

**Evaluation of the
Thermochemical Code -
CHEETAH 2.0 for Modelling
Explosives Performance**

Jing Ping Lu

DSTO-TR-1199

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Jing Ping Lu

Weapons Systems Division
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ABSTRACT

The Lawrence Livermore National Laboratory CHEETAH 2.0 program has been used to analyse a number of conventional ideal explosive ingredients, ideal explosive compositions, non-ideal explosive compositions, and new and proposed explosives. It has also been used to study the effect of heats of formation and different types of binders on the predicted performance of explosive formulations. It is shown that the CHEETAH 2.0 program using the traditional Chapman-Jouget thermodynamic detonation theory can accurately model and predict performance of new explosive materials and of ideal explosives. It can also predict reasonably accurately experimental results for mildly non-ideal explosives. It is also shown that the CHEETAH 2.0 program based on the Wood-Kirkwood detonation theory can successfully model both mildly non-ideal explosives and moderate non-ideal explosives. It can replicate many of the features of non-ideal explosives such as detonation velocities and sonic reaction zone widths, and explosive properties such as detonation velocities as a function of the charge radius. In attempting to apply CHEETAH 2.0 to PBXW-115(Aust) using the estimated radius of curvature for the detonation front built into the code, difficulties were initially encountered in achieving convergence to a self-propagating detonation velocity. However, if an experimentally determined radius of curvature is used, good results are achieved from "Kinetic" CHEETAH, reflecting non-ideal features such as detonation velocities dependent on charge radius. Finally, in view of the strengths and limitations of CHEETAH, recommendations for the future work are made.

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Executive Summary

To establish and maintain a technology base of R&D in new and advanced explosives to satisfy the requirements of the Australian Defence Force, DSTO's current explosive research programs are focused on explosive formulations with enhanced performance for specific applications. In order to evaluate the performance and properties of new explosive compositions efficiently without resorting to expensive tests and trials, there is a continuing need in the energetic materials field for reliable prediction models. Lawrence Livermore National Laboratory's CHEETAH is a descendent of the TIGER thermochemical code that is widely used both to predict the performance of propellants and explosives and to evaluate formulations of new energetic materials. It also allows researchers to vary ingredients and compositions to optimise the desired performance properties. This report assesses the scope and applicability of CHEETAH for predicting performance of new explosive ingredients and of established and new, ideal and non-ideal, explosive compositions. A study of the effect of heats of formation and different types of binders on the predicted performance of explosive formulations has also been carried out. The objective is to determine whether CHEETAH can be used by DSTO as an everyday tool for new explosive formulations. On the basis of evaluation of ideal explosive ingredients and compositions, non-ideal explosive compositions, and new and proposed explosives, it is concluded that CHEETAH will be a useful everyday tool in DSTO research into advanced explosives. A number of technical conclusions and recommendations for future work are also made.

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Jing Ping Lu was awarded a PhD in Civil Engineering at University of Wollongong in 1991. She spent 10 years in the Division of Building, Construction and Engineering, CSIRO where she was in charge of modelling aspects of projects related to the structural use of different materials. She joined the Explosive Group, WSD at DSTO in March 2000 and is currently conducting research into the performance prediction of explosive materials and the mathematical modelling and computer simulation of explosive behaviour.

