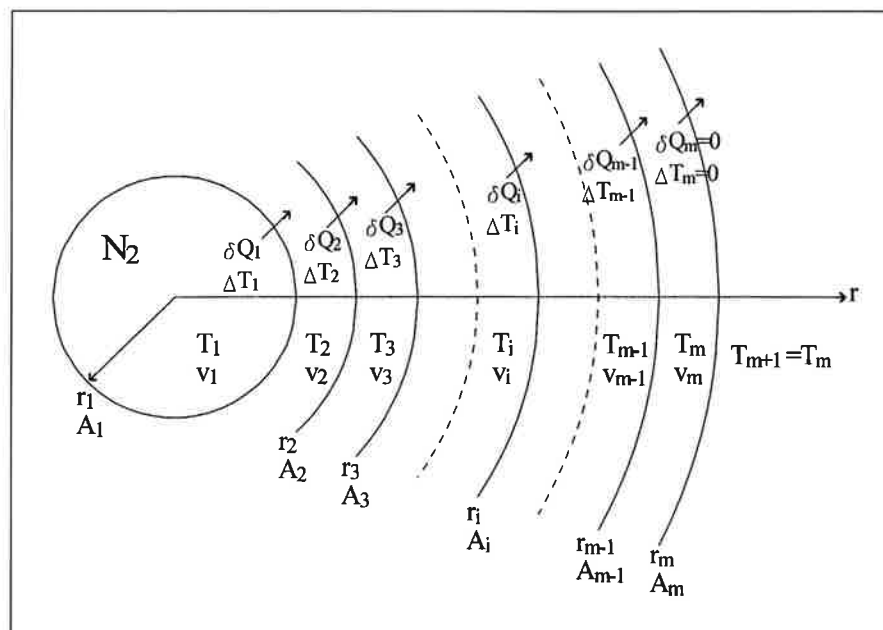




DYNAMIC DEAD-PRESSING OF A CHEMICALLY GASSED EMULSION EXPLOSIVE

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SWEDISH ROCK ENGINEERING RESEARCH
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**DYNAMIC DEAD-PRESSING
OF A CHEMICALLY
GASSED EMULSION EXPLOSIVE**

**Dynamisk dödpressning av ett kemiskt
gasat emulsionssprängämne**

Shulin Nie, Li Chen, SveBeFo

FÖRORD

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

Inom detoniken är en huvuduppgift att öka kunskaperna om sprängämnens verkningsätt, dvs att kunna beskriva detonationsförloppet i civila sprängämnen i sådan detalj att växelverkan mellan det detonerande sprängämnet och berget kan återges oberoende av håldiameter, bergegenskaper osv. För detta syfte har en brinnmodell tagits fram i form av en brinnekvation med materialdata för civila sprängämnen av emulsionstyp.

En annan huvuduppgift är att ge underlag till användning och utveckling av sprängämnen som är mindre känsliga för den tryckpåverkan som tidigare laddningar i en sprängsalva utsätter sprängämnet i ett borrhål för innan intieringstidpunkten. Sådana sprängämnen är en viktig del i att säkerställa att sprängsalvor uppnår avsedd funktion. Under perioden 1993-96 har SveBeFos arbete främst gällt dödpressning av gasade emulsioner och deras förmåga att återfå sin förmåga att detonera. Tidigare har motsvarande egenskaper studerats hos mikrosfärkänsliggjorda emulsionssprängämnen och ANFO.

I föreliggande rapport avrapporteras SveBeFo projekt 182. Instrumenterade dödpressnings- och återhämtningsförsök på en gasad emulsion i stålrör har utförts och simulerats genom en ny förklaringsmodell. I modellen upphettas sprängämnet runt gasbubblorna vid trycksättning dels av visköst arbete i matrisen, dels av adiabatisk komprimering av gasen. Det viskösa arbetet dominerar helt. När sprängämnet uppnår en kritisk temperatur startar en reaktion som leder till detonation.

Dödpressningen förklaras av gasbubblornas volymminskning när sprängämnet trycksätts och värmeledningen till matrisen vilka medför att sprängämnet vid ny stötvågspassage inte kan uppnå erforderlig initieringstemperatur. Detta tar några ms. Vid momentan tryckavlastning sker återhämtningen 10-100 gånger snabbare när gasen i bubblorna, som under expansion först kyla under matrisen temperatur, genom värmeledning återtar sin utgångstemperatur. Förklaringsmodellen stöds av försöken och kan härigenom medverka till att förstå och åtgärda bl.a. dödpressningsproblem.

En referensgrupp bestående av representanter för Nitro Nobel, Kimit och FOA har följt forskningsarbetet och givit värdefulla bidrag till det.

Stockholm i januari 1997

Finn Ouchterlony

SUMMARY

The detonability of a chemically gassed emulsion explosive has been studied in recent tests, after the study of three micro-balloon-sensitized emulsion explosives. Blasting experiments in steel pipes and computer simulations have been carried out. This study showed that the tested explosive can tolerate a pressure of 17 MPa before it is dead-pressed. The explosive can also recover its detonability after the pressure vanishes. Furthermore, the computer simulation showed that the dead-pressing and the detonability recovery are very rapid processes, approximately 2 ms for the dead-pressing and 50 ns for the detonability recovery. These simulation results are consistent with the experimental evidence. This report describes the study of the chemically gassed emulsion explosive. The properties of the explosive, experimental design and procedure, simulation principle and algorithm as well as the final results are described.

Keywords: Emulsion explosive, dead-pressing, pressure desensitization, chemical gassing, initiation mechanism, detonability recovery.

SAMMANFATTNING

Initierbarheten av ett kemiskt gasat emulsionssprängämne har studerats i den senaste försöksserien, efter att tre mikroballengkänsliggjorda emulsionssprängämnen tidigare har studerats. Sprängförsök i stålrör och datasimulering har utförts. Studien visade att detta sprängämne kan klara av ett tryck av 17 MPa innan det blir dödpresat. Sprängämnet kan också återhämta sin initierbarhet när trycket är förbi. Dessutom har simuleringen visat att både dödpresnings- och återhämtningsprocessen är mycket snabba. Det tar ca 2 ms för dödpresning och 50 ns för återhämtning. Dessa simuleringsresultat överensstämmer väl med försöket. Rapporten beskriver undersökningen av det kemiskt gasade emulsionssprängämnet. Sprängämnets egenskaper, den experimentella uppställningen och proceduren, simuleringsprincipen och algoritmen samt slutresultaten redovisas.

Nyckelord: emulsionssprängämne, dödpresning, kemisk gasning, initieringsmekanism, återhämtning.

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1. INTRODUCTION

The phenomenon of pressure desensitization of industrial explosives such as ANFO and emulsion explosives has been studied at SveBeFo in a series of research projects. The problem has been approached from two major aspects, namely, a) how much pressure an explosive may be exposed to in rock blasting practice and b) how much pressure the explosive can stand without being dead-pressed. Meanwhile the mechanism of dead-pressing and detonability recovery was also studied.

Results have been obtained in both research areas. In the first area, a pressure gage has been developed /1/ and pressure profiles in boreholes have been measured /2/. In the second aspect, testing methods for ANFO and emulsion explosives respectively have been developed /3, 4/. One ANFO and three emulsion explosives sensitized by glass micro-balloons have been studied /3, 5/.

After the studies of the three micro-balloon sensitized emulsions, a further study has been carried out on a chemically gassed emulsion explosive, which will be described in this report. The experimental technique, the computer simulation and the results achieved are described.

2. PREPARATION AND PROPERTIES OF THE GASED EMULSION EXPLOSIVE

2.1 Preparation and the physical properties of the gassed emulsion explosive

The tested explosive is the fourth emulsion explosive in our testing series. The main difference between this explosive and the other three explosives is the different sensitizer used. Namely, this explosive is sensitized by the means of chemical gassing instead of micro-balloons. The matrix of this explosive is essentially the same as those in the previous three explosives /5/. However, since the chemical gassing process introduces a small amount of water into the explosive, the water content of the matrix is reduced accordingly during the manufacturing, which was carried out by Nitro Nobel AB. Therefore, the density of this matrix is slightly higher than the previous ones. The properties of this chemically gassed emulsion explosive are listed in Table 1, together with other three tested explosives for the convenience of comparison.

Table 1: Properties of the tested explosives.

Explosive	Matrix density (kg/m ³)	Explosive density (kg/m ³)	Sensitizer			VOD in ϕ 52 mm steel pipe (m/s)
			Type	Wt-%	Vol-%	
1	1320	1200	Q-CEL 719	1.70	10.7	5812
2	1320	1210	Q-CEL 723	2.05	10.7	—
3	1320	1210	B37/2000	3.26	10.7	6249
4	1360	1200	Gassing	0.011*	11.76*	—

*: see the calculation in Section 5.2.4.

A batch of matrix of about 200 kg was manufactured for this experiment. Then, the matrix was chemically gassed using the technique provided by the Nitro Nobel AB. The gassing agent is essentially a solution of sodium nitrite (NaNO_2).

The final density of the explosive after 24 hours of gassing was designed to be 1200 kg/m^3 . In the normal blasting practice, the gassing process takes only few minutes. However, in this study, we had to retard the reaction, since it is desirable to charge the explosive mixture into the pipe before the gas bubbles are formed. In such a way, the gassing reaction takes place inside the pipe and the bubbles are protected from possible damages caused by the charging processes. Also, the viscosity of the explosive is much lower before the forming of the bubbles, which facilitates the charging process. Thus, preliminary laboratory experiments have been carried out in order to achieve the right gassing speed and the designed final density. The amount and the concentration of the gassing agent have been determined by these laboratory experiments. Figure 1 is a typical gassing diagram which shows the decrease of the explosive density with time after the addition of the gassing agent. It was found that the gassing technique is reliable and the gassing process is very reproducible.

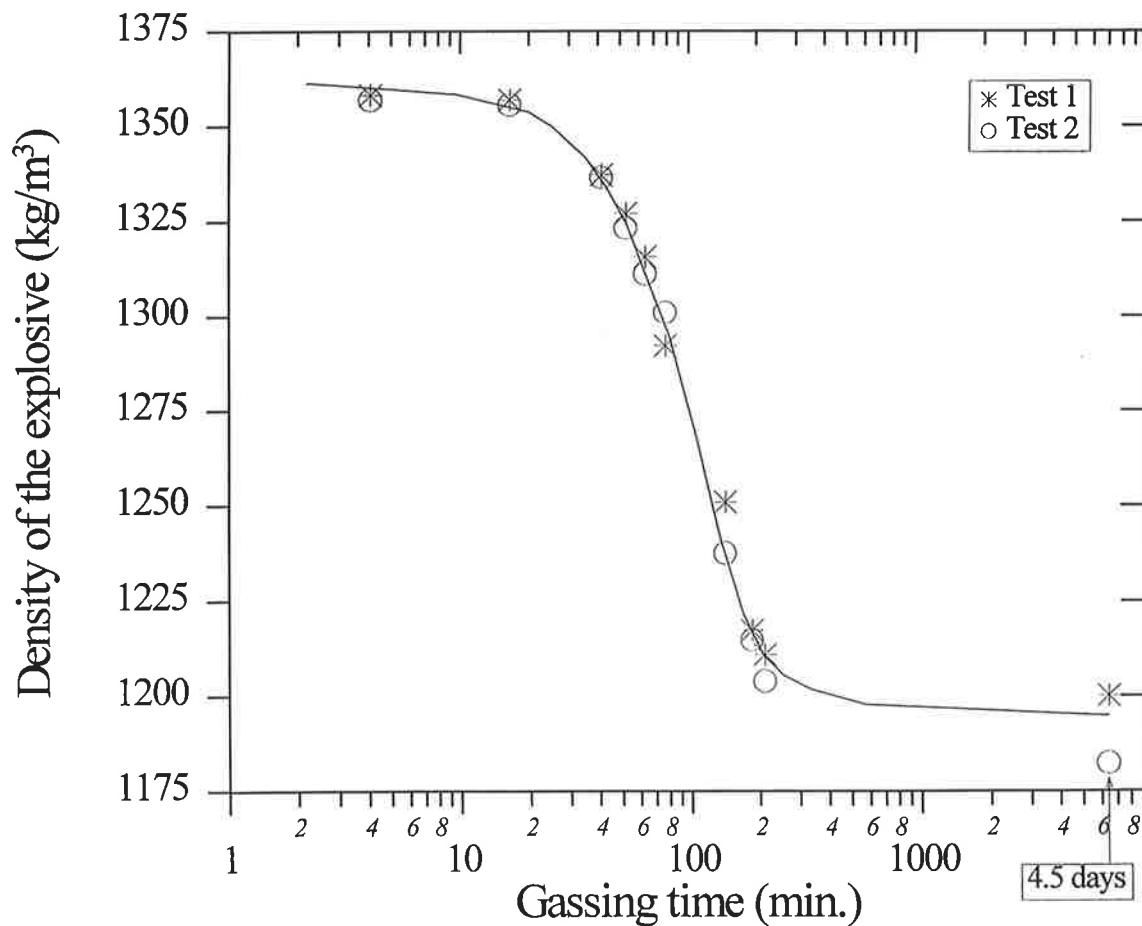


Fig. 1: A typical gassing diagram achieved in the laboratory experiments.

2.2 The critical density of the matrix

Besides the properties mentioned in Table 1, the critical density of the matrix was determined. The "critical density" is defined as the maximum density of the explosive containing this matrix, at which the explosive may be detonable. In other words, if the density of the explosive exceeds this critical density, it will not detonate. If the density of the explosive is below the critical density, it will be detonable.

The critical density of the matrix was determined by a series of initiation tests, in which the explosives were confined in the same type of steel pipes and initiated by the same kind of primer as used in all other detonability experiments described in /5/. The size of the steel pipes is 52 mm in inner diameter and about 1.5 m in length. The velocity of detonation was measured continuously along the whole charge length using the VODR-1 instrument. The signals together with the regression lines can be seen in APPENDIX I.

The explosives in this test series were prepared by mixing the matrix with various amount of Q-CEL 719 glass micro-balloons (GMB) to achieve different densities.

The critical density of the matrix was determined to be 1270 kg/m³. The detailed results can be seen in Table 2 and Fig. 2. It means that if an emulsion explosive containing this matrix is compressed to a density of 1270 kg/m³, it will lose its detonability, even in the confinement of a steel pipe.

Table 2: Determination of the critical density of the matrix.

Test No.	Explosive density (kg/m ³)	Velocity of detonation (m/s)
1	1249	4704
2	1257	5724
3	1260	5660
4	1262	5018
5	1263	6056
7	1266	0
8	1267	5955
9	1270	5493
10	1276	0

3. TESTING METHOD AND PROCEDURE

The set-up of the experiment is actually the same as used in the earlier tests /5/. However, it is still shown in Fig. 3. The steel pipe measures 52 mm in inner diameter, 4 mm in wall thickness and approximately 1.5 m in length. After the clay buffer was placed in the right position, the matrix was properly mixed with the gassing agent according to the recipe determined by the laboratory experiments, see Section 2.1. Then the mixture was charged into the steel pipe with the help of a vacuum pump, as illustrated in Fig. 4. Since the viscosity of the mixture is low before the gassing process starts, this charging method worked excellently.

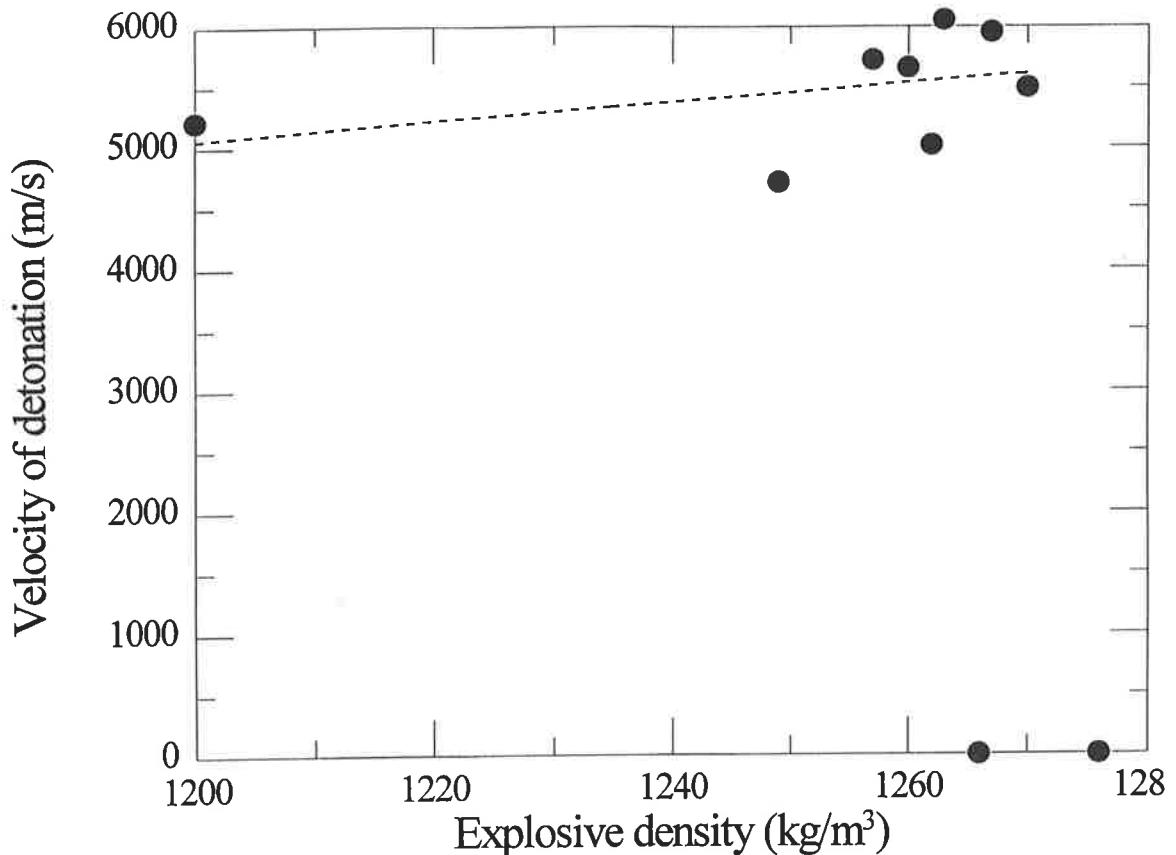


Fig. 2: Dependence of the velocity of detonation on the density of the explosive containing the testing matrix and Q-CEL 719 micro-balloons.

After the charging, the mixture was left for the gassing process for approximately 24 hours. The explosive obtained then has a density around 1200 kg/m³.

Just before the blasting experiment, the pressure gages, black powder and a primer were sequentially loaded. The signals from the piezo ceramic pressure gages /1/ were recorded by a LeCroy digital oscilloscope. The primer consisted of a No. 8 electrical delay detonator and a booster of 50 g pressed PETN and TNT.

After the initiation of the black powder and the detonator, the detonability of the emulsion explosive was determined by visual examinations on the test site. If the explosive was dead-pressed, a length of steel pipe, usually about 1 m, could be recovered and the explosive was spread around. Otherwise, neither the pipe nor the explosive could be recovered.

Attempts have been made to measure the velocity of detonation (VOD) continuously along the steel pipe using the VODR-1 instrument. However, since some damages had occurred to the VODR-1 instrument at that time, no meaningful information of VOD was obtained. Thus, the performance of the explosive in different blasts could not be quantified. Nevertheless, it has been observed that the performance of the explosive was different in different blasts in terms of ground vibration and shock wave in the air, depending on the pressure it has been exposed to.

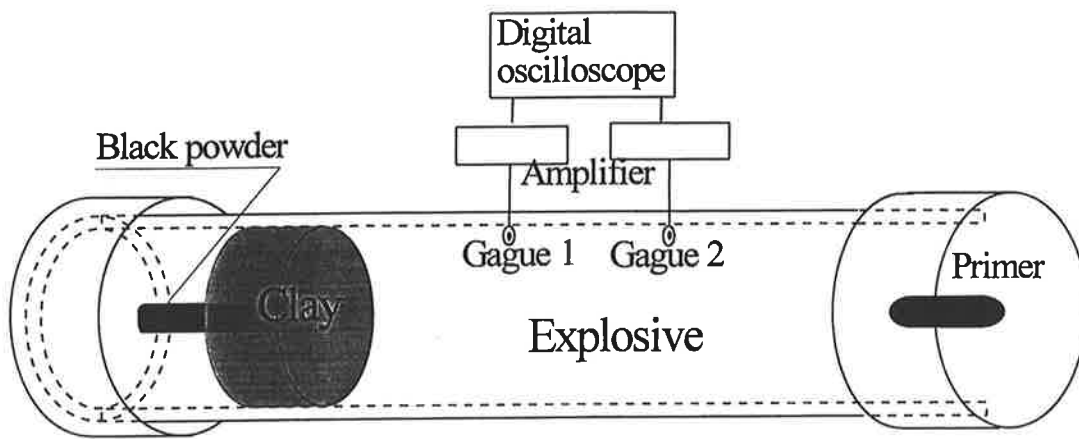


Fig. 3: Method used to test the detonability of emulsion explosives under dynamic pressure in steel pipe.

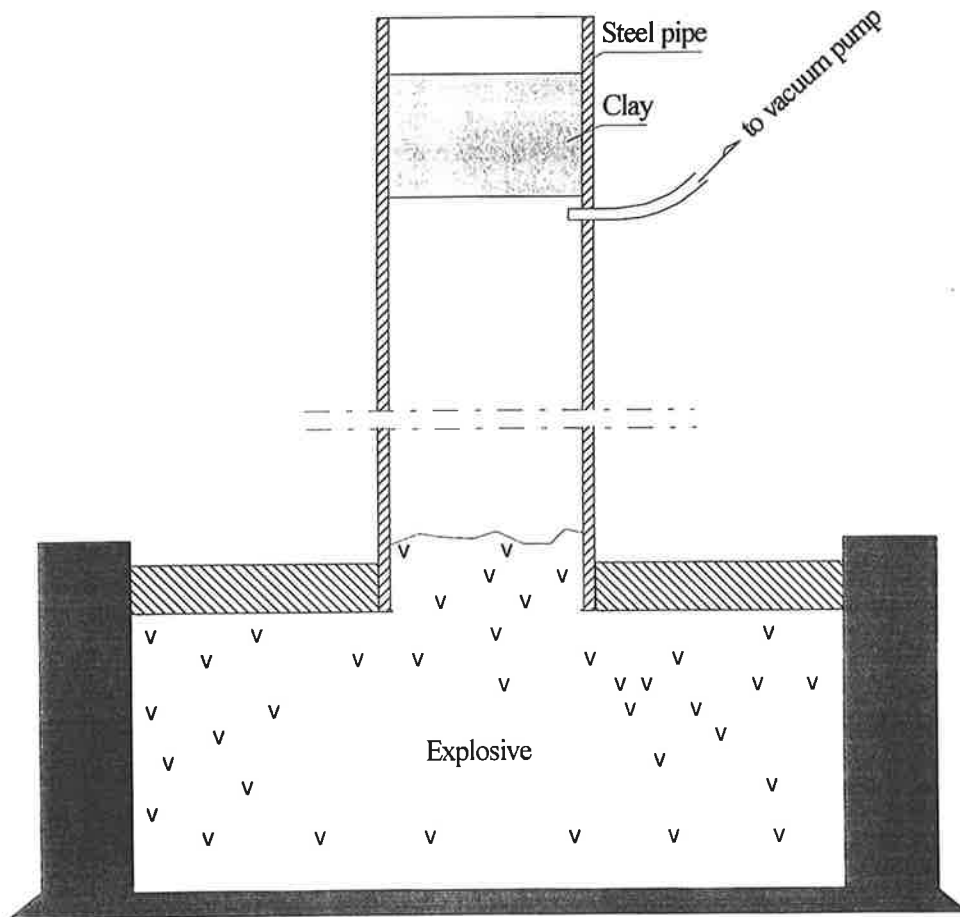


Fig. 4: Illustration of the charging method based on a vacuum pump.

4. DETONABILITY OF THE GASED EMULSION EXPLOSIVE

4.1 Analysis of the testing results

The testing results regarding the detonability of the gassed emulsion explosive are gathered in Table 3. Records of the pressure histories are shown in APPENDIX II. The detonability results are plotted as a function of the peak compression pressure and the waiting time in Fig. 5 or as a function of the momentary compression pressure (as defined below) and the waiting time in Fig. 6.

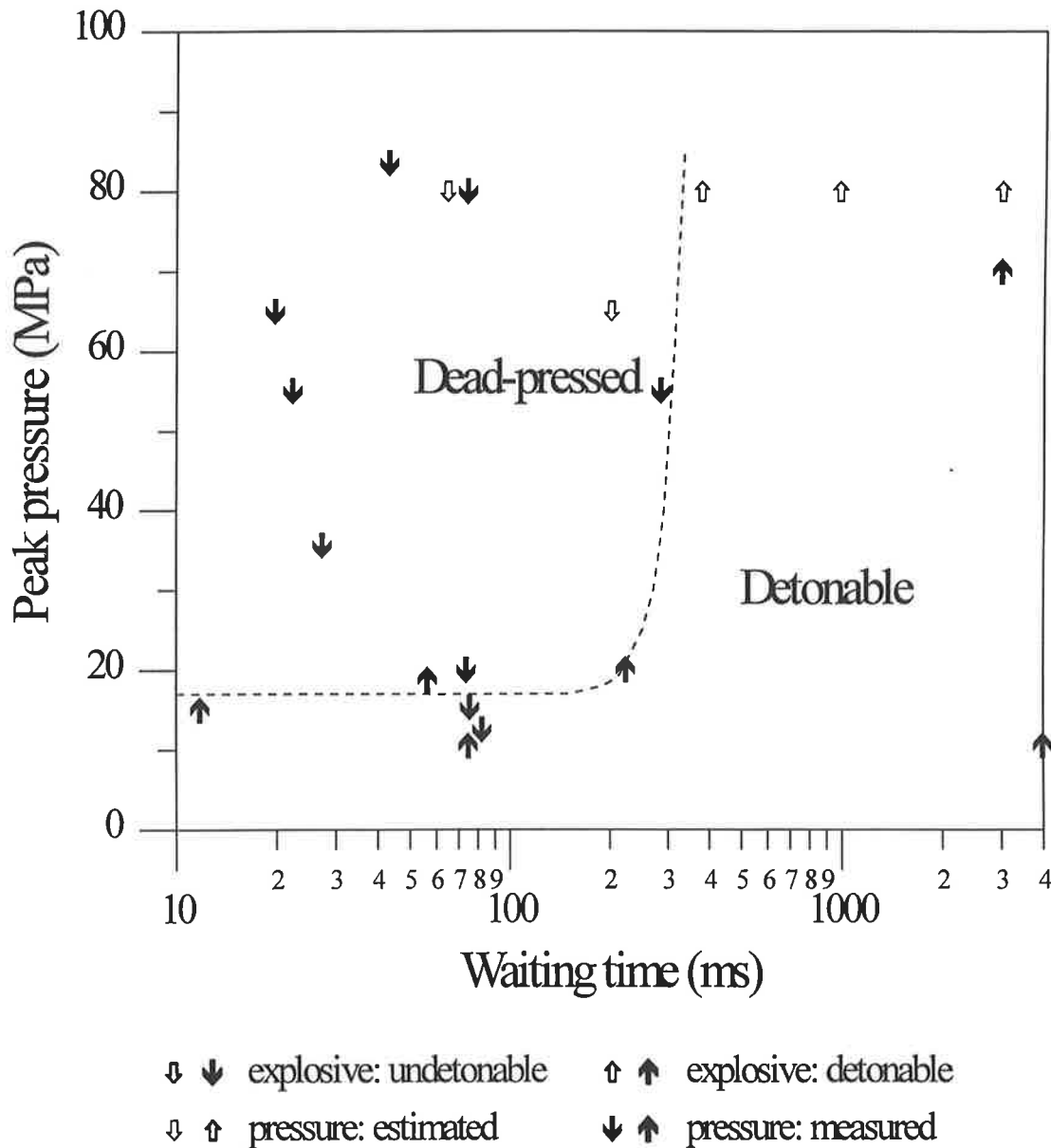


Fig. 5: Detonability of the chemically gassed emulsion explosive under dynamic pressure, plotted as a function of the peak compression pressure and waiting time.

