Detonation reaction zone in nitromethane: Experimental and numerical studies

Barbara Štimac[a], Martin Künzel[b], Muhamed Sućeska[a], Siniša Stanković[a], Jindrich Kucera[c]

a) University of Zagreb, Faculty of Mining, Geology, and Petroleum Engineering, Pierottijeva 6, Croatia
b) OZM Research s.r.o., Blížňovice 32, Hrochův Týnec, Czech Republic
c) University of Pardubice, Faculty of Chemical Technology, Institute of Energetic Materials, Doubravice 41, Pardubice, Czech Republic

bstimac@rgn.hr

Abstract

The detonation reaction zone in nitromethane (NM) sensitised with 1% of ethylene diamine (EDA) and mixture of nitromethane and 10 % EDA is studied experimentally and by numerical modelling. The experiments involved measuring of the particle velocity history using impedance window technique instrumented with photonic Doppler velocimetry. Numerical modelling was done by EXPLO5 thermochemical code using its kinetic detonation module. The module includes slightly divergent Wood-Kirkwood detonation theory and the pressure-dependent reaction rate model, and it enables modelling of time dependent phenomena in the detonation reaction zone.

Impedance window technique allows us to partially resolve the reaction zone profile. The measured particle velocity profiles of nitromethane agree with the ZND theory: A sharp spike followed by rapid drop in particle velocity over first 10 ns, and then a slower decrease toward the CJ point, which is reached after 60 ns for NM/1%EDA and 77 ns for NM/10% EDA.

The reaction rate parameters are calibrated based on experimentally obtained particle velocity profiles and detonation reaction zone width. Using so obtained kinetic parameters, time distribution of parameters within detonation driving zone (including flow parameters, fraction of unreacted explosive, concentration of individual products, thermodynamic parameters of unreacted explosive and reaction products, pressure, temperature, density, etc.) is calculated starting from the von Neumann spike down to the CJ point. A sufficient agreement between experimental and calculated detonation velocities and particle velocity and pressure profiles is obtained.

Keywords: nitromethane, reaction zone, Doppler velocimetry, numerical modeling

1   Introduction

Nitromethane (NM) is a liquid explosive mostly studied as an example of a homogenous condensed phase explosive, such as liquid TNT and single-crystal PETN. Since homogenous liquid explosives and perfect crystal solid explosives contain no voids, there is no hot spot initiation during shock compression. Shock initiation of such explosives is governed completely by strong compression of thin layer of explosive and obeys temperature-dependant reaction rate laws [1]. By adding small amount of impurities or additives, initiation properties may change from homogenous to heterogeneous explosive [2].

Chemical reaction zone (CRZ) is a spatial distance between the shock wave and the sonic locus in a steady propagating one-dimensional detonation (Figure 1). The shock wave initiates

the chemical reactions at von Neumann spike and at the sonic locus most, but not all, chemical reactions have occurred, and chemical heat release rate is zero [3].
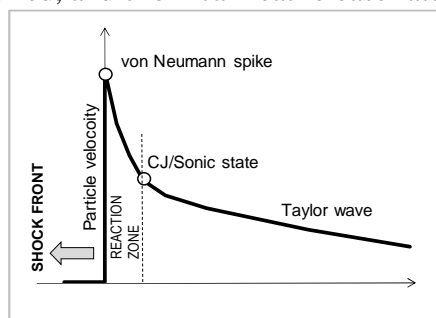

Figure 1.   Particle velocity profile of the reaction zone

It is difficult to accurately measure detonation wave reaction zone of NM. Many different techniques are used for direct or indirect measurements of the CRZ of homogeneous explosives, like plate push experiments, detonation front curvature experiments, emitted light measurements and laser velocity interferometry [4]. Since the requirement for successful experiment is high time resolution, laser velocity interferometry has proven to be one of the most useful and reliable methods. Laser velocity interferometry excels if applied in impedance window experiments where a block of transparent material ("window") is attached to a front surface of cylindrical explosive charge. This technique provides particle velocity-time profiles which makes it directly applicable for measurement of length of the CRZ of liquid explosives. Depending on variations (Fabry-Perot, VISAR, ORVIS, PDV), time resolution ranges from 10 ns to less than 1 ns.

