the emulsion matrices are listed in Table A2-2.

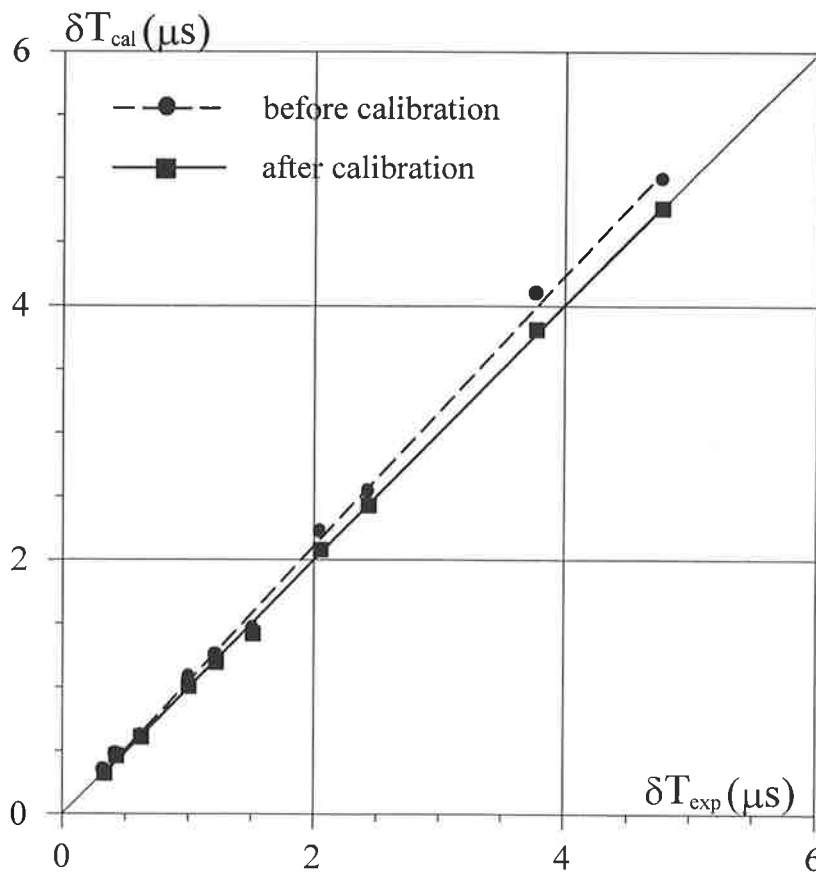


Figure A2-5: The comparison of the shock arrival times before and after calibration.

Table A2-2: Hugoniot of the inert emulsion matrices:

Matrix	Density ρ_{0m} , g/cm ³	Hugoniot
k1a	1,38	$U_s = 2,260 + 1,554U_p$ (km/s)
k1f	1,40	$U_s = 2,20 + 1,788U_p$ (km/s)
k1g	1,37	$U_s = 1,964 + 1,536U_p$ (km/s)

2. Hugoniot of the unreacted emulsion explosives

The emulsion explosive is a mixture of the matrix and the microballoons. Therefore it can be regarded as a "porous" matrix. Knowing the Hugoniot of the matrix, the Hugoniot of the porous material may be calculated by the method suggested by Voskoboinikov et al. (1976). This method is based on the following two assumptions (see also Deng et al. 1995):

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

Assume that the Hugoniot of the matrix is known as

$$U_{sm} = C_{0m} + S_{1m}U_{pm} \quad (\text{A2-7})$$

This can be rewritten in the following form:

$$\frac{U_{sm}}{a_0} = \alpha_1 + \alpha_2 \frac{U_{pm}}{a_0} \quad (\text{A2-8})$$

Where U_{sm} and U_{pm} are the shock wave velocity and the particle velocity of the matrix respectively, a_0 is the sound velocity of the matrix, $\alpha_1 = C_{0m}/a_0$ and $\alpha_2 = S_{1m}$.

For the emulsion explosive (the mixture of the matrix and the ideal gas), there is a linear relation between the shock wave velocity U_{se} and the particle velocity U_{pe} :

$$\frac{U_{se}}{a_0} = \sigma + \xi \frac{U_{pe}}{a_0} \quad (\text{A2-9})$$

Here σ and ξ are constants that are functions of the initial densities of the matrix and the emulsion explosive as follows:

$$\sigma = \frac{\rho_{0m}}{\rho_{0e}}(B_1 + 1,141B_3), \quad \xi = \frac{\rho_{0m}}{\rho_{0e}}(B_2 - 0,2958B_3). \quad (\text{A2-10})$$

Here ρ_{0m} and ρ_{0e} are the initial densities of the matrix and the emulsion explosive. The constants B_1 , B_2 and B_3 are calculated by the following equations

$$B_1 = \frac{\alpha_1}{(\beta\alpha_2 + 1)^{3/2}}, \quad B_2 = \frac{\alpha_2}{\beta\alpha_2 + 1} \quad \text{and} \quad B_3 = \frac{-\alpha_1^2}{2(\beta\alpha_2 + 1)^2}. \quad (\text{A2-11})$$

Here β is a function of the ratio of the specific heats of the ideal gas γ and the initial densities of the matrix and the emulsion explosive ρ_{0m} and ρ_{0e} :

$$\beta = \frac{2}{\gamma + 1} \left(\frac{\rho_{0m}}{\rho_{0e}} - 1 \right). \quad (\text{A2-12})$$

The Hugoniot coefficients of the emulsion explosive are obtained from Equation A2-7:

$$C_{0e} = \sigma a_0 \quad \text{and} \quad S_{1e} = \xi \quad (\text{A2-13})$$

As an approximation, the constant C_{0m} is used as a substitute for the sound velocity of the matrix a_0 . Using the Hugoniot of the matrices (Table A2-2) and the equations above, the Hugoniot of the emulsion explosives can be calculated. The results are listed in Table A2-3.

Table A2-3: Hugoniot of the unreacted emulsion explosives:

Explosive (matrix)	density ρ_{0e} , g/cm ³	Hugoniot
k1a (k1a)	1,165	$U_s = 1,788 + 1,503U_p$ (km/s)
k1b (k1a)	1,250	$U_s = 1,969 + 1,523U_p$ (km/s)
k1c (k1a)	1,090	$U_s = 1,635 + 1,486U_p$ (km/s)
k1f (k1f)	1,184	$U_s = 1,674 + 1,679U_p$ (km/s)
k1g' (k1g)	1,240	$U_s = 1,712 + 1,507U_p$ (km/s)
K1g'' (k1g)	1,086	$U_s = 1,434 + 1,475U_p$ (km/s)

A2.2 JWL Parameters of the Unreacted (inert) Explosives

We have to express the equation of state of the unreacted explosive in the JWL form, since the DYNA2D code uses this form. This has been performed in two steps. First the isentrope of the unreacted explosive between the initial state and the von Neumann pressure was calculated based on the explosives Hugoniot and an assumed constant Grüneisen γ . The von Neumann pressure was taken as twice the C-J pressure, which was calculated by the TIGER (later by the Cheetah) code (see section A2.3). Then a JWL equation was fitted to the isentrope. The curve fitting was carried out using a computer program ANPASS (Almström 1994).

In the following, the derivation of the isentrope will be outlined and the final JWL equation for the unreacted explosive will be presented in the next section, together with the relevant parameters for the fully reacted products.

Since the Hugoniots of the explosives are known (Table A2-3), the equation of state of the explosive can be expressed in the Grüneisen form (Hallquist 1990):

$$P = \frac{\rho_0 C_0^2 \mu [1 + (1 - \gamma/2)\mu]}{[1 - (S_1 - 1)\mu]^2} + \gamma E. \quad (\text{A2-14})$$

Using $\mu = v_0/v - 1$, the above equation can be transformed into:

$$E = E[P(s, v), v] = \frac{P - F(v)}{\gamma}. \quad (\text{A2-15})$$

Here s is the entropy, P is the pressure, v is the specific volume, E is the internal energy, and γ is the Grüneisen constant. The function $F(v)$ is in the following:

$$F(v) = \frac{\rho_0 C_0^2 [(1 - \gamma/2)v_0^2 + (\gamma - 1)v_0 v - \gamma/2 v^2]}{[(1 - S_1)v_0 + S_1 v]^2}. \quad (\text{A2-16})$$

The isentrope can be derived accordingly, since on the isentrope we have $ds = 0$, or:

$$dE/dv = -P. \quad (\text{A2-17})$$

By Equation A2-15, we have:

$$\frac{dE}{dv} = \frac{1}{\gamma} \frac{dP}{dv} - \frac{1}{\gamma} \frac{dF}{dv}. \quad (\text{A2-18})$$

Combining Equations A2-17 and A2-18, we obtain the following differential function:

$$\frac{dP}{dv} + \gamma P = \frac{dF}{dv} = f(v). \quad (\text{A2-19})$$

Here:

$$f(v) = \frac{a_1 + a_2 v}{[(1 - S_1)v_0 + S_1 v]^3}, \quad (\text{A2-20})$$

where:

$$\left. \begin{aligned} a_1 &= -C_0^2 (S_1 + 1 - \gamma) v_0 \\ a_2 &= C_0^2 (S_1 - \gamma) v_0 \end{aligned} \right\}. \quad (\text{A2-21})$$

The solution to Equation A2-19 is:

$$P(v) = k(v) e^{-\rho_0 v}, \quad (\text{A2-22})$$

where:

$$k(v) = \int \frac{a_1 + a_2 v}{[(1 - S_1)v_0 + S_1 v]^3} e^{\rho_0 v} dv + C. \quad (\text{A2-23})$$

Here C is an integration constant, which is determined by the boundary condition, i.e. $P = 0$ at $v = v_0$.

The following JWL form is fitted to the generated isentrope curve (P - V relation):

$$P = A \left(1 - \frac{\omega}{R_1 V}\right) e^{-R_1 V} + B \left(1 - \frac{\omega}{R_2 V}\right) e^{-R_2 V} + \frac{\omega E}{V}. \quad (\text{A2-24})$$

Here P is the pressure, $V = \rho_0 / \rho$ is the relative volume, where ρ_0 and ρ are the initial and the current densities of the explosive. A , B , R_1 , R_2 and ω are fitting constants. An initial condition, saying that $E(V_0, P_0) = 0$, is used to constrain the fitting. Otherwise, the initial internal energy for the inert emulsion could have a non-zero value, which would change the computational internal energy of the mixture of the unreacted emulsion and the fully reacted products.

The calculated JWL parameters for the unreacted explosives are listed in Table A2-4.

A2.3 JWL Parameters of the Fully Reacted Products

The reaction products and their isentropic expansion from the CJ-state were calculated by the thermodynamic code Tiger (later Cheetah) using the BKWR equation of state. Then the same JWL form of Equation A2-24 was fitted to the calculated isentrope for the reaction products. This time, the fitting is constrained by the CJ-state. The JWL parameters for the fully reacted explosives, the CJ-states and the initial internal energy of the reaction products E_0 are listed in Table A2-4.

Finally, the heat capacities for both the unreacted emulsions and the reacted products need to be determined. These two parameters are required by the DYNA2D code as constants. The equation of state A2-1 is used to calculate the two constants. For the unreacted emulsions, the value is calculated by applying the initial conditions to the equation, while for the fully reacted products, the value is calculated by applying the CJ-conditions to the equation. The results are also listed in the Table A2-4. The heat capacities for the fully reacted products obtained here are between the minimum and maximum values calculated by the Tiger code.

Table A2-4: JWL parameters for the tested emulsion explosives:

explosive	k1a	k1b	k1c	k1g'	k1g''
JWL parameters of the unreacted explosive					
density ρ_0 , g/cm ³	1,165	1,250	1,090	1,240	1,086
A , Mbar	132,86	295,78	66,884	179,70	84,843
B , Mbar	-0,07104	-0,13027	-0,04498	-0,07153	-0,03608
R_1	13,842	15,016	13,0	14,433	14,097
R_2	0,97716	1,2784	0,85629	0,8765	0,79653
ω	0,9728	1,2755	0,850	0,87385	0,79362
C_v , bar/°K	91,792	95,209	74,829	113,96	68,511
JWL parameters of the reaction products					
A , Mbar	4,4423	6,7671	3,8012	6,7941	6,0
B , Mbar	0,1547	0,2257	0,1303	0,2309	2,0839
R_1	6,1054	6,2450	6,002	6,4037	3,7619
R_2	2,2733	2,2710	2,090	2,40	0,1262
ω	0,9395	0,8820	0,7140	0,9990	0,7223
C_v , bar/°K	15,557	15,091	12,711	15,446	12,347
E_0 , Mbarcm ³ /cm ³	0,03348	0,03948	0,03333	0,03645	0,03152
CJ states by Tiger (or Cheetah) code					
temperature, °K	1919	1862	1961	1808	1870
VOD, km/s	6,179	6,622	5,844	6,515	5,774
pressure, Mbar	0,10925	0,13148	0,09319	0,12581	0,09004
compression, ρ_0/ρ	0,7547	0,7602	0,7497	0,7610	0,7513
particle velocity, km/s	1,518	1,588	1,463	1,557	1,436

Appendix 3: Determination of the Burning Rate Parameters

A3.1 DYNA2D Setups

1. 1D setup: the detonation with infinite diameter

The DYNA2D computations of our 'rate-stick' experiments have been carried out with different setups. The simplest one is the 1D setup consisting of one element column with a 20 mm long donor explosive and a 100 mm long main charge. The element size is 0,02×0,02 mm. The model contains 6000 elements and takes about 15 minutes to run on a 400 MHZ Pentium II PC. If necessary, even finer cells can be used for the computations.