Table 3: Detonability of the chemically gassed emulsion explosive.

Test No.	T1 ^① (ms)	T2 ^② (ms)	V12 ^③ (m/s)	Tp ^④ (ms)	Tf ^⑤ (ms)	Waiting Time ^⑥ (ms)	Black powder (g)	Peak pressure (MPa) ^⑦			Momentary pressure (MPa) ^⑧			Detonable (Y/N)
								Gage 1	Gage 2	Estimated	Gage 1	Gage 2	Estimated	
1	29.94	32.11	138.2	35.73	100*	64	10.0	>6	>6.4	80	—	—	—	N
2	21.8	23.97	138.2	27.59	400*	372	10.0	>34	>37	80	—	—	—	Y
3	22.98	25.16	137.6	28.79	3000*	2971	10.0	>22	>18.5	80	—	—	—	Y
4	24.93	26.75	164.8	29.78	3000*	2970	15.0	70	?	70	—	—	—	Y
5	23.75	25.42	179.6	28.20	1000*	972	15.0	>72	>74	80	—	—	—	Y
6	19.94	22.21	132.2	25.99	82.19	56.20	7.5	20	17.5	18.8	19.5	15.4	17.5	Y
7	21.50	23.51	149.3	26.86	110.26	73.40	10.0	>90	80	80	>90	75.5	75.5	N
8	19.72	21.72	150.0	25.05	100.47	75.42	8.5	12.5	18	15.3	7	13	10	N
9	21.92	24.23	129.9	28.08	101.60	73.52	7.5	?	20	20	?	13.5	13.5	N
10	22.43	25.02	115.8	29.34	111.36	82.02	6.0	12.5	12.5	12.5	11.6	11.1	11.4	N
11	24.59	27.28	111.5	31.76	106.37	74.61	5.0	10.5	10.5	10.5	9.9	9.4	9.7	Y
12	19.90	22.47	116.7	26.75	4000*	3973	6.0	10.5	>10.5	10.5	—	—	—	Y
13	18.59	20.99	125.0	24.99	247.41	222.42	7.5	>20	20	20	>20	15.3	15.3	Y
14	—	—	—	—	200*	200*	9.0	—	—	65	—	—	—	N
15	21.31	23.22	157.1	26.40	69.09	42.69	10.0	86	81	83.5	84	58.5	71.3	N
16	25.21	27.03	164.8	30.06	52.25	22.19	12.0	50	60	55	44	54	49	N
17	29.78	31.82	147.1	35.22	54.87	19.65	9.0	65	?	65	48	?	48	N
18	20.27	22.46	137.0	26.11	53.36	27.25	8.0	32	39	35.5	32	35	33.5	N
19	25.54	28.21	112.4	32.66	44.40	11.74	6.0	14	16	15	13	12.7	12.9	Y
20	24.72	26.29	191.1	28.91	—	—	15.0	93	?	93	—	?	—	—
21	24.33	26.09	170.5	29.02	311.36	282.34	12.0	?	55	55	?	33	33	N

①: T1 = pressure arrival time at Gage 1.

②: T2 = pressure arrival time at Gage 2.

③: V12 = average velocity of the pressure wave between Gage 1 and 2 where the distance is 300 mm.

④: Tp = pressure arrival time at the primer. The distance from Gage 2 to the primer is 500 mm and the pressure wave velocity is assumed to be V12, i.e. $Tp = T2 + 500/V12$.

⑤: Tf = primer firing time.

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⑥: Waiting Time = $Tf - Tp$.

⑦: Peak pressure = the maximum pre-compression that the explosive had subjected to

⑧: Momentary pressure = the pre-compression that the explosive was subjected to at the initiating moment.

*: When these times can not be measured from the pressure signals, they are taken as the nominal delay times in the detonators.

?: The pressure history did not give useful information. In some cases, the reason could be identified as damage in the cable.

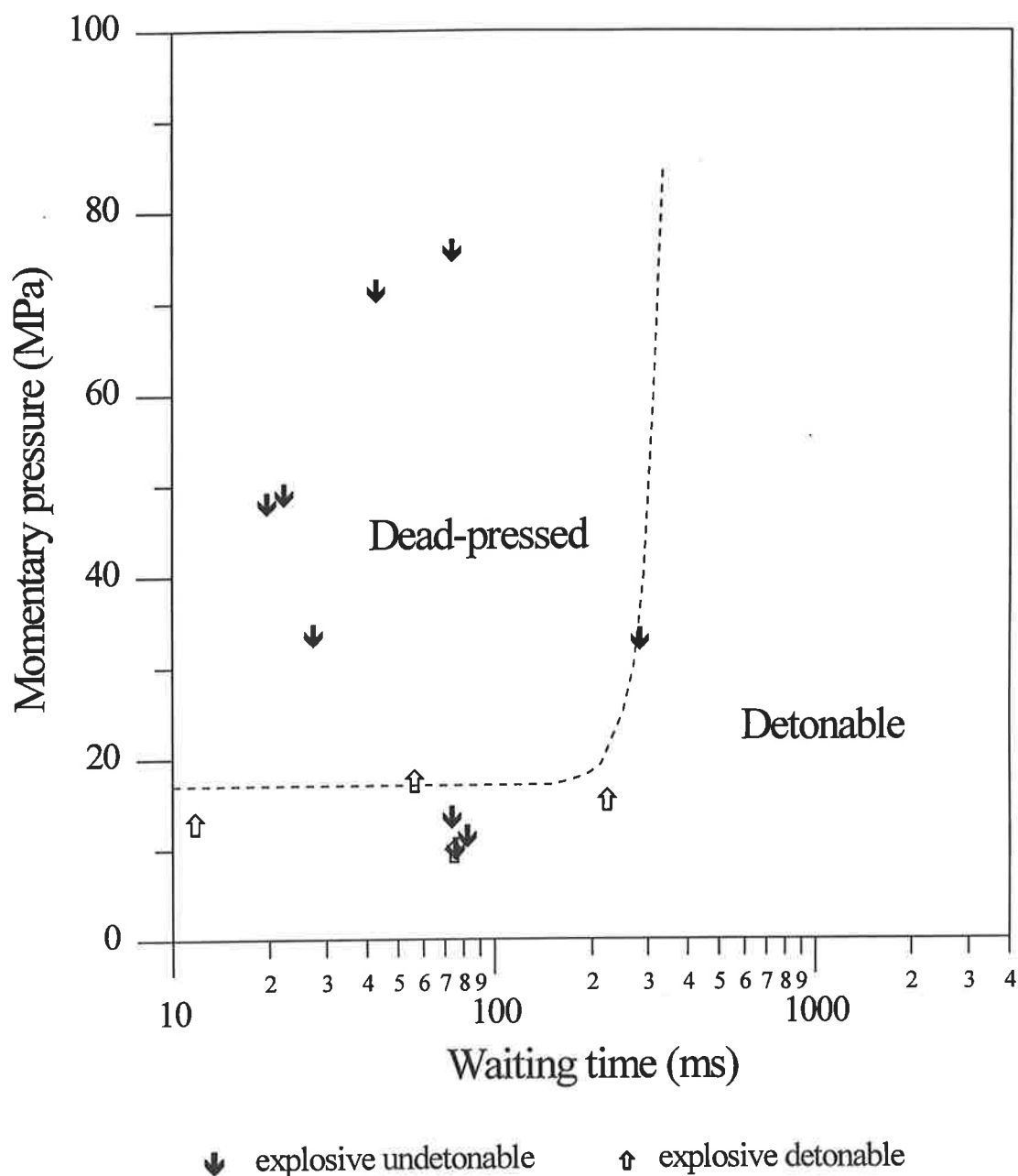


Fig. 6: Detonability of the chemically gassed emulsion explosive under dynamic pressure, plotted as a function of the momentary compression pressure and waiting time.

The same definitions of waiting time and peak pressure were used for the analysis of this test series as used for the three explosives tested earlier /5/. Namely, the waiting time is the time delay between the arrival of the pressure at the explosive and the initiation of the explosive by the primer, see also Table 3.

The concepts of the peak pressure and the momentary pressure are illustrated in Fig. 7. The momentary pressure is defined as the pre-compression on the explosive at the moment of initiation. This momentary pressure was read from the pressure history. No consideration has been taken of the time constant of the recording system. However, in those blasts where the momentary pressure could be measured, the corresponding waiting times are short, less than

80 ms for most of them, see Table 3 and Fig. 6. Therefore, the influence of the time constant is little for them.

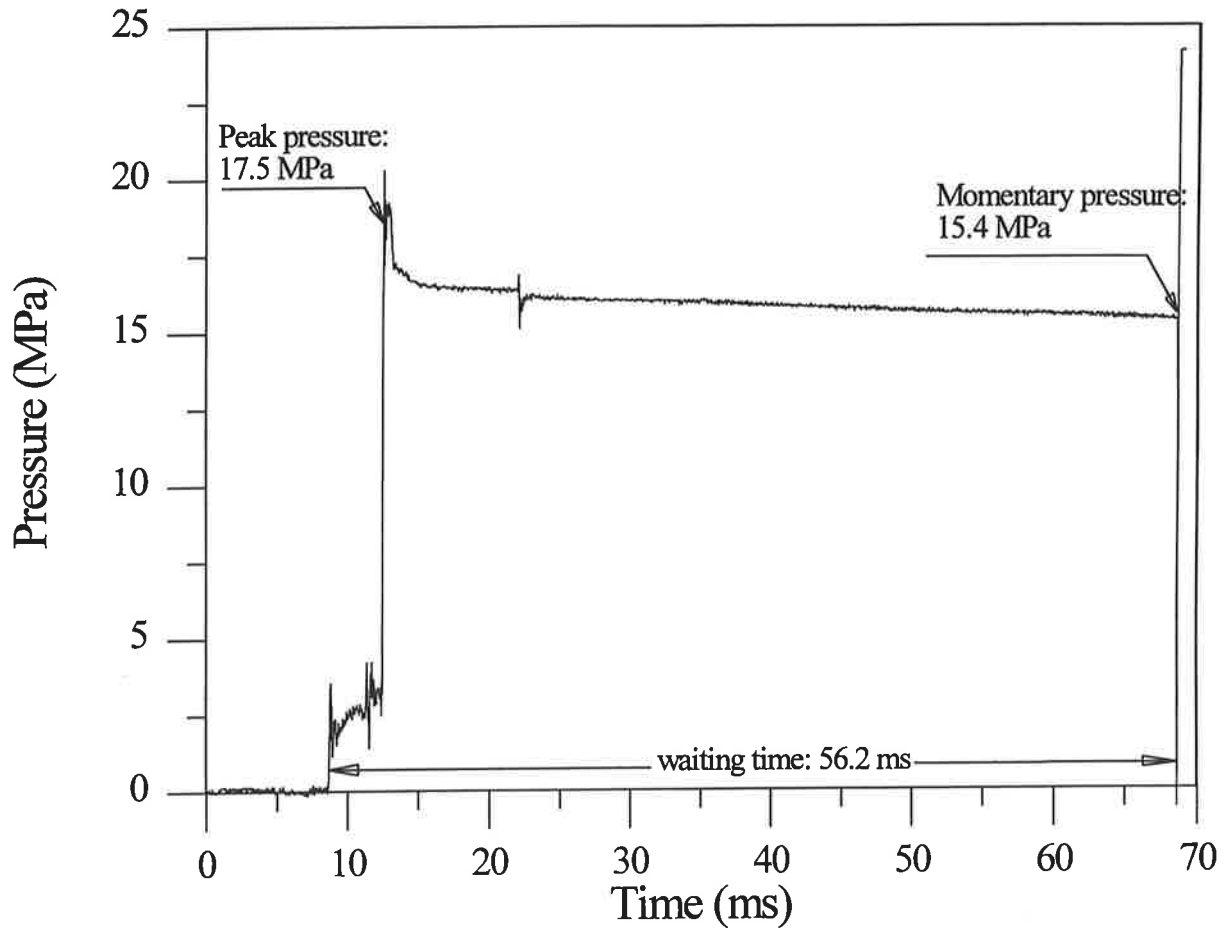


Fig. 7: Definition of the peak pressure and the momentary pressure. The pressure history shown is from Gage 2 in Test No. 6, see Appendix II.

As can be seen from Table 3, 21 blasts have been carried out. However, in one blast, test No. 14, the oscilloscope did not trigger. Therefore, the pressure signals were not registered. In some other cases, the recording levels were set too low and overflows occurred during the registrations. In both cases, the peak pressures were estimated based on the weight of the black powder and the existing registrations, if any. When the detonability results were plotted in the peak pressure - waiting time diagram, Fig. 5, such estimated pressure values were distinctly symbolized.

In another blast, test No. 20, the steel pipe burst by the pre-compression. The explosive and the primer were thrust out of the pipe before being initiated. Therefore, the detonability could not be determined in this test.

4.2 Detonability of the tested explosive

Comparing the detonability in the peak pressure - waiting time plot (Fig. 5) and in the momentary pressure - waiting time plot (Fig. 6), the same dividing line may be constructed between the detonable explosive and the dead-pressed explosive. In other words, the momentary pressure or the pressure on the explosive at the initiation moment can also determine the detonability of the explosive. When the momentary pressure decreases to a level below 17 MPa, the explosive can be detonable.

The fact that the momentary pressure can determine the detonability of the explosive implies that the explosive may be detonable even if it has been subjected to a pressure higher than 17 MPa, as long as the momentary pressure at the initiation moment is lower than 17 MPa. Test No. 13, see Table 3, is such an example. The explanation is that the explosive has been dead-pressed by the higher pressure, but it recovered its detonability before the initiation when the pressure fell below 17 MPa. Therefore, the explosive must have a very short recovery time. However, this recovery time could not be determined exactly in the experiment, since the minimum delay interval of the detonator is 25 ms.

The rapid detonability recovery of the gassed emulsion explosives has also been observed by other researchers. For example, in a half scale test in a sand bed, Huidobro and Austin /6/ observed that their chemically gassed emulsion explosive is fully recovered if the delay time between the donor and the acceptor charges is longer than approximately 50 ms.

Compared with the other two emulsion explosives containing glass micro-balloons (GMBs) as shown in Fig. 8, there are similarities in the detonability of the gassed explosive and the ones with GMB Q-CEL 719. However, the recovery time is much shorter for the gassed explosive.

Based on the above analysis, the following conclusions can be drawn on the detonability of the chemically gassed emulsion explosive:

- 1) It can tolerate a pressure of as high as 17 MPa, which is even higher than the explosive containing the GMB Q-CEL 719 /5/.
- 2) The momentary pressure determines the detonability of the explosive, rather than the peak pressure or waiting time.
- 3) The recovery of the detonability occurs very rapidly. As soon as the momentary pressure decreases below 17 MPa, the explosive is detonable. On the contrary, once the explosive containing GMBs is dead-pressed, it is permanently dead in rock blasting practice /5/.
- 4) The dead-pressing of gassed explosives may be avoided in rock blasting practice by adequate timing of the initiation sequences.

As a by-product of the experiment, the pressure wave velocity in the gassed emulsion explosive was found to be very low, only between 100 - 200 m/s, see V12 in Table 3.

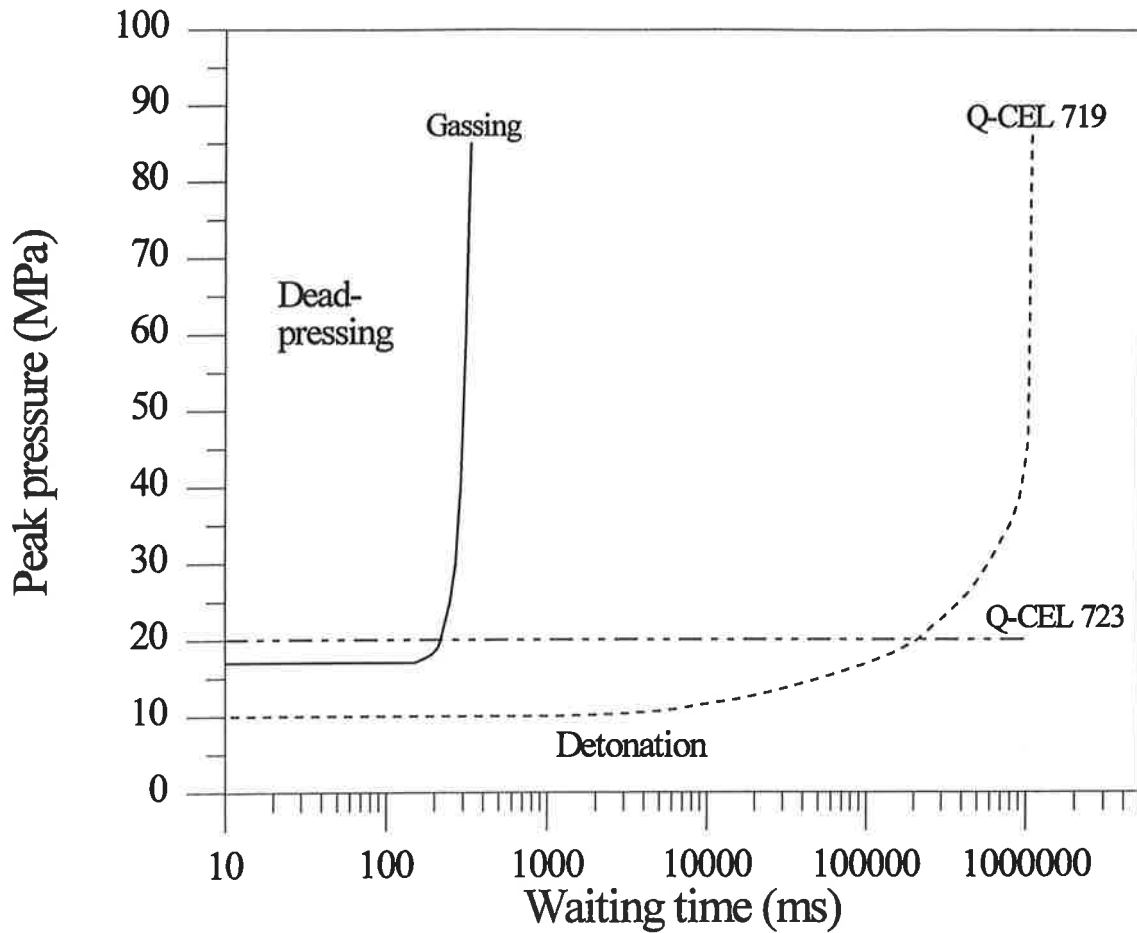


Fig. 8: Detonability of three emulsion explosives, two sensitized by glass micro-balloons (GMBs) /5/ and one by chemical gassing. In the area above the respective dividing line, the explosive is dead-pressed. The fourth tested explosive which is sensitized by GMB B37/2000 did not show any dead-pressing for pressures up to 100 MPa /5/.

5. SIMULATION OF THE DYNAMIC DEAD-PRESSING AND DETONABILITY RECOVERY

In order to understand the dynamic processes of the dead-pressing and the detonability recovery in the gassed emulsion explosive, a computer program has been written and numerical simulations have been carried out. From the simulations, the times necessary for dead-pressing the explosive and for the recovery of detonability after the dead-pressing are estimated.

In the following, the simulation principle, algorithm and results will be described. However, it should be stated that this simulation was not intended to simulate all the details rather to provide an engineering estimate of the dynamic processes. Therefore, necessary assumptions and simplifications have been employed in the calculations to avoid too complicated algorithms.

5.1 Mechanism of initiation and dead-pressing

5.1.1 Initiation mechanism

Several initiation mechanisms can be involved during the initiation of a high explosive, e.g. the hydrodynamic mechanism, adiabatic gas compression in the cavities and visco-plastic heating in the vicinity of cavities. A good discussion of those mechanisms has been given by Frey /7/. However, the viscous heating of matrix in the vicinity of cavities (glass micro-balloons or gas bubbles) is the dominant mechanism responsible for the shock initiation of an emulsion explosive, as can be concluded from reference /7/.

In the simulation, the initiation mechanism is assumed to be the viscous work and the isentropic compression of the gas bubbles. These two mechanisms together heat up the matrix surrounding the gas bubbles, since the matrix can receive heat from the hot gas bubbles while it is heated up by the viscous work. When the matrix reaches a critical temperature, it starts to burn and an initiation results. This critical temperature is determined to be 300 °C, according to Engström /8/.

For reference reasons, the critical environmental temperature for self-heating ignition of some high explosives are 253 °C for HMX, 215 °C for RDX, 287 °C for TNT, 200 °C for PETN and 331 °C for TATB /9/.

However, even if a matrix starts to burn at 300 °C, there is no guaranty for the detonation, as indicated by Perlid /10/. Nevertheless, in the steel pipe experiment, the confinement of and the pressure on the explosive are high, which is favourable for the burning to detonation transition. Thus the above initiation temperature is judged to be reasonable and is used as the initiation criterion in the simulation.

It should be emphasised that the viscous heating of the matrix in the vicinity of a gas bubble is largely dependent on the bubble size. If the bubble is too small, the viscous heating may be negligible /11/.

5.1.2 Dead-pressing mechanism

The dead-pressing is a failure of initiation by the above-mentioned initiation mechanism. During the pre-compression, the matrix flows inwards towards the centres of the gas bubbles. This flow results in a viscous heating in the matrix itself and a compression of the bubbles. The bubble volume decreases. However, the bubble temperature increases accordingly, determined by the equation of state of that gas, and will in all probability be higher than the temperature in the surrounding matrix. Therefore, heat dissipation from the gas bubbles to the matrix takes place. This heat loss will lower the bubble temperature and further decrease the bubble volume, provided that the pressure is kept constant.

If the explosive is shocked by a primer while the gas bubbles are "cold" and small, the explosive may not be initiated because of insufficient viscous heating and gas compression. In other words, the shock-induced temperature in the matrix may be lower than the critical ignition temperature. When the highest temperature in the matrix caused by the viscous heating and the gas compression is lower than 300 °C, the explosives is not detonable or it is dead-pressed. This is the dead-pressing criterion used in the simulation.

5.1.3 Mechanism of detonability recovery

According to the dead-pressing criterion, the mechanism of detonability recovery can be depicted. After the pre-compression is released, the gas bubbles will expand. Meanwhile, as the bubble volume increases, the temperature decreases correspondingly. When the temperature in the bubbles is lower than the ambient matrix temperature, the bubbles will regain heat from the matrix. Gradually, the bubble temperature and the bubble size will return to such a state that the explosive is detonable again.

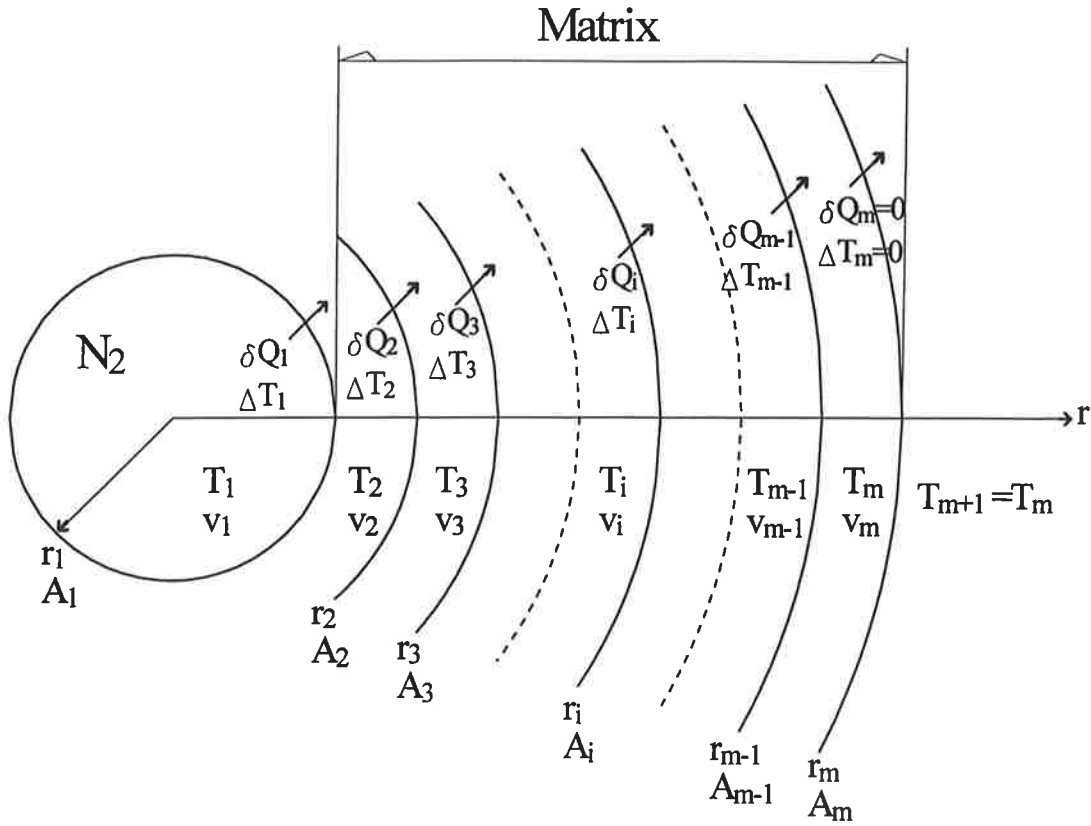
5.2 Calculation algorithm

In the following description of the simulation algorithm, the element geometry, program flow chart, governing equations and input data are outlined.