The CRZ length of NM varies for different authors and different experimental and numerical modelling techniques applied [3,4,5]. Most studies agree with the existence of faster and slower chemical reactions in the CRZ. First, mostly used and referenced, and thus most reliable experiment on length of CRZ of nitromethane was done by Engelke et al. [3]. They used front curvature measurements on NM and estimated the length of CRZ approximately 6 ns (36 µm). Both Bouyer et al. [5] and Sheffield et al. [4] based their experiments on this one and used laser-based interferometry to measure particle velocity profiles of the steady state detonation wave at NM/PMMA interface and to determine the CRZ length in NM. In their experiments, time resolution varied from 8 ns to 1 ns. Their results confirmed previous work. Rapid decrease in particle velocity profile in first 5-10 ns is followed by a much slower decrease in particle velocity with time, until it reaches estimated CJ conditions at approximately 50 ns (300 µm) [4,5]. Besides previously mentioned high time resolution needed in the experimental setup, one of the main problems in determination of the CRZ in NM is the uncertainty in identifying the CJ state from the reaction zone profile. Slower chemical reactions after approximately first 10 ns result in a flatter profile with no distinctive drop which makes it difficult to determine the end of reaction zone [6].

Particle velocity at von Neumann spike is measured in most experiments at the NM/PMMA interface [3, 4, 5] and shows a range of 2.2 to 2.45 mm/µs. It should be emphasized that the measured peaks are 10 to 20% below theoretically estimated values due to insufficient time resolution of most experimental setups [5]. On the other hand, Menikoff and Shaw`s [6] theoretical calculations placed particle velocity at von Neumann spike closer to 2.8-2.9 mm/µs, which is in correspondence with earlier work of Tarver and Urtiew [6,1].

Besides experimental studies, some authors [1,6] attempted to numerically model CRZ of NM using different chemical kinetics models and equations of state for reactants and products. Some authors [6, 7] also dealt with modelling shock initiation of NM or liquid homogenous explosives in general. Menikoff and Shaw [6], for example, used temperature-

based reaction rate. Their work showed different mechanisms for gas-phase reactions and for liquid-phase reactions. Nunziato and Kipp (cited in [6]) have numerically modelled detonation and the CRZ of NM with a reaction rate corresponding to the two reaction mechanisms running parallelly.

In this work, we studied NM reaction zone structure by both numerical modelling and experiment.

2 Theoretical calculation of reaction zone parameters

Numerical modelling of reaction zone was done using thermochemical computer code EXPLO5. The code uses Wood-Kirkwood (WK) slightly divergent detonation theory coupled with pressure-dependent chemical kinetics. The WK theory solves Euler hydrodynamic flow equations along the central streamline of the cylindrical explosive charge and treats radial expansion as a first order perturbation of perfect one-dimensional flow [8]. Those two aspects together allow the prediction of detonation velocity as a function of rate of chemical reactions and the rate of radial expansions, which makes it more accurate than standard ZND model in the case of so-called "non-ideal" explosives. Numerical solution of ordinary differential equations gives flow properties behind the shock front; i.e. between the von Neumann spike and sonic point.

Implementation of the WK model into thermochemical code requires a lot of input information on explosive charge studied; e.g. reaction rate model, radial expansion rate, equation of state of unreacted explosive, equation of state of detonation products and thermodynamic properties of all compounds as a function of temperature [9]. As mentioned above, EXPLO5 has a built-in pressure-dependent reaction rate model given by equation [10]:

$$\frac{d\lambda}{dt} = k\lambda^B(1-\lambda)^C\left(\frac{p}{p_0}\right)^D \tag{1}$$

where k is the reaction rate constants, B, C, D are constants in the rate equation, λ is conversion of fraction reacted and p_0 is reference pressure in GPa.

Detonation velocities and reaction zone width of many explosives can be satisfactory reproduced with $B = 0$, $C = 1$ and $D = 2$ parameters [9]. Radial expansion rate is calculated with the following equation [11]:

$$\omega_r = \frac{D-u}{R_c} \tag{2}$$

where ω_r is radial expansion rate, u is particle velocity in the shock front and R_c is radius of shock curvature. That radius of shock curvature is estimated from a relationship between charge radius, failure radius and curvature radius.

The state of unreacted explosive is described by Murnaghan equation [12]:

$$p = \frac{1}{\kappa n}\left[\left(\frac{v_0}{v}\right)^n - 1\right] \tag{3}$$

where v_0 is the molar volume of the product, κ is the inverse of the bulk modules and n is a derivative of [$dB(p,T)/dp$]. Similar Murnaghan equation of state is used for the state of condensed detonation products.

The state of gaseous detonation products is described by BKW equation of state in a following form:

$$\frac{pV}{RT} = 1 + xe^{\beta x} = f(x) \tag{4}$$

where: $x = \dfrac{K}{\left[V(T+\theta)^{\alpha}\right]}$, V is the volume occupied by gaseous products (molar volume

of gases), k_i covolume of *i*-th detonation product, $K = \kappa \sum\limits_{i=1}^{N} x_i k_i$, $x_i = n_i / n_T$ (mol fraction of

i-th detonation product), α, β, κ and θ adjustable constants.