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1. Introduction

To establish and maintain a technology base of R&D in new and advanced explosives to satisfy the requirements of the Australian Defence Force, DSTO's current explosive research programs are focused on explosive formulations with enhanced performance for specific applications. An additional aim is to develop new formulations with reduced response to hazards stimuli in order to satisfy Insensitive Munitions (IM) requirements. In order to evaluate efficiently the performance and properties of new explosive compositions without resorting to expensive tests and trials, there is a continuing need in the energetic materials field for reliable prediction models. The usual starting point for any investigation into a new explosive composition is the prediction of its ideal detonation velocity and Chapman-Jouget (C-J) state properties using a thermodynamic equilibrium code [Kennedy 2000]. "Back of the envelope" empirical methods such as those of Rothstein [1979, 1981] and Kamlet [1968] offer limited accuracy and reliability, whereas *ab initio* methods are too sophisticated and demanding of computational resources for preliminary screening purposes. Thermochemical codes are considered a compromise balancing acceptable accuracy with affordable resources. In general terms, the code solves thermodynamic equations between product species to find chemical equilibrium by minimising the free energy [Fried et al. 1998]. Many thermochemical codes such as BKW [Mader 1998], IDeX [Freeman et al. 1991], JAGUAR [Stiel and Baker 1999] and TIGER [Cowperthwaite and Zwisler, 1973] have been developed all over the world. CHEETAH [Fried et al. 1998] is a descendent of the TIGER thermochemical code that is widely used both to predict the performance of propellants and explosives and to evaluate formulations of new energetic materials. It also allows researchers to vary ingredients and compositions to optimise the desired performance properties. CHEETAH 2.0 was made available to DSTO by Lawrence Livermore National Laboratory through the US Navy Insensitive Munitions Office, under Annex No N-99-AT-5851 to the Mutual Weapons Development Data Exchange Agreement between the US Department of Defense and the Australian Department of Defence. This report assesses the scope and applicability of CHEETAH for predicting performance of new explosive ingredients and of established and new, ideal and non-ideal, explosive compositions. The objective is to determine whether CHEETAH can be used by DSTO as an everyday tool for new explosive formulations.

2. Brief Description of CHEETAH Code

2.1 How CHEETAH operates

CHEETAH is a thermochemical code that predicts the results from detonation of a mixture of specified reactants. It operates by solving thermodynamic equations to predict detonation products and properties such as temperature, pressure, volume, and total energy released.

2.2 Code features

CHEETAH 2.0 has incorporated a number of improvements over its antecedent TIGER, as listed below.

- **User convenience.** CHEETAH has been made simpler and easier to use, with much enhanced user convenience.
- **Algorithmic improvements.** CHEETAH has replaced all of TIGER's solvers with new algorithms, and can handle multiple condensed phases.
- **Reactant library.** CHEETAH 2.0 includes a reactant library which contains 366 ingredients. In addition CHEETAH can perform calculations using new reactants, given a knowledge of chemical composition, density and heat of formation.
- **Equation of state improvements.** In the product libraries, CHEETAH currently implements the Becker-Kistiakowski-Wilson (BKW) and JCZ3 equation of state (EOS), and a new intermolecular potential exp-6 gaseous EOS. (Please note the acronym BKW has been used variously to describe the thermodynamic code, the EOS and even the parameter set, occasionally leading to some confusion.) CHEETAH also contains new solid (Murnaghan) and liquid (Grover) EOS, and a virial non-ideal gas EOS in order to produce the same output as the BLAKE code for evaluation of gun propellants. There have been a number of different parameter sets proposed for the BKW EOS.
- Finger et al. [1976] proposed the renormalised BKWR parameters based on 10 measured detonation velocities, 10 measured detonation pressures and four measured detonation temperatures in CHNOF explosives.
- NEWC1 is another renormalised BKW library with a three-phase carbon equation of state. Hobbs and Baer [1993] derived the BKWS parameter set which uses a large number of product species (61) containing C, N, O and H. The BKWS library was also tested for aluminised explosives.
- Fried et al. [1998] employed a modern stochastic optimisation algorithm to find the new parameters referred to as BKWC using 17 product species which is modestly greater than the 12 species used in BKWR but much less than the 61 species of BKWS.

Therefore, the BKWC library is recommended for using as an everyday tool for explosive formulators.

- **Kinetic CHEETAH.** In earlier versions of CHEETAH, calculations were based on traditional Chapman-Jouguet thermodynamic theory, which assumes that the thermodynamic equilibrium of the detonation products is reached instantaneously and that all reactants are consumed completely. It is also assumed that flow is one-dimensional, the reaction zone is infinitely thin, and that completion of reaction coincides with the sonic point in the flow. This is true for ideal explosives that release the energy very quickly. However, for non-ideal explosives certain reaction rates are slow, and these slow chemical reactions require a long time to achieve thermochemical equilibrium. In order to model these time dependent phenomena considering partial combustion and detonation in composite explosives with large reaction zones, a new chemical kinetics model has been added to CHEETAH 2.0. This model is based on the slightly divergent detonation theory of Wood and Kirkwood [1954], which considers detonation in composite explosives with large reaction zones, and the interplay between the energy produced by kinetically controlled reactions and the energy lost due to radial expansion of the product gases.