5.2.1 Symmetry and element layout

A spherical symmetry was assumed and the calculations are performed in spherical co-ordinates, of which the origin is located at the centre of the gas bubbles. This symmetry simplifies the calculation into one-dimensional.

Each gas bubble is simulated by one element while the matrix surrounding the gas bubble is divided into 100 elements of spherical shells, see Fig. 9, where the total number of elements, m , is 101.



m = total number of elements = 101.

T_i = temperature in each spherical element, $i = 1, \dots, m$.

v_i = volume of each spherical element, $i = 1, \dots, m$.

r_i = radius of each spherical element, $i = 1, \dots, m$.

A_i = outer surface area of each spherical element, $i = 1, \dots, m$.

δQ_i = heat dissipated between two adjacent elements, $i = 1, \dots, m$.

ΔT_i = temperature difference between two adjacent elements, $i = 1, \dots, m$.

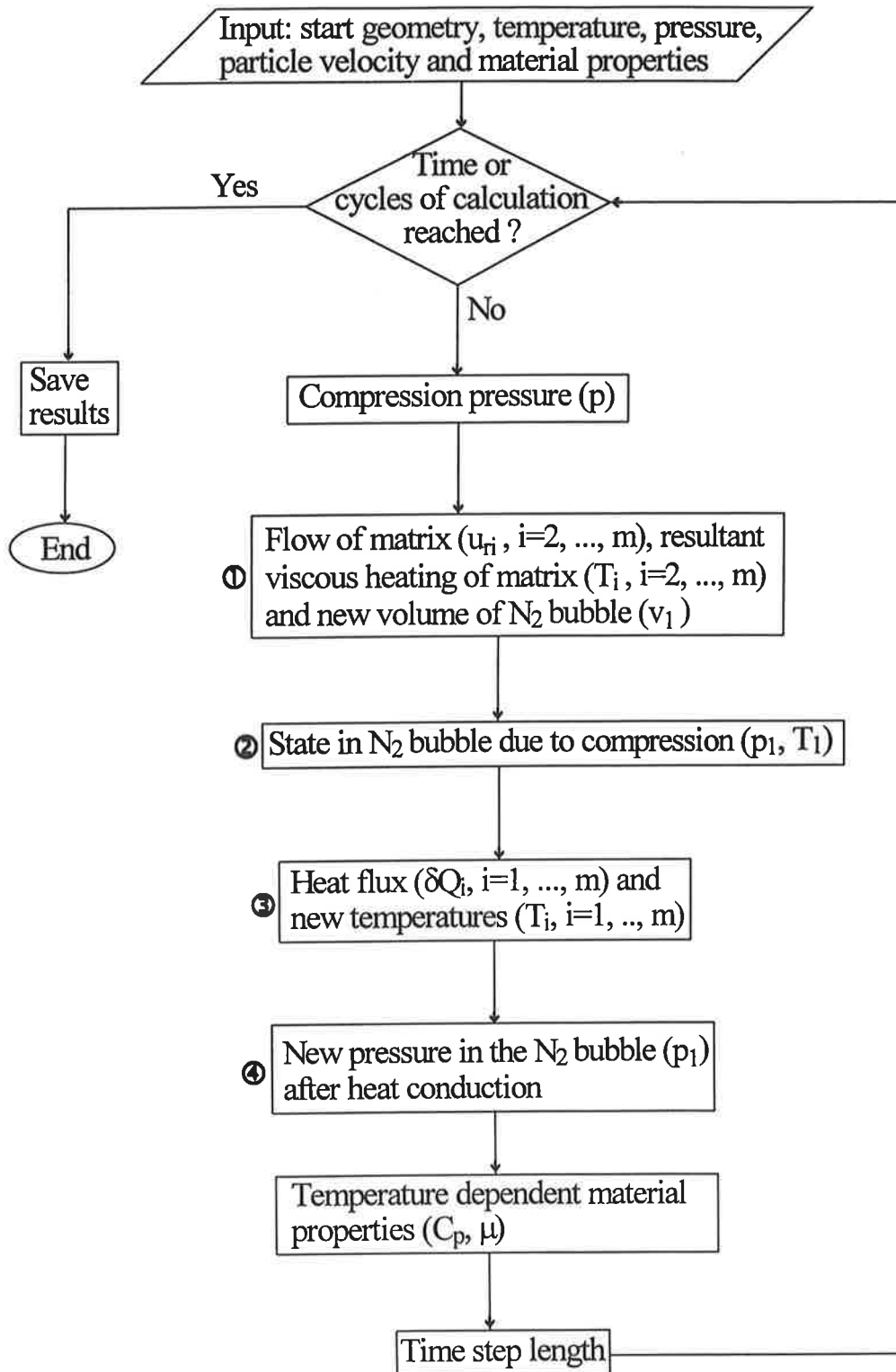
Fig. 9: Element net of the simulation viewed in a plane.

At the start of the simulation, the widths of all matrix elements are equal, $1.04 \mu\text{m}$, see details in Section 5.2.4. During the pre-compression, the element widths increase due to the matrix movement inwards towards the centre of the gas bubble.

The elements of such sizes have been judged to be sufficiently fine for the simulation. Simulations have been carried out using smaller element sizes, e.g. $m = 201$, but the results do not differ within the numerical precision.

5.2.2 Program flow chart

The program flow chart is shown below. Four major calculations are carried out in each time step as marked by ①, ②, ③ and ④ in the flow chart. The governing equations for these calculations are described in Section 5.2.6.



5.2.3 Pressure profile for pre-compression, initiation and detonability recovery

The pressure for the pre-compression is assumed to have a simplified profile as shown in Fig. 10. The amplitude is 17 MPa. The rise edge is linear and the pressure increases from 1 atm to 17 MPa in 0.1 ms.

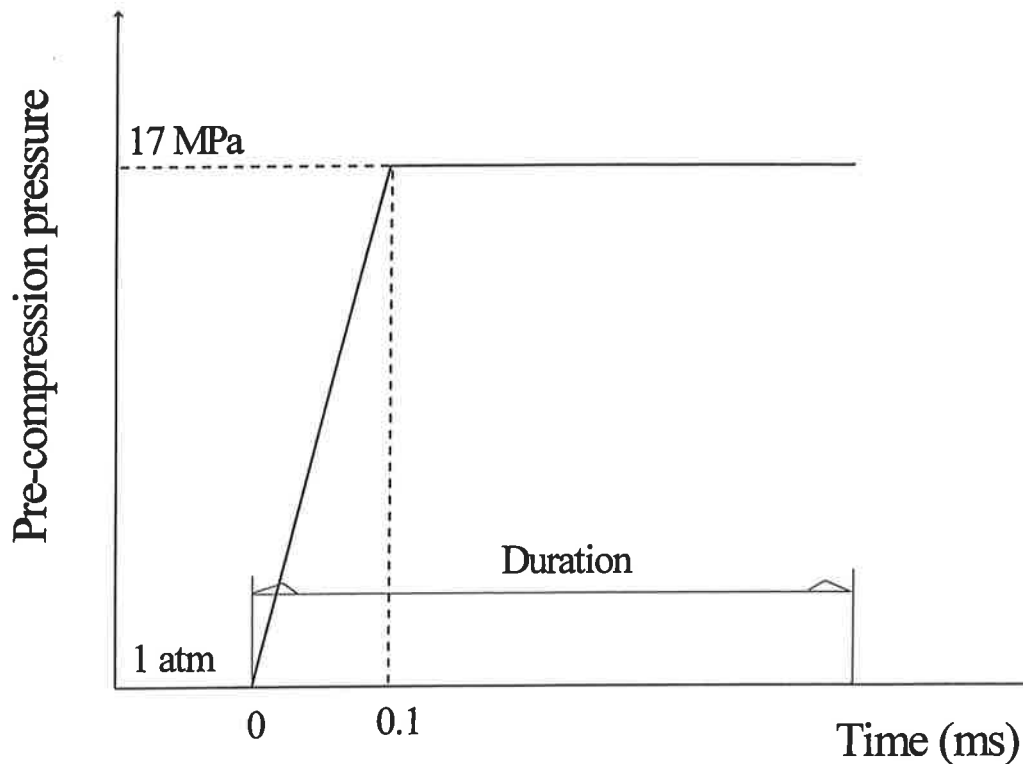


Fig. 10: The simplified pressure profile responsible for the pre-compression in the simulation.

The selection of such a pressure profile is based on the pressure measurements from the experiments, as explained in the following.

The pressure histories recorded in the experiments in the steel pipes have various appearances. Both rise time and amplitude can vary significantly. However, since 17 MPa is the dead-pressing pressure determined by the experiments, this 17 MPa was decided to be the amplitude of the pre-compression pressure in the simulation. Then, a representative pressure signal, from Gage 2 in Test No. 6, was selected from the records, see Fig. 7 or Appendix II. The rise edge of this pressure, zoomed in Fig. 11, is approximately 0.1 ms long. Thus, this pressure is further simplified into Fig. 10 and used as the pre-compression pressure in the simulation.

The initiation pressure is a shock wave with an amplitude of 24.8 GPa, which is the theoretical detonation pressure of the primer used in the experiments, calculated by Eq. 1 below.

$$p_{\text{init}} = \rho_e \cdot \text{VOD}^2 / 4 \quad \dots\dots\dots (1)$$

Where: p_{init} = the detonation pressure of the primer, (Pa)

ρ_e = density of the explosive in the primer = 1550 kg/m³ /12/

VOD = velocity of detonation of the explosive = 8000 m/s /12/

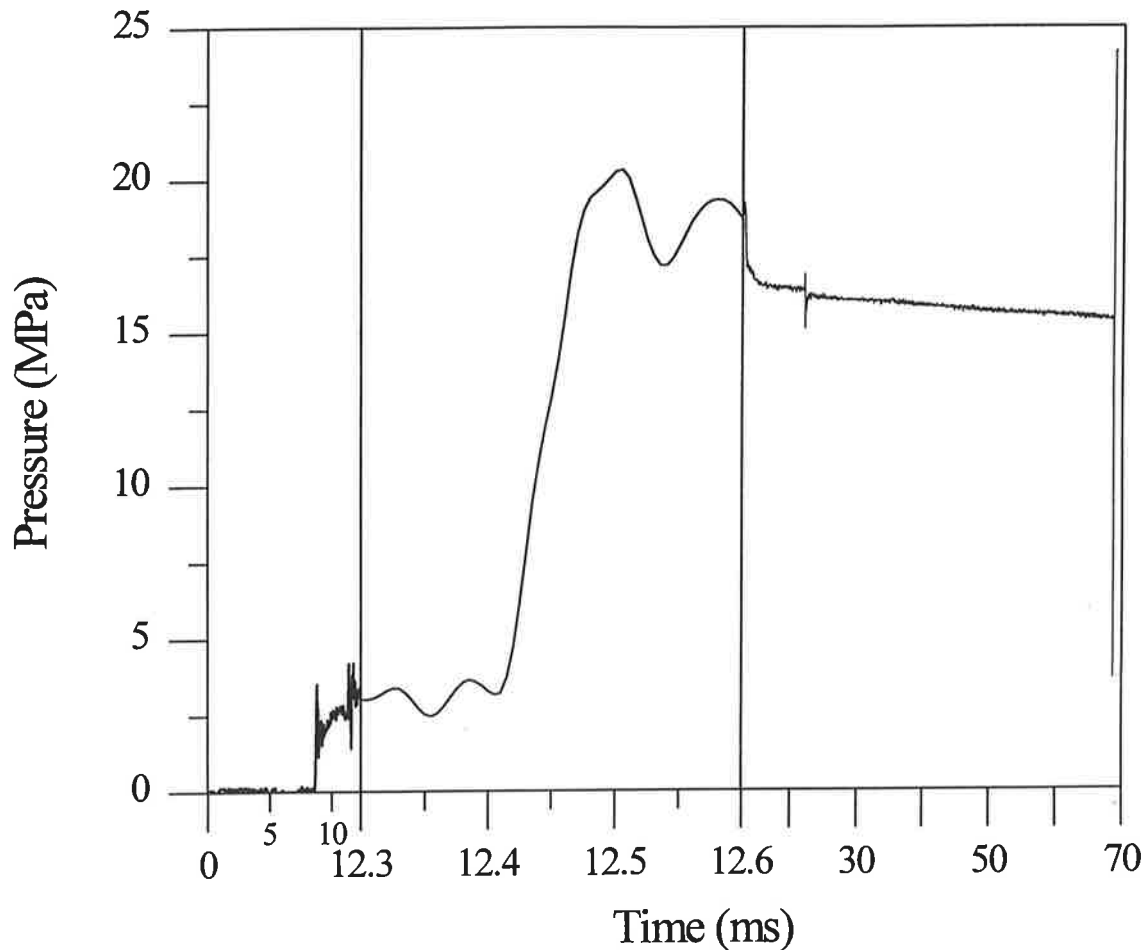


Fig. 11: Pressure record from Gage 2 in Test No. 6. The rise edge is zoomed.

Fig. 12 shows the pressure history when the explosive is initiated while it is still under pre-compression. The figure defines also the concept of "waiting time".

To simulate the recovery of detonability, the pre-compression is suddenly released from 17 MPa to 1 atm after 20 ms, see Fig. 13. As will be described later in this paper, Section 5.3.1, after a waiting time of 20 ms, the pre-compression can no longer harm the explosive significantly, in terms of decreases in the bubble volume and temperature. However, this pressure release is an artificial case. In the reality, there always exists a decay time. Nevertheless, using this hypothetical pressure release, a theoretical detonability recovery time can be calculated.

Earlier pressure measurements carried out in blast holes in rock showed a pressure duration of 5 to 40 ms [2]. Thus a pressure duration of 20 ms in the simulation is also relevant to the blasting practice.

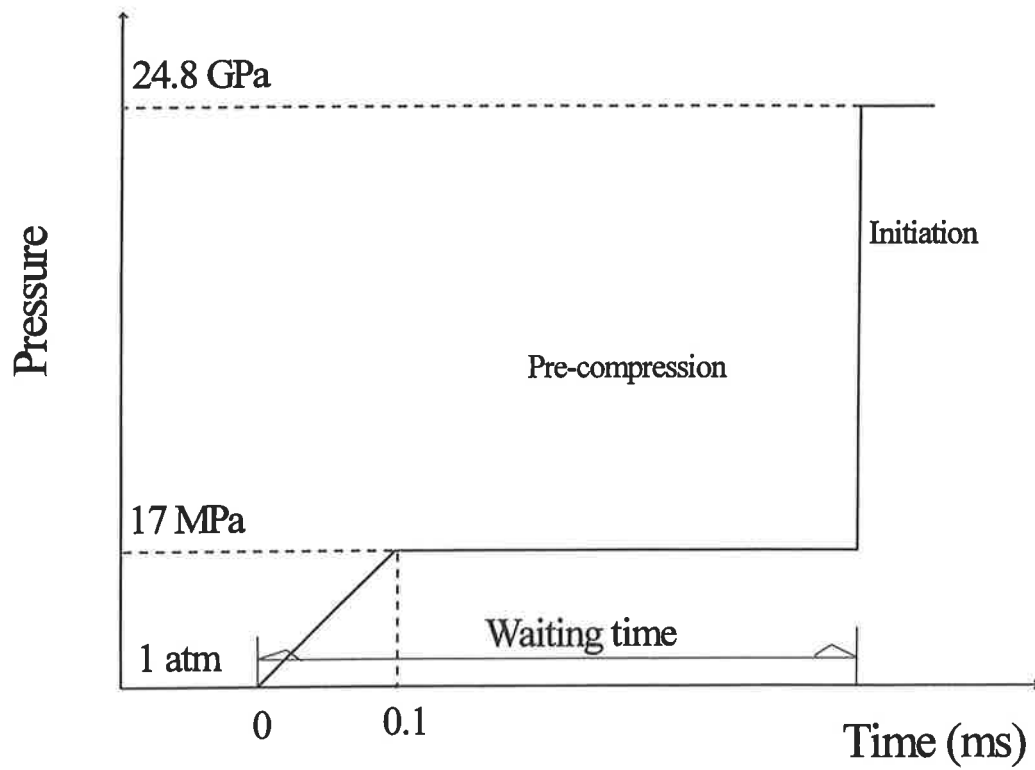


Fig. 12: Pressure profile when the explosive is initiated while it is still under pre-compression.

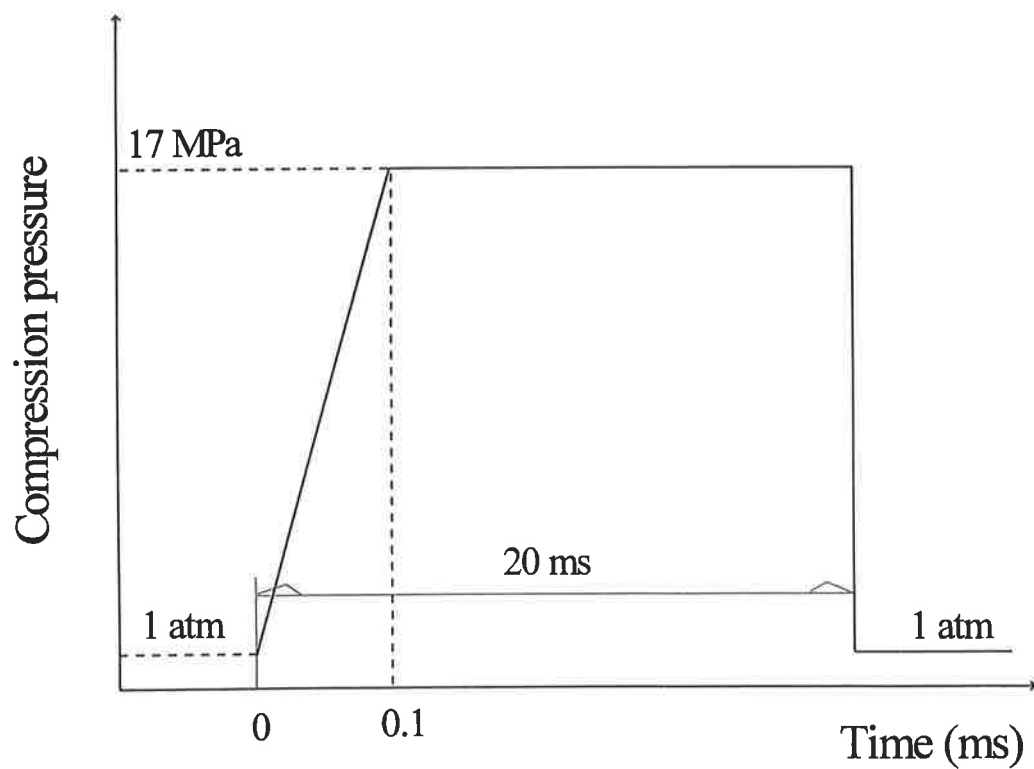


Fig. 13: Artificial pressure profile simulating the release of the pre-compression.

5.2.4 Geometric data of the gas bubbles and matrix at the start of simulation

Physically, a gassed emulsion explosive can be considered as a compound of the aqueous matrix and gaseous bubbles. Owing to the gassing technique used, the gas content in the tested explosive is essentially Nitrogen gas (N_2), a stable and well-known gas.

Fraction of the N_2 gas bubbles in the explosive

In Table 4, the densities of the gassed explosive and its components are listed.

Table 4: Densities of the gassed explosive and its components.

Material	Density (kg/m ³)	Specific volume (m ³ /kg)
Matrix	$\rho_M = 1360$ at 20 °C	—
Explosive	$\rho_e = 1200$ at 20 °C	$v_e = 0.833 \cdot 10^{-3}$
N_2 gas	$\rho_N = 1.25$ at 0 °C /13/ = 1.165 at 20 °C (by ideal gas law)	—

According to the physical composition of the explosive, Equations 2 and 3 can be established:

$$\rho_e = (\rho_M v_M + \rho_N v_N) / v_e \quad \dots\dots\dots (2)$$

$$v_e = v_M + v_N \quad \dots\dots\dots (3)$$

Where: v_M and v_N are the volume of matrix respective N_2 gas in 1 kg of the explosive.

Based on the data in Table 4, the solutions of the Eqs. 2 and 3 are:

$$v_M = 0.735 \cdot 10^{-3} \text{ m}^3/\text{kg explosive}$$

$$v_N = 0.098 \cdot 10^{-3} \text{ m}^3/\text{kg explosive}$$

Therefore: the volume-% of the N_2 bubbles = $v_N / v_e = 11.76 \%$.

the weight-% of the N_2 bubbles = $\rho_N v_N / \rho_e v_e = 0.011 \%$.

The diameter of the N_2 gas bubbles

It is assumed that the gas bubbles have the spherical shape and are equal in size. The diameter lies between 100 and 300 μm /8/ and is taken as 200 μm in the simulation. Thus, the radius of the N_2 bubbles at the ambient condition is: $r_0 = 100 \mu\text{m}$.

The amount of matrix surrounding each N_2 gas bubble

Assume that the N_2 bubbles are uniformly and cubically distributed in the matrix. In other words, the distance between any two adjacent bubbles in any one of three orthogonal directions is equal. It is also to say that each N_2 bubble is immersed in the centre of a matrix cube, of which the side length is equal to the distance between the centres of two adjacent bubbles or $2 \cdot r_b$ in Fig. 14.

If the matrix surrounding each N_2 bubble is averaged out into a shell of the same volume, the outer radius of this equivalent shell, r_M in Fig. 14, can be obtained by Eq. 4:

$$\frac{r_0}{r_M} = \left(\frac{v_N}{v_e} \right)^{1/3} \quad \dots\dots\dots (4)$$

Therefore:

$$r_M = 204.11 \text{ } \mu\text{m}.$$

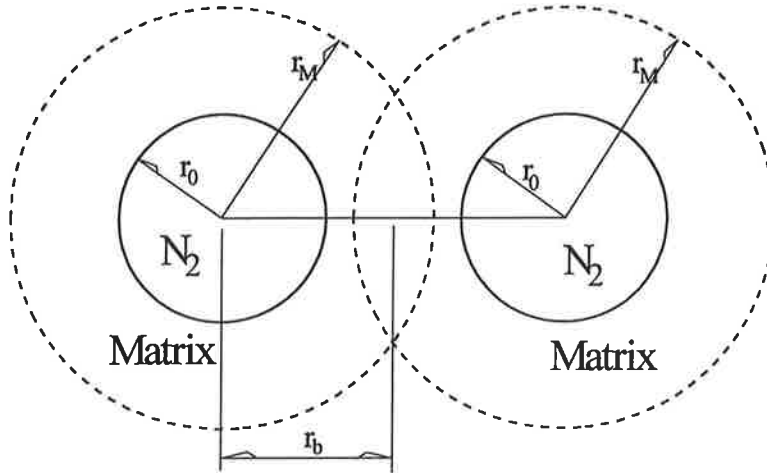


Fig. 14: Distances between two adjacent N_2 bubbles.

If this equivalent matrix shell is equal-spaced divided into 100 shells according to Section 5.2.1, the shell width is: $(r_M - r_0)/100 = 1.04 \text{ } \mu\text{m}$.

During the compression, the volume (v_0) and the radius (r_0) of the N_2 bubbles decrease. The outer radius of the equivalent matrix shell around each N_2 bubble, r_M in Fig. 14, will be changed accordingly. This dynamic process is calculated in Sections 5.2.6.2 and 5.2.6.4.

Comparing Fig. 14 with Fig. 9, it can be seen that: $r_M = r_m = r_{101}$.

5.2.5 Material properties, units and symbols

For the convenience of reading, the material properties and the principal symbol set-up used in the simulation are summarized below, although they are also explained in the places they appear in this report. The SI units are used throughout this report except that the conventional pressure unit of atm is used in several places for convenience.

Property of the emulsion explosive

- Density at 20 °C: $\rho_e = 1200 \text{ kg/m}^3$

Properties of the emulsion matrix

- Density at 20 °C: $\rho_M = 1360 \text{ kg/m}^3$
- Specific heat: $C_{pM} = 1080 \text{ J/kg/K}$ /14/
- Critical ignition temperature = 300 °C
- Viscosity: $\mu = 1.608 \cdot 10^{12} / T^{4.255} \text{ Pa}\cdot\text{s}$, see values in Table 5 /8/.

Table 5: Viscosity of the matrix /8/.

Temperature (°C)	Temperature (K)	Viscosity, μ (Pa·s)
60	333	30
20	293	50
10	283	60
0	273	70

Properties of N₂ gas

- Molar weight = 0.028 kg/mol
- Density at 1 atm and 20 °C: $\rho_N = 1.25 \text{ kg/m}^3$
- Specific heat in J/K/mol
 - at constant pressure: $C_p = 28.58 + 3.77 \cdot 10^{-3} \cdot T - 0.5 \cdot 10^5 / T^2$ /13/
 - at constant volume: $C_v = 20.414 + 2.693 \cdot 10^{-3} \cdot T - 0.3571 \cdot 10^5 / T^2$
- Ratio of the specific heat: $C_p/C_v = 1.4$ /13/
- Van der Waal equation of state: $(p + a n^2 / v^2)(v - nb) = nRT$
 - for N₂ gas: $a = 0.140835 \text{ m}^6 \cdot \text{Pa/mol}^2$ /13/
 - $b = 3.913 \cdot 10^{-5} \text{ m}^3/\text{mol}$ /13/
- Radius of gas bubbles at 1 atm and 20 °C: $r_0 = 100 \text{ }\mu\text{m}$

Thermal conduction constants

- Coefficient of heat transfer between N₂ gas and the matrix: $\alpha = 4190 \text{ W/m}^2/\text{K}$ /14/
- Thermal conductivity of the matrix: $\lambda = 0.209 \text{ W/m/K}$ /14/

Principal symbol set-up

- State variables
 - p = pressure, (Pa)
 - T = temperature, (K)
 - v = volume, (m³)
 - e = internal energy, (J)
 - S = entropy, (J)
- Physical properties
 - A = area, (m²)
 - r = radius, (m)
 - n = number in moles
 - u = particle velocity, (m/s)
 - μ = viscosity, (Pa·s)
 - ρ = density, (kg/m³)

- Thermal properties
 - C_p = specific heat at constant pressure, (J/K/mol)
 - C_v = specific heat at constant volume, (J/K/mol)
 - E_v = rate of viscous heating, (J/m³/s)
 - Q = heat, (J)
 - α = coefficient of heat transfer between N₂ gas and the matrix, (W/m²/K)
 - λ = thermal conductivity of the matrix, (W/m/K)
- Subscripts
 - $_0$ = initial values for the N₂ gas, before pre-compression
 - $_i$ = element number
 - $i = 1$ for N₂ gas
 - $i = 2, \dots, 101$ for matrix
 - $_e$ = explosive
 - $_M$ = matrix
 - $_m = 101$
 - = element number of the matrix element which is located farthest from the N₂ bubble, see Fig. 9,
 - $_N$ = N₂ gas
 - $_v$ = viscous heating
- Differentials
 - δ = time differential
 - Δ = spatial differential

5.2.6 Governing equations and their applications in the program

During the pre-compression, the matrix moves inwards towards the centre of the gas bubbles and compresses the gas bubble. When the pre-compression is released, the movement of the matrix will reverse its direction and the gas bubbles expand. However, the governing equations for both the compression and expansion phases are the same. And in both phases, the viscous flow of the matrix increases its temperature. In the following, the governing equations and numerical solutions for the pre-compression phase are described in the same sequence as the processes appear in the program flow chart, see Section 5.2.2.