Numerical solution of the WK differential flow equations gives flow properties behind the shock front, provided the initial conditions (state variables $t = 0$) are known. Initial conditions for the WK equations are the state variables ($p, v, E, \lambda(i)$) at the shock front, i.e. at the von Neumann spike. Finding of the von Neumann spike, values of the state variables at the von Neumann spike and behind the shock front down to the sonic point, is done in EXPLO5 in the following way:

- Detonation velocity is treated as known (specified) parameter
- Reacted fraction of explosive, i.e. initial concentration of products, is taken to be zero
- Intersection of the Rayleigh line for specified detonation velocity and the pressure on shock Hugoniot of unreacted explosive gives von Neumann spike and corresponding pressure and volume (p, v)
- For a given p, v and λ condition, EXPLO5 performs thermodynamic equilibrium calculations to determine concentrations of all species and the energy:
- $E(p, v, \lambda) = E_u(p, v, \lambda) + E_p(p, v, \lambda) - Q(p, v, \lambda)$
- where subscript u and p mean unreacted explosive and reaction products, respectively,
- as well other flow parameters required for the further calculations (temperature, entropy, particle velocity, sound velocity, sonic parameter, fraction reacted, etc.)
- Integration of differential equations is carried out applying the Runge-Kutta method. Integration starts at the von Neumann spike (initial conditions) and continues toward the sonic point. In this way a structure of shock wave behind the shock front is obtained. For the self-sustaining detonation velocity integration terminates at the sonic point.

3 Experimental

3.1 Materials

Liquid explosive mixtures were composed of nitromethane (97+% purity) and 1,2-diamminoethane (EDA, ethylenediammine, 99.5% purity) in the mass ratios of 90:10 and 99:1. The liquid explosives were loaded in polypropylene (PP) tubes with 22.5 mm inner diameter and wall thickness of 4.2 mm. The length to diameter ratio of the charges was $l/d = 10$. The tube was closed by a 3d-printed detonator holder at one end and by a disc made of 6 mm thick polymethylmethacrylate (PMMA) plate at the other end. The charges were initiated by industrial detonators with a base charge of 0.72 g of RDX packed in aluminium shell. The tube with the tested explosive was fixed in a vertical position with the detonator pointed downwards (Figure 2).
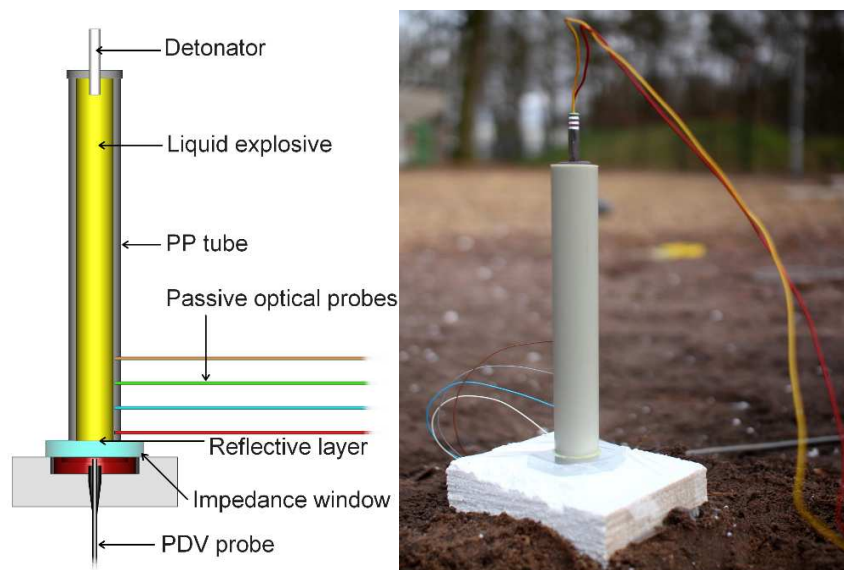
Figure 2. Scheme (cross-section) and photograph of the experimental arrangement

3.2 Detonation velocity measurements

The velocity of detonation was measured using a series of passive fibre optic probes perpendicular to the charge axis. Four glass optical fibres with outer jacket diameter of 0.9 mm were inserted to wells drilled in the charge casing 30 mm apart. The depth of the wells was such that the tips of the probes were still separated from the liquid explosive by 0.5 mm thick layer of plastic to avoid any leakage. The light signals generated by the explosive were transmitted by the optical fibres and recorded using OPTIMEX-8 light acquisition system (manufactured by OZM Research). The detonation velocity was determined as a slope of the distance-time data.