- *JWL fitting program.* CHEETAH incorporates a program to fit the output to an empirical JWL EOS.

2.3 CHEETAH outputs

CHEETAH generates two output files. The main output file records detailed information about thermodynamic states calculated. The second output file is a single sheet summary of the run, which details the C-J condition (including pressure, volume, energy, temperature and detonation velocity), cylinder expansion and an empirical fit of the results to a JWL EOS. Details of detonation velocity and pressure are most readily measured and are generally available for most explosives. Measurement of detonation velocity generally has an experimental accuracy of 1%, while that for detonation pressure is typically only 10% [Fried et al. 1998]. Other parameters are not so readily measured and are not determined on a routine basis, and data are therefore unavailable for many materials. In this report, therefore, attention is focussed on detonation velocity and C-J pressure to evaluate the usefulness and effectiveness of the CHEETAH code.

3. Evaluation of CHEETAH Code

In order to evaluate CHEETAH, a number of cases were analysed using CHEETAH 2.0 with reference to the following categories. These are nominally ideal explosives (both individual explosive ingredients and ideal explosive compositions) and non-ideal explosive compositions (aluminised explosives) using "standard" BKW, kinetic calculations on non-ideal explosives, new and proposed explosives, and the effects of heat of formation and different binders on the explosive performance. There are six parts in this section. The first part gives the computed results from standard runs based on the traditional Chapman-Jouget thermodynamic detonation theory. The second part describes the calculations on non-ideal explosives using kinetic detonation theory. The third part presents the results for new and proposed explosives. The fourth part summarises the study of the influence of heats of formation on the predicted performance of explosives. The fifth part is focused on the effect of different binders on the explosive performance. The last part reports on the current development in the application of CHEETAH.

3.1 Chapman-Jouget detonation

Tables 1 to 3 give the details of the predicted performance properties, based on the traditional Chapman-Jouget thermodynamic detonation theory, for representative explosive ingredients, ideal explosive compositions and non-ideal explosive compositions, respectively. For comparison purposes, the available experimental data are also included. It should be noted that the recommended BKWC LLNL product library has generally been used. The BKW EOS has the following form [Fried et al. 1998]:

$$\frac{pv}{RT} = 1 + \frac{K}{v(T+\Theta)^\alpha} \exp \frac{\beta K}{v(T+\Theta)^\alpha} \text{ where } K = \kappa \sum x_i k_i \quad (1)$$

Here, p is the pressure, v is the molar gas volume, R is the gas constant, x_i is mole fraction and κ_i the individual geometrical covolume. The four global adjustable parameters for BKWC are as follows: $\alpha=0.5$, $\beta=0.40266$, $\Theta=5441$, $\kappa=10.864$. Variations in equations of states and their parameters, together with different product libraries and heats of formation used, will all contribute to differences in the calculations. Therefore, these should always be quoted.

Table 1. Detonation properties for individual explosive ingredients

Name	Density (g/cm ³)	P (GPa)			VoD (m/s)		
		Cal.	Exp. ⁺	Err. %	Cal.	Exp. ⁺	Err. %
HMX	1.89	38.6	38.7	-2.6	9244	9110	1.5
PETN	1.76	30.84	31	-0.5	8274	8260	0.17
RDX	1.80	34.47	34.1	1.1	8920	8754	1.9
	1.77	33.12	33.79	-2.0	8807	8639	1.9
TATB	1.847	27.03	25.9	4.4	7814	7660	2.0
Tetryl	1.61	22.11	22.64	-2.3	7361	7580	-2.9
	1.36	15.41	14.2**	8.5	6616	6680**	-0.96
TNT	1.64	19.17	19	0.9	6843	6950	-1.5
	1.61	18.32	18.7	-2.0	6752	6780	-0.41

⁺ Data from [Hall and Holden, 1988]

** Data obtained at charge diameter of 40mm.

The computed detonation properties for individual ingredients listed in Table 1 are in excellent agreement with available experimental data, as is to be expected since most belong to the performance database from which the BKWC product library was derived. Thus detonation velocities are within 2% of experimental values, while detonation pressures are generally within 5%. The largest deviations are with the insensitive TATB, which has a strong detonation-diameter dependence, and for detonation pressure of Tetryl at low density.