5.2.6.1 Viscous flow of the matrix and the resultant heating

Governing equations

Compared with the gas bubbles, the compressibility of the matrix is negligible. Therefore, the matrix is assumed to be incompressible in the simulation. For a viscous and incompressible fluid, the flow is governed by the Navier-Stoke equation (Eq. 5) and the continuity equation (Eq. 6) below /15/.

$$\frac{\partial \mathbf{u}_r}{\partial t} + (\mathbf{u} \bullet \nabla) \mathbf{u}_r = -\frac{1}{\rho_M} \cdot \frac{\partial p}{\partial r} + \frac{\mu}{\rho_M} \left[\nabla^2 \mathbf{u}_r - \frac{2\mathbf{u}_r}{r^2} \right] \dots\dots\dots(5)$$

$$\nabla \bullet \mathbf{u} = 0 \dots\dots\dots(6)$$

Where: u_r = velocity component in the radial direction, (m/s)

t = time, (s)

$\mathbf{u}$ = velocity vector = $\{u_r, 0, 0\}$ in a spherically symmetric flow

ρ_M = density of the matrix, (kg/m³)

p = pressure in the matrix, (Pa)

r = radial co-ordinate

μ = viscosity, (Pa.s)

$$\text{Since: } \nabla \cdot \mathbf{u} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \cdot u_r) \quad \dots\dots\dots(7)$$

Eqs. 5 and 6 can be transformed into Eqs. 8 and 9:

$$\frac{\partial u_r}{\partial t} + \frac{1}{\rho_M} \cdot \frac{\partial p}{\partial r} - \frac{2u_r^2}{r} = 0 \quad \dots\dots\dots(8)$$

$$\frac{\partial u_r}{\partial r} + \frac{2u_r}{r} = 0 \quad \dots\dots\dots(9)$$

The energy dissipated as viscous heat per unit volume and unit time, E_v , is /15/:

$$E_v = 2\mu(e_{rr}^2 + e_{\theta\theta}^2 + e_{\phi\phi}^2 + 2e_{\theta\phi}^2 + 2e_{\phi r}^2 + 2e_{r\theta}^2) \quad \dots\dots\dots(10)$$

Where: e_{rr}^2 to $e_{r\theta}^2$ are components of the rate-of-strain tensor.

In the spherical symmetry:

$$e_{rr} = \partial u_r / \partial r \quad \dots\dots\dots(11)$$

$$e_{\theta\theta} = e_{\phi\phi} = u_r / r \quad \dots\dots\dots(12)$$

$$e_{\theta\phi} = e_{\phi r} = e_{r\theta} = 0 \quad \dots\dots\dots(13)$$

With the help of Eqs. 11, 12, 13 and 9, Eq. 10 can be reduced to:

$$E_v = 12\mu \left(\frac{u_r}{r} \right)^2 \quad \dots\dots\dots(14)$$

Thus, Eqs. 8 and 9 determine the flow of the matrix and Eq. 14 determines the viscous heating in the matrix.

Numerical solutions

Solving Eq. 9, the flow of the matrix elements can be described by:

$$u_{ri} = (r_{a2}/r_{ai})^2 \cdot u_{r2} \quad \dots\dots\dots(15)$$

Where: u_{ri} = velocity of the i :th matrix element for $i = 3, \dots, 101$, (m/s)
 u_{r2} = velocity of the first matrix element, i.e. the one closest to the N_2 gas bubble, refer to Fig. 9, (m/s)
 r_{ai} = intermediate radius of the i :th matrix element for $i = 3, \dots, 101$
 $= (r_{i-1} + r_i)/2$, (m)
 r_{a2} = intermediate radius of the first matrix element
 $= (r_1 + r_2)/2$, (m)

Meanwhile, the velocity of the first matrix element, u_{r2} , can be solved by Eqs. 15 and 8:

$$\frac{\partial u_{r2}}{\partial t} - \frac{2u_{r2}^2}{r_{a2}} + \frac{1}{\rho_M} \frac{\partial p}{\partial r} = 0 \quad \dots\dots\dots(16)$$

Or:

$$\delta u_{r2} = \left(\frac{2u_{r2}^2}{r_{a2}} - \frac{1}{\rho_M} \frac{p_2 - p_1}{r_2 - r_1} \right) \cdot \delta t \quad \dots\dots\dots(17)$$

Where: δu_{r2} = increment of u_{r2} in one time step, (m/s)
 δt = length of the time step, (s)
 p_2 = compression pressure on the first matrix element determined by the pressure profiles in Section 5.2.3, (Pa)
 p_1 = pressure in the N_2 gas bubble, (Pa)
 r_2 = outer radius of the first matrix element, refer to Fig. 9, (m)
 r_1 = radius of the N_2 gas bubble, (m)

The viscous heating in each matrix element, E_{vi} for $i = 2, \dots, m$, is:

$$E_{vi} = 12\mu \left(\frac{u_{ri}}{r_{ai}} \right)^2 \quad \dots\dots\dots(18)$$

Consequently, the temperature increment in each matrix element during each time step owing to the viscous heating is:

$$\delta T_{vi} = \frac{E_{vi}}{\rho_M \cdot C_{pM}} \quad \dots\dots\dots(19)$$

Where: δT_{vi} = temperature increment in i :th matrix element during one time step, (K)
 E_{vi} = viscous heating of i :th matrix element during one time step, (J/m³/s)
 ρ_M = density of matrix, (kg/m³)
 C_{pM} = specific heat of matrix at constant pressure, (J/K/kg)

At the initial step of the simulation, the pressure in the matrix equals to the compression pressure, see Fig. 10, while the pressure in the N_2 gas bubble equals to the atmosphere pressure, 1 atm.

5.2.6.2 State in the gas bubbles due to the compression

Since the matrix flows, the N_2 gas bubbles are compressed. The compression is simulated by an isentropic process followed by a heat transmission from the bubble to the surrounding matrix. This section describes the calculation of the state in the gas bubble (v_1 , p_1 and T_1) caused by the isentropic compression while the heat transmission is described in the next section, Section 5.2.6.3.

The initial state of the N_2 gas bubble prior to the beginning of the simulation:

radius $r_0 = 100 \mu\text{m} = 10^{-4} \text{ m}$, see Section 5.2.4.

volume $v_0 = 4\pi r_0^3/3 = 4.1888 \cdot 10^{-12} \text{ m}^3$.

temperature $T_0 = 20 \text{ }^\circ\text{C} = 293 \text{ K}$.

pressure $p_0 = 1 \text{ atm} = 1.0132 \cdot 10^5 \text{ Pa}$.

Calculation of v_1 :

The gas compression is determined by the matrix flow and the decrease in the bubble radius during one time step is calculated by:

$$\delta r_1 = u_{r1} \cdot \delta t \quad \dots\dots\dots(20)$$

Where: δr_1 = change of the N_2 bubble radius during one time step, (m)

u_{r1} = velocity of the N_2 bubble wall in this time step, (m/s)

δt = length of the time step, (s)

At the end of each time step, the bubble radius, r_1 , is:

$$r_1 = (r_1)_{\text{old}} + \delta r_1 \quad \dots\dots\dots(21)$$

Where $(r_1)_{\text{old}}$ is the bubble radius at the beginning of each time step.

The bubble volume, v_1 , at the end of each time step is therefore:

$$v_1 = 4\pi r_1^3/3 \quad \dots\dots\dots(22)$$

Calculation of p_1 and T_1 :

The isentropic process, $dS_1 = 0$, means:

$$de_1 + p_1 dv_1 = 0 \quad \dots\dots\dots(23)$$

Where S_1 and e_1 are the entropy and internal energy in a gas bubble respectively.

On the other hand:

$$de_1 = n \cdot C_v dT_1 + [T_1 (\partial p_1 / \partial T_1)_{v1} - p_1] dv_1 \quad \dots\dots\dots(24)$$

By equating Eq. 23 and Eq. 24, Eq. 25 is derived.

$$n \cdot C_v dT_1 + T_1 (\partial p_1 / \partial T_1)_{v_1} dv_1 = 0 \quad \dots\dots\dots(25)$$

Where: n = amount of N_2 gas in a bubble
 $= \rho_N v_0 / 0.028 = 1.7428 \cdot 10^{-10}$ mole
 C_v = the specific heat of the N_2 gas at constant volume, (J/K/mol)

Since $C_p/C_v = 1.4$ for N_2 /13/, the temperature dependence of C_v can be expressed by:

$$C_v = C_p/1.4 = A + B \cdot T_1 + C/T_1^2 \quad \dots\dots\dots(26)$$

Where constants: $A = 20.414$ J/K/mol /13/
 $B = 2.693 \cdot 10^{-3}$ J/K²/mol /13/
 $C = -3.571 \cdot 10^4$ J·K/mol /13/

Furthermore, the state in the N_2 bubble can be described by the Van der Waal equation of state:

$$(p_1 + a n^2 / v_1^2)(v_1 - nb) = nRT_1 \quad \dots\dots\dots(27)$$

Where constants: $a = 0.140835$ m⁶·Pa/mol² /13/
 $b = 3.913 \cdot 10^{-5}$ m³/mol /13/
 R = gas constant = 8.31451 J/K/mol

From the Van der Waal gas equation, Eq. 27, it can be derived:

$$(\partial p_1 / \partial T_1)_{v_1} = nR / (v_1 - nb) \quad \dots\dots\dots(28)$$

Substituting Eqs. 28 and 26 into Eq. 25, the following equation is obtained:

$$(A/T_1 + B + C/T_1^3) dT_1 = [R/(nb - v_1)] \cdot dv_1 \quad \dots\dots\dots(29)$$

Or:

$$A \cdot \ln T_1 + B \cdot T_1 - \frac{C}{2T_1^2} + R \cdot \ln(v_1 - nb) - k = 0 \quad \dots\dots\dots(30)$$

Where: the integration constant, $k = \ln \left[T_0^A \cdot (v_0 - nb)^R \right] + B \cdot T_0 - \frac{C}{2T_0^2}$, and v_0 and T_0 are the initial volume (m³) and temperature (K) in the gas bubbles.

Giving volume v_1 , determined by Eq. 22, T_1 can be solved from Eq. 30 and thereafter p_1 by Eq. 27.

Equation 30 has been solved numerically by the Newton-Raphson method. Program 3 in Appendix III is a subroutine for this purpose.

5.2.6.3 Heat flux between elements and the resultant temperature changes

The gas compression and the viscous flow of the matrix create an uneven temperature field and cause heat conduction between elements.

Heat flux between N₂ gas and matrix

The heat transmission from the bubble to its surrounding matrix occurs on the whole bubble surface and is calculated by Eq. 31, a linear function of the temperature difference.

$$\delta Q_1 = \alpha \cdot A_1 \cdot \Delta T_1 \cdot \delta t \quad \dots\dots\dots(31)$$

Where: δQ_1 = heat transferred from N₂ bubble to the matrix during time δt , (J), see Fig. 9

α = coefficient of heat transfer = 4190 W/m²/K /14/

A_1 = surface area of the N₂ bubble = $4\pi r_1^2$, (m²)

r_1 = radius of the N₂ bubble, (m)

$\Delta T_1 = T_1 - T_2$, (K), see Fig. 9

T_1 = temperature in the N₂ bubble, (K), see Fig. 9

T_2 = temperature in the matrix element adjacent to the N₂ bubble, (K), see Fig. 9

δt = length of one time step, (s)

Heat flux between adjacent matrix elements

The conservation of energy in each matrix elements implies:

$$v_i \rho_M C_{pM} \cdot \frac{\partial T_i}{\partial t} = Q_{\text{gain}} - Q_{\text{loss}} + v_i \cdot E_{vi} \quad \dots\dots\dots(32)$$

Where: i = element number = 2, ..., 101

Q_{gain} = heat gained from the neighbour elements, (J/s)

Q_{loss} = heat lost to the neighbour elements, (J/s)

E_{vi} = heat produced by the viscous work, (J/m³/s), see Eq. 18

Meanwhile, the heat conduction between any adjacent two matrix elements is calculated by:

$$\delta Q_i = \lambda \cdot A_i \cdot \frac{\Delta T_i}{\Delta r_i} \cdot \delta t \quad \dots\dots\dots(33)$$

Where: i = element number = 2, ..., 101 for the matrix, see Fig. 9

δQ_i = heat flux from i :th to the $(i+1)$:th element during time δt , (J), see Fig. 9

Δr_i = distance between the i :th and the $(i+1)$:th element, see Fig. 9

= $(r_{i+1} - r_{i-1})/2$, (m)

ΔT_i = temperature difference between the i :th and the $(i+1)$:th element, see Fig. 9

= $T_i - T_{i+1}$, (K)

λ = thermal conductivity of the matrix = 0.209 W/m/K /14/

A_i = area of the outer surface of the i :th element

= $4\pi r_i^2$, (m²)

δt = length of the time step, (s)

Therefore, during each time step, Eq. 32 can be re-written into:

$$v_i \rho_M C_{pM} \cdot \delta T_i = \delta Q_{i-1} - \delta Q_i + v_i \cdot E_{vi} \cdot \delta t \quad \dots\dots\dots(34)$$

Where: v_i = volume of the i :th element

$$= 4\pi(r_i^3 - r_{i-1}^3)/3, (m^3)$$

δT_i = temperature increment in i :th matrix element during one time step, (K)

The boundary conditions are, referring to Fig. 9:

$$\delta Q_{101} = 0 \quad \dots\dots\dots(35)$$

$$\Delta T_{101} = 0 \quad \dots\dots\dots(36)$$

Temperature in the elements after the heat conduction

The temperature change during one time step, δT , in an element can be calculated as follows.

For the N_2 gas bubble:

$$\delta T_1 = -\delta Q_1 / (n \cdot C_p) \quad \dots\dots\dots(37)$$

For the matrix, by solving Eq. 34:

$$\delta T_i = \frac{\delta Q_{i-1} - \delta Q_i + v_i \cdot E_{vi} \cdot \delta t}{v_i \rho_M C_{pM}}, \text{ for } i = 2, \dots, 101 \quad \dots\dots\dots(38)$$

Therefore, the new temperature in all elements at the end of one time step is:

$$(T_i)_{\text{new}} = (T_i)_{\text{old}} + \delta T_i, \text{ for } i = 1, \dots, 101 \quad \dots\dots\dots(39)$$

5.2.6.4 Calculation of other time dependent variables

Through the calculations in the above sections, i.e. Sections 5.2.6.1 to 5.2.6.3, the following variables have been solved for one time step:

- volume (v_1) and temperature (T_1) of the N_2 gas bubble at the end of the time step
- temperature in all matrix elements (T_i for $i = 2, \dots, 101$)

However, several other variables must be calculated before the simulation can continue to the next time step. These variables are:

- pressure (p_1) in the N_2 gas bubble at the end of the time step
- co-ordinates of the matrix elements (r_i for $i = 2, \dots, 101$) at the end of the time step
- temperature dependent material properties (C_p and μ)

In this section, calculations of those variables are described.

Final pressure in the N₂ bubble

According to Section 5.2.6.2, the pressure in the N₂ bubble after the isentropic compression phase can be solved. However, after the transmission of heat from the N₂ bubble to the surrounding matrix, the temperature in the N₂ bubble decreases, see Section 5.6.2.3. Thus, the pressure in the N₂ bubble will decrease accordingly.

During this sub-step of the simulation, the N₂ bubble undergoes an isochoric process, since the volume of the bubble has been determined by the viscous flow of the matrix. Therefore, the final pressure in the N₂ bubble can be solved again by Eq. 27, after the temperature is solved in Section 5.2.6.3.

Co-ordinates of the matrix elements

Because of the matrix movement inwards towards the centre of the N₂ bubble, the radii of the matrix elements decrease. However, since the matrix is assumed to be incompressible, the volume of each element is constant, i.e.:

$$v_i = \text{constant, for } i = 2, \dots, 101 \quad \dots\dots\dots(40)$$

or:

$$\frac{4\pi}{3}(r_{i\text{new}}^3 - r_{i-1\text{new}}^3) = \frac{4\pi}{3}(r_{i\text{old}}^3 - r_{i-1\text{old}}^3) \quad \dots\dots\dots(41)$$

Recursive manipulation of Eq. 41 gives the solution of the matrix radii at the end of the time step:

$$r_{i\text{new}} = \sqrt[3]{r_{i\text{old}}^3 + r_{i-1\text{new}}^3 - r_{i-1\text{old}}^3} \quad \dots\dots\dots(42)$$

In Eqs. 41 and 42, "i" is the element number ($i = 2, \dots, 101$), subscript "new" stands for the value at the end of the present time step while subscript "old" stands for the value at the end of the last time step. r_i is the radius of the gas bubble.

Accordingly, the values of the surface areas, $A_{i\text{new}}$, and the radial distances, $\Delta r_{i\text{new}}$, in Eq. 33 can be calculated.

The temperature dependent material properties, C_p and μ

The temperature dependence of C_v , the specific heat of N₂ gas, has already been taken into account in the reduction of Eq. 30. However, C_p should be re-calculated after each time step using Eq. 26 based on the final temperature of the N₂ gas. The viscosity of the matrix, μ , is re-calculated by Eq. 43 below, which is the regression result of viscosity in Table 5, see Section 5.2.5, using an empirical viscosity-temperature relation /16/:

$$\mu = 1.608 \cdot 10^{12} / T^{4.255} \quad \dots\dots\dots(43)$$

5.3 Results of the simulation

5.3.1 Radius and temperature of the gas bubbles and temperature in the surrounding matrix during the pre-compression

As the pre-compression (Fig. 10) is applied on the explosive, the N_2 bubbles are compressed. Their temperature rises while the radius decreases. Because of the higher temperature in the N_2 bubbles, heat will dissipate to the surrounding matrix. This heat dissipation lowers the temperature in the N_2 bubbles, diminishes the radius of the N_2 bubbles and warms up the matrix, as time elapses.

Fig. 15 and Fig. 16 show the radius of the gas bubble respective the temperature in the gas bubble during the pre-compression. Fig. 17 shows the temperature in the matrix in the immediate vicinity of the gas bubble. Fig. 18 shows how the temperature in the N_2 bubble and in the matrix evens out with time due to the heat flow.

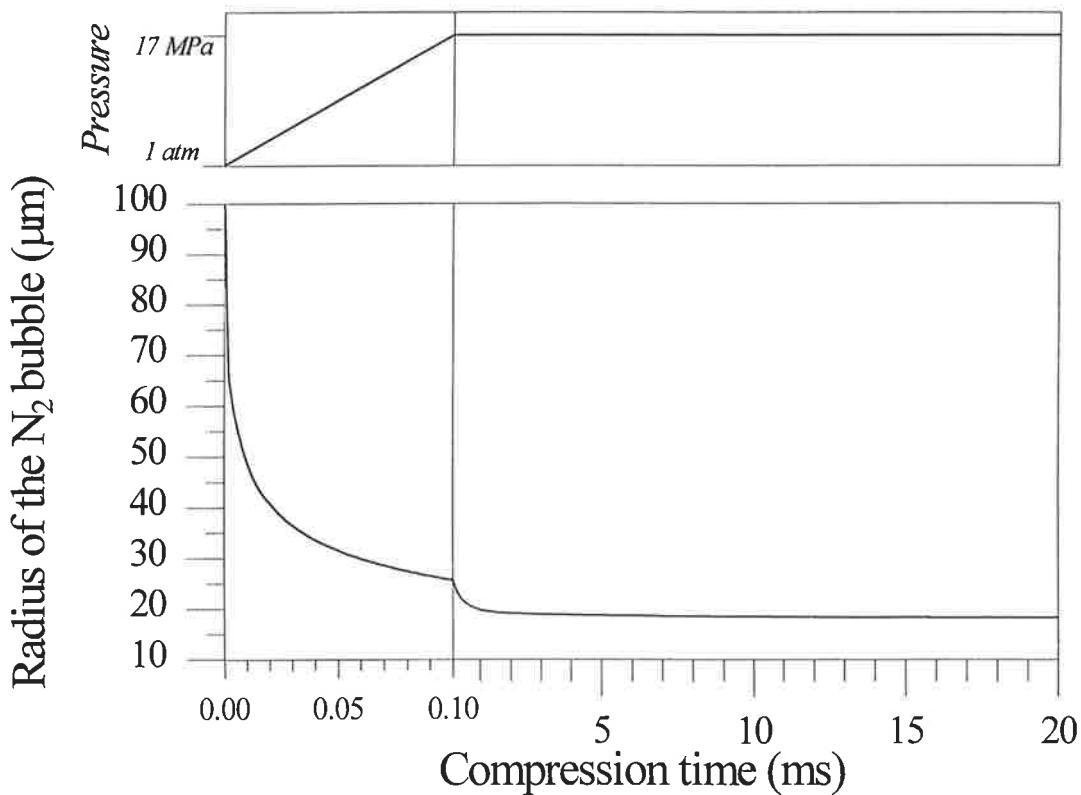


Fig. 15: Radius of the N_2 gas bubble during the pre-compression, corresponding pressure profile in the upper figure or in Fig. 10. Note the dual time scales.

As can be seen from Figs. 15 and 16, when the pressure rises from 1 atm to 17 MPa in the time period 0 to 0.1 ms, the compression causes a very rapid decrease in the bubble radius and simultaneously a very rapid increase in the bubble temperature. At the end of the pressure rise, i.e. at 0.1 ms, the bubble radius has decreased from 100 μm to 25.6 μm while the bubble temperature increased from 20 $^{\circ}C$ to 514 $^{\circ}C$. Therefore, the pressure rise reduced the bubble radius by 74.4 μm while increased the bubble temperature by 494 $^{\circ}C$.

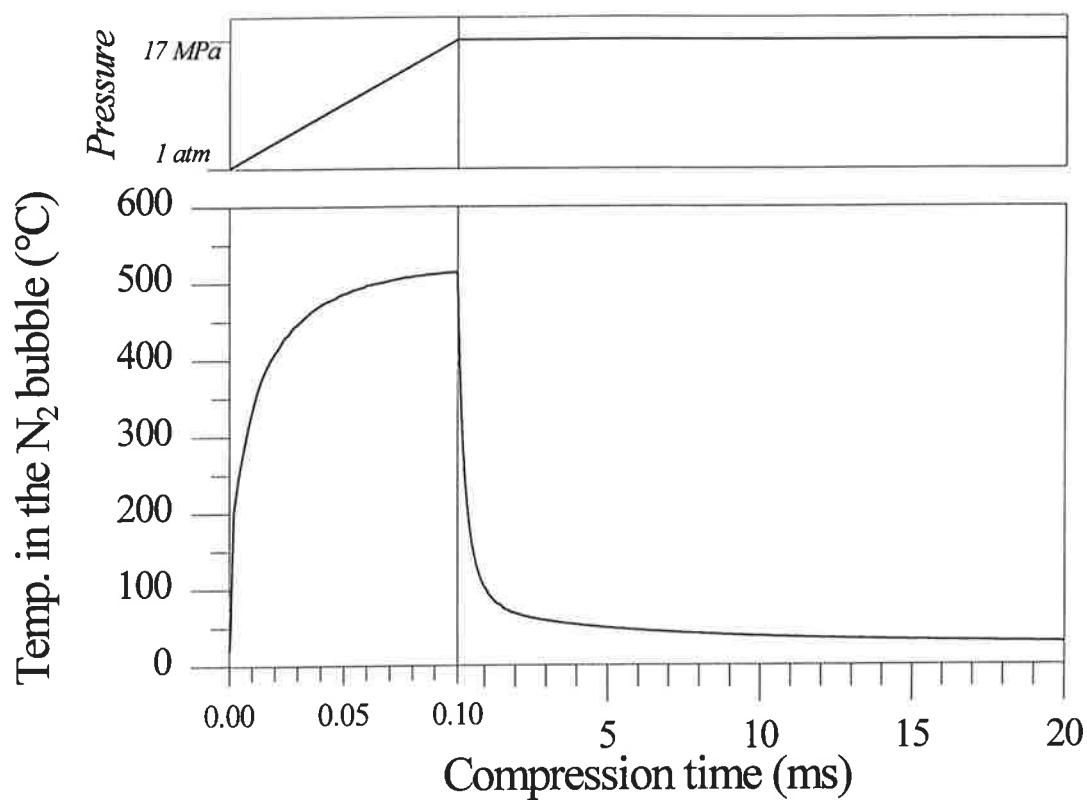


Fig. 16: Temperature in the N₂ gas bubble during the pre-compression, corresponding pressure profile in the upper figure or in Fig. 10. Note the dual time scales.