A programmed-burning model of the JWL Equation A2-24 is used for the donor explosive PETN (Pentaerythritol Tetranitrate). The parameters of the donor explosive are listed in Table A3-1 (Murphy 1995).

Six monitoring nodes along the axis near the charge end are used for the steady-state VOD evaluations. The shock is assumed to reach a node when the node velocity exceeds 300 m/s (Deng et al. 1995). The VOD value is calculated by the slope of a linear fitting of the data in the distance-time space. The stability of the VOD value can also be checked. Figure A3-1 shows an example of the running distance over the 6 nodes.

One monitoring element is needed to analyse the other properties of the detonation, for example, the pressure and reaction extent trajectories (Figure A3-2). As we can see from the figure, the reaction zone is resolved relatively well. Further studies show that little improvement can be achieved by using finer cells (see the section A3.6).

Table A3-1: JWL EOS parameters for the donor explosive PETN:

Variable and unit	Parameter	variable and unit	Parameter
Density ρ_0 (g/cm ³)	1,77	A (Mbar)	6,170
CJ pressure (Mbar)	0,335	B (Mbar)	1,693
VOD (km/s)	8,30	R_1	4,4
Initial internal energy E_0 (Mbar cm ³ /cm ³)	0,101	R_2	1,2
		ω	0,25

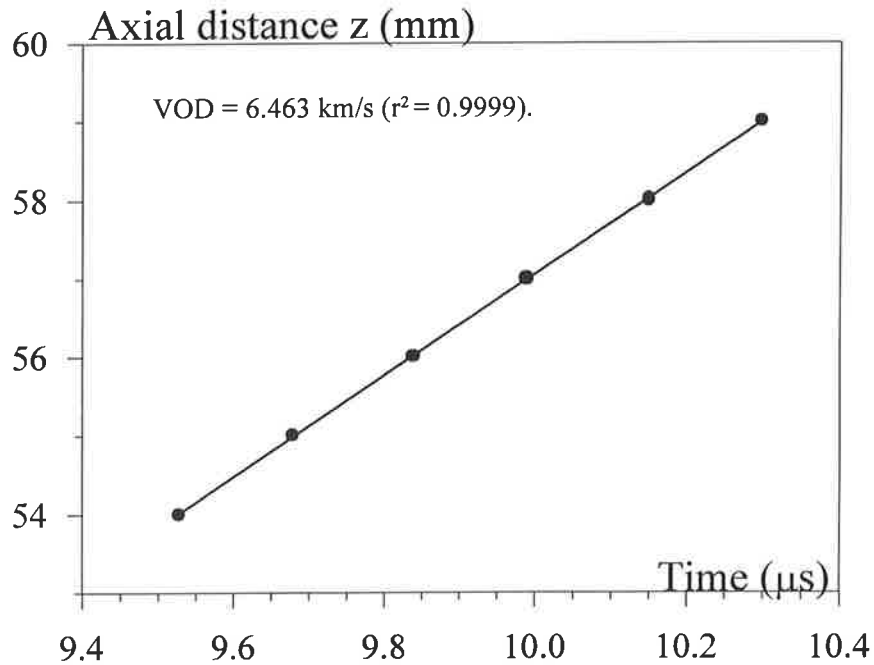


Figure A3-1 A VOD evaluation from the running distance data of a DYNA2D calculation for emulsion k1g' using the 1D setup. The high value of the correlation coefficient r^2 shows that the VOD has stabilised over these nodes.

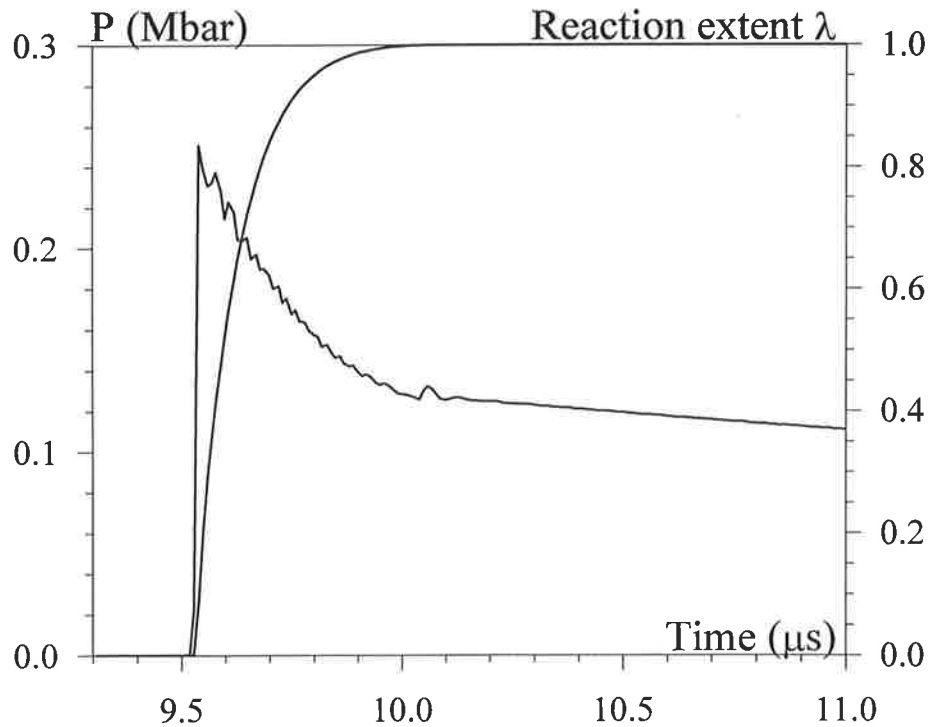


Figure A3-2 The pressure and extent of the reaction profiles for a steady detonation (for emulsion k1g' and the 1D-setup, VOD = 6,463 km/s).

2. 2D setups: the detonations with finite diameters

A DYNA2D setup of the cylindrical charge is shown in Figure A3-3. A total of 3 materials are involved in the computation: the donor explosive PETN, the explosive to be calibrated and the confining material PVC (or PMMA). In order to simplify the computation, two material regions were used for the PVC (PMMA for k1a emulsion) tube. After a certain computation time, the first part (PVC1 in the Figure) 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 PVC tube. Axially symmetric geometry is used.

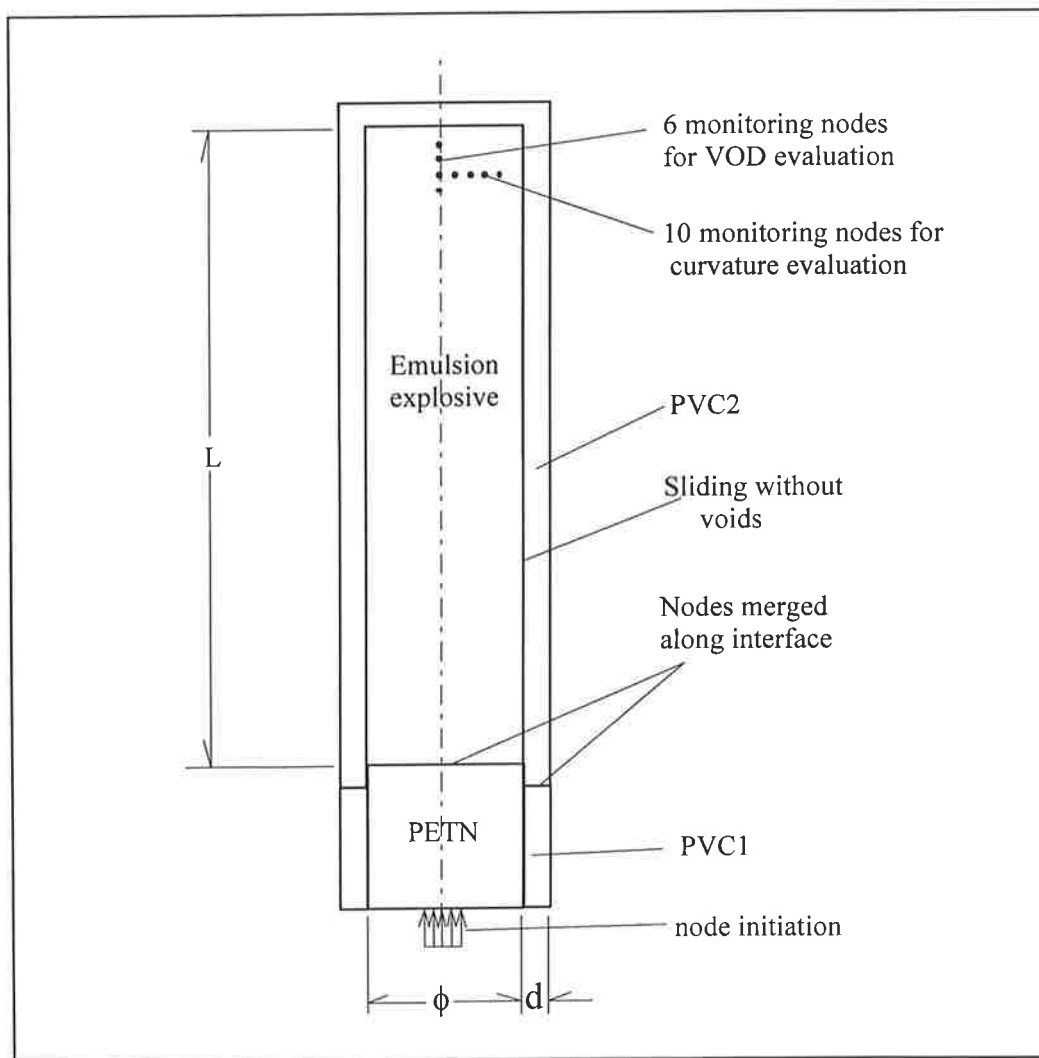


Figure A3-3 DYNA2D computation setup for the cylindrical charges.

Totally 4 computational setups were used for the simulation of each parameter set. The inner charge diameters range from 20 to 80 mm and the main charge lengths range from 80 to 320 mm. The length/diameter ratio is 4, which has proven sufficient to obtain a stable detonation. The thickness values of the PVC (or PMMA) tubes are the average ones of the individual tubes used in the experiments. The dimensions of the computation setups are listed in Table A3-2. Element sizes range from 0,2×0,2 to 0,8×0,8 mm. This is sufficient to obtain the stabilised VOD values and the curvature radii of the detonation fronts, but not sufficient to resolve the detonation zone completely (see discussions below). An example of the DYNA2D computation is shown in Figure A3-4. The straight expansion lines of the PVC tube shows that the detonation is already stabilised.

Table A3-2: Dimensions for the DYNA2D computation setups (see Figure A3-3):

No.	charge diameter ϕ (mm)	PVC (or PMMA) tube thickness d (mm)	charge length L (mm)	element size in emulsion explosive (mm×mm)
1	20	1,9	80	0,2×0,2
2	40	2,3	160	0,4×0,4
3	60	3,1	240	0,6×0,6
4	80	3,8	320	0,8×0,8

The computation starts with the initiation of PETN of the same kind as used in the 1D setup (see the Table A3-1). A strong shock is generated for initiation of the emulsion explosive. The PETN donor has the same diameter as the main charge and has a length of about 10~15% of the main charge. This has proven sufficient to initiate the emulsion explosive. With these setups, we are not testing the initiation (or shock to detonation) properties of the emulsion explosives. We assume that all measurements from the experiments were obtained from steady-state detonations, i.e. that both the VOD values and the curvature radii of the detonation fronts are independent of time.

The Ignition and Growth model is used for the main charges. The parameters of the equations of state for both the unreacted explosive and the reaction products are listed in Table A2-4. The burning rate parameters were calibrated and that will be discussed in the next section.