Table 2. Detonation properties for representative ideal explosive compositions

Name	Density (g/cm ³)	P (GPa)			VoD (m/s)		
		Cal.	Exp.*	Err. %	Cal.	Exp.*	Err. %
Composition A-3 (RDX/Paraffin 91/9)	1.59	22.46	26.0	-2.3	7566	8100	-6.6
		24.81 ⁺⁺		-1.2	8064 ⁺⁺		-0.4
Composition B (RDX/TNT/WAX 59.5/39.5/1)	1.67	24.77	26.4	-6.2	7630	7860	-2.9
Cyclotol(65/35)	1.715	27.5	29.2	-5.8	8036	8036	0.0
Cyclotol(75/25)	1.62	24.92	26.5	-6.0	7950	7950	0.0
NTO/TNT 50/50	1.71	22.5	22.6	-0.4	7418	7370	0.65
Octol (60/40)	1.80	30.33	32.0	-5.2	8227	8160	0.82
Octol (75/25)	1.81	32.25	34.37	-6.2	8506	8364	1.70
Pentolite (PETN/TNT 50/50)	1.68	24.19	24.6	-1.7	7677	7750	-0.9

* Data from [Hall and Holden, 1988]

** Calculations are based on BKWS library

Computed detonation properties for representative ideal explosive compositions in Table 2 also show excellent agreement with experimental data. With the exception of Composition A-3, detonation velocities agree within about 2% and detonation pressures within about 6%. It is interesting that, in common with most equilibrium codes, CHEETAH systematically underestimates C-J pressures. The BKWC product library significantly underestimates the detonation velocity of Composition A-3, but the BKWS library gives much better correlation with experimental data. The reason for this discrepancy is not clear.

Table 3. Detonation properties for representative non-ideal explosive compositions

Name	Density (g/cm ³)	P (GPa)			VoD (m/s)			
		Cal.	Exp.	Err. %	Cal.	Exp.	Ref.	Err. %
Amatol (AN/TNT 60/40)	1.56	19.67			7367	6840	Hall and Holden 1988	7.7
Baratol (Ba(NO ₃) ₂ /TNT 76/24)*	2.61	20.46	14	31.6	6680	4925	Hall and Holden 1988	26
H6 (RDX/TNT/Al/Paraffin 44.15/29.31/20/6.54)	1.76	20.77	24.5	-19.7	7000	7367	Hall and Holden 1988	-5.0
Tritonal (TNT/Al 80/20)	1.72	16.47			6105	6475	Mader 1979	-5.7
Torpex (RDX/TNT Al 42/40/18)	1.81	23.82			7177	7495	U.S. Army 1971	-4.2
AFX-645 (TNT/NTO/Al/PEG 32/48/12/8)	1.63	16.98			6512	6540	Corely 1995	-0.4
ARX-2002 (RDX/Al/HTPB 61/20/19)	1.65	18.35			7000	7273	Cliff 2000	-3.8
PBXN-109 (RDX/Al/HTPB 67/20/13)	1.70	20.50			7194	7630	Hall and Holden 1988	-5.7
PBXN-109 (RDX/Al/HTPB 67/20/13)	1.681	19.95	23.7	-15.8	7118	7602	Hall and Holden 1988	-6.4
AFX-770 (RDX/AP/Al/NQ/HTPB /IDP 27/27/16/12/9/9)	1.616	18.19			6915	6050	Bocksteiner et al 1999	14.3
ARX-2010 (RDX/Al/AP/HTPB 41/20/20/19)	1.64	17.66			6798	6724	Cliff 2000	1.1
PBXW-115 (AP/Al/RDX/HTPB 43/25/20/12)	1.79	20.78			7046	5910	Bocksteiner et al 1994	19.2

* The calculations were based on BKWS product library as Baratol contains an "unusual" element 'Ba'.