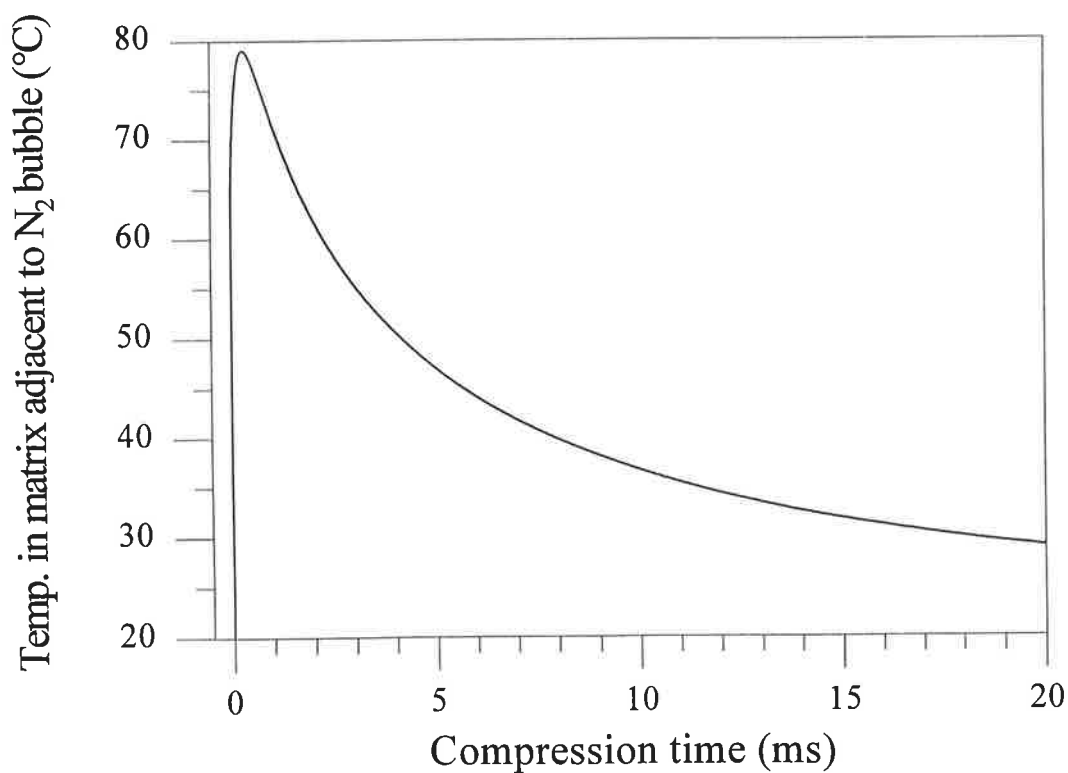


Fig. 17: Temperature in the matrix element closest to the N₂ bubble during pre-compression.

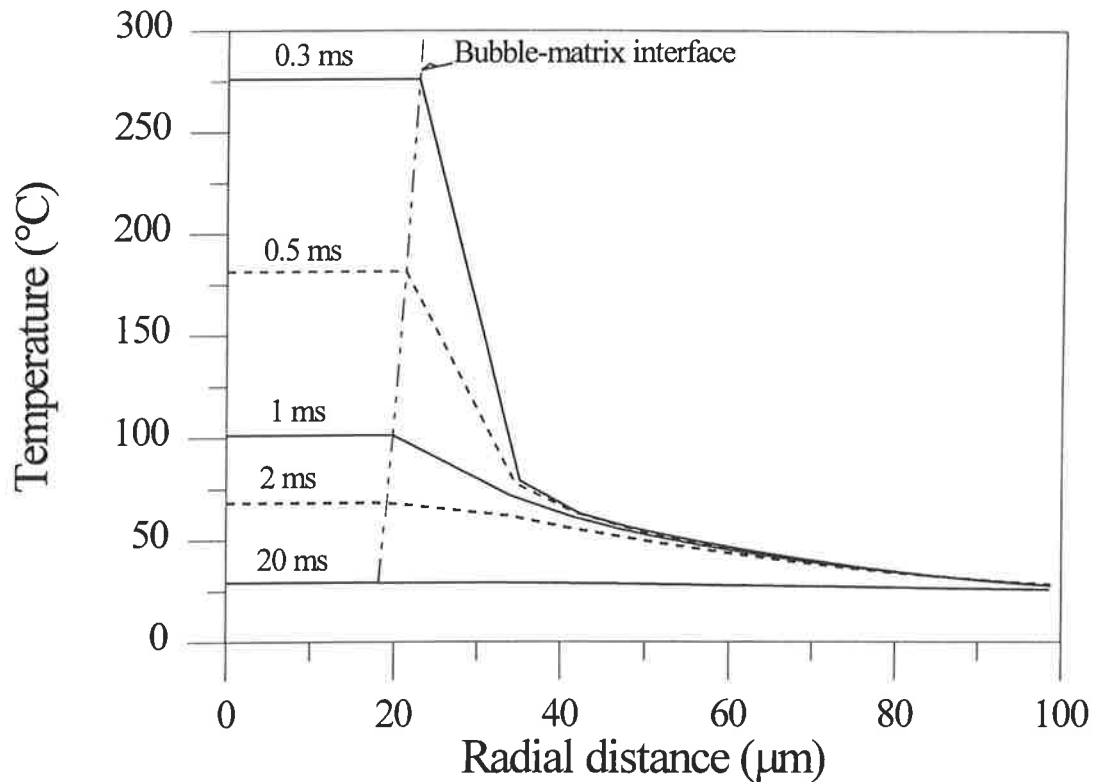


Fig. 18: Spatial temperature distribution in the N_2 bubble and the matrix, after different compression time. The original bubble radius before the compression is $100\ \mu\text{m}$.

After 0.1 ms, the pressure stops rising but stays constant, see Fig. 10. This time, the bubble temperature decreases very rapidly in the beginning owing to the heat transmission from the bubble to the matrix. However, in the same time, the bubble radius decreases quite slowly. After 2 ms of compression, the bubble radius decreased to $19.1\ \mu\text{m}$ while the bubble temperature decreased to $68.2\ ^\circ\text{C}$.

Within a compression time of 2 ms, the bubble radius has decreased from $100\ \mu\text{m}$ to $19.1\ \mu\text{m}$, a total diminution of $80.9\ \mu\text{m}$, see Fig. 15. Of this $80.9\ \mu\text{m}$ total diminution, $74.4\ \mu\text{m}$ or 92% was caused by the pressure rise from 0 to 0.1 ms. During this time, the effect of heat transmission may be disregarded, since the time period of 0.1 ms is very short compared to 2 ms. Thus, it can be concluded that the compression is the overwhelming reason for the bubble size diminution.

It can also be seen that after 1 ms of compression, the radius and the temperature decrease very slowly. After 10 ms, they no longer decrease significantly. After 20 ms, there are almost no changes.

The temperature in the matrix element adjacent to the N_2 bubble, Fig. 17, first rises to a maximum of $79\ ^\circ\text{C}$ in 0.3 ms due to the overwhelming effects of the viscous heating and the heat gained from the N_2 bubble. Then it decreases due to the heat conduction to farther matrix elements.

5.3.2 Dead-pressing of the gassed emulsion explosive

If, at different waiting times during the compression, the explosive is initiated by the primer, see pressure profile in Fig. 12, the explosive will be subjected to a shock from the primer. This shock causes an intensive viscous flow of the matrix, compresses the N_2 bubbles to a high temperature and leads to a higher temperature in the matrix as a result. The matrix may be initiated, according to the initiation criterion described in Section 5.1.1. The temperature in the matrix element closest to the N_2 bubble determines whether the explosive will be initiated, since the highest matrix temperature occurs there.

However, the resulting temperature in the matrix is dependent on the radius and temperature of the N_2 bubbles at the initiating moment, which in their turns depend on the pre-compression period or the waiting time, as shown in Figs. 15 and 16.

Fig. 19 shows how this shock-induced temperature in the matrix element adjacent to the N_2 bubble decreases with the waiting time. According to this figure, the explosive is dead-pressed at waiting times longer than 2 ms. At the waiting time of 2 ms, the shock induced temperature in the matrix reaches 297.4 °C as the highest, which is very close to the initiation temperature of 300 °C. At this dead-pressing moment, the radius of the N_2 bubble has been compressed to 19.1 μm and the internal temperature is 68 °C

For comparison reasons, the temperature in the matrix has been calculated for the case of a direct initiation by the primer, i. e. without pre-compression or at waiting time 0. The highest temperature in the matrix or the temperature in the matrix element closest to the N_2 bubbles rises to 993 °C in 8.5 ns, see Fig. 19 at waiting time 0. The initiation of the explosive is apparent in this case.

5.3.3 Recovery of the detonability of the gassed emulsion explosive

If the pre-compression vanishes after a certain time as shown in Fig. 13, the N_2 bubbles will expand and the temperature inside them decreases accordingly. Gradually, the temperature in the surrounding matrix will be higher than that in the N_2 bubbles. The matrix flow and the heat flux will reverse their directions. That is, the matrix flows away from the N_2 bubbles while the heat flux goes into the N_2 bubbles. Therefore, the N_2 bubbles start to regain some heat lost during the pre-compression. This heat regain compensates some of the temperature decrease caused by the bubble expansion.

The bubble expansion process, in which the radius increases and temperature decreases, is shown in Figs. 20 and 21 respectively. If initiation attempts are applied at different times, different temperatures will be induced in the matrix in the same manner as described in Section 5.3.2, see results in Fig. 22.

As described in Section 5.2.3, Fig. 13, the pressure release occurs after 20 ms of pre-compression. At this time, the temperature in the N_2 bubbles is as low as 29.2 °C and the bubble radius is as small as 18.2 μm . Longer waiting time can not harm the explosive much more, see Section 5.3.1.

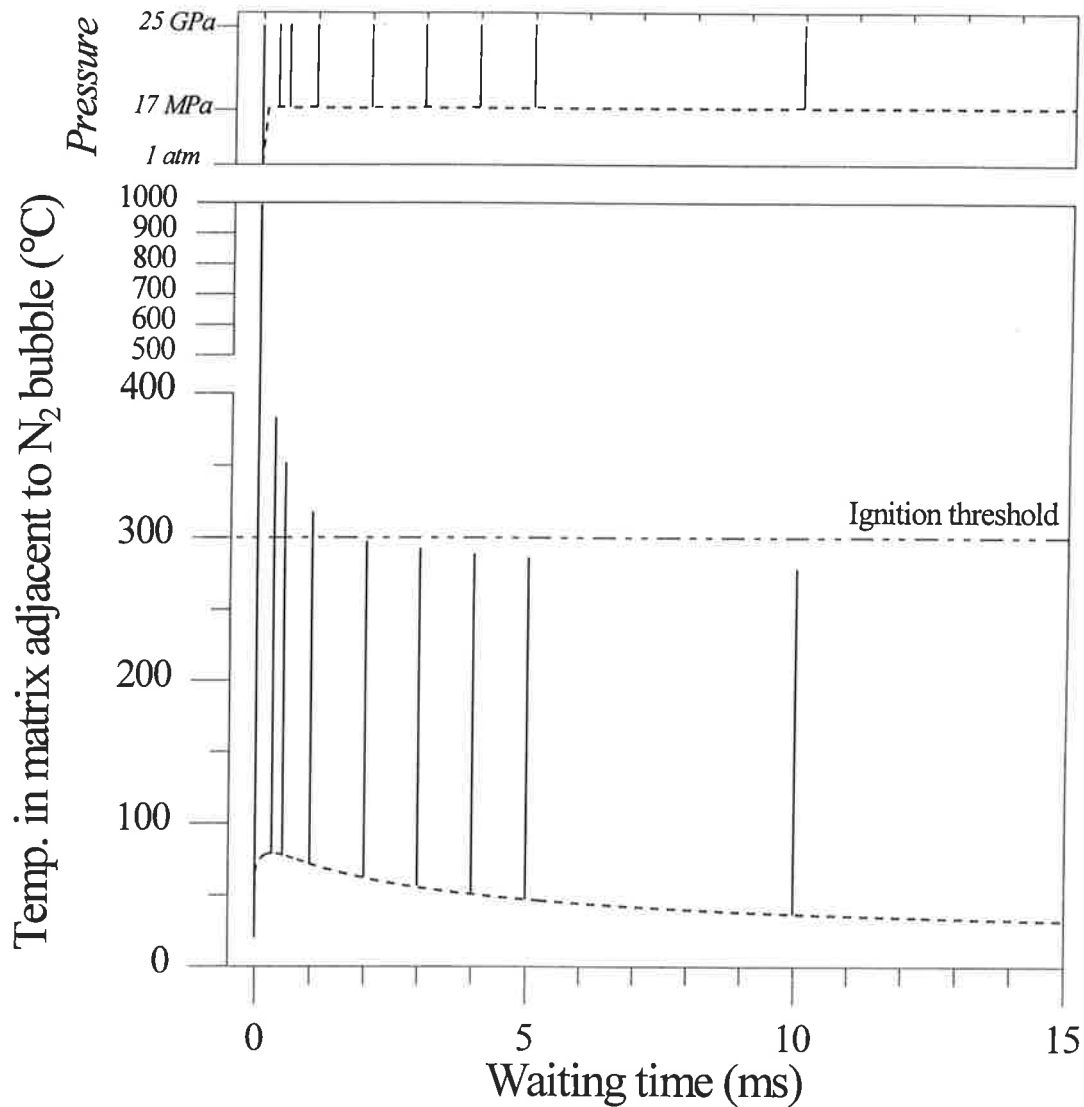


Fig. 19: Temperature in the matrix element adjacent to the N₂ bubble induced by initiation attempts using the primer at different waiting times, when the explosive is still under compression. The corresponding pressure profile is shown in the upper figure. The dashed lines correspond to the pre-compression.

Based on the initiation criterion in Section 5.1.1 and the results in Fig. 22, the explosive is detonable again 50 ns after the pressure release. In other words, the explosive recovers its detonability in 50 ns, which is a rapid process. At this recovery moment, the N₂ bubble has expanded to 19.2 μm , see Fig. 20. However, the internal temperature has decreased to 3.6 °C, see Fig. 21.

5.3.4 Initiation and dead-pressing mechanism

The initiation mechanism has been applied twice in the simulation, first in determining the dead-pressing and then in determining the detonability recovery of the explosive. In the following, the initiation process in both cases will be studied in more detail.

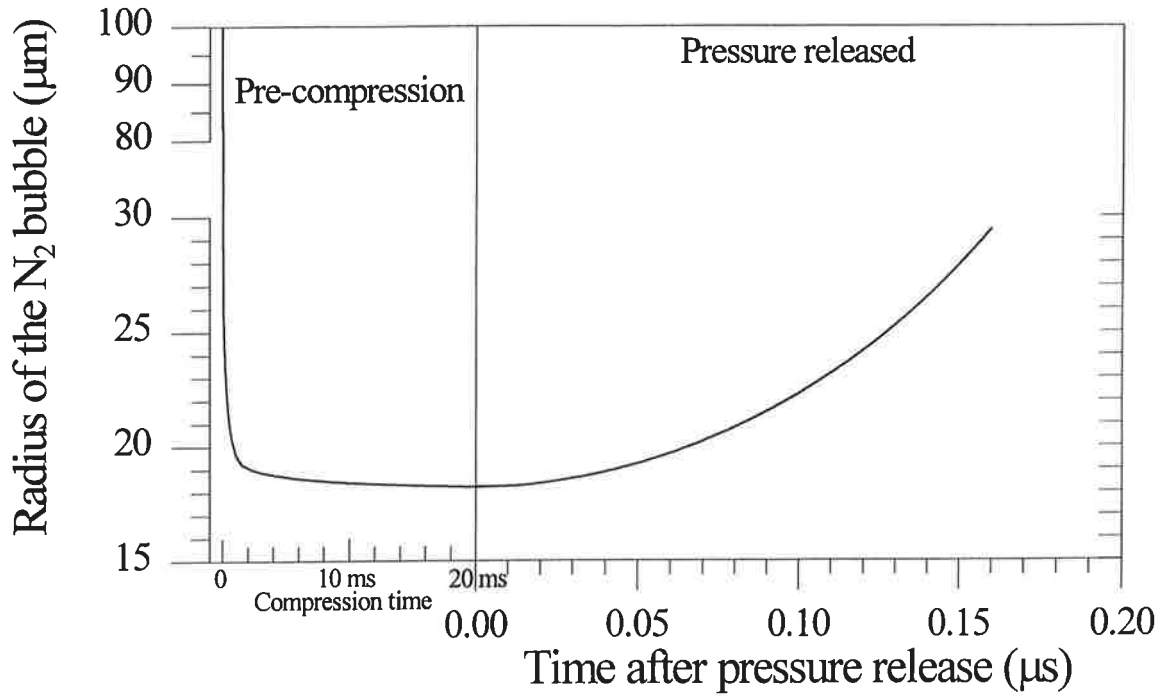


Fig. 20: Radius of the gas bubbles during and after the pre-compression, corresponding to the pressure profile in Fig. 13.

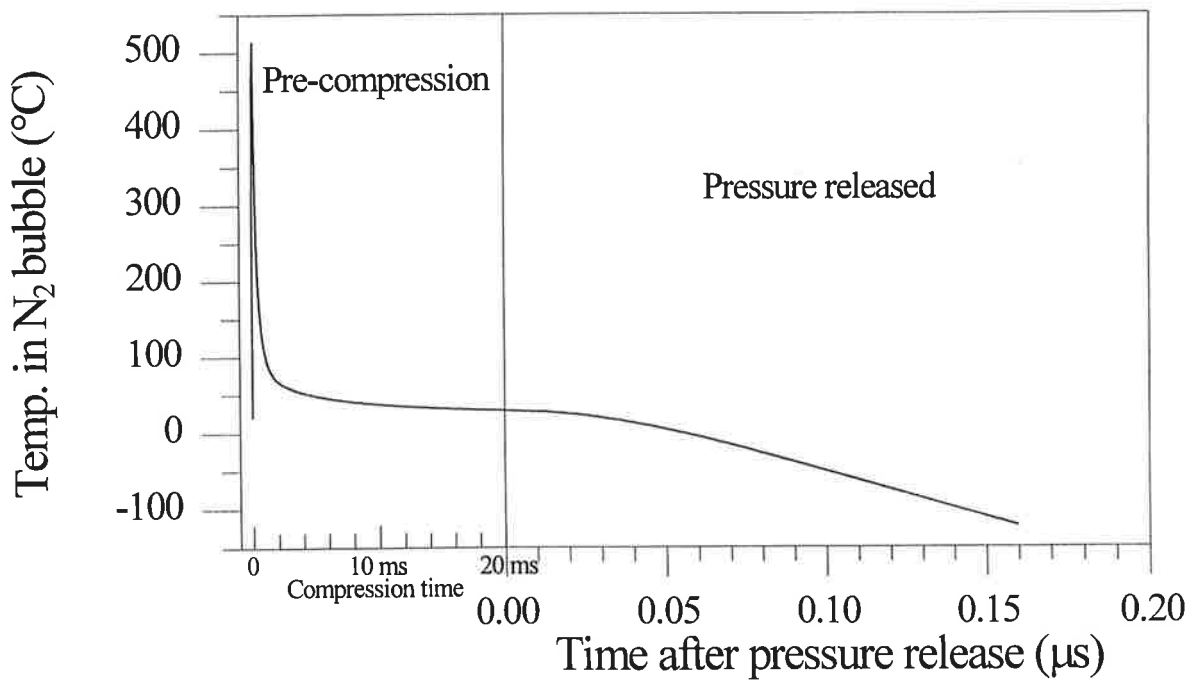


Fig. 21: Temperature in the gas bubbles during and after the pre-compression, corresponding to the pressure profile in Fig. 13.

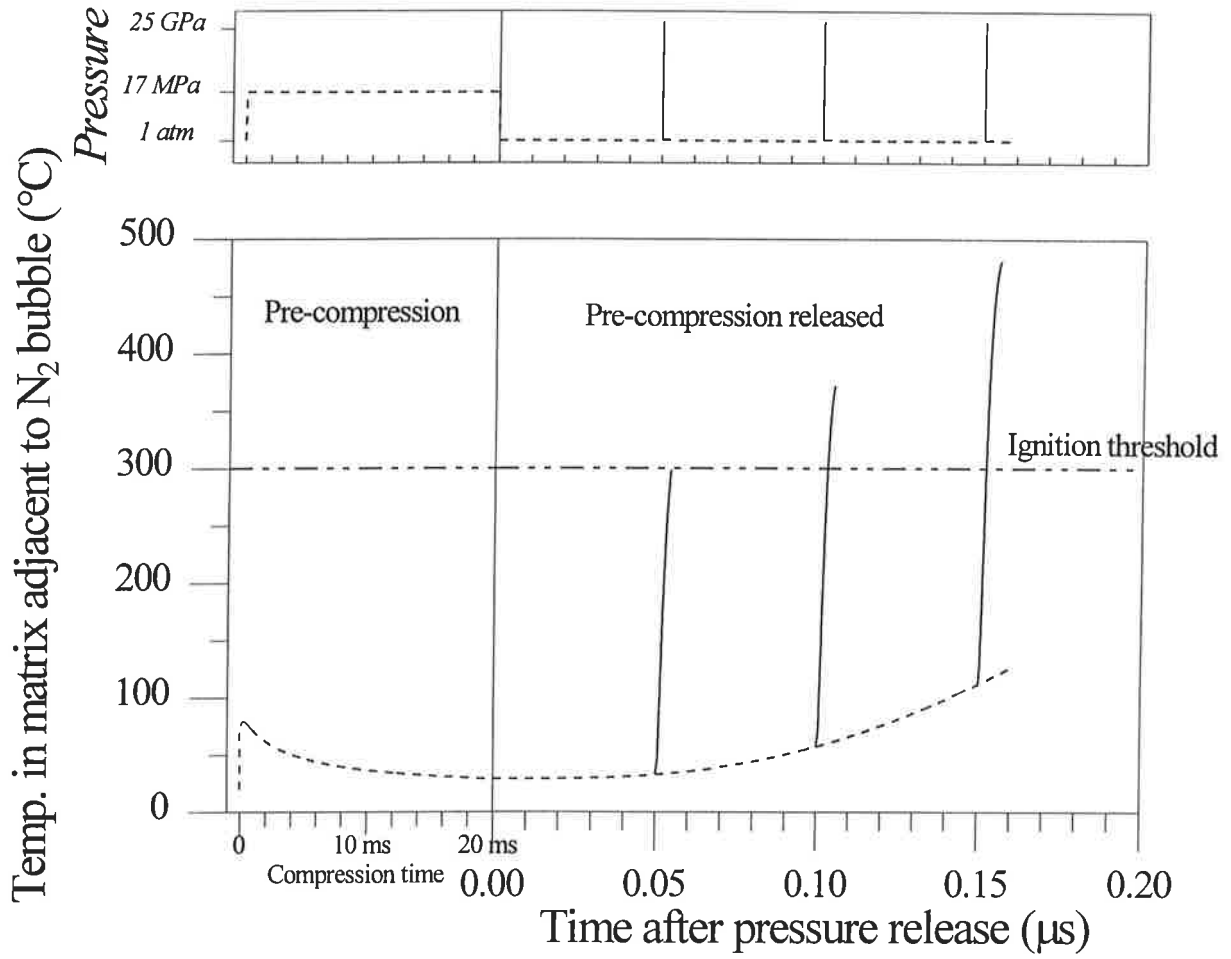


Fig. 22: Temperature in the matrix element adjacent to the N₂ bubble induced by initiation attempts using the primer at different time after the pre-compression vanishes. The corresponding pressure profile is shown in the upper figure as well as in Fig. 13. The dashed lines correspond to compression at 17 MPa or 1 atm.

Fig. 23 is a close-up of Fig. 19 at the waiting time 2 ms. It shows that the temperature in the matrix in the vicinity of the N₂ bubble is shocked from 62 to 297.4 °C in approximately 4 ns. The temperature increase in the N₂ bubble in the same period is shown in Fig. 24.

The temperature increase in the matrix is caused by the viscous flow of the matrix itself and the heat transferred from the N₂ bubble into the matrix, as described in Section 5.1.1. The transferred heat can be calculated by Eq. 44 and its resultant temperature increase in the matrix element by Eq. 45 below, if heat conduction from this matrix element to other elements is disregarded.

$$Q_1 = \int_0^{4\text{ns}} \alpha \cdot A_1 \cdot (T_1 - T_2) \cdot dt \quad \dots\dots\dots(44)$$

$$\delta T_2 = \frac{Q_1}{V_2 \cdot \rho_M \cdot C_{pM}} \quad \dots\dots\dots(45)$$

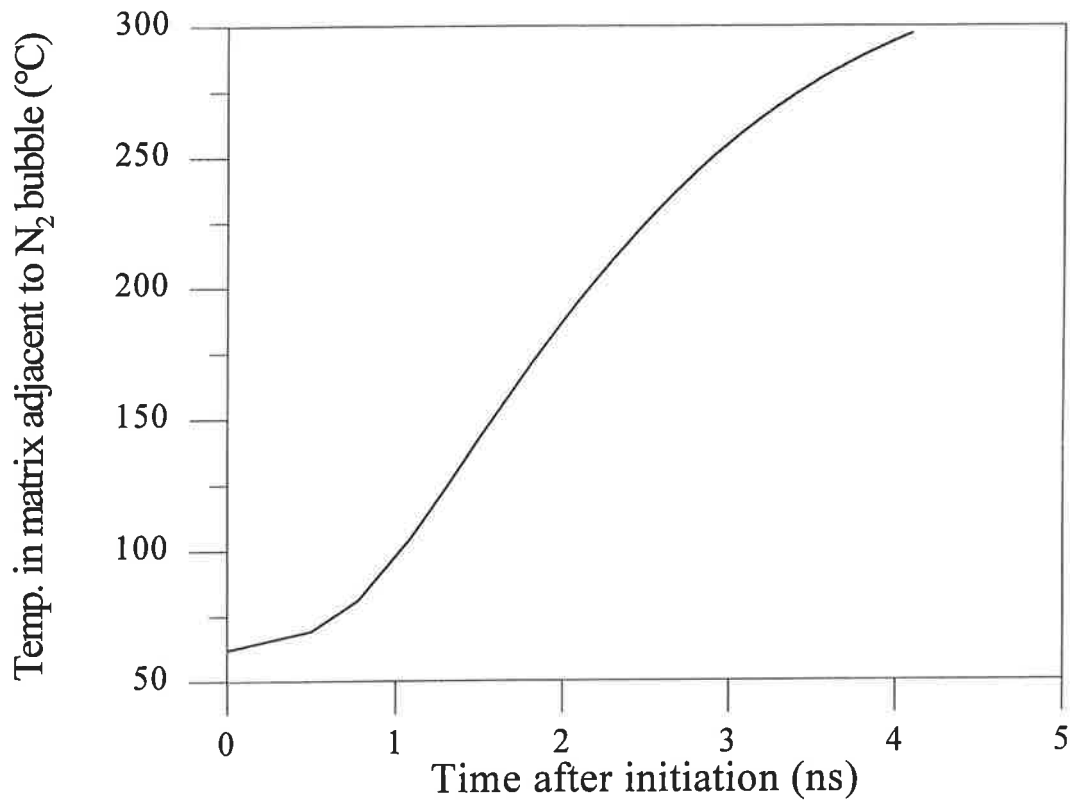


Fig. 23: The temperature rise in the matrix element adjacent to the N₂ bubble caused by the initiation attempt at waiting time 2 ms, cf. Fig. 19.