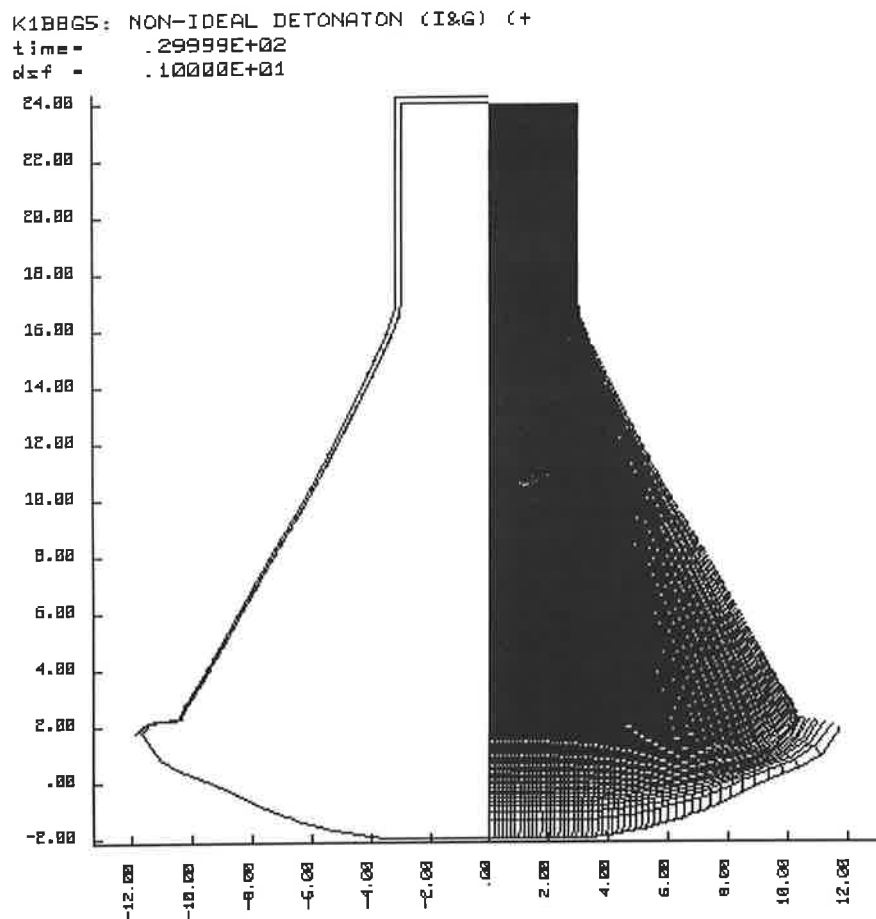


Figure A3-4 A DYNA2D simulation of the steady-state detonation. The donor explosive PETN and the first part of the PVC (or PMMA) tube (PVC1, see Figure A3-3) have already been deleted (k1b emulsion, $\phi = 60$ mm, VOD = 5,95 km/s and $R_0 = 107,5$ mm).

Both the VOD values and the curvature radii of the detonation fronts will be evaluated. The same method is used for the VOD evaluations as in the 1D computations. Ten monitoring nodes along a radial line near the charge end are used for the curvature evaluations. Thus totally 21 points were used for the curvature data fits. The node velocity of 300 m/s is still used as the trigger for the shock arrivals. Under the condition of a constant VOD value for all nodes, the locus of the detonation front can be determined by the shock arrival time differences to these nodes and the VOD value (Deng et al. 1995). Then an ellipse is fitted to the detonation front. The radius at the

charge axis can be calculated accordingly. Figure A3-5 shows an example of the calculated detonation front and the fitted ellipse.

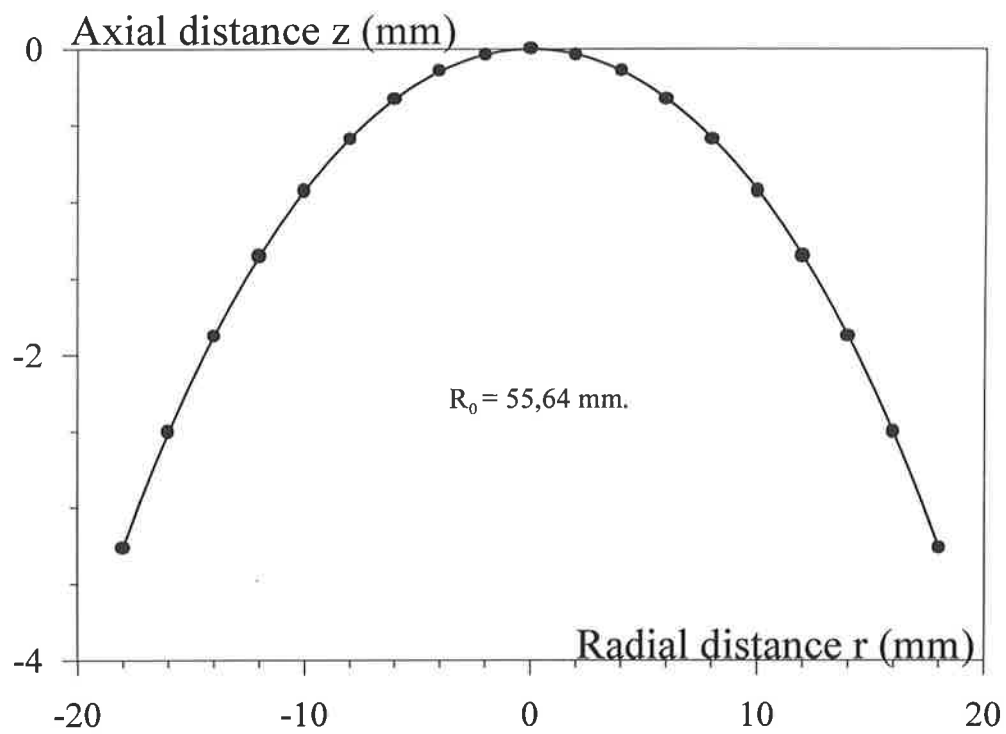


Figure A3-5 A calculated detonation front and the fitted ellipse (emulsion k1g', $\phi = 40$ mm, VOD = 5,81 km/s and $R_0 = 55,64$ mm).

A3.2 The Burning Rate Function and the Calibration Method

The burning rate function used for the emulsion explosives is of the following form:

$$\frac{d\lambda}{dt} = ig(1 - \beta\lambda)^2 (\mu_e - \mu_c)^4 + gr(1 - \lambda)^{2/3} \lambda^{2/9} P^y. \quad (\text{A3-1})$$

Here λ is the reaction extent (the fraction of the explosive that has reacted, kg/kg), t is the time, P is the pressure, $\mu_e = \rho_e / \rho_0 - 1$ is the relative compression of the explosive, ρ_e / ρ_0 is the ratio of the current density to the initial density of the explosive and μ_c is the critical relative compression. The parameters ig , gr , β and y are calibration constants.

The reaction starts when the relative compression μ_e exceeds the critical value μ_c . In order to get a smoother transition from the ignition phase (the ig -term) to the growth phase (the gr -term), a new parameter β was introduced into the ignition term (Deng et al. 1995), where β is greater than 1. The ignition phase terminates when $\beta\lambda = 1$ (or $\lambda_{mxig} = 1/\beta$, compared with the original burning rate function). Thus when $\lambda \geq 1/\beta$, the first ignition term stops contributing to the reaction. This could also have been expressed by adding a step function to A3-1.

In our earlier study on the emulsion k1a (Deng et al. 1995), the following form of the burning rate function was used:

$$\frac{d\lambda}{dt} = ig(1 - 2\lambda)^{2/9} (\mu_e - \mu_c)^2 + gr(1 - \lambda)^{2/3} \lambda^{2/9} P^2. \quad (\text{A3-2})$$

Comparing with the Equation A3-1, the constant β in the ignition term and the pressure exponent y have become free variables in this study. We have found that the detonation front curvature is sensitive to the constant β (see discussion below) and that the pressure exponent y is very important for the calculated VOD values.

In the earlier study, the initial internal energy for the fully reacted products was included as an adjustable parameter, which has proven incorrect.

In this study, larger values for the exponents on the $(1 - \beta\lambda)$ and the $(\mu_e - \mu_c)$ terms are used, which results in larger calibrated values of the ignition coefficient ig . Besides, this yields a smooth reaction rate surface in the λ - P plane

The critical diameter has proven important for determining the critical relative compression μ_c for the first emulsion k1a (Deng et al. 1995). In this study, this value has not been used for the calibration and the μ_c values are only roughly estimated by the experimental critical diameters.

Therefore, we have totally four free parameters. The burning models are calibrated for each explosive by varying the four parameters against the 2D cylinder test results.

The quantities used for the calibration are the VOD values and the curvature radii of the detonation fronts at the charge axis. The calculated VOD values and the curvature radii have been compared with those from experiments and the best burning rate parameters have been determined by minimising the following quantity:

$$Q = \sum_{i=1}^n \left[\left(\frac{VOD_{com,i} - VOD_i}{VOD_i} \right)^2 + \left(\frac{R_{0com,i} - R_{0i}}{R_{0i}} \right)^2 \right]. \quad (A3-3)$$

Here $VOD_{com,i}$ and $R_{0com,i}$ are the computed VOD values and the detonation front radii at the charge axis of different charge diameters. n is the number of DYNA2D computation set-ups (calibration number). VOD_i and R_{0i} are the VOD values and the detonation front radii corresponding to the charge diameters for the computation setups on the experimental curve-fitted lines in the following equations:

$$D(\phi) = a - b/\phi \quad (A3-4)$$

and

$$R_0(\phi) = c_0 + c_1\phi + c_2\phi^2 \quad (A3-5)$$

where ϕ is the (inner) charge diameter in mm, a , b and c_i are fitting constants.

The procedure was to manually search the parameter space over a coarse mesh before concentrating on the interesting areas (see the next section). Each step was evaluated manually. This made the calibration relatively difficult and time consuming.

A3.3 Preliminary Calibrations

There would be too many parameter combinations if we consider the four adjustable parameters at the same time. We calibrated these parameters in two steps: a preliminary and a final calibration. In the preliminary stage, we tried to use the special properties of the parameters and the 1D setup to search the parameter space over a coarse mesh. Then, the final calibrations were more easily made within a small parameter space. In this way, the calibrations could be carried out more efficiently.

1. Preliminary determination of the lower bound of ig and gr with 1D setup

A DYNA2D computation of the 1D detonation is simple and easy to run. The extrapolated experimental VOD values at the infinite diameter agree very well with those by the Tiger code (see Table 3-3). The DYNA2D code must be able to reproduce these results. Therefore, the VOD values from the 1D detonation can be used for the calibrations of the burning rate parameters. Besides, one can use very fine cells and make more accurate calculations.

The results of the 1D computation show that there is an upper bound for the VOD value as well as for the other CJ parameters (see Appendix 4). The upper bounds for the VOD values are close to those extrapolated from experiments and by the Tiger code and are independent of the burning rate parameters.

By the Equation A3-1, we know that the reaction rate increases with the two linear coefficients ig and gr . The upper bounds of the two parameters can not be determined from the VOD values, because the upper bounds for the VOD values (and other detonation parameters) are determined by equations of state for the fully reacted products (see Appendix 4), not by the burning rate function. The lower bounds of the two parameters however can be tested by decreasing the two values, until the calculated VOD values become much smaller than the experimental one (or the one obtained by the Tiger code). Figure A3-6 shows that the lower bound of the gr is between 50 and 100. Of course, at the same time, the search area for other parameters must be properly determined within a large range (not necessarily accurate). For this example, the parameter space for other parameters is $\beta = 2$, $ig = 5 \sim 100$ and $\gamma = 2 \sim 2.4$. We can do the same to the parameter ig to find its lower bound. The final burning rate parameters for

the explosive (k1b) became $\beta = 1,2$, $ig = 60$, $gr = 90$ and $y = 2,2$.

The upper bounds of these parameters can be checked using the 2D setups (the setups with finite diameters). It is not always easy to find these limit values. In fact, we used both 1D and 2D setups several times to make the search space of the parameters smaller.

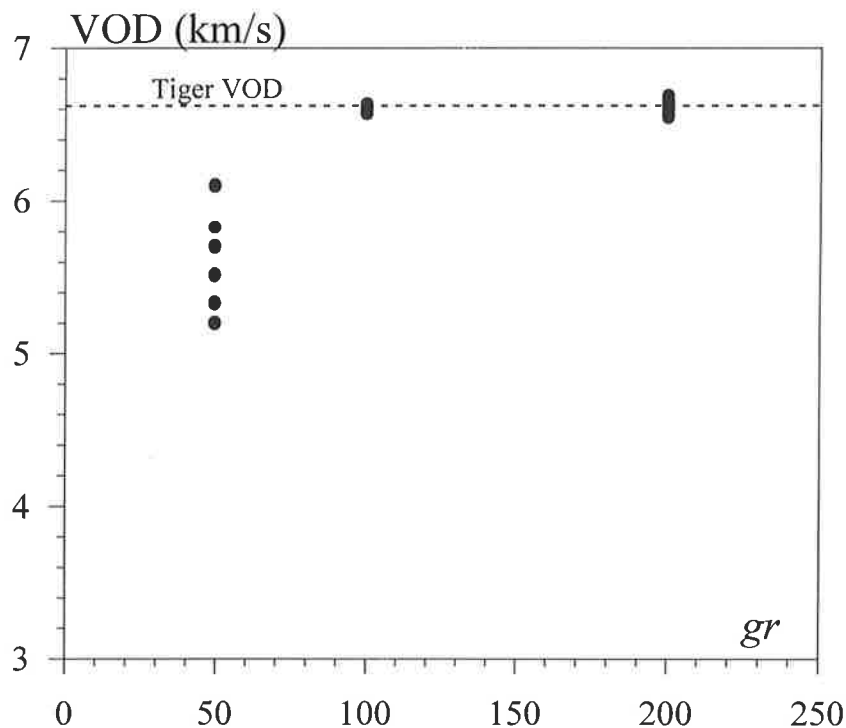


Figure A3-6 An example of determination of the lower bounds for the two linear coefficients of the burning rate function ig and gr . A lower bound range from 50 to 100 for the parameter gr can be determined (1D computation for emulsion k1b).