3.3 Particle velocity measurements

Particle velocity-time profiles were inferred from impedance window experiments. The photonic Doppler velocimetry [13] measurements were performed using a single measurement channel of the four-channel OPTIMEX-PDV photonic Doppler velocimeter manufactured by OZM Research. The resulting electrical signal was recorded using a high bandwidth Tektronix oscilloscope (DPO70000 series). The laser (1550 nm) was operated at an optical power output of 16 mW. The laser light was pointed to the target by means of a simple flat end fibre probe which was fixed in position perpendicular to the impedance window surface. A reflective layer made of aluminized polypropylene tape was fixed between the explosive and the PMMA window. The oscilloscope records were analysed using short-time Fourier transform (STFT) with a Hamming window. The window parameters were set in a way that the time and velocity resolution based on the STFT uncertainty principle [14] was 5 ns and 30 m/s respectively.

The measured particle velocity profiles at the explosive-PMMA interface were used to estimate the NM particle velocities using an assumption that even partially reacted explosive is described by the Cooper's generalized isentrope for detonation products [15].

4 Results and discussion

To understand the measured particle velocity profile, one must understand detonation wave and PMMA window interface interaction. When detonation wave impacts PMMA

window, shock will be created by the impact and travel into PMMA, while reflected shock wave will travel back into detonation products. Since conservation laws must be preserved at the interface, it follows that pressure and particle velocities at the interface are the same in both NM and PMMA. Thus, equating the Hugoniots of both NM and PMMA one can calculate pressure and particle velocity at the interface.

Graphical solution of interaction problem is illustrated by so-called cross-plot given in Figure 3. To determine parameters in reaction zone of NM we need to know the equation of states (EOS) of both the unreacted NM and its detonation products, as well as detonation velocity. To construct cross plot we used the following input data:

- Measured detonation velocity of NM equals 6.3 mm/μs, for $\rho_0 = 1.13$ g/cm^3
- The Rayleigh line ($p = \rho_0 D u_p$) is calculated using measured detonation velocity of 6.3 mm/μs and $\rho_0 = 1.13$ g/cm^3
- The Hugoniot curve of unreacted NM is calculated by equation $U_s = C + S \cdot u_p$, where $C = 1.76$ mm/μs and $S = 1.56$ [4]
- The PMMA Hugoniot is calculated by equation $U_s = C + S \cdot u_p$, where $C = 2.598$ mm/μs, $S = 1.516$; the density used was 1.186 g/cm^3 [15]
- The NM products Hugoniot is calculated by EXPLO5. Obtained pressure-particle velocity dependence is approximated by quadratic function: $p = 1.5434 \cdot u_p^2 + 1.7139 \cdot u_p + 4.7665$
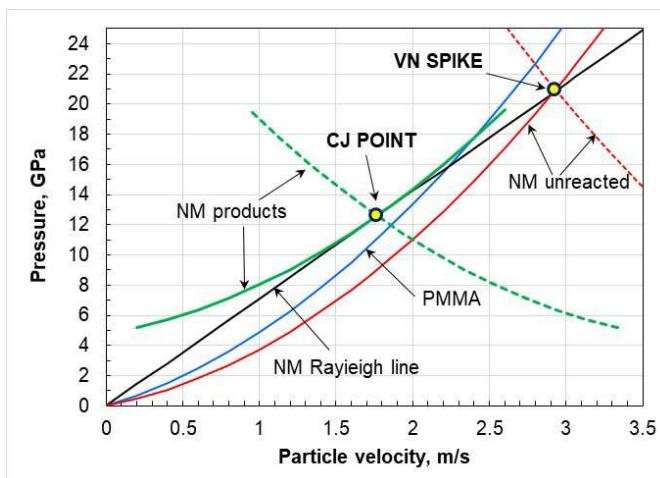

Figure 3.   Cross plot of Hugoniots of unreacted NM and its detonation products, Rayleigh line for NM, and Hugoniot of PMMA used to describe reaction zone measurements in this study

Using the above described approach and experimentally determined detonation velocities, we calculated pressure and particle velocity at the CJ state and von Neumann spike for two NM compositions; NM containing 1% and 10% of EDA. The calculation is done for NM/PMMA interface and for NM compositions. The calculation results are presented in Table 1.

Based on the results given in Table 1. we should expect measured VNS interface particle velocity to be 2.78 mm/μs for NM with 1% EDA and 2.69 mm/μs for NM with 10 % EDA, and interface particle velocity at the CJ point to be 1.855 mm/μs for NM with 1% EDA and 1.75 mm/μs for NM with 10 % EDA. These values of interface particle velocities at the CJ points are used for determination of reaction zone duration time/width from experimentally measured particle velocity-time profiles (Figure 4). It should be noted that the measured detonation velocity for NM with 1% EDA agrees with the previously published literature

values [14], as well as with theoretically predicted values using EXPLO5 thermochemical code.