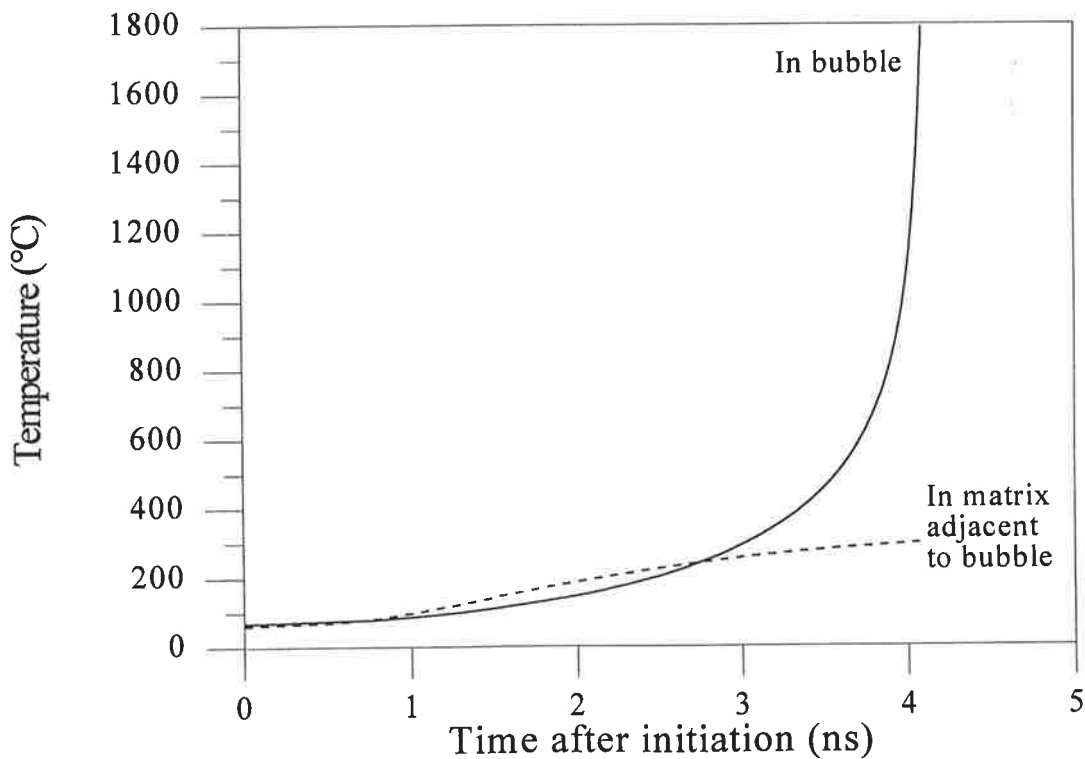


Fig. 24: The temperature increase in the matrix element adjacent to the N₂ bubble and in the N₂ bubble caused by the initiation attempt at waiting time 2 ms, cf. Fig. 23.

Where: Q_1 = heat transferred from N_2 bubble to the matrix during initiation, i.e. 4 ns, (J)

α = coefficient of heat transfer = 4190 W/m²/K /14/

A_1 = surface area of the N_2 bubble, (m²)

T_1 = temperature in the N_2 bubble, (K), refer to Fig. 9

T_2 = temperature in the matrix element adjacent to the N_2 bubble, (K), refer to Fig. 9

t = time, (s)

δT_2 = temperature increase in the matrix adjacent to the N_2 bubble, (K or °C)

v_2 = volume of the matrix element, (m³), refer to Fig. 9

ρ_M = density of the matrix = 1360 kg/m³

C_{pM} = specific heat of the matrix = 1080 J/K/kg /14/

The results obtained from those two equations are:

$$Q_1 = 2.315 \cdot 10^{-12} \text{ J}$$

$$\delta T_2 = 1.193 \cdot 10^{-5} \text{ } ^\circ\text{C}$$

If the heat conduction to other matrix elements is concerned, then δT_2 is even smaller. This implies that the gas compression mechanism has contributed with a temperature increase less than $1.193 \cdot 10^{-5} \text{ } ^\circ\text{C}$ to the total increment of 235 °C for the initiation. Or, it can be concluded that the viscous heating alone is responsible for the initiation.

The same conclusion can be drawn from the study of the initiation attempt applied 50 ns after the pre-compression is released, Fig. 25.

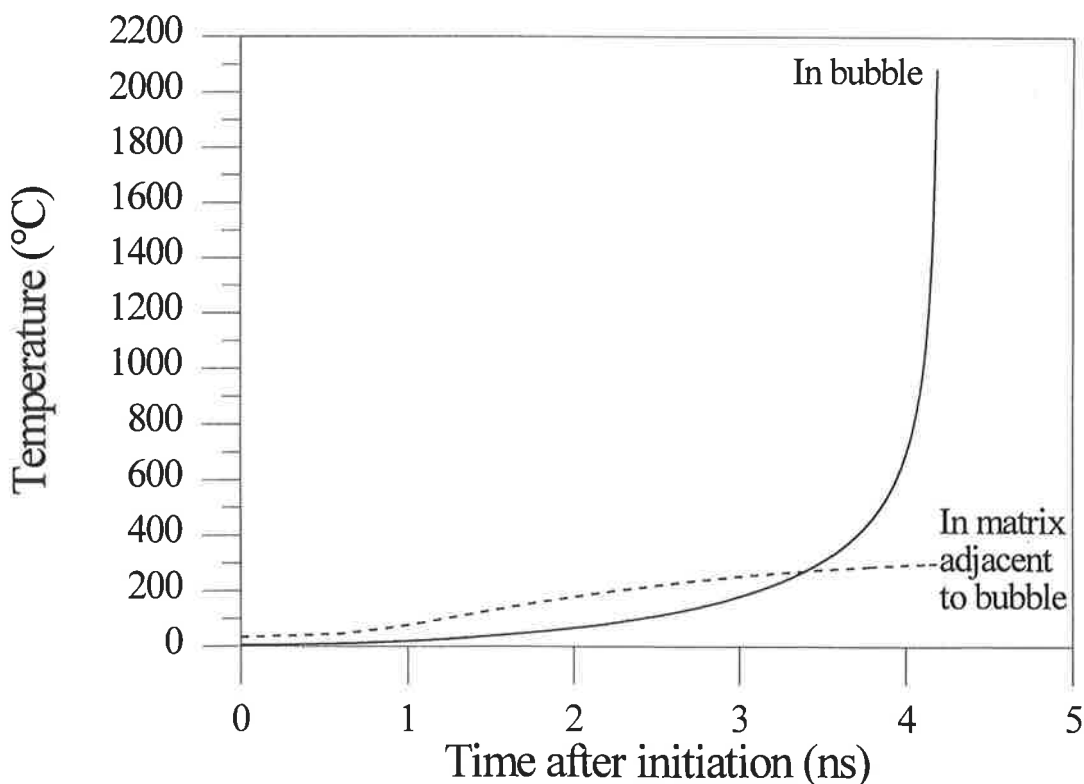


Fig. 25: Temperature increase in the N_2 bubble and in the matrix element closest to the bubble during the initiation attempt 50 ns after the pre-compression vanishes, cf. Fig. 22.

According to Eqs. 8, 9 and 14, the viscous heating is dependent on the density and viscosity of the matrix, the amplitude of the shock pressure and the bubble size, assuming that the particle velocity of the matrix at the initiation moment is zero. Since the matrix density, matrix viscosity and shock amplitude are constant in the initiation simulations, the viscous heating is therefore only dependent on the bubble size. Hence, it can be further concluded that it is the bubble size which determines the detonability of the gassed emulsion explosive in these simulations.

The above study of two initiations confirmed this conclusion. The explosive is dead-pressed when the bubble radius decreased to 19.1 μm , at waiting time 2 ms, and the explosive recovers its detonability when the bubble radius expanded to 19.2 μm , at 50 ns after the pressure release, see Fig. 20. A critical bubble radius exists around 19.1 μm , provided that the initiation pressure is 24.8 GPa and the ignition temperature of the matrix is 300 °C. However, in the two initiating moments, the temperature of the bubble was much different, see Fig. 21. These facts show that despite the different temperatures in the N_2 bubbles, the explosive is detonable as long as the bubble radius is larger than the critical radius.

Furthermore, the analysis in Section 5.3.1 showed that the compression is the overwhelming reason for the diminution of the bubble size. The heat transmission from the bubbles to the surrounding matrix has a minor effect.

As a conclusion of the above analysis, it can be stated that the viscous heating is the initiation mechanism for shock initiation and that the diminution of the bubble size, due to the compression and heat loss of the bubbles, is the cause of the dead-pressing.

5.3.5 Extension of the simulation results

The simulation has demonstrated that the size diminution of the gas bubbles due to compression and heat loss is responsible for the dead-pressing of the chemically gassed emulsion explosive. According to this mechanism, the following results are expected.

The larger the gas bubbles are, the more sensitive the explosive is to initiation and the longer dead-pressing time the explosive has.

The faster the compression pressure rises, or the shorter rise time the pressure has, the higher amplitude the pressure can reach before the explosive is dead-pressed. The reason is that the shorter the rise time is, the less the heat loss from the gas bubbles is. The less heat loss means a higher bubble temperature and a larger bubble volume. Therefore, the explosive should be able to tolerate a higher rapid-rising pressure than a slow-rising pressure before the bubbles are sufficiently small and the explosive is dead-pressed.

The calculated recovery time is based on a hypothetical pressure profile, where the pressure release happens abruptly in no time. In the rock blasting practice, this kind of pressure falling hardly exists. Instead, the pressure decay processes very slowly [2]. Therefore, the visible recovery time in practice is determined by the speed of the pressure decay. Nano-seconds after the pressure decreases to a certain level, the explosive is detonable again.

As observed in the experiments, see Section 4.2, the momentary pressure on the explosive at the initiation moment can determine the detonability of the explosive. This phenomenon can be explained by the fast dead-pressing and detonability recovery processes. In the experiments where the momentary pressure could be measured, the waiting times were very long, from 20 to 282 ms, see Fig. 6 and Table 3, compared to the dead-pressing time of 2 ms. Therefore, the explosive has been dead-pressed for a long time and waiting for the pressure decay which occurred very slowly, see pressure histories in Appendix II. However, immediately after the pressure decreased to a level below approximately 17 MPa, the N₂ bubbles expanded to a size larger than the critical radius. If the explosive were initiated by the primer at this moment, the explosive would detonate.

5.3.6 Conclusions of the simulation

Although this simulation has included several assumptions and simplifications, it does explain the dead-pressing and detonability recovery of the gassed emulsion explosives. Furthermore, the simulation showed that the dead-pressing and the detonability recovery are very rapid processes, which coincides with the experimental results. At a pressure of 17 MPa, the dead-pressing of the explosive takes 2 ms, while the detonability recovery takes 50 ns. The rapid dead-pressing and detonability recovery processes explain why the detonability of the gassed explosive is determined by the momentary pressure rather than the maximum pressure, as shown by the experiments.

The simulation also indicated that the viscous heating of matrix in the vicinity of the gas bubbles is responsible for the shock initiation of the gassed emulsion explosive. Since the viscous heating is determined by the bubble radius at the initiation moment, the bubble radius actually determines the detonability of the explosive. The minimum bubble radius for initiation is 19.1 μm for the tested explosive, provided that the initiation pressure is 24.8 GPa and the ignition temperature of the matrix is 300 °C.

Thanks to the rapid detonability recovery, misfires may be avoided in the rock blasting practice by designing adequate delay time between holes.

To obtain an even better understanding of the dead-pressing and detonability recovery processes, more sophisticated ignition models and more realistic pressure profiles may be helpful.

6. CONCLUSIONS

The study described in this report can be concluded as follows.

- A chemically gassed emulsion explosive has been studied by experiments and simulation.
- The simulation resulted in good agreement with the experimental work.
- The explosive studied can tolerate a pressure of 17 MPa, which is higher than some low strength micro-balloon-sensitized emulsions.

- The dead-pressing occurs very rapidly and takes about 2 ms.
- The diminution of the gas bubbles is the cause for dead-pressing. Both the compression and the heat loss of the gas bubbles contribute to the size diminution of the bubbles. However, the compression is the overwhelming cause.
- The minimum bubble radius for initiation is 19.1 μm for the tested explosive, provided that the initiation pressure is 24.8 GPa and the ignition temperature of the matrix is 300 °C.
- According to the experiments, the detonability of the gassed explosive can be recovered very rapidly. According to the simulation, the recovery takes about 50 ns, should the pre-compression be released abruptly. This rapid recovery is a unique feature of the gassed emulsions, which the micro-balloon-sensitized emulsions do not have.
- The viscous heating in the vicinity of the gas bubbles is the dominant mechanism for shock initiation of the gassed emulsion explosive.
- In rock blasting practice, the malfunction of the gassed explosive due to dead-pressing may be avoided by proper design of the initiation sequences.

ACKNOWLEDGEMENT

This study included both experiments and simulations. The experiments were carried out by Shulin Nie and Li Chen while the simulations were carried out by Shulin Nie.

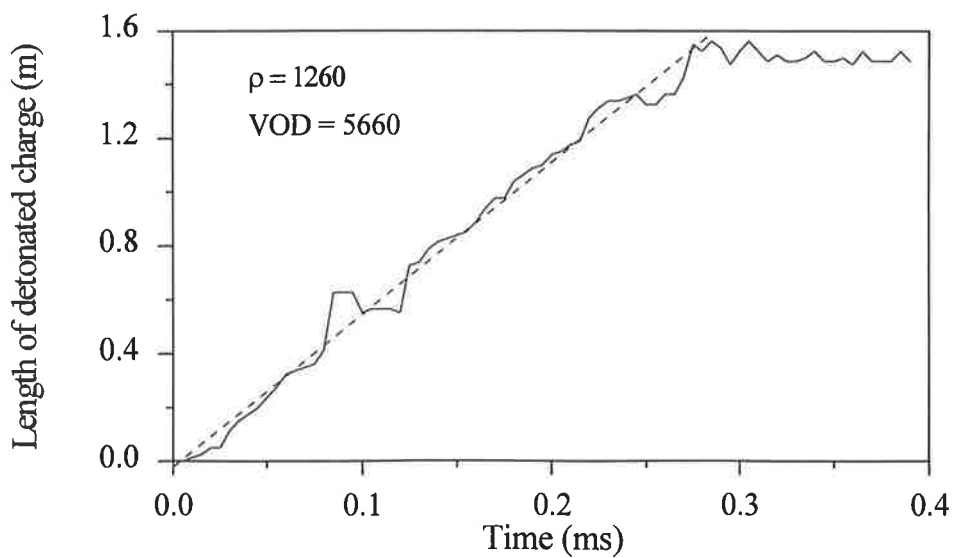
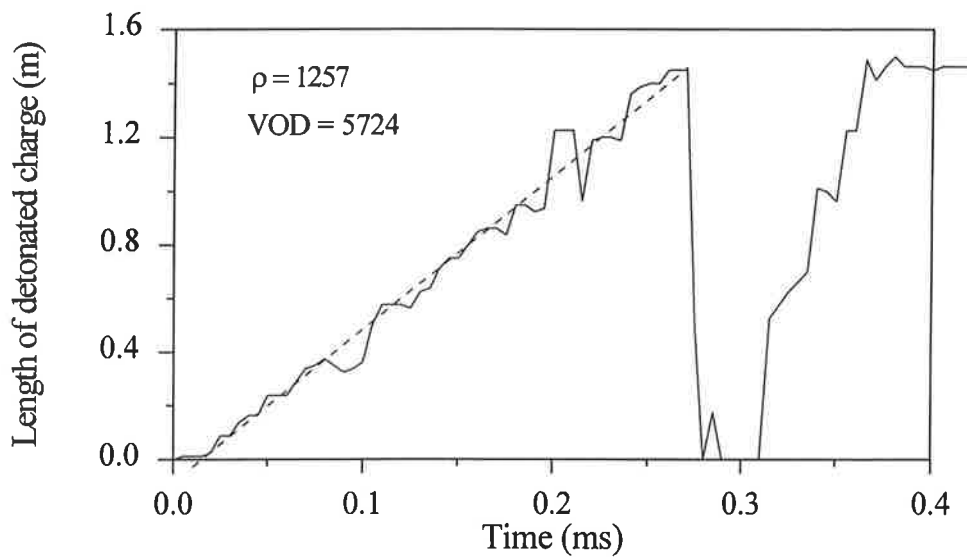
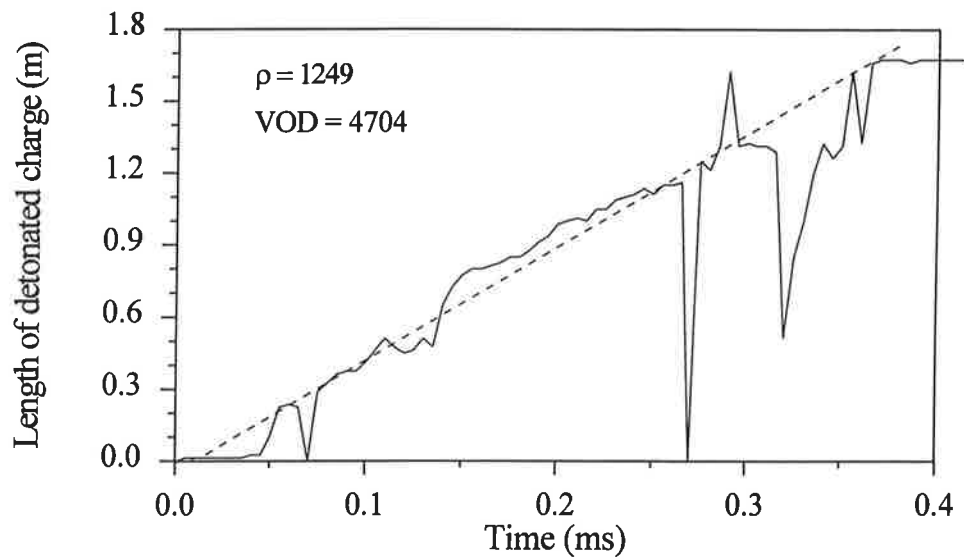
The FoU Division of the Nitro Nobel AB, particularly, Mr. B Engstråten, is gratefully acknowledged for providing us with the chemical gassing technique of emulsion explosives and some property data of the explosive, for the manufacturing of all the steel pipes used in the experiments and for the manufacturing of the matrix of the studied explosive.

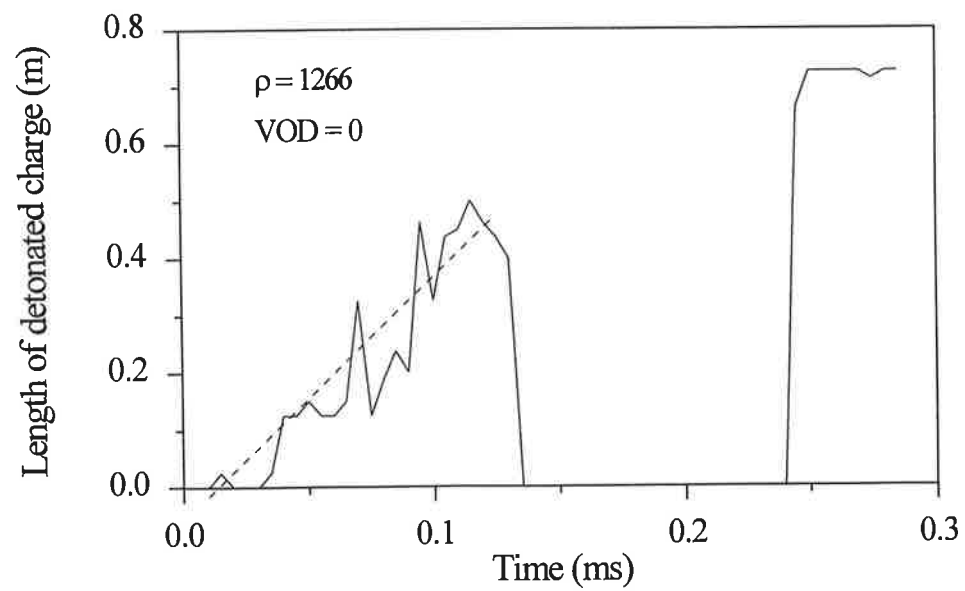
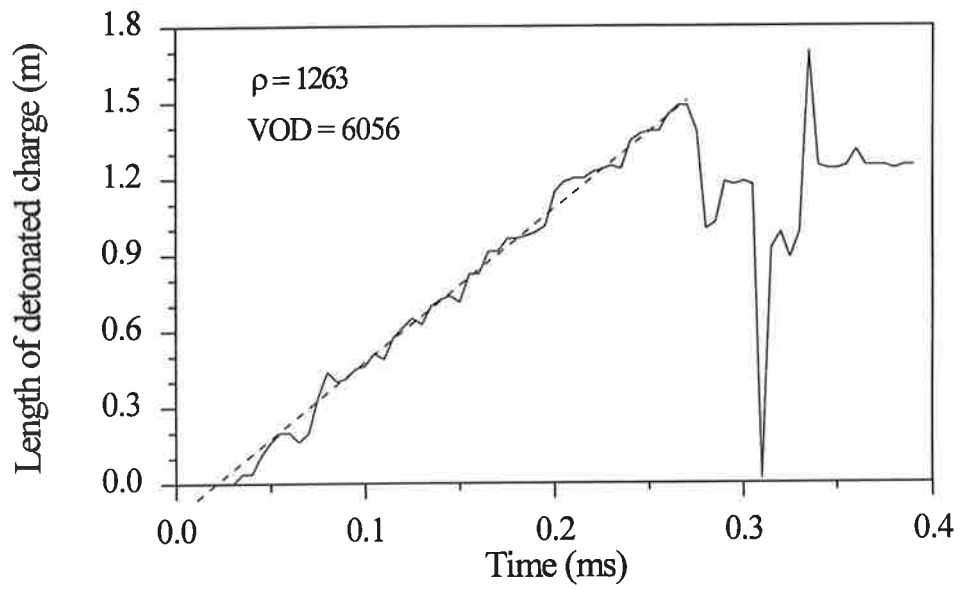
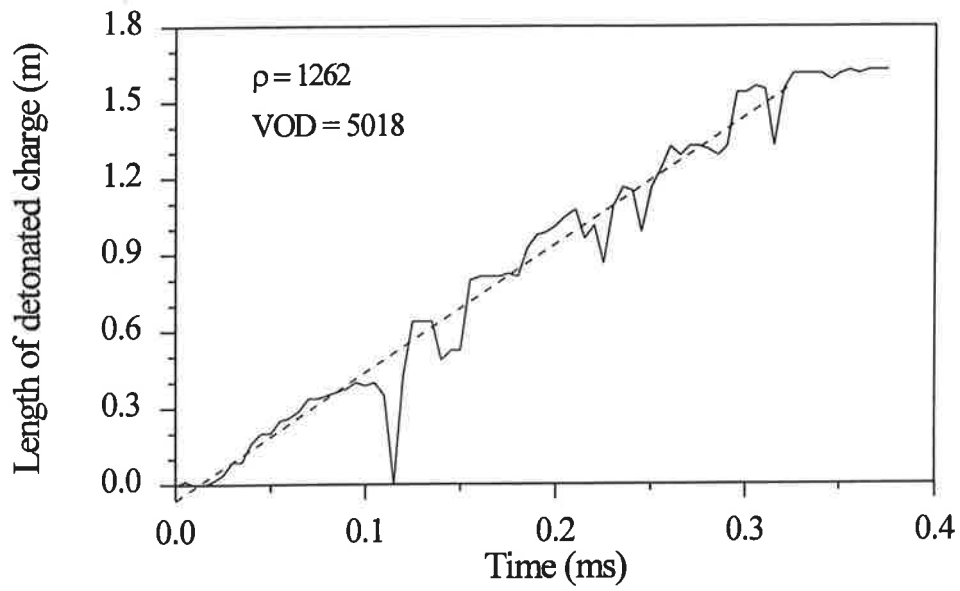
Thanks are also directed to Dr. F Ouchterlony at SveBeFo and Dr. H Almström at FOA for their valuable discussions and comments on the computer simulation.