2. Determination of the pressure exponent y by the VOD values of the small diameter charges

It has been proven that the pressure is very important to the burning process of an explosive (Lee & Tarver 1980). This is represented by the pressure exponent y in the burning rate function.

With the help of the linear relation of the VOD values vs. the inverse charge diameter in Appendix 1, we need to control only two points: the VOD values of the infinite diameter

(the 1D case) and a relatively small charge diameter. The 2D setups of small diameter charges are used to calibrate the pressure exponent. At the same time, the two linear coefficients ig and gr are also be calibrated, since the 1D detonation yields the same results for relative large values of the two parameters.

Figure A3-7 shows an example of the effect of the pressure exponent γ on the VOD values at constant ig and gr . The proper γ value of the explosive (emulsion k1g'') was calibrated to be 1,79 ($ig = 37$ and $gr = 150$).

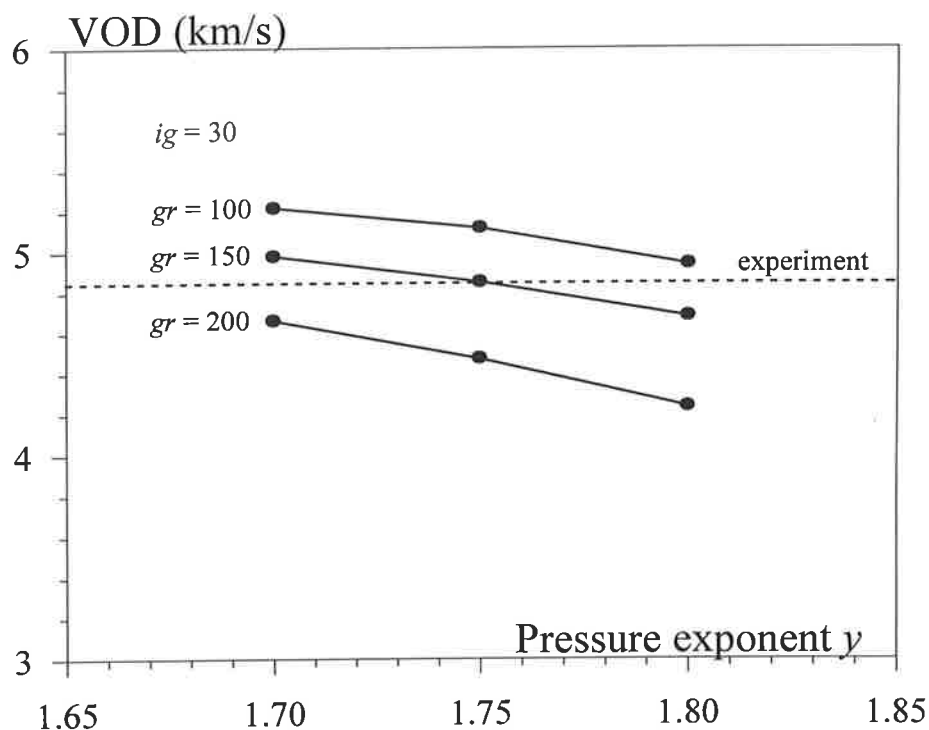


Figure A3-7 An example of determination of the pressure exponent γ by the 2D computation model with a k1g'' emulsion charge of 20 mm diameter.

3. Determination of the constant β by the curvature radii of the detonation fronts of the relatively large diameter charges

The earlier experience from the calibration of emulsion k1a (Deng et al. 1995) showed that the ratio of the detonation radius to the VOD value, R_0/D , was affected more by the initial internal energy E_0 than by the ratio of the two linear coefficients gr/ig . As already commented on, E_0 can not be varied at will however. The present study shows that the R_0/D value is affected by both the constant β and the coefficient ratio gr/ig .

Figure A3-8 shows the R_0/D value increases slightly with the coefficient ratio gr/ig . This means that the detonation front becomes more flat. The R_0/D value increases also with a decreasing β value. Figure A3-9 shows the combined effects of these parameters on the ratio R_0/D . The results show also that the effect of the constant β depends also on the other three parameters. For example, for the case of $\gamma = 1,90$, $gr = 200$ and $ig = 20\sim 30$, the constant has almost no influence on the R_0/D value.

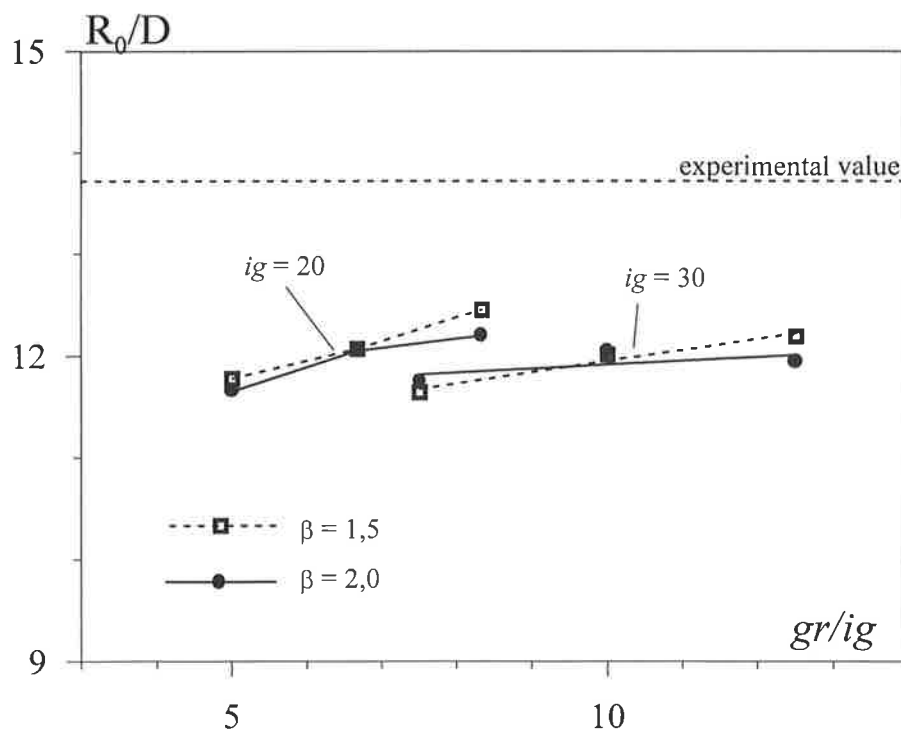


Figure A3-8 Effects of the coefficient ratio gr/ig on the ratio R_0/D for a k1g" emulsion charge of 40 mm diameter.

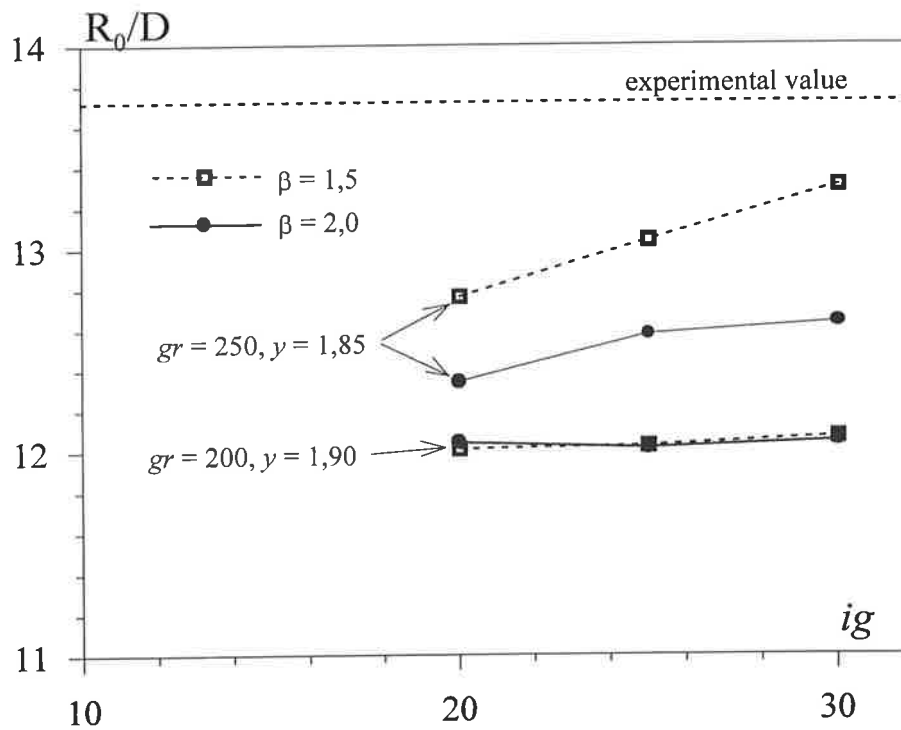


Figure A3-9 The combination effects of the coefficient ratio gr/ig and the constant β on the ratio R_0/D for a k1g'' emulsion charge of 40 mm diameter.

In our calibrations, the constant β is used in the preliminary stage and its value is determined by the experimental curvature radii. The detailed fittings of the detonation fronts are carried out by the three parameters, ig , gr and y in the final stage.

A3.4 Final Calibrations

After determining the value of the constant β and the interesting area of the other three parameters, ig , gr and y , further calculations were made with much smaller variations of the three parameters. The best parameter set is easily determined by minimising the Q value in the Equation A3-3. The final results of these burning rate parameters are listed in Table A3-3. The comparisons between the experiments and the DYNA2D predictions are shown in Figures A3-10 through A3-14.

As we can see from these figures, the finally calculated radii of the detonation fronts are in very good agreement with those from the experiments. The predicted VOD values are in good agreement with those from experiments for the 1D case and the smaller diameter charges. For the larger diameter charges, the computed values are higher than the experimental ones. The average VOD difference between computations and experiments is 0,28 km/s, while the average radius difference is 7,5 mm. This corresponds to only 4,6% and 6,6% respectively. The reason for the higher predicted VOD values for large diameter charges is probably the larger elements used. For example, for the 80 mm diameter charges, elements of 0,8×0,8 mm were used, which usually yields higher VOD values. Because of the RAM memory limitations, it was impossible to use smaller elements for the computations of the large diameters on our computers.

Table A3-3: The calibrated burning rate parameters for five emulsion explosives:

Emulsion	ig	gr	y	β	(μ_c)	$\lambda_{mxi} (=1/\beta)$
k1a	18	190	1,92	1,5	0,08	0,6667
k1b	60	90	2,20	1,2	0,08	0,8333
k1c	18	120	1,80	1,0	0,05	1,0
k1g'	20	220	2,10	2,5	0,09	0,40
k1g''	37	150	1,79	1,2	0,05	0,8333

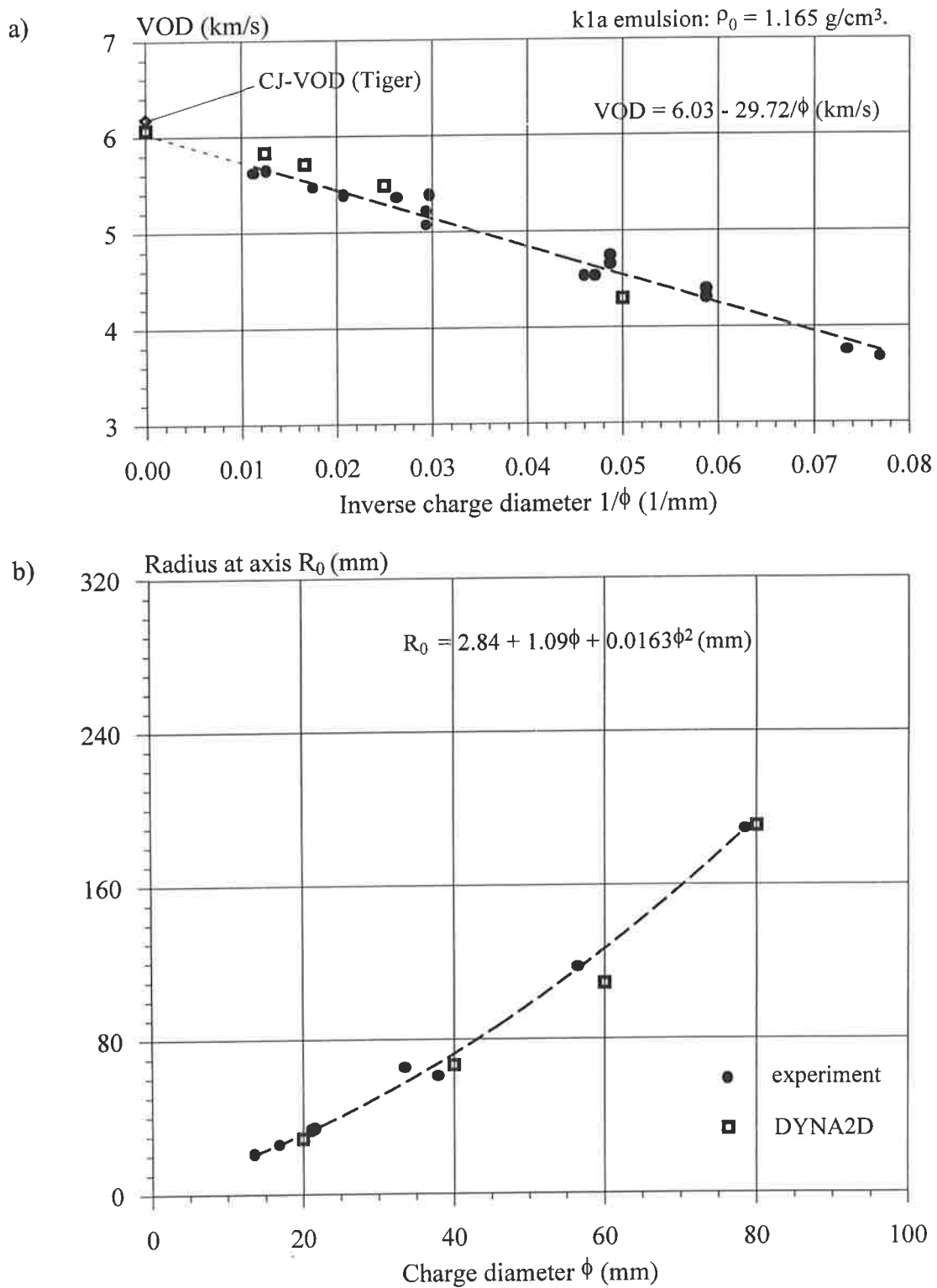


Figure A3-10 Comparisons of the VOD values (a) and the curvature radii at charge axis (b) by the DYNA2D computations with the experiments (k1a emulsion)