Table 1. Particle velocity and pressure data predicted using the cross plot, Explo5 with EXP-6 EOS and experimentally determined values of detonation velocity (last column)

Test	Explosive	ρ_0, g/cm^3	Von Neumann spike			CJ state			
			$u_{VNS-PMMA}$ mm/µs	$u_{VNS,}$ mm/µs	$P_{VNS,}$ GPa	$u_{CJ-PMMA}$ mm/µs	u_{CJ} mm/µs	P_{CJ} GPa	D_{exp} mm/µs
1	NM +	1.13	2.79	2.93	20.96	1.86	1.77	12.6	6.31
2	1%EDA	1.13	2.77	2.90	20.50	1.85	1.76	12.6	6.28
3	NM +	1.10	2.70	2.87	19.40	1.76	1.68	11.4	6.14
4	10%EDA	1.10	2.68	2.85	19.30	1.75	1.68	11.4	6.12

Measured NM/PMMA interface particle velocities profiles are shown in Figure 4. The results show that measured VNS velocities (at $t = 0$ µs) for the two NM mixtures equal 2.12 mm/µs and 2.04 mm/µs, respectively. Based on the cross plot (Figure 3) these values are much lower (~25%) than expected (2.78 and 2.69 mm/µs). This is consequence of insufficient time resolution of the STFT evaluated PDV data (5 ns), which causes the front to be truncated. Some recent measurements, that have time resolution 1-2 ns [4,5], give VNS particle velocities about 2.20-2.45 mm/µs, which is still insufficient to fully resolve initial stage of the chemical reaction zone of NM (the VNS particle velocity is still 15 % lower than expected).

The reaction zone width is determined from the measurements taking average value of interface particle velocity at the CJ point to be 1.855 mm/µs for NM with 1% EDA and 1.75 mm/µs for NM with 10 % EDA (Figure 4).
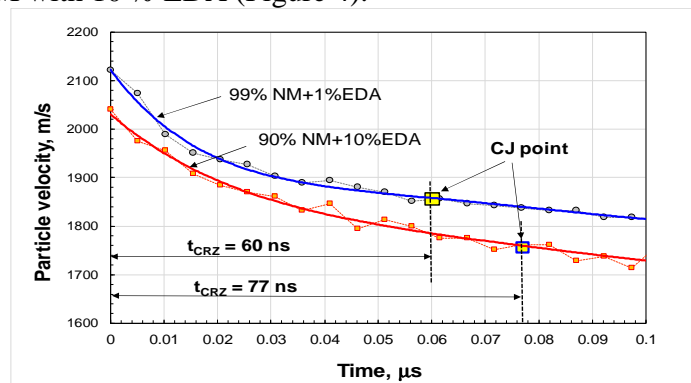

Figure 4.   Measured particle velocity profiles at the NM/PMMA interface for NM mixtures containing 1% and 10 % EDA

The reaction zone duration time, i.e. time to reach the CJ point, in the case of NM with 1% EDA equals 60 ns, and for NM with 10% EDA 77 ns. This gives approximate width of the reaction zone of 272 µm and 342 µm, respectively (calculated as $(D-u_{p, CJ})$ t_{CRZ}). It should be mentioned that accurate determination of t_{CRZ} is difficult since the slope of particle velocity -time curve in vicinity of the CJ point is small, so a small variation in particle velocity results in large variation in the reaction time. For example, decrease of interface particle velocity for 30 mm/µs (which is measuring uncertainty) will result in increase of the reaction time by almost two times (from 50 to 90 ns).

The obtained width of the reaction zone for NM with 1% EDA (60 ns and 270 µm) is close to recently reported data [4,5]. The authors reported reaction time of 50 ns and width of

reaction zone of about 300 μm. Mochalova et al. [2] studied NM/diethylenetriamine (DETA) mixtures and found that the reaction time decreases by adding small amount of DETA (from 50 to 30 ns with 2% DETA). Above 2% DETA reaction time again slowly increases but remains less than 50 ns up to 25% DETA. It is to be expected that addition of EDA in our experiment will also give shorter reaction time, however our results suggest that 10% of EDA increases reaction time from 50 to 77 ns. However, more detailed study is required to draw reliable conclusion.

4.1   Reaction zone modeling

Numerical modeling of the reaction zone is performed using kinetic module of EXPLO5 code, which is based on the Wood-Kirkwood slightly divergent detonation theory described in Section 2. The calculation is done using the following input parameters:

- The state of unreacted NM and EDA is described by the Murnaghan EOS (Eq. 3). The parameters in the Murnaghan EOS for NM are: $V_0 = 54.02$ cm^3/mol, $\kappa = 5.03 \cdot 10^{-5}$ 1/bar, n = 6.97 and $V_0 = 66.85$ cm^3/mol, $\kappa = 7.5 \cdot 10^{-5}$ 1/bar, n = 6.0 for EDA. The values of parameters for NM are derived from linear U-up dependence [11], while parameters for EDA are estimated following Souers et al. [16] approach and takin sound velocity to be 1200 m/s

- Input parameters for explosive charge: Unconfined charge, $d = 22.5$ mm, $R_f = 2$ mm, $R_c = 104$ mm for both NM mixtures

- Thermodynamic functions of unreacted NM are derived from heat capacity *vs*. temperature values reported by [17], and for EDA taking constant heat capacity of 172.59 J/mol K and entropy of 202.42 J/mol K. Temperature dependence of thermodynamic functions is described by four-degree polynomial.