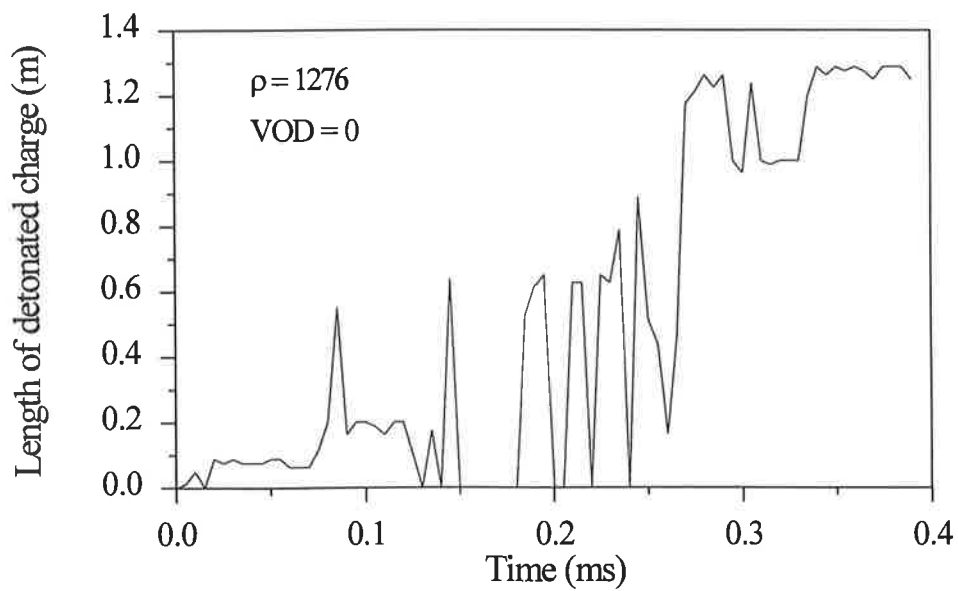
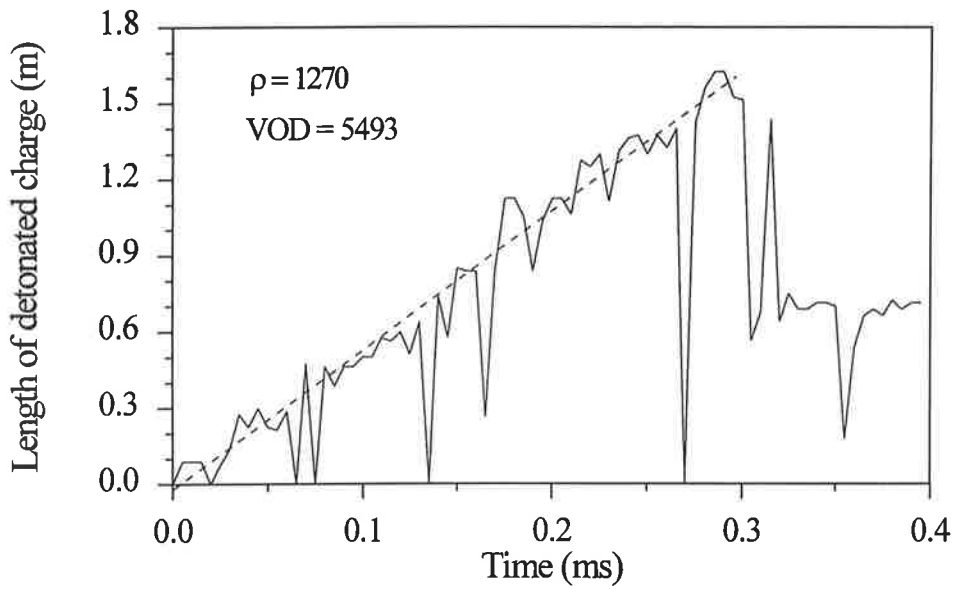
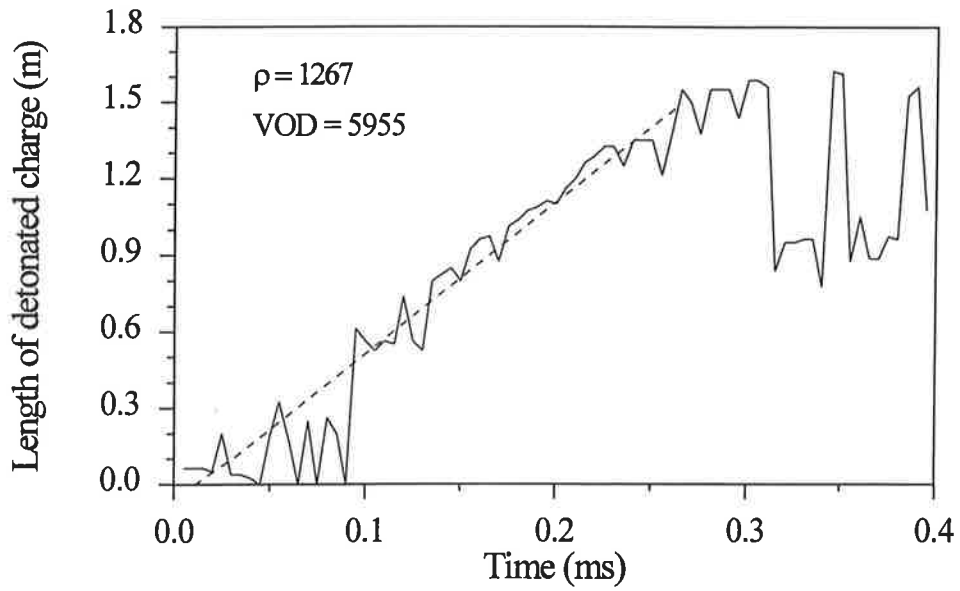
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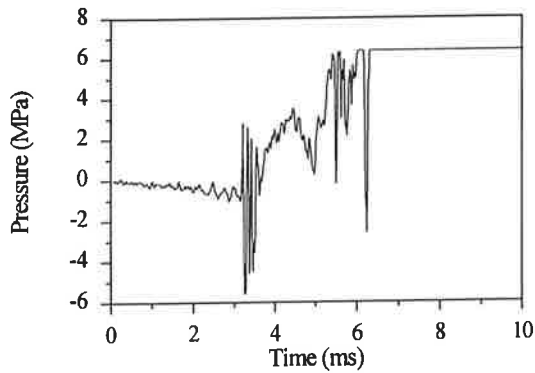
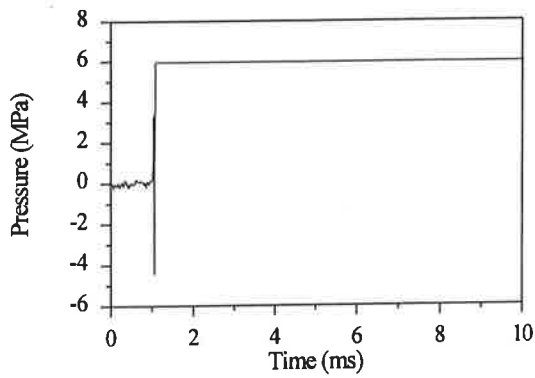
APPENDIX I: Signals from the continuous measurement of the velocity of detonation during the determination of the critical density of the matrix.



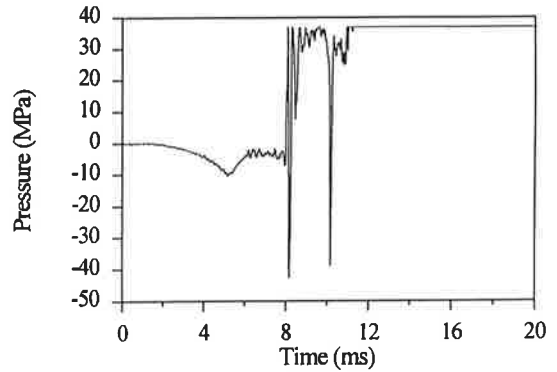
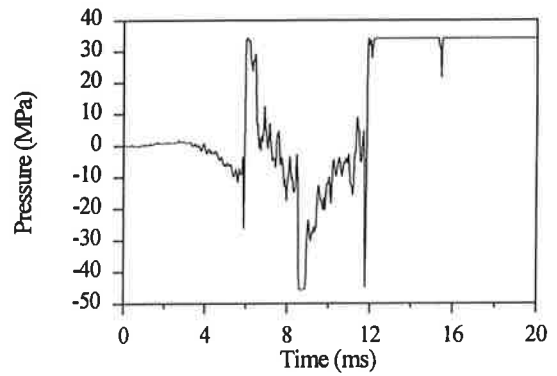




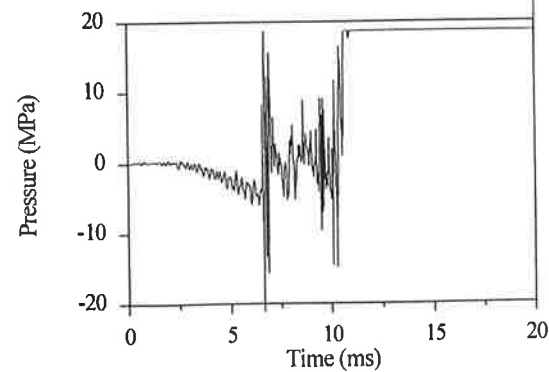
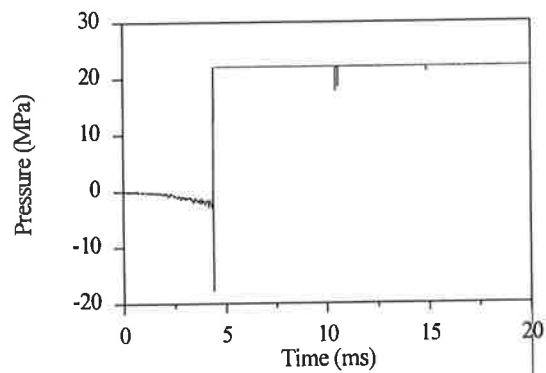
APPENDIX II: Pressure histories recorded in the detonability tests of the chemically gassed emulsion explosive.



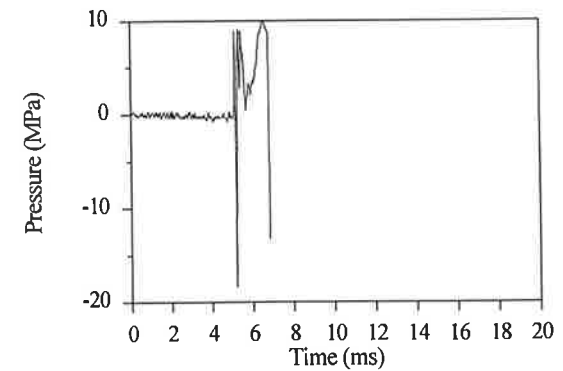
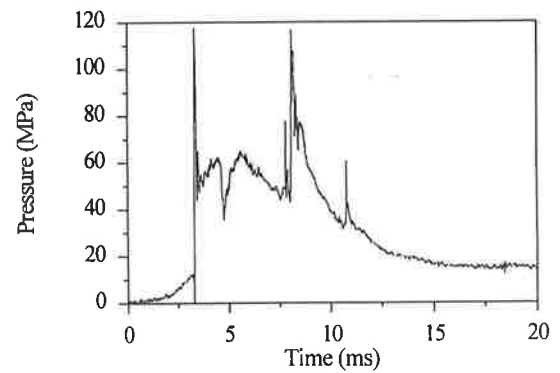
Upper: Test No. 1, Gage 1.
Lower: Test No. 1, Gage 2.



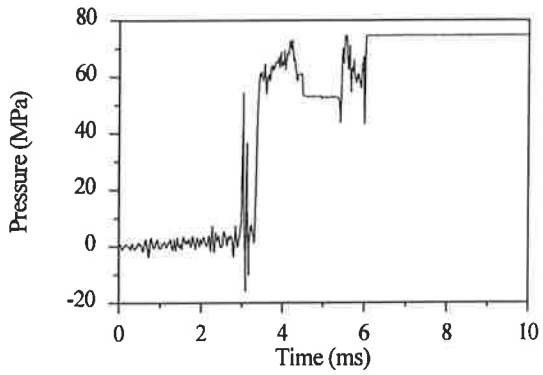
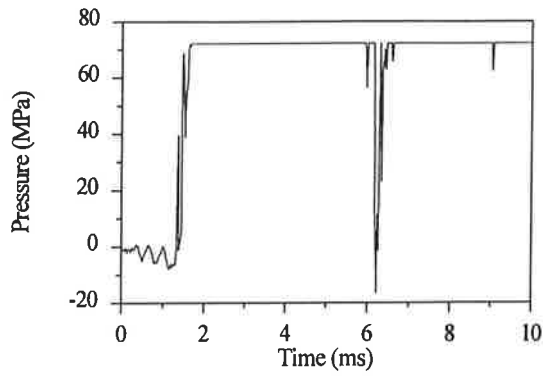
Upper: Test No. 2, Gage 1.
Lower: Test No. 2, Gage 2.



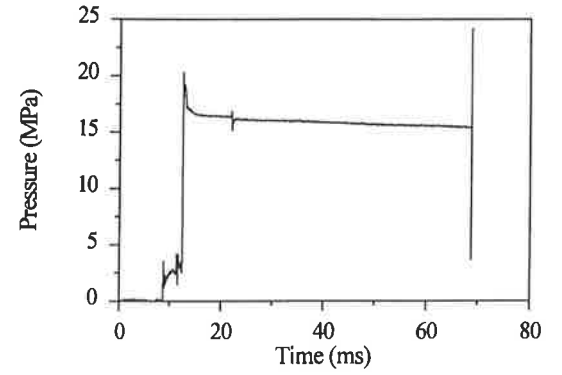
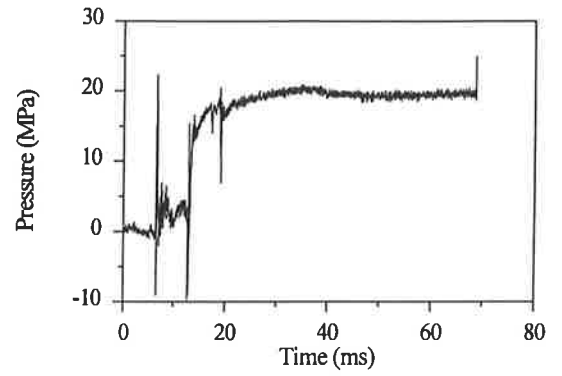
Upper: Test No. 3, Gage 1.
Lower: Test No. 3, Gage 2.



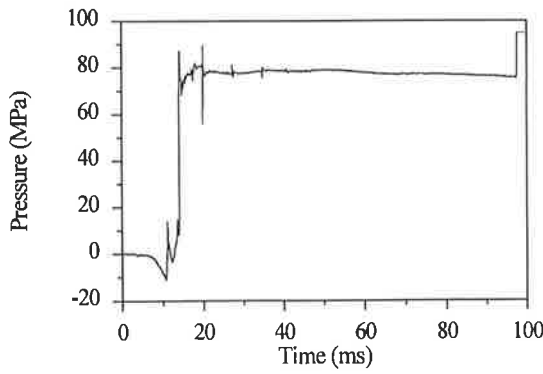
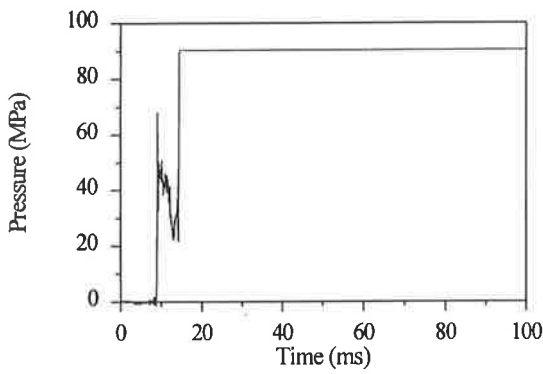
Upper: Test No. 4, Gage 1.
Lower: Test No. 4, Gage 2.



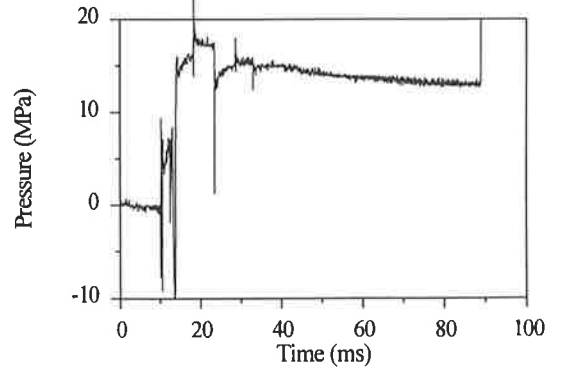
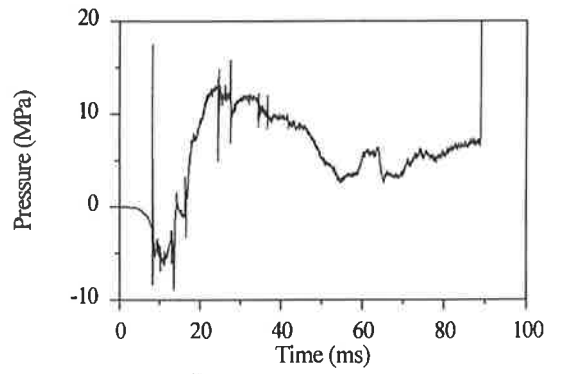
Upper: Test No. 5, Gage 1.
Lower: Test No. 5, Gage 2.



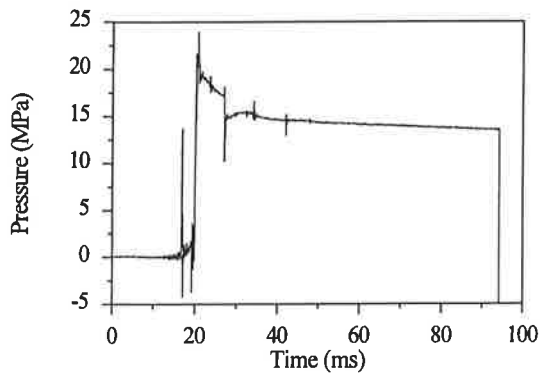
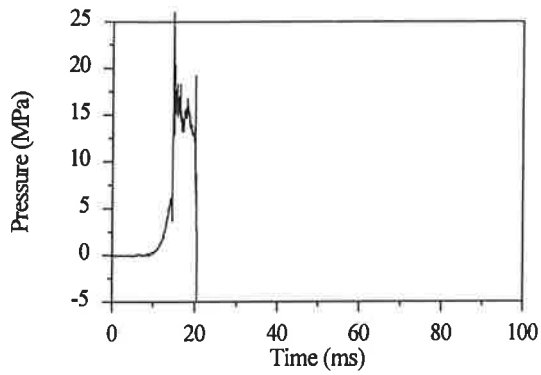
Upper: Test No. 6, Gage 1.
Lower: Test No. 6, Gage 2.



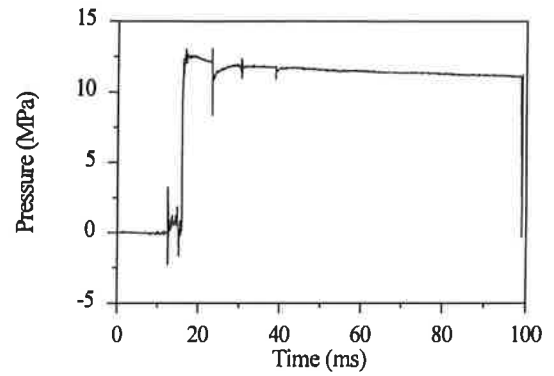
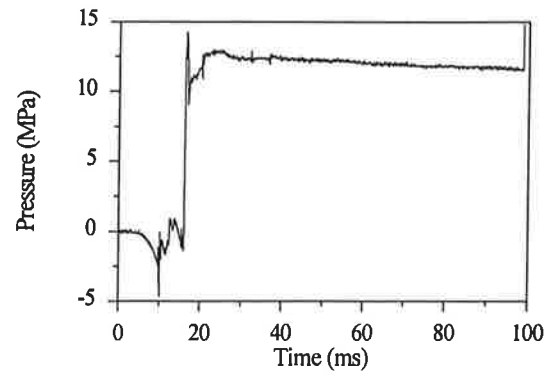
Upper: Test No. 7, Gage 1.
Lower: Test No. 7, Gage 2.



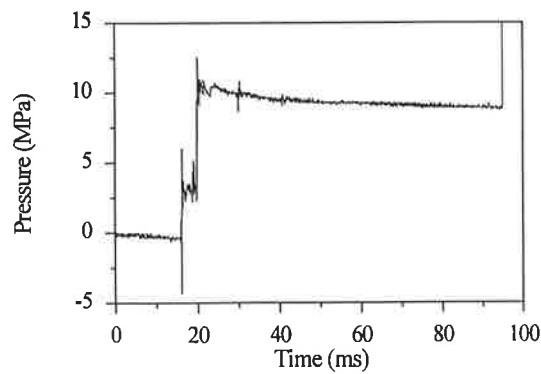
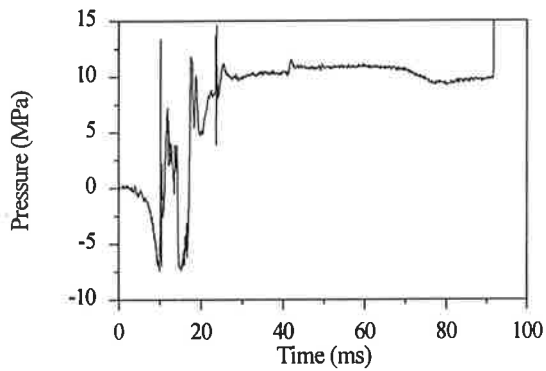
Upper: Test No. 8, Gage 1.
Lower: Test No. 8, Gage 2.



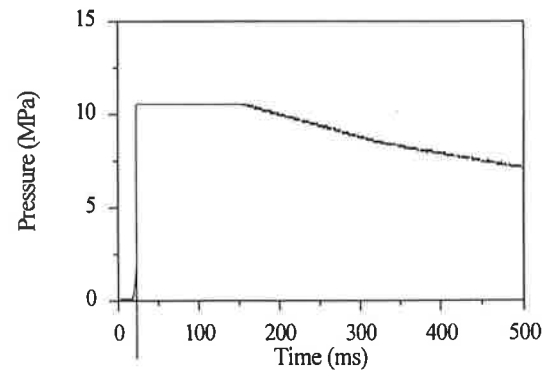
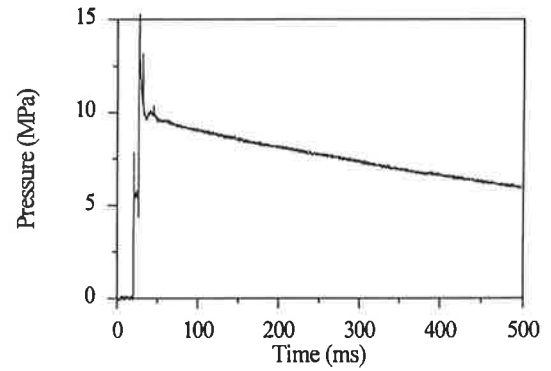
Upper: Test No. 9, Gage 1.
Lower: Test No. 9, Gage 2.



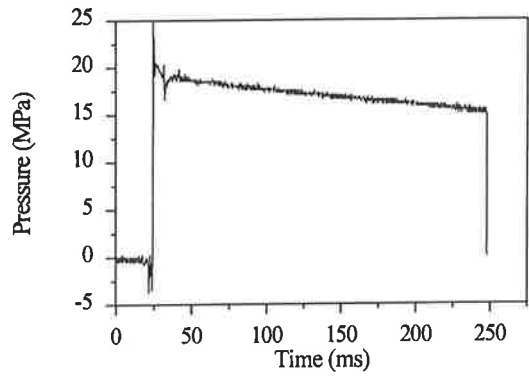
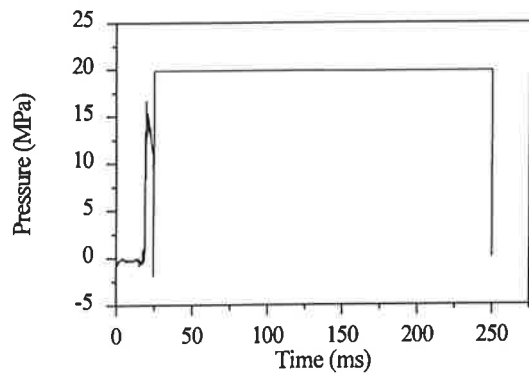
Upper: Test No. 10, Gage 1.
Lower: Test No. 10, Gage 2.



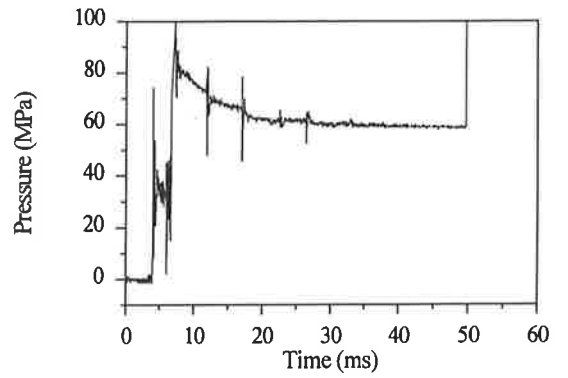
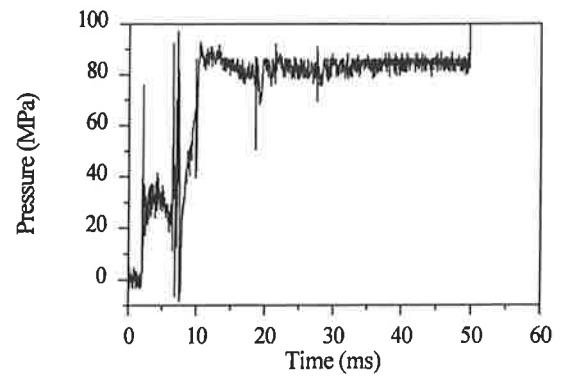
Upper: Test No. 11, Gage 1.
Lower: Test No. 11, Gage 2.



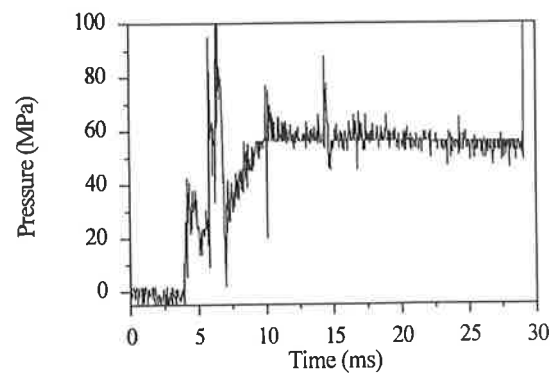
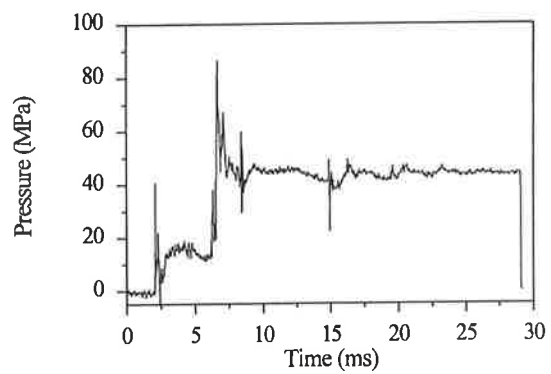
Upper: Test No. 12, Gage 1.
Lower: Test No. 12, Gage 2.



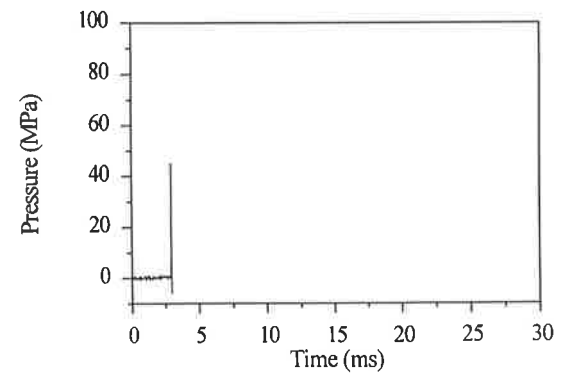
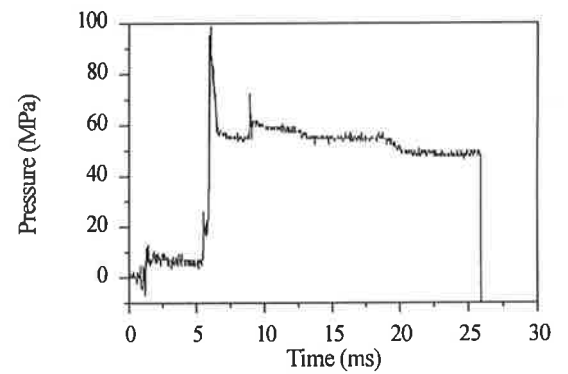
Upper: Test No. 13, Gage 1.
Lower: Test No. 13, Gage 2.