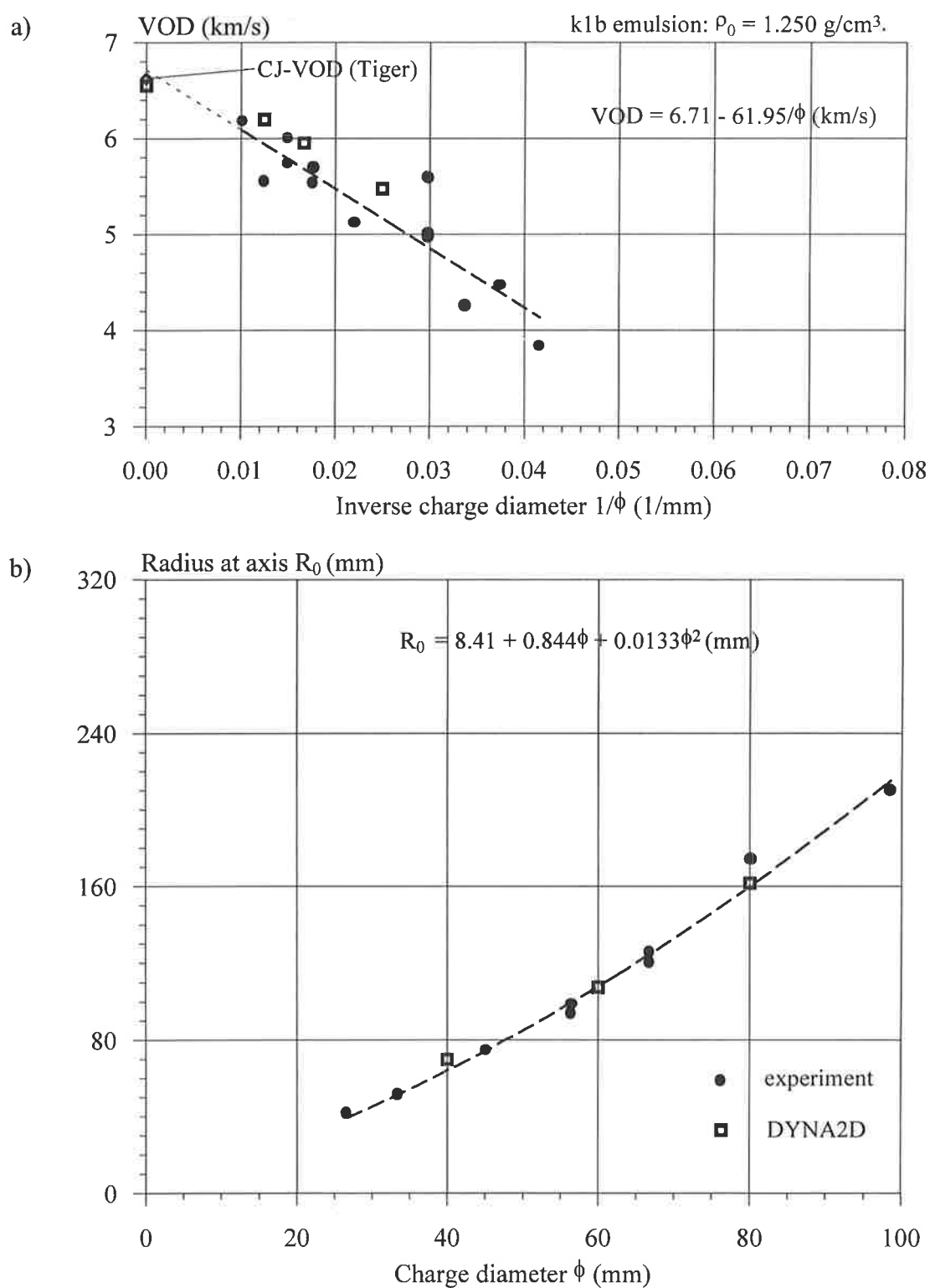


Figure A3-11 Comparisons of the VOD values (a) and the curvature radii at charge axis (b) by the DYNA2D computations with the experiments (k1b emulsion)

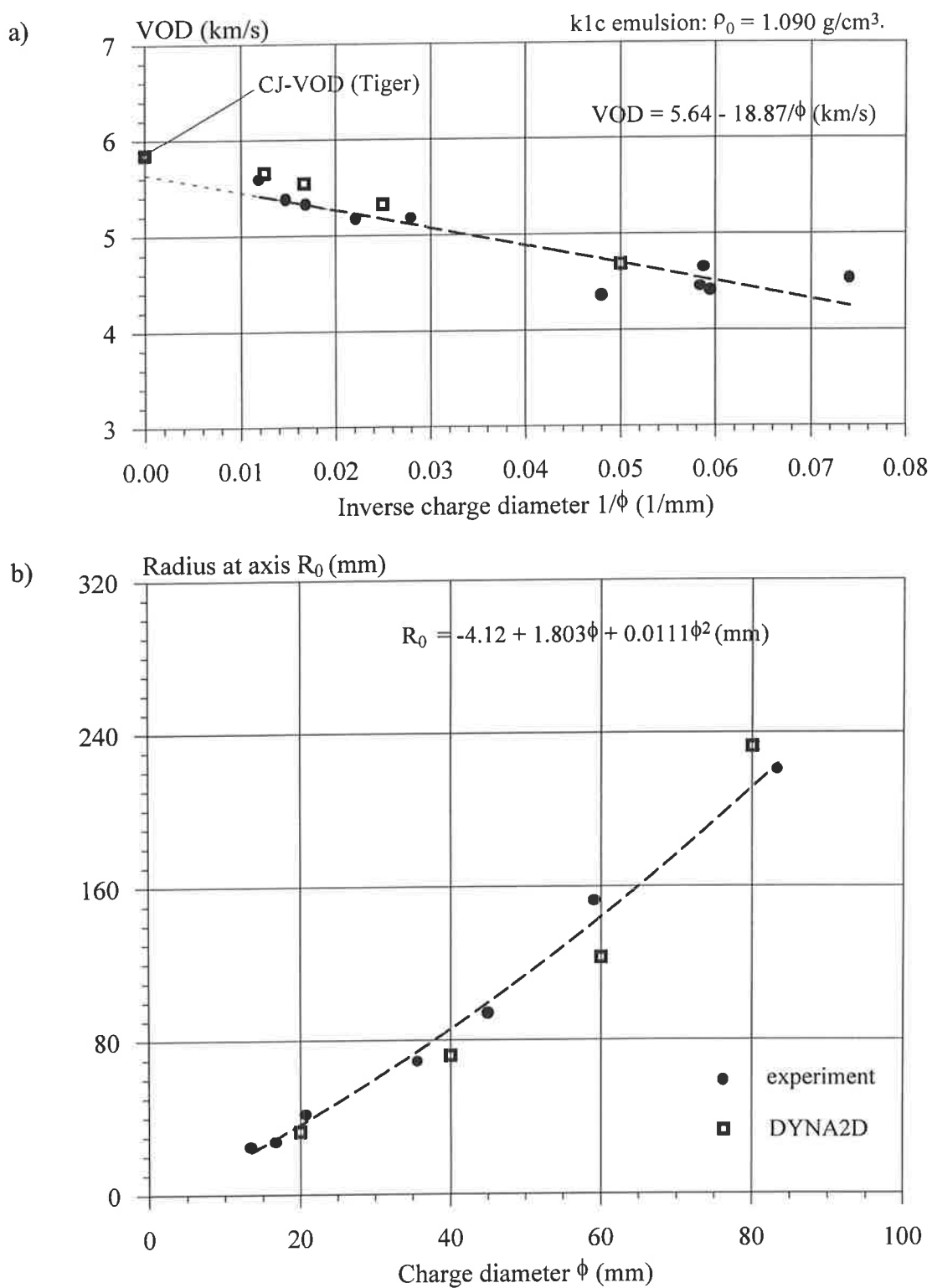


Figure A3-12 Comparisons of the VOD values (a) and the curvature radii at charge axis (b) by the DYNA2D computations with the experiments (k1c emulsion)

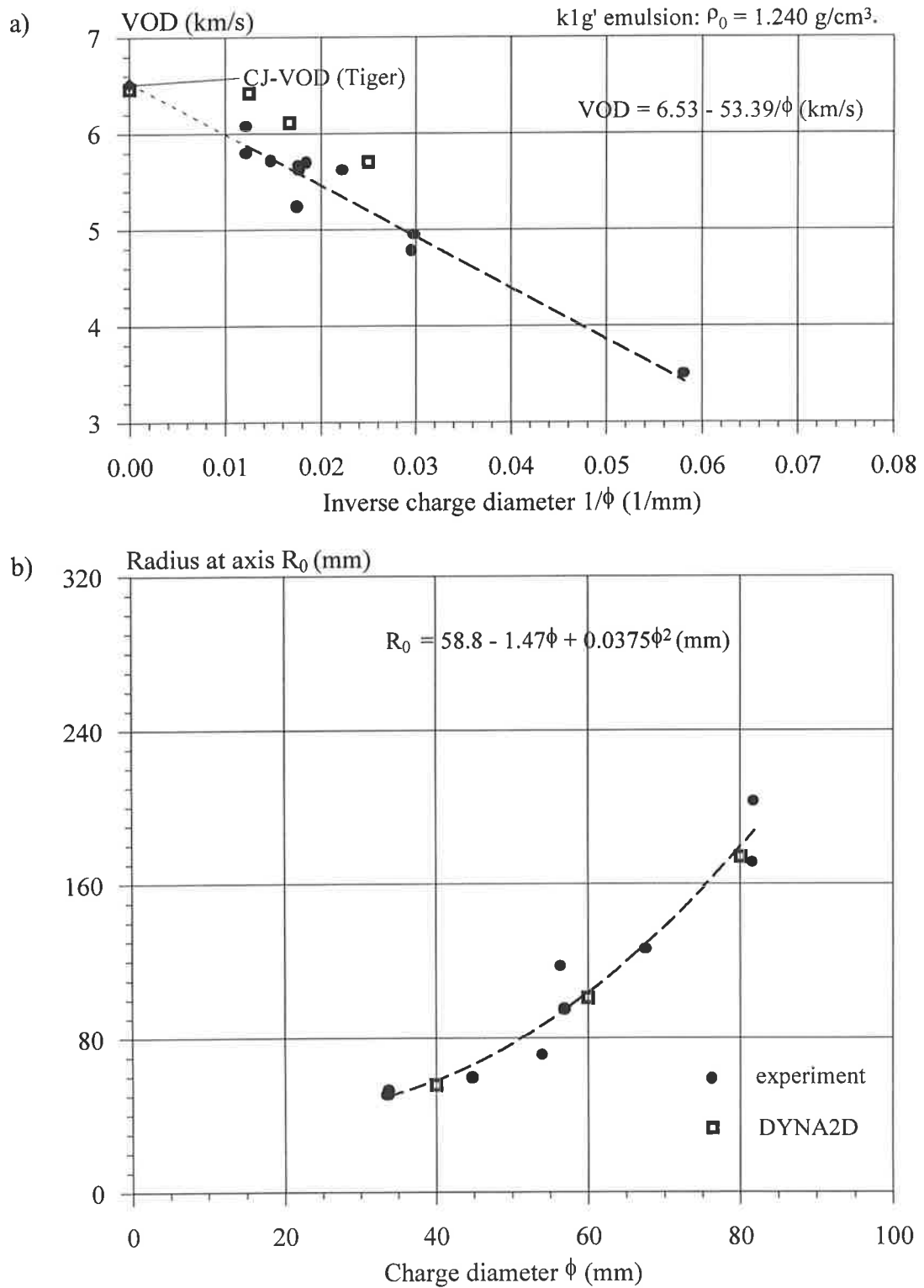


Figure A3-13 Comparisons of the VOD values (a) and the curvature radii at charge axis (b) by the DYNA2D computations with the experiments (k1g' emulsion)