- Based on preliminary thermochemical calculations we considered the following detonation products: H_2O, N_2, H_2, NH_3, CO_2, CO, CH_4, CH_2O_2, and C(gr) are created in NM detonation process.

- Rate of chemical decomposition of NM compositions in the chemical reaction zone is described by pressure-dependent model (Eq. 1). Kinetic parameters in the model (*k, B, C, D*) are adjusted so to reproduce experimentally obtained reaction time and particle velocity-time profile. We found that the second-order pressure-dependent model can satisfactory describe experimental results:

- $$\frac{d\lambda}{dt} = k\,(1-\lambda)^2 \left(\frac{p}{p_0}\right)^2 \quad (5)$$

- where the rate constant (*k*) equals 10.35 (1/μs) (1/GPa^D) for both NM compositions.

As mentioned earlier, integration of the Wood-Kirkwood flow equations gives flow parameters, reacted fraction and concentration of individual products along the Rayleigh line, starting from the von Neumann spike, down to the sonic point/CJ point (Figure 5). Calculation results are summarised in Table 2.

Since our intention was also to compare experimentally obtained particle velocity-time profiles with the profiles obtained by numerical modelling using EXPLO5 kinetic module, we converted measured interface particle velocities within the reaction zone (i.e. between the VNS and the CJ point) in particle velocities in NM products. This is done assuming Cooper's generalised isentrope for detonation products is applicable even in the case when explosive is partially reacted. This assumption does not affect significantly calculation results since the Huguenot curves of PMMA and NM are quite close to each other. Based on this calculation we found almost linear correlation between u_{PMMA} and u_{NM}: $u_{PMMA} = 0.78\ u_{NM} + 490$ within the reaction zone of NM with 1 % EDA.
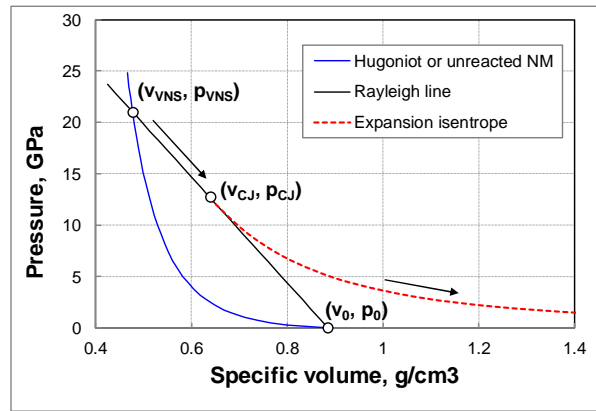
Figure 5.   Graphical presentation of calculation process (NM, D = 6300 m/s)

Table 2. Summary of calculation results

Parameter	NM with 1%EDA, $\rho = 1.13$ g/cm^3, $d = 22.5$ mm	NM with 10% EDA $\rho = 1.10$ g/cm^3, $d = 22.5$ mm
CJ point		
D, mm/µs	6358	6182
P_{CJ}, GPa	12.34	11.16
T_{CJ}, K	3184	2911
u_{CJ}, mm/µs	1.714	1.638
ρ_{CJ}, g/cm^3	1.542	1.491
$C_{o,CJ}$, mm/µs	4.644	4.548
Von Neumann spike		
E_{VNS}, MJ/kg	4.280	3.949
u_{VNS}, mm/µs	2.925	2.810
P_{VNS}, GPa	21.02	19.11
T_{VNS}, K	1598	1401
ρ_{VNS}, g/cm^3	2.093	2.017
$C_{o,VNS}$, mm/µs	8.395	8.094
Reaction zone width		
t_{CRZ}, ns	59.7	78
w_{CRZ}, µm	267	341
Fraction reacted (λ_{reac})	0.991	0.992