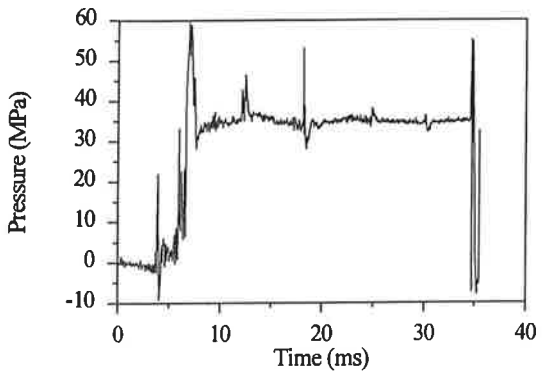
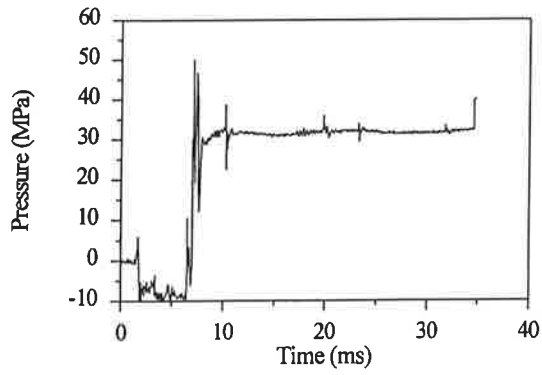
Upper: Test No. 15, Gage 1.
Lower: Test No. 15, Gage 2.



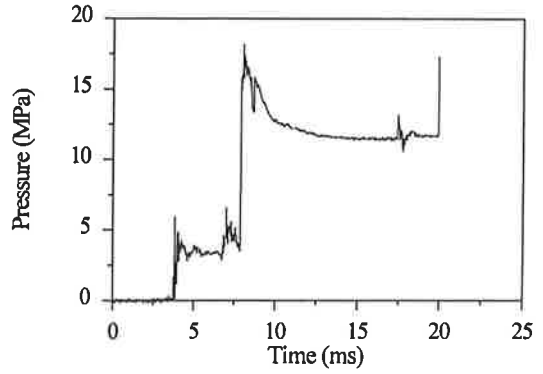
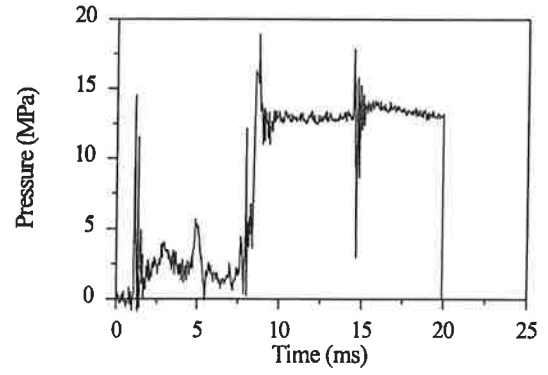
Upper: Test No. 16, Gage 1.
Lower: Test No. 16, Gage 2.



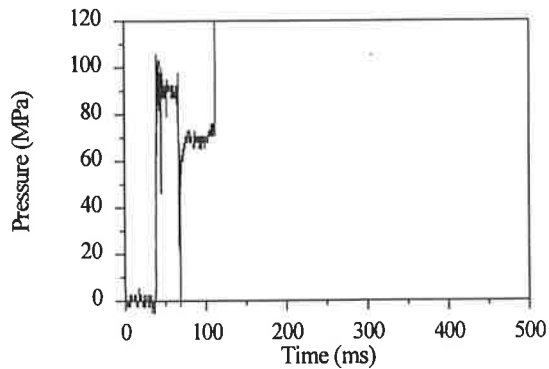
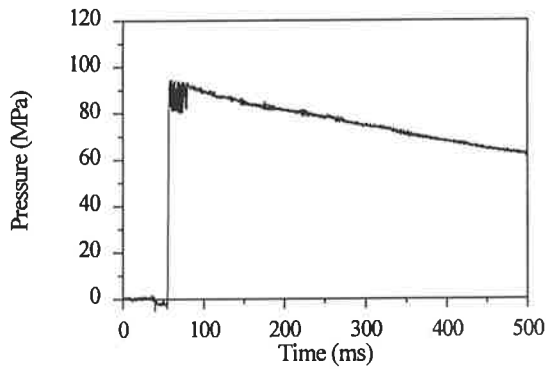
Upper: Test No. 17, Gage 1.
Lower: Test No. 17, Gage 2.



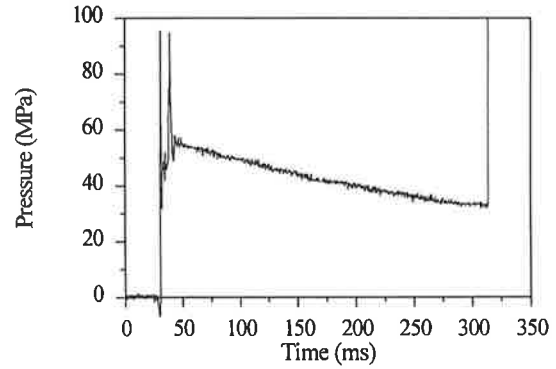
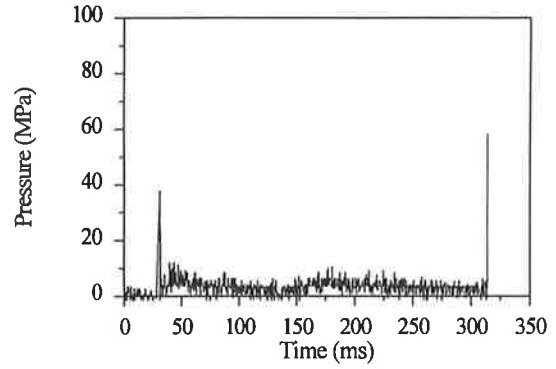
Upper: Test No. 18, Gage 1.
Lower: Test No. 18, Gage 2.



Upper: Test No. 19, Gage 1.
Lower: Test No. 19, Gage 2.



Upper: Test No. 20, Gage 1.
Lower: Test No. 20, Gage 2.



Upper: Test No. 21, Gage 1.
Lower: Test No. 21, Gage 2.

APPENDIX III: Programs and subroutines for the simulation.

Program 1: Calculation of temperature in the N₂ bubble, temperature in the surrounding matrices and radius of the N₂ bubble, when the N₂ bubble is adiabatically compressed from 1 atm. to 17 MPa while heat conducted into the surrounding matrix. Pressure duration = 1 ms, see pressure profile in Fig. 10.

```
clear;
%-----start geometry, velocity, pressure and energy data-----
m=101;
r(1)=100e-6; %bubble's initial radius (m)
r(m)=(r(1)^3+7.5034e-12)^(1/3); %radius of the equivalent matrix shell (m)
dr=(r(m)-r(1))/(m-1); %start radial distance between elements (m)
for i=2:1:m; r(i)=r(1)+(i-1)*dr; %out-radius of the matrix elements (m)
    v(i)=4*pi/3*(r(i)^3-r(i-1)^3); %volume of matrix elements
    ur(i)=0; E(i)=0; %velocity resp energy
end
r1v=r(1); %radius of N2
ur2v=ur(2); %velocity of 1st matrix
p1=1.0132e5; %start pressure in N2, Pa
%-----starting temperature-----
for i=1:1:m+1; T(i)=293; end %start temperature of matrix and N2 bubble
T1v=T(1); T2v=T(2); %temperature of N2 resp 1st matrix
%-----material data-----
R=8.31451;
aa=0.140835; %von der waal's constant
bb=3.913e-5; %von der waal's constant
alfa=4190; %w/K/m2
lambda=0.209; %w/K/m
rhoe=1360; %kg/m3
Cpe=1080; %J/K/kg
a=28.58; %J/K/mol
b=3.77e-3; %J/K2/mol
c=-0.5e5; %JK/mol
n=1.7428e-10; %amount of N2 in a bubble in mol
%-----flow calculation-----
r1old=r(1); %save old r(1) for future use
dt=1e-7; %time step in s
t=0; tv=t; %start time and real time
for j=0:20:9980 %stop time = 1e-3 s
    for k=1:1:20
        t=(j+k)*dt
        if t<1e-4, p=1.69e11*t+1.0132e5;
        else p=1.7e7; end
        dp=p-p1;
        [ur(1),r(1)]=flow(ur(1),r(1),r(2),dp,dt); %velocity ur(1) and r of N2
    %-----viscous heating-----
    for i=2:1:m
        r(i)=(r(i)^3+r(1)^3-r1old^3)^(1/3); %out-radius of the matrix element
        rm(i)=(r(i)+r(i-1))/2; %mid-radius of matrix elements
        mu(i)=1.60765e12*T(i)^(-4.25477); %viscosity of matrix (Pa*s)
```

```

E(i)=12*mu(i)*dt*r(1)^4*ur(1)^2/rm(i)^6;           %J/m^3
T(i)=T(i)+E(i)/rhoe/Cpe;                             %new T due to viscous heating
end
%-----state in the N2 after matrix flow-----
[T(1),p1]=pn1(T(1),r(1),r1old);
%-----heat flow between N2 and matrix-----
dT(1)=T(1)-T(2);
A(1)=4*pi*r(1)^2;                                     %momentary surface area of the bubble
v(1)=4*pi/3*r(1)^3;                                   %momentary volume of the bubble
dQ(1)=alfa*A(1)*dT(1)*dt;                             %heat from N2 to matrix
%-----heat flow between matrices-----
for i=2:1:m
    A(i)=4*pi*r(i)^2;                                   %area of the matrix elements
    T(m+1)=T(m);                                         %since dT(m)=0 and dQ(m)=0, boundary
    dT(i)=T(i)-T(i+1);
    r(m+1)=r(m);                                         %assign any value to r(m+1)
    dQ(i)=A(i)*dT(i)*lambda*dt^2/(r(i+1)-r(i-1)); %heat flow between matrix elements
    T(i)=(dQ(i-1)-dQ(i))/rhoe/Cpe/v(i)+T(i); %new T in the matrix duo to heat flow
end
%prepare for next cycle
Cp=a+b*T(1)+c/T(1)^2;                                   %new Cp in J/K/mol due to T change
T(1)=T(1)-dQ(1)/n/Cp;                                   %new T in the N2 bubble after heat dissipation
r1old=r(1);
p1=n*R*T(1)/(v(1)-n*bb)-aa*n^2/v(1)^2; %new p in N2 after heat dissipation
end %end of k
%-----save results for analyse, time between saved data = 1e-5 s-----
ur(2)=(r(1)/rm(2))^2*ur(1); %velocity of 1st matrix elements
tv=[tv
    t];
r1v=[r1v
    r(1)];
ur2v=[ur2v
    ur(2)];
T2v=[T2v
    T(2)];
T1v=[T1v
    T(1)];
end %end of j
trTTu=[tv,r1v,T1v,T2v,ur2v];
save trTTu1.dat trTTu -ascii;
%-----save results for further calculation-----
v(102)=v(101); %assign any value for v(102)
rTv=[r',T',v'];
u12p1=[ur(1),ur(2),p1];
save rTv1ms.dat rTv -ascii
save u12p11ms.dat u12p1 -ascii

```

Program 2: Subroutine "flow" solving the Navier-Stoke equation for the viscous flow of the matrix and determining the radius of the N₂ bubbles.

```
%subroutine to calculate the flow of matrix          flow.m
function[ur,r]=flowf(ur1,r1,r2,dp,dt)      %ur1: initial value
rhoe=1360;
dr=r2-r1;
durd=2*ur1^2/r1-dp/dr/rhoe;
dur=durd*dt;                                     %change of ur(1) during the time
ur=ur1+dur;
r=r1+ur*dt;                                     %new r(1) for N2 due to ur(1)
```

Program 3: Subroutine "pn1" using the Newton-Raphson method to solve the temperature and pressure in the N₂ bubbles during the isentropic compression.

```
% Newton-Raphsons subroutine to solve T and p of N2 in each time step      pn1.m
function [tn2,p]=pn1(T0,r,r0)      %T0,r0=initial T and r for N2 in each time step
n=1.165*4*pi*1e-12/3/0.028;      %N2 gas in a bubble in mol
v0=4*pi*r0^3/3;      %old N2 volume before each time step
v=4*pi*r^3/3;      %new N2 volume after each time step
a=0.140835;
b=3.913e-5;
R=8.31451;
a1=20.414;
b1=2.693e-3;
c=-3.571e4;
k=log(T0^a1*(v0-n*b)^R)+b1*T0-c/2/T0^2;      %integration constant
T=T0;      %initial T for iteration
h=1;      %initial h for iteration
while abs(h)>1.0e-10*abs(T),
    f=a1*log(T)+b1*T-c/2/T^2+R*log(v-n*b)-k;
    fp=a1/T+b1+c/T^3;
    h=f/fp;
    T=T-h;
end
p=n*R*T/(v-n*b)-a*n^2/v^2;      %final p in N2 bubble
tn2=T;
```

Program 4: Calculation of temperature in the N₂ bubble, temperature in the surrounding matrices and radius of the N₂ bubble, when the N₂ bubble is pre-compressed from 1 atm. to 17 MPa for a period of 1 ms (or, waiting time = 1 ms), then shocked to 24.8 GPa (See pressure profile in Fig. 12).

```

clear;
load rtv1ms.dat
load ul2p11ms.dat
%-----start geometry, velocity, pressure, temperature and energy data-----
m=101;
r=rtv1ms(:,1)';
T=rtv1ms(:,2)';
v=rtv1ms(:,3)';
ur=[]; E=[]; %velocity resp energy
r1v=[]; %radius of N2
ur2v=[]; %velocity of 1st matrix
ur(1)=ul2p11ms(1,1);
ur(2)=ul2p11ms(1,2);
p1=ul2p11ms(1,3);
T1v=[]; T2v=[]; %temperature of N2 resp 1st matrix
%-----material data-----
R=8.31451;
aa=0.140835; %von der waal's constant
bb=3.913e-5; %von der waal's constant
alfa=4190; %w/K/m2
lambda=0.209; %w/K/m
rhoe=1360; %kg/m3
Cpe=1080; %J/K/kg
a=28.58; %J/K/mol
b=3.77e-3; %J/K2/mol
c=-0.5e5; %JK/mol
n=1.7428e-10; %amount of N2 in a bubble in mol
%-----flow calculation-----
r1old=r(1); %save old r(1) for future use
dt=1e-10; %time step in s
t=dt; %t=time after initiation
tv=[]; %real time
for j=0:50:9950
    for k=1:1:50
        p=2.48e10; %initiation pressure = 24.8 GPa
        dp=p-p1;
        [ur(1),r(1)]=flow(ur(1),r(1),r(2),dp,dt); %collase velocity, ur(1), and r of N2
        %-----viscous heating-----
        for i=2:1:m
            r(i)=(r(i)^3+r(1)^3-r1old^3)^(1/3); %out-radius of the matrix element
            rm(i)=(r(i)+r(i-1))/2; %mid-radius of matrix elements
            mu(i)=1.60765e12*T(i)^(-4.25477); %viscosity of matrix (Pa*s)
            E(i)=12*mu(i)*dt*r(1)^4*ur(1)^2/rm(i)^6; %J/m^3
            T(i)=T(i)+E(i)/rhoe/Cpe; %new T due to viscous heating
        end
        %-----state in the N2 after matrix flow-----
        [T(1),p1]=pn1(T(1),r(1),r1old);
    end
end

```

```

%-----heat flow between N2 and matrix-----
dT(1)=T(1)-T(2);
A(1)=4*pi*r(1)^2; %momentary surface area of the bubble
v(1)=4*pi/3*r(1)^3; %momentary volume of the bubble
dQ(1)=alfa*A(1)*dT(1)*dt; %heat from N2 to matrix
%-----heat flow between matrices-----
for i=2:1:m
    A(i)=4*pi*r(i)^2; %area of the matrix elements
    T(m+1)=T(m); %since dT(m)=0 and dQ(m)=0, boundary
    dT(i)=T(i)-T(i+1);
    r(m+1)=r(m); %assign any value to r(m+1)
    dQ(i)=A(i)*dT(i)*lambda*dt*2/(r(i+1)-r(i-1)); %heat flow between matrix elements
    T(i)=(dQ(i-1)-dQ(i))/rhoe/Cpe/v(i)+T(i); %new T in the matrix duo to heat flow
end
    T2=T(2);
%prepare for next cycle
Cp=a+b*T(1)+c/T(1)^2; %new Cp in J/K/mol due to T change
T(1)=T(1)-dQ(1)/n/Cp; %new T in the N2 bubble after heat dissipation
r1old=r(1);
p1=n*R*T(1)/(v(1)-n*bb)-aa*n^2/v(1)^2; %new p in N2 after heat dissipation
if ur(1)<0, dt=abs((r(1)-(3*n*bb/4/pi)^(1/3))*1e-3/ur(1)); end
t=t+dt
[T2,p1,ur(1)]
end %end of k
%-----save results for analyse, time between saved data = 1e-5 s-----
ur(2)=(r(1)/rm(2))^2*ur(1); %velocity of 1st matrix elements
tv=[tv
    t];
r1v=[r1v
    r(1)];
ur2v=[ur2v
    ur(2)];
T2v=[T2v
    T(2)];
T1v=[T1v
    T(1)];
end %end of j
trTTu=[tv,r1v,T1v,T2v,ur2v];
save trTTu1f.dat trTTu -ascii;
%-----save results for further calculation-----
v(102)=v(101); %assign any value for v(102)
rTv=[r',T',v'];
u12p1=[ur(1),ur(2),p1];
save rtv1f.dat rTv -ascii
save u12p11f.dat u12p1 -ascii

```

Program 5: Calculation of the temperature in the N₂ bubble and the radius of the N₂ bubble, when it is pre-compressed by a pressure of 17 MPa for 20 ms and then the pressure releases. (See pressure profile in Fig. 13).

```

clear;
load rtv20ms.dat
load u12p120m.dat
%-----start geometry, velocity, pressure, temperature and energy data-----
m=101;
r=rtv20ms(:,1)';
T=rtv20ms(:,2)';
v=rtv20ms(:,3)';
ur=[]; E=[]; %velocity resp energy
r1v=[]; %radius of N2
ur2v=[]; %velocity of 1st matrix
ur(1)=u12p120m(1,1);
ur(2)=u12p120m(1,2);
p1=u12p120m(1,3);
T1v=[]; T2v=[]; %temperature of N2 resp 1st matrix
%-----material data-----
R=8.31451;
aa=0.140835; %von der waal's constant
bb=3.913e-5; %von der waal's constant
alfa=4190; %w/K/m2
lambda=0.209; %w/K/m
rhoe=1360; %kg/m3
Cpe=1080; %J/K/kg
a=28.58; %J/K/mol
b=3.77e-3; %J/K2/mol
c=-0.5e5; %JK/mol
n=1.7428e-10; %amount of N2 in a bubble in mol
%-----flow calculation-----
r1old=r(1); %save old r(1) for future use
dt=1e-9; %time step in s
t=dt; %real time = 20 ms +t
tv=[]; %time sequence
for j=0:20:2980
while t<5e-8
for k=1:1:20
while t<5e-8
p=1.0132e5; %pressure released to 1 atm
dp=p-p1;
[ur(1),r(1)]=flow(ur(1),r(1),r(2),dp,dt); %collase velocity, ur(1), and r of N2
%-----viscous heating-----
for i=2:1:m
r(i)=(r(i)^3+r(1)^3-r1old^3)^(1/3); %out-radius of the matrix element
rm(i)=(r(i)+r(i-1))/2; %mid-radius of matrix elements
mu(i)=1.60765e12*T(i)^(-4.25477); %viscosity of matrix (Pa*s)
E(i)=12*mu(i)*dt*r(1)^4*ur(1)^2/rm(i)^6; %J/m^3
T(i)=T(i)+E(i)/rhoe/Cpe; %new T due to viscous heating
end
%-----state in the N2 after matrix flow-----

```

```

[T(1),p1]=pn1(T(1),r(1),r1old);
%-----heat flow between N2 and matrix-----
dT(1)=T(1)-T(2);
A(1)=4*pi*r(1)^2; %momentary surface area of the bubble
v(1)=4*pi/3*r(1)^3; %momentary volume of the bubble
dQ(1)=alfa*A(1)*dT(1)*dt; %heat from N2 to matrix
%-----heat flow between matrices-----
for i=2:1:m
    A(i)=4*pi*r(i)^2; %area of the matrix elements
    T(m+1)=T(m); %since dT(m)=0 and dQ(m)=0, boundary
    dT(i)=T(i)-T(i+1);
    r(m+1)=r(m); %assign any value to r(m+1)
    dQ(i)=A(i)*dT(i)*lambda*dt*2/(r(i+1)-r(i-1)); %heat flow between matrix elements
    T(i)=(dQ(i-1)-dQ(i))/rhoe/Cpe/v(i)+T(i); %new T in the matrix duo to heat flow
end
%prepare for next cycle
Cp=a+b*T(1)+c/T(1)^2; %new Cp in J/K/mol due to T change
T(1)=T(1)-dQ(1)/n/Cp; %new T in the N2 bubble after heat dissipation
r1old=r(1);
p1=n*R*T(1)/(v(1)-n*bb)-aa*n^2/v(1)^2; %new p in N2 after heat dissipation
dt=0.01*(r(2)-r(1))/(10+ur(1))^2;
t=t+dt;
tdt=[t,dt]
T1p1ur1=[T(1),p1,ur(1)]
end %end of k
end %end of while
%-----save results for analyse, time between saved data = 1e-5 s-----
ur(2)=(r(1)/rm(2))^2*ur(1); %velocity of 1st matrix elements
tv=[tv
    t];
r1v=[r1v
    r(1)];
ur2v=[ur2v
    ur(2)];
T2v=[T2v
    T(2)];
T1v=[T1v
    T(1)];
end %end of while
end %end of j
trTTu=[tv,r1v,T1v,T2v,ur2v];
save trTTu4r.dat trTTu -ascii;
%-----save results for further calculation-----
v(102)=v(101); %assign any value for v(102)
rTv=[r',T',v'];
u12p1=[ur(1),ur(2),p1];
save rTv4r.dat rTv -ascii
save u12p14r.dat u12p1 -ascii
save tdt4r.dat tdt -ascii

```

Program 6: Calculation of temperature in the N₂ bubble, temperature in the surrounding matrices and radius of the N₂ bubble, when the N₂ bubble is first pre-compressed from 1 atm. to 17 MPa for a period of 20 ms and then, 50 ns after the pre-compression is released, shocked to 24.8 GPa. (See pressure profile in Fig. 13).

```

clear;
load tdt4r.dat
load rtv4r.dat
load u12p14r.dat
%-----start geometry, velocity, pressure, temperature and energy data-----
m=101;
r=rtv4r(:,1)';
T=rtv4r(:,2)';
v=rtv4r(:,3)';
ur=[]; E=[]; %velocity resp energy
r1v=[]; %radius of N2
ur2v=[]; %velocity of 1st matrix
ur(1)=u12p14r(1,1);
ur(2)=u12p14r(1,2);
p1=u12p14r(1,3);
T1v=[]; T2v=[]; %temperature of N2 resp 1st matrix
%-----material data-----
R=8.31451;
aa=0.140835; %von der waal's constant
bb=3.913e-5; %von der waal's constant
alfa=4190; %w/K/m2
lambda=0.209; %w/K/m
rhoe=1360; %kg/m3
Cpe=1080; %J/K/kg
a=28.58; %J/K/mol
b=3.77e-3; %J/K2/mol
c=-0.5e5; %JK/mol
n=1.7428e-10; %amount of N2 in a bubble in mol
%-----flow calculation-----
r1old=r(1); %save old r(1) for future use
dt=tdt4r(2); %time step in s
t=tdt4r(1)+dt; %t=time after pressure release
tv=[]; %real time
for j=0:20:49980
    for k=1:1:20
        p=2.48e10; %initiation pressure = 24.8 GPa
        dp=p-p1;
        [ur(1),r(1)]=flowf(ur(1),r(1),r(2),dp,dt); %collase velocity, ur(1), and r of N2
        %-----viscous heating-----
        for i=2:1:m
            r(i)=(r(i)^3+r(1)^3-r1old^3)^(1/3); %out-radius of the matrix element
            rm(i)=(r(i)+r(i-1))/2; %mid-radius of matrix elements
            mu(i)=1.60765e12*T(i)^(-4.25477); %viscosity of matrix (Pa*s)
            E(i)=12*mu(i)*dt*r(1)^4*ur(1)^2/rm(i)^6; %J/m^3
            T(i)=T(i)+E(i)/rhoe/Cpe; %new T due to viscous heating
        end
    end
    %-----state in the N2 after matrix flow-----

```

```

[T(1),p1]=pn1(T(1),r(1),r1old);
%-----heat flow between N2 and matrix-----
dT(1)=T(1)-T(2);
A(1)=4*pi*r(1)^2;           %momentary surface area of the bubble
v(1)=4*pi/3*r(1)^3;         %momentary volume of the bubble
dQ(1)=alfa*A(1)*dT(1)*dt;   %heat from N2 to matrix
%-----heat flow between matrices-----
for i=2:1:m
    A(i)=4*pi*r(i)^2;        %area of the matrix elements
    T(m+1)=T(m);             %since dT(m)=0 and dQ(m)=0, boundary
    dT(i)=T(i)-T(i+1);
    r(m+1)=r(m);             %assign any value to r(m+1)
    dQ(i)=A(i)*dT(i)*lambda*dt^2/(r(i+1)-r(i-1)); %heat flow between matrix elements
    T(i)=(dQ(i-1)-dQ(i))/rhoe/Cpe/v(i)+T(i); %new T in the matrix duo to heat flow
end
    T2=T(2);
%prepare for next cycle
Cp=a+b*T(1)+c/T(1)^2;       %new Cp in J/K/mol due to T change
T(1)=T(1)-dQ(1)/n/Cp;       %new T in the N2 bubble after heat dissipation
r1old=r(1);
p1=n*R*T(1)/(v(1)-n*bb)-aa*n^2/v(1)^2; %new p in N2 after heat dissipation
dt=0.01*(r(2)-r(1))/(10+ur(1))^2;
if ur(1)<0, dt=abs((r(1)-(3*n*bb/4/pi)^(1/3))*1e-3/ur(1)); end
t=t+dt;
tdt=[t,dt]
T2p1ur1=[T2,p1,ur(1)]
end %end of k
%-----save results for analyse, time between saved data = 1e-5 s-----
ur(2)=(r(1)/rm(2))^2*ur(1); %velocity of 1st matrix elements
tv=[tv
    t];
r1v=[r1v
    r(1)];
ur2v=[ur2v
    ur(2)];
T2v=[T2v
    T(2)];
T1v=[T1v
    T(1)];
end %end of j
trTTu=[tv,r1v,T1v,T2v,ur2v];
save trTTu4rf.dat trTTu -ascii;
%-----save results for further calculation-----
v(102)=v(101); %assign any value for v(102)
rTv=[r',T',v'];
u12p1=[ur(1),ur(2),p1];
save rTv4rf.dat rTv -ascii
save u12p14rf.dat u12p1 -ascii
save tdt4rf.dat tdt -ascii

```