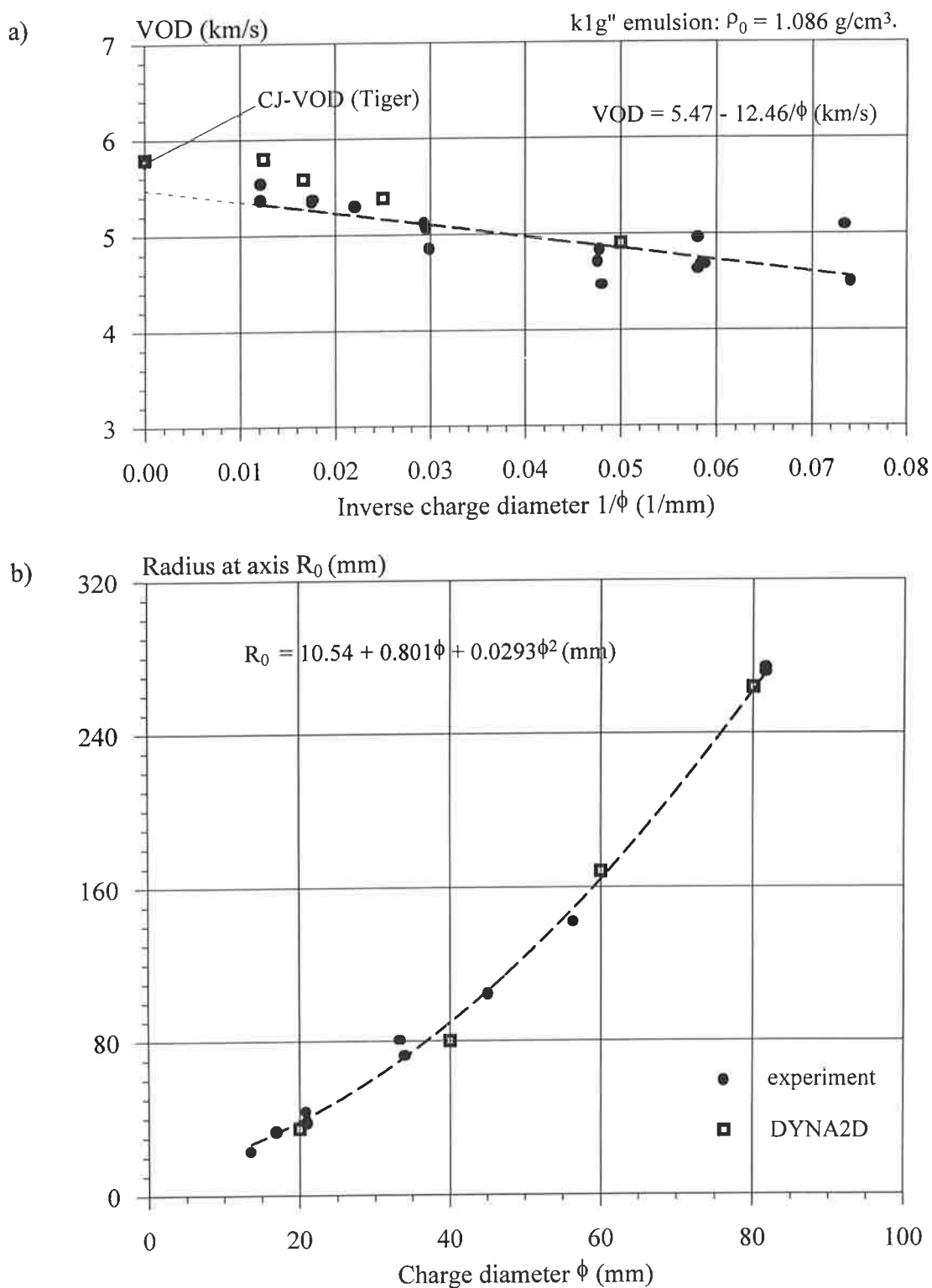


Figure A3-14 Comparisons of the VOD values (a) and the curvature radii at charge axis (b) by the DYNA2D computations with the experiments (k1g" emulsion)

A3.5 Relation between the Pressure Exponent γ and the Slope of $VOD(1/\phi)$

We have studied the relations between the experimental variables and the physical properties of the explosives in Appendix 1. To know the relationship among the burning rate parameters, the physical properties of the explosives and the experimental variables is very important for understanding the physics of the explosive burning process. Such relations will make the calibration of the burning rate parameters more efficient. Unfortunately very little has been done on this area.

We have found that the pressure exponent γ in the burning rate function A3-2 depends on the slope b in the experimental relation $D(1/\phi)$ (Equation A1-5). Figure 3-8 shows a linear relation between the two variables. Using this relation, the pressure exponent for a new emulsion explosive can probably be estimated relatively accurately before the actual calibration of the burning rate parameters takes place. This, according to our experience, will save much time during the calibration. It is our intention to see if this relationship holds for new emulsion explosives that we are going to test.

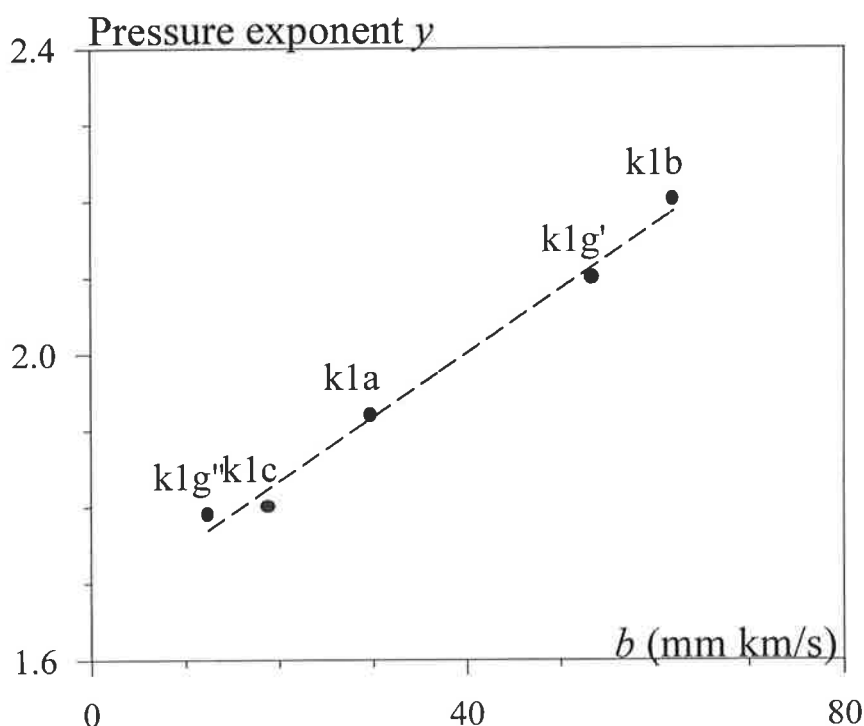


Figure A3-15 The pressure exponent γ in the burning rate function as a function of the slope b in the experimental function $D(1/\phi)$.

A3.6 Accuracy of the Computations by DYNA2D

The accuracy of the DYNA2D computations is determined by the accuracy of the input parameters for the emulsion explosives and by the element size. Here only the errors caused by using coarse cells in the computation models are going to be discussed.

1. The accuracy of the VOD values and the detonation front radii

We used uniform meshes with element sizes from 0,2×0,2 to 0,8×0,8 mm for charge diameters from 20 to 80 mm. This has proven enough to obtain stabilised VOD values and curvature radii. For the charges of 40 mm diameter, for example, 0,4×0,4 mm elements were used for the calibration computations. When smaller elements are used, the changes of the evaluated steady-state VOD values and curvature radii at the charge axis are negligible (see Table A3-4). Therefore, the element size used is sufficient for the calibrations when only the steady-state VOD values and the curvature radii of the detonation fronts are concerned. For the setups with smaller elements, we used shorter charges, with a constant length/diameter ratio, for the computations. Otherwise, the problem would be too large for our DYNA2D code to handle.

The charge with 80 mm diameter, where 0,8×0,8 mm elements were used, is the worst case. For most computations, the VOD values and the curvature radius of the detonation fronts stabilise within the given mesh limits. In some cases, they did not stabilise within the narrow intervals for the burning rate parameters. The reason is probably that the element size was too large and/or that the burning rate parameters were not properly chosen.

We have tested that smaller elements such as 0,5×0,5 mm will improve the computation stability for the charge of 80 mm diameter, but to use them throughout is beyond the capacity of our computer.

Table A3-4: Effects of element size on the calculated VOD and detonation front radii for emulsion k1a:

Element size (mm×mm)	0,4×0,4	0,2×0,2	0,1×0,1
VOD (km/s)	5,492	5,518	5,502
Radius at charge axis (mm)	65,17	64,75	65,37

2. Detonation zones

To resolve the detonation zone is another requirement for the element size. The detonation zones are resolved well for the computations of the 1D setups (see Figure A3-2), since smaller elements ($0,02 \times 0,02$ mm) are used. It is easy to evaluate the detonation zone lengths on these curves. Figure A3-16 shows that the detonation zone lengths are almost constant with element sizes from $0,01 \times 0,01$ to $0,05 \times 0,05$ mm.

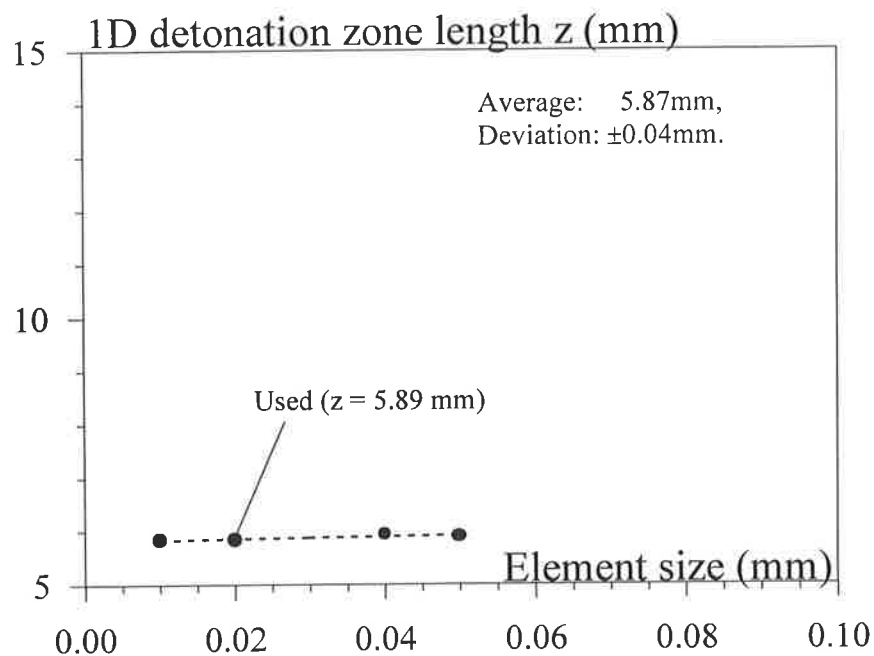


Figure A3-16 The evaluated detonation zone lengths for the computations with different element sizes (the 1D detonation).

For the detonations with finite diameters, larger elements were used for the computations. The detonation zones are not resolved completely. Figure A3-17 shows the oscillating pressures from the computations with the 40 mm diameter charges and $0,4 \times 0,4$ mm elements. The results show that the coarse elements used in the computations are not the sole reason for the oscillation, since the oscillation exists even for the case of $0,1 \times 0,1$ mm elements. The oscillation is probably caused by the boundary effect. The oscillation by the boundary effect is a physical phenomenon and can probably be enlarged by the coarse elements used.