Calculated particle velocity-time data for NM, converted in this way to the NM/PMMA interface particle velocity-time data are shown in Figure 6, along with our experimental data and experimental data reported by Sheffield et al. [4] obtained with time resolution of 1 ns. Our analysis showed that the experimental data can be reproduce better if we shift calculated *u-t* curve along time axis. The shift roughly corresponds to time resolution used in experimental studies. In the same way we converted experimental NM/PMMA interface velocity data into NM particle velocity data ($u_{NM} = 1.28$ u_{PMMA} - 628) and compared them with calculated data (Figure 6b). The experimental data match calculated very well when they are shifted along time axis for the same time.
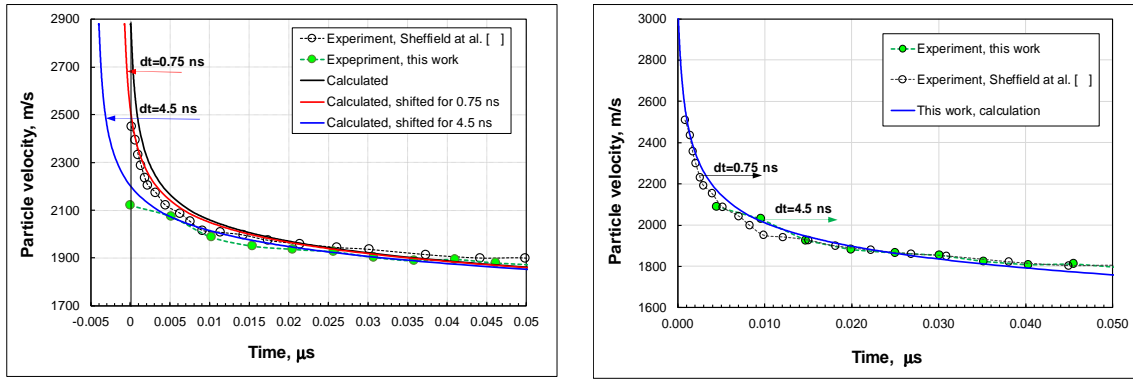
Figure 6. Calculated and experimental interface particle velocities profiles for NM;
a) calculated NM/PMMA interface particle velocities shifted to reproduce experimental data,
and b) experimental NM particle velocities of shifted to reproduce calculation results

Calculated von Neumann spike is very sharp (Figure 6b), followed by a rapid drop in particle velocity over first 10 ns (from 2.94 to 2.00 mm/µs) and much slower decrease from 10 ns to the CJ point. As stated by some authors [4,5] this is evidence of existence of fast reactions in early stage, which are followed by slow reactions in the vicinity of the CJ state. The analysis given in Figure 6b shows that calculated NM particle velocity at the von Neumann spike equals 2.94 mm/µs, while NM particle velocity measured at time resolution of 1 nm equals 2.51 mm/µs and 2.1 mm/µs at 5 ns time resolution. In other words, even at 1 ns time resolution, measured von Neumann spike particle velocity is 15% lower than calculated. This means that measured spike particle velocity is the velocity at some distance from the von Neumann spike. Truncated von Neumann spike obtained by measurements is the consequence of limited time resolution of experimental techniques and a very sharp drop in particle velocity in the vicinity of the spike (about 15% for 1 ns). However, combining experimental data with numerical modelling one can restore the entire von Neumann spike, provided reaction rate model and parameters are properly calibrated. Some calculated detonation parameters within NM reaction zone are shown in Figure 8.
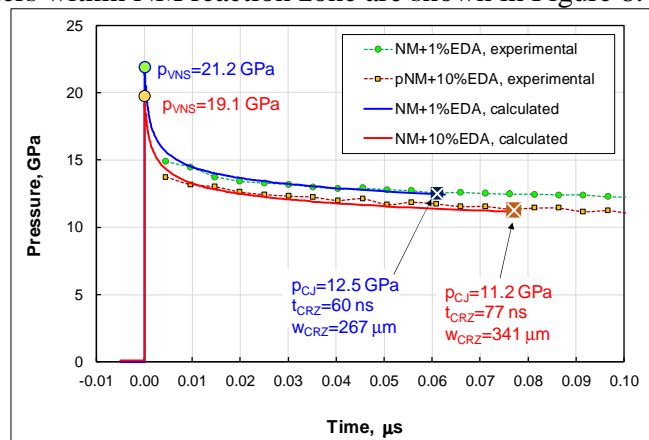