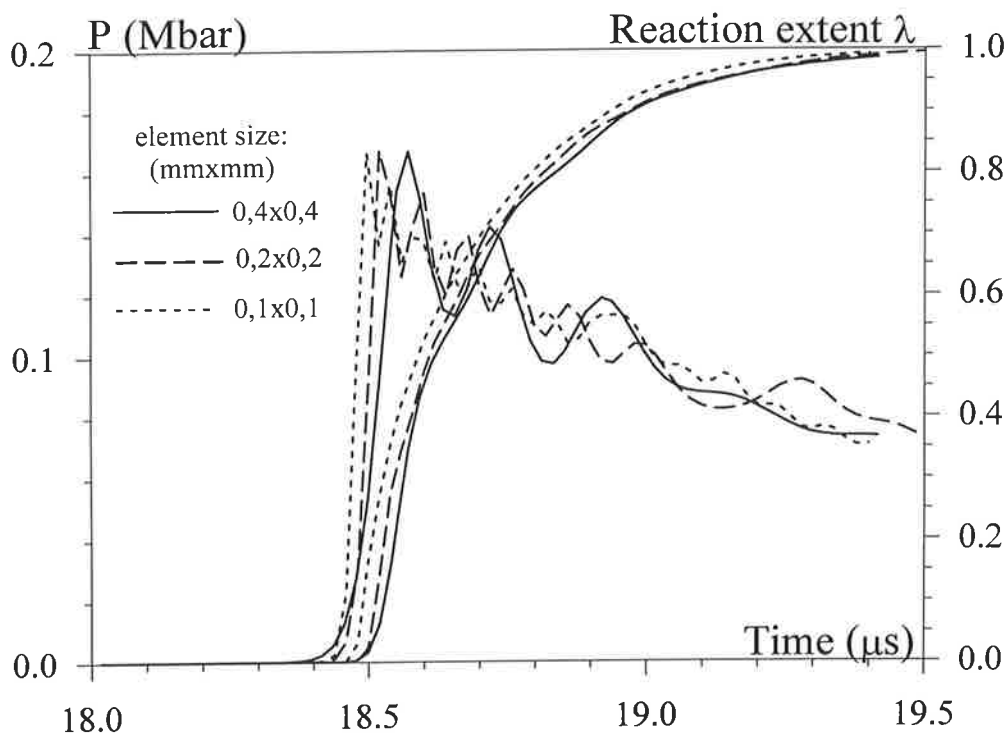


Figure A3-17 Pressures and reaction extents for steady-state detonations using different element sizes (k1a emulsion and $\phi = 40$ mm).

According to Kennedy (1995), about 20 elements along the detonation zone are needed to resolve the detonation zone completely. Our later analyses show that the detonation zone length is approximately 3 mm for the $\phi 40$ mm charge. The proper element size thus is 0,15×0,15 mm. Using such small elements is beyond the capacity of our computer.

For the finite diameter charges, the evaluation of the detonation zone length becomes more difficult, because of the oscillations of the computational quantities. The results, thus, are relatively inaccurate. This is discussed in Appendix 4.

A large number of the elements takes a long time to compute and more easily causes the computations unstable. Therefore, the 1D setup is still useful for the calibration even when a more powerful computer is available. The simple 1D setup takes a very short time to run. We have used 1D setup during the preliminary stage of the calibration, which would otherwise take much more time.

Appendix 4: Analyses of the Burning Models

After the burning rate models have been built, it is possible to study them closely. Here we will discuss some important features of our burning model, in comparison with other burning models.

A4.1 The 1D and 2D Detonations

In an ideal-detonation model like the CJ theory, an equation of state is used to describe the state of the fully reacted products. In the Ignition and Growth model, the reactive flow is described with the mixture of the unreacted emulsion and the fully reacted products. The way to describe the state of the reactive flow during detonation distinguishes the detonation theories.

For the truly 1D case, the Ignition and Growth model simulates the same process as the Tiger or Cheetah code does (using CJ theory), although different methods are used for the two codes. The JWL parameters used by the DYNA2D code are obtained from the Tiger/Cheetah computation. Therefore, the 1D detonations by the two codes should be the same, at least very close to each other. This characteristic can be used to check the accuracy of the DYNA2D computations.

In Figure A4-1, the Hugoniot of the unreacted emulsion and the isentrope of the fully reacted products (emulsion k1b) are plotted using the input parameters for the DYNA2D code. The one for the fully reacted products represents the 1D detonation by the Tiger code. The P - V curve by the DYNA2D computation of a real-life detonation is between those two curves and the points on the curve represent the states of the mixture of the inert emulsion and the fully reacted products. The burning rate parameters used in the DYNA2D calculation are listed in Table 3-1.

Table A4-1 shows a good agreement of CJ states by the Tiger and the DYNA2D codes.

The DYNA2D curve (the solid line) starts from the initiation point (on the Hugoniot of the unreacted explosive) and ends on the Tiger isentropic curve of the fully reacted products. The DYNA2D curve consists of three parts: the compression part, the rapid burning part and the isentropic expansion part. During the compression, the explosive

starts to burn (ignition) and the state point moves up rapidly to its top value but not the von Neumann point as in the ZND detonation. As the chemical reaction proceeds, the point moves down, along the Rayleigh line, to the CJ-state. After the CJ-state, the products expand along the isentropic curve.

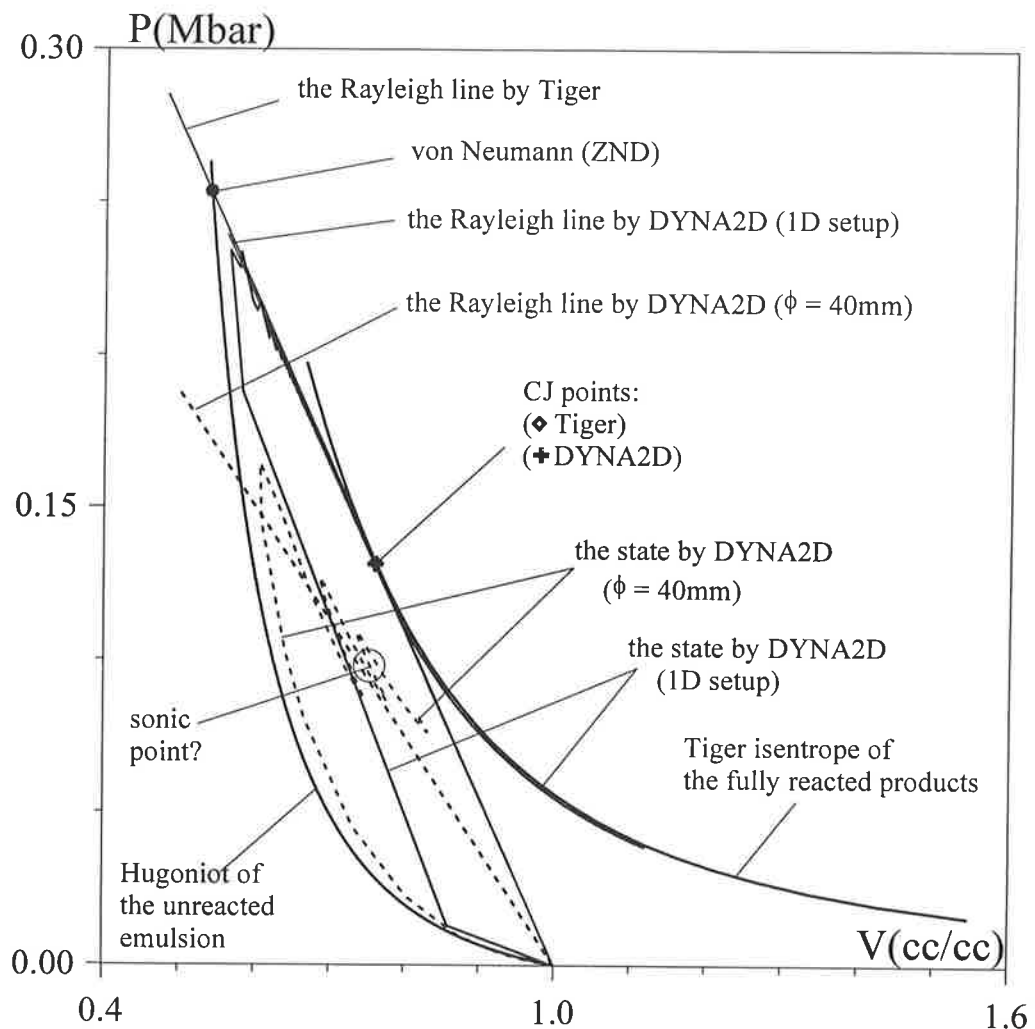


Figure A4-1 The P-V diagram for the steady detonation in emulsion k1b.

Table A4-1: Comparison of CJ states by the Tiger and the DYNA2D codes:

Code	VOD (km/s)	pressure (Mbar)	volume (cm ³ /g)	density (g/cm ³)
Tiger	6,622	0,1325	0,7602	1,315
DYNA2D	6,593	0,1305	0,7599	1,316

The differences of the non-ideal and ideal burning models can be seen from the 1D diagram. The CJ theory is the simplest one and no chemical reaction gets involved. The ZND theory simplifies the compressing ignition process by introducing the von Neumann point. The burning process is simply described by the states along the Rayleigh line from the von Neumann point, where $\lambda = 0$, to the CJ point, where $\lambda = 1$. Both theories describe the 1D detonation only.

It has been proven that the detonation of an explosive starts at a relatively low pressure, not at the von Neumann point (Lee & Tarver 1980).

The non-ideal detonation model (here, with help of the Ignition and Growth burning function) simulates the whole burning process, from the ignition by the shock compression to the isentropic expansion of the fully reacted products. In this burning function, the chemical reaction starts at a relatively low pressure, not at the von Neumann pressure like in the ZND theory. Thus this burning model describes the detonation process better than the other two models, simply because it simulates the non-ideality of the detonation process.

The differences between the non-ideal and ideal models are clearly demonstrated by the detonation with a charge of 40 mm diameter (the dot-lines). The pressure built in the explosive is rather low because of the radial loss of energy. The “Rayleigh line”, which is determined by the initial density of the explosive and the steady VOD value, is away from that in the 1D detonation. An ideal model can not simulate the 2D or 3D detonations correctly.

The relatively large elements used in the DYNA2D models and the charge boundary effects are responsible for the oscillation of the state curve, which causes the difficulties in defining the sonic point (see the next section).

Figure A4-1 shows also that the state of the 1D detonation, its sonic pressure, its steady-state VOD value and its isentropic expansion curve form the upper bounds of all 2D or 3D detonations.

A4.2 Detonation Zone Lengths

Detonation zone is the area between the shock front surface and the sonic surface. This is the area where conditions are subsonic and in which the high-pressure flow can catch up to the shock front and do work on it. Behind the sonic surface, the conditions are supersonic. Within the supersonic region, the flow has no influence on the shock front.

It is difficult to measure the detonation zone length, especially for non-ideal explosives such as emulsion explosives (Kirby and Leiper 1985). The concept is however very important in the study of the detonation properties of an explosive. Using the burning models, the detonation zone can be computed relatively easily. In the following, we have examined the 1D detonation zone length (the CJ set-up) and the zone length on the charge axis for the charges with finite diameters.

1. Detonation zone for the 1D detonation

For 1D set-ups, it is rather easy to locate the sonic point by examining the following condition (Johansson and Persson 1970):

$$D = C + U_p, \quad (\text{A4-1})$$

where D is the detonation velocity, C , the local sound velocity and U_p , the particle velocity. Since the DYNA2D code does not give the sound velocity as an output, it is calculated by the following equation:

$$C = \sqrt{-\frac{V}{\rho} \left(\frac{dP}{dV} \right)}, \quad (\text{A4-2})$$

where P is the pressure and $V = \rho_0 / \rho$ is the relative volume, where ρ_0 and ρ are the initial and the current densities of the explosive. From the sonic point, the detonation zone length can be calculated. Figure A4-2 shows an example of the determination of the sonic point for the 1D detonation. The estimated detonation zone lengths for the 1D detonation are listed in Table A4-2. Figure A4-3 shows that the detonation zone length is linear related to the VOD value for the infinite diameter, with an exception of emulsion k1b.

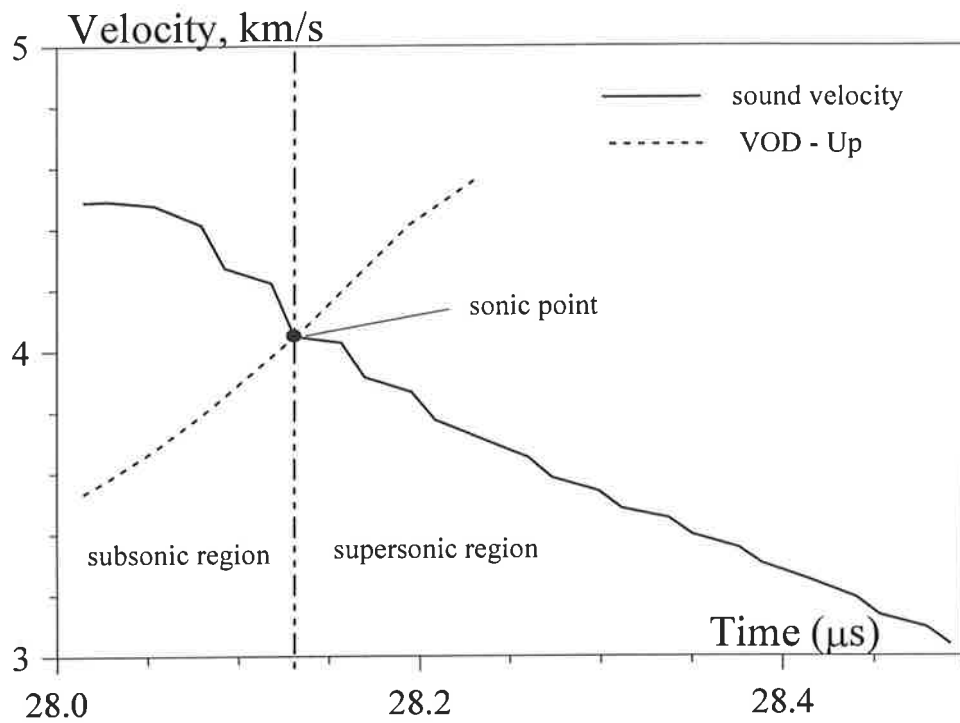


Figure A4-2 Determination of the sonic point for the 1D detonation (k1b emulsion).

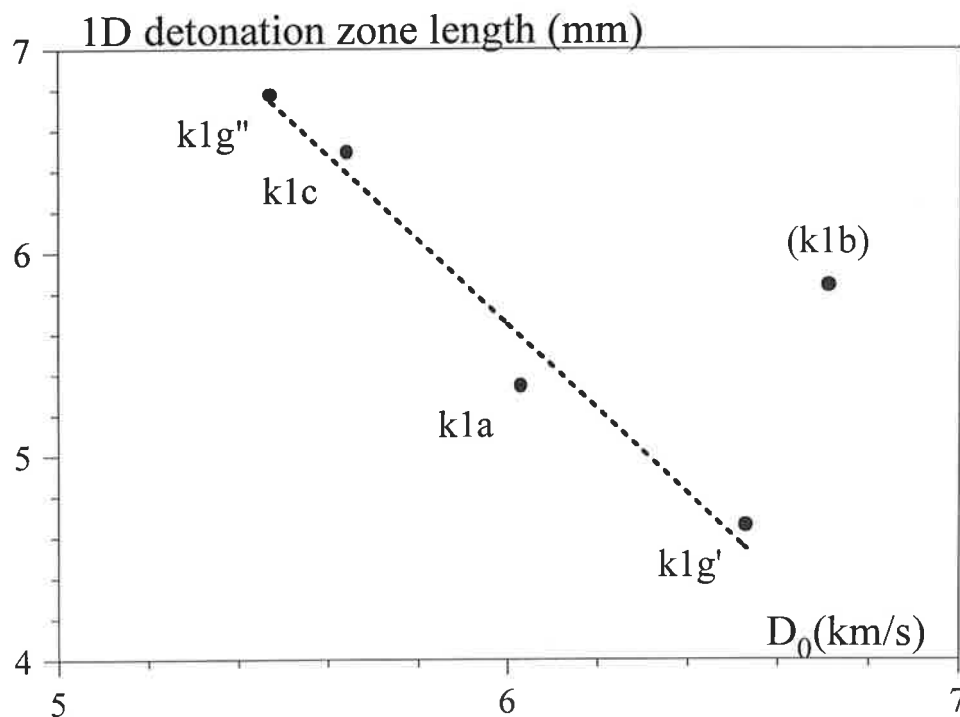


Figure A4-3 The relation between the detonation zone length and the VOD value for the 1D detonation.

2. Detonation zone for the 2D detonations

For the charges with finite diameters, it is more difficult to define the sonic point, since the pressure trajectories oscillate. The oscillations are probably caused by the relatively large elements used in the DYNA2D computations and the charge boundary effects. For example, elements of $0,8 \times 0,8$ mm were used for the charges of 80 mm diameter. It is not possible to use finer elements with this version of the DYNA2D code.

These oscillating pressure curves sometimes display two sonic points. This is a spurious numerical phenomenon, not a physical one. We use the last one as the sonic point, since the first one usually yields an incredibly thin detonation zone. The sonic point is then determined by Equation A4-1. The detonation zone lengths estimated for the finite diameter charges are thus relatively inaccurate.

For the 1D case, there is a unique detonation zone length everywhere. For the finite diameter cases, the zone length is a function of the distance from the charge axis and the zone lengths shown in the figure are those on the charge axes. The calculated detonation zone lengths at the charge axis are listed in Table A4-2. The results show that the detonation zone length generally decrease with decreasing charge diameter.

Table A4-2: The evaluated detonation zone lengths at the charge axis (mm):

explosive	ρ_0 (g/cm ³)	$\phi \rightarrow \infty$	$\phi = 80$ mm	$\phi = 60$ mm	$\phi = 40$ mm	$\phi = 20$ mm
k1a	1,165	5,339	5,657	3,713	3,404	-
k1b	1,250	5,840	5,398	5,765	3,964	-
k1c	1,090	6,490	6,575	3,843	3,517	2,720
k1g'	1,240	4,652	2,563	4,701	2,583	2,459
k1g''	1,086	6,773	2,746	3,744	3,482	-

3. Average detonation zone length for cylindrical charges

Based on 56 curvature measurements for 26 explosives, Souers (1997) has presented simplified expressions for the average detonation zone length. The simplest one is that it

is approximately equal to the edge lag of the detonation front on the charge surface:

$$\langle x_e \rangle \approx L_0, \quad (\text{A4-3})$$

where $\langle x_e \rangle$ is the average the detonation zone length and L_0 is the edge lag of the detonation front on the charge surface. The following equation is used to fit the experimental fronts:

$$L(r) = Ar^2 + Br^6, \quad (\text{A4-4})$$

where, r is the radial distance to the charge axis, L is the detonation front lag at distance r , and A and B are fitting constants. Thus the edge lag on the charge boundary is calculated as $L_0 = L(r_0)$, where r_0 is the charge radius.

The other is a functional relation between VOD size effect and detonation zone length in the following:

$$\frac{D}{D_0} = 1 - \frac{\langle x_e \rangle}{\sigma r_0}, \quad (\text{A4-5})$$

where D/D_0 is the ratio of the VOD value of the charge to the VOD value at the infinite diameter. For an unconfined charge, σ is a function of the variables $\langle x_e \rangle$ and r_0 (Souers 1997). Later Souers proposed another formula to calculate variable σ through the concept of the average angle of the detonation front $\langle \Theta \rangle$ (Souers & Garza 1998):

$$\sigma = \frac{1}{\cos\langle \Theta \rangle \sin\langle \Theta \rangle}, \quad (\text{A4-6})$$

where $\langle \Theta \rangle$ is the average angle between the direction normal to the detonation front and the charge axis at the average radius $\langle r \rangle = r_0/\sqrt{2}$. Combining Equations A4-5 and A4-6, the average detonation zone length can be expressed in the following:

$$\langle x_e \rangle = \frac{r_0(1 - D/D_0)}{\cos\langle \Theta \rangle \sin\langle \Theta \rangle}. \quad (\text{A4-7})$$

Using Equations A4-3 and A4-7 to the k1a emulsion, we obtain the calculated average detonation zone lengths for different charge diameters. The results are listed in Table A4-3. Figure A4-4 also shows the average detonation zone lengths for k1a using Equations A4-3 and A4-7.

Table A4-3: The average detonation zone lengths evaluated by Souers methods (k1a):

r_0 (mm)	D (km/s)	A	B	$\langle \Theta \rangle$ (deg)	$1 - D/D_0$ ¹⁾	σ	$\langle x_e \rangle$ ²⁾ (mm)	$\langle x_e \rangle$ ³⁾ (mm)
6,8	3,74	0,0247	$1,73 \times 10^{-6}$	24,5	0,364	3,08	1,28	10,2
8,5	4,35	0,0201	$6,76 \times 10^{-7}$	27,6	0,260	3,45	1,71	8,69
10,6	4,53	0,0158	$3,53 \times 10^{-7}$	31,7	0,230	3,59	2,28	9,18
10,85	4,53	0,0163	$8,85 \times 10^{-8}$	23,4	0,230	3,59	2,06	10,1
16,8	5,37	0,0084	$1,89 \times 10^{-8}$	23,4	0,087	4,97	2,78	6,80
19,0	5,35	0,0082	$9,63 \times 10^{-9}$	24,4	0,090	4,91	3,41	7,40
28,3	5,45	0,0047	$1,39 \times 10^{-9}$	22,5	0,073	5,26	4,44	10,2
39,3	5,64	0,0027	$4,18 \times 10^{-10}$	24,3	0,041	6,39	5,77	8,59

¹⁾: The VOD value at the infinite diameter $D_0 = 5,88$ km/s;

²⁾: The average detonation zone length by Equation A4-3;

³⁾: The average detonation zone length by Equation A4-7.

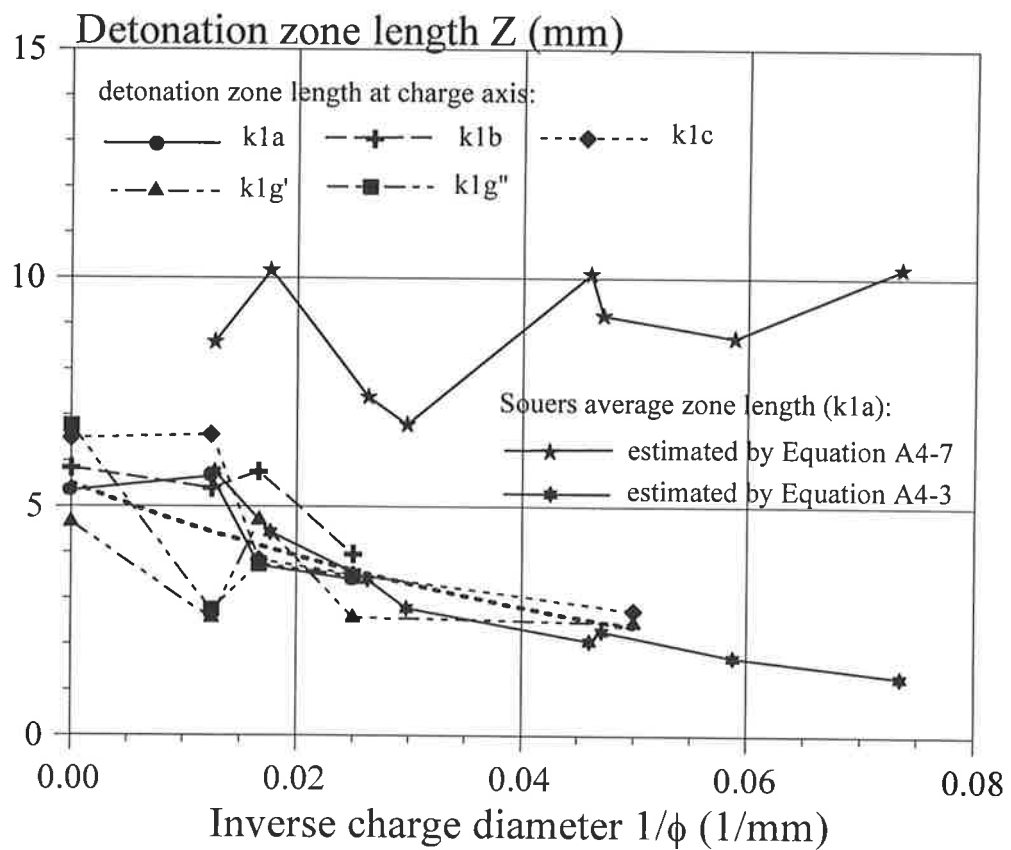


Figure A4-4: Relation of detonation zone length and inverse charge diameter.

The results show that the average detonation zone length is measured better by the edge lag L_0 (Equation A4-3) than that by the Equation A4-7. The interest thing is that the edge lag method was found only “approximately true” (Souers & Garza 1998). The new proposed ratio of the variables $\langle x_e \rangle$ and L_0 equals to $2,3 \pm 1,6$ instead of 1. Thus considerably longer detonation zone lengths can be expected. The detonation zone lengths estimated by Equation A4-7 are considerably longer than our values and show no overall influence of the charge size. This discrepancy demonstrates the necessity of a detailed description of the detonation process.

A4.3 Reaction Zone

The concepts of detonation zone and reaction zone are different. The reaction zone of a detonation ends on the surface where the chemical reaction is complete. For an ideal or 1D detonation, the chemical reaction is complete at the sonic surface, while for the non-ideal detonation, the reaction is not necessarily complete there. Table A4-4 shows that reaction extents at the sonic point on the charge axis lie within 68–99 % for charge diameters between 40 and 80 mm. In general the value decreases for small diameter charges where Table A4-4 shows a different tendency one may suspect that the routine used to determine the sonic surface lacks in accuracy.

The reaction zone for a non-ideal explosive, therefore, is usually longer than the detonation zone (Dussell 1997). This can be seen clearly by comparing the reaction zone lengths in Table A4-5 with the detonation zone lengths in Table A4-2.

Table A4-4: Reaction extents at the sonic point on the charge axis:

explosive	ρ_0 (g/cm ³)	$\phi = 80\text{mm}$	$\phi = 60\text{mm}$	$\phi = 40\text{mm}$
k1a	1,165	0,998	0,968	0,916
k1b	1,250	0,859	0,848	0,679
k1c	1,090	0,992	0,927	0,899
k1g'	1,240	0,938	0,983	0,926
k1g''	1,086	0,917	0,989	0,896

Table A4-5: The evaluated reaction zone lengths of the emulsion explosives (mm):

explosive	ρ_0 (g/cm ³)	$\phi = 80\text{mm}$	$\phi = 60\text{mm}$	$\phi = 40\text{mm}$
k1a	1,165	7,862	7,124	5,601
k1b	1,250	8,178	7,165	5,713
k1c	1,090	7,585	6,850	5,468
k1g'	1,240	8,369	7,302	6,039
k1g''	1,086	7,676	6,711	5,502