Figure 7. Calculated and experimental pressure-time profiles
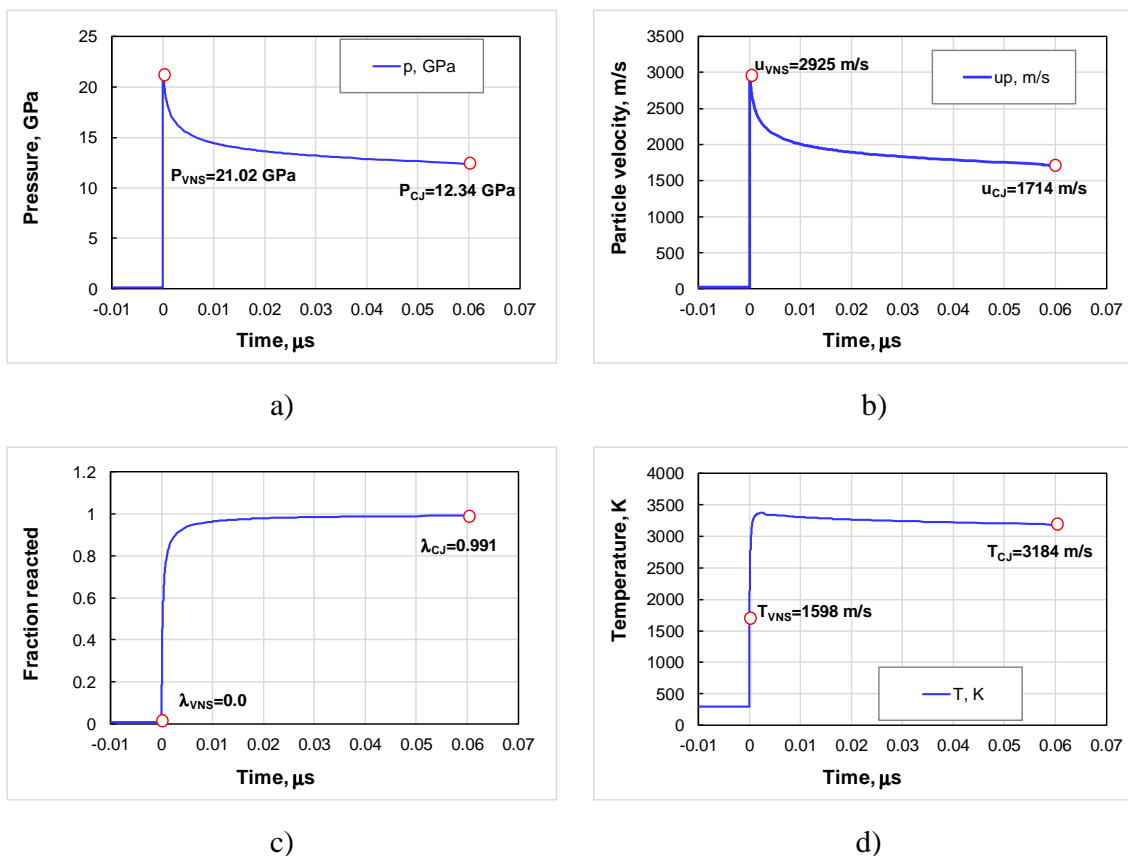in NM with 1% EDA reaction zone

Figure 8.　Calculated parameters in reaction zone of NM with 1% EDA

The calculated parameters at the von Neumann spike ($p = 21.02$ GPa, $V = 0.478$ cm^3/kg, $u_p = 2925$ m/s) are close to expected from cross plot Hugoniots calculation (Figure 3) and Menikoff et al. [6] calculations. Temperature at the von Neumann spike equals 1598 K and reaches its maximum of 3375 K after 2.5 ns, followed by slow decrease toward the CJ point (3184 K).

The results of calculation confirm existence of sharp von Neumann spike where all parameters studied (p, u_p, T, etc.) quickly change in the first 10 ns. For illustration, 95% of NM reacts in the first 6.7 ns, followed by slow change that ends at the CJ point.

5 Conclusions

The results presented show that PDV technique can be used for determination of the detonation wave width and the reaction time; however, it cannot resolve the von Neumann spike entirely. As the consequence of very sharp spike and insufficient time resolution (5 ns), experimentally obtained spike is truncated.

Experimentally determined reaction time for NM sensitised with 1% EDA equals 60 ns (width 267 µs) is close to the values of 50 nm reported by some other authors [4]. The reaction time for NM containing 10% EDA is slightly longer and equals 85 nm (width 361 µs).

The results also show that the structure of detonation reaction zone can be modelled by EXPLO5 kinetic module based on the Wood-Kirkwood detonation model. The pressure-dependent reaction rate model, incorporated in EXPLO5, is calibrated to reproduce experimental reaction time and NM particle velocity-time profile. Such calibrated model is used to model detonation reaction zone.

The results of calculation confirm experimentally observed structure of the reaction zone; existence of very fast reactions in the early stage (80% of material react in the first 1 ns and 95% in first 7 ns), followed by slow stage (from 7 ns to the CJ state, 60 ns). Also, calculated pressure and particle velocities at the von Neumann spike and the CJ point for both studied NM compositions, agree with the data calculated from the Hugoniots of NM (reacted and unreacted) and the Rayleigh line (cross plot shown in Figure 3).

Combining experimental measurements of particle velocity and numerical modelling proved to be a useful approach in resolving von Neumann spike and detailed structure of the reaction zone of explosives.

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