Detonation velocities in Table 3 computed using the BKWC product library for "mildly non-ideal" aluminised explosives are up to 6% lower than experimental data. (Calculations for Amatol, which contains ammonium nitrate, exceed experimental results by nearly 8%.) However calculations for "grossly non-ideal" explosives, containing both aluminium and ammonium perchlorate, overestimate detonation velocities by 15-20%. For the few non-ideal explosives for which experimental data are available, CHEETAH using the BKWC library substantially underestimates C-J

pressures. Further, BKWC was unable to handle Baratol because of the presence of barium. Estimates using the BKWS library overestimated performance of this composition by a wide margin.

These results indicate limitations in the usefulness of CHEETAH and the BKWC product library for modelling non-ideal explosives. Indeed, LLNL note that the BKWS library has been used most systematically tested for aluminised explosives, whereas BKWC and BKWR have not been tested in this context. To investigate possible improvement of CHEETAH, calculations were performed on selected formulations using the alternative product libraries BKWS and NEWC1. The four "global adjustable" parameters in the BKW EOS are listed in Table 4 for the BKWS and NEWC1 product libraries, together with those for BKWC. "Kinetic" CHEETAH was later investigated, and the results are detailed in the next section (3.2).

Table 4. Global parameters for BKW EOS

Library	α	β	κ	Θ
BKWC	0.50	0.403	10.86	5441
BKWS	0.50	0.298	10.50	6620
NEWC1	0.52	0.402	12.31	3827

Table 5 summarises the pressure and velocity of detonation predicted with different product libraries and the available experimental data for a few aluminised explosives. To obtain some insight into the role of aluminium, two runs were conducted for each library, firstly treating the aluminium as a normal reactive ingredient, and secondly treating the aluminium as an inert solid.

Table 5. Detonation properties predicted for representative non-ideal explosive using different product libraries

Name	Density (g/cm ³)	Al	Product Library											
			BKWC				BKWS				NEWC1			
			P (GPa)	VoD (m/s)			P (GPa)	VoD (m/s)			P (GPa)	VoD (m/s)		
				Cal.	Cal.	Exp. Err. %		Cal.	Cal.	Exp. Err. %		Cal.	Cal.	Exp. Err. %
Tritonal	1.72	Reactive	16.47	6105	6475	-5.7	17.3	6449	6475	-0.4	15.28	5951	6475	-8.1
		Inert	15.3	6500	6475	0.4	16.77	6872	6475	6.1	15.02	6202	6475	-4.2
PBXN-109	1.7	Reactive	20.50	7194	7630	-5.7	21.20	7277	7630	-4.6	16.92	6388	7630	-16.3
		Inert	17.69	7005	7630	-8.2	21.21	7703	7630	1.0	18.59	6837	7630	-10.4
ARX-2010	1.64	Reactive	17.66	6798	6724	1.1	18.80	7031	6724	4.6	13.37	5692	6724	-15.3
		Inert	14.31	6394	6724	-4.9	19.29	7389	6724	9.9	14.08	6064	6724	-9.8
PBXW-115	1.79	Reactive	20.51	7046	5910	19.2	21.19	7450	5910	26.1	16.10	5955	5910	0.8
		Inert	17.89	7048	5910	19.3	23.77	7683	5910	30.0	17.38	6378	5910	7.9

The results in Table 5 are not very consistent, and no general trend can be discerned. The BKWS product library is recommended for aluminised explosives, and gives satisfactory results for the "mildly non-ideal" Tritonal and PBXN-109 and acceptable results for ARX-2010. However, in the case of Tritonal and ARX-2010 best correlation with experimental results is achieved when the aluminium is treated as a reactive ingredient, whereas for PBXN-109 the aluminium is better treated as inert. For PBXW-115, detonation velocities predicted using the BKWS product library were substantially higher than experimentally determined, regardless of the treatment for aluminium. Although not tested or recommended for aluminised explosives, the BKWC product library performed well for Tritonal and for PBXN-109 (at least if the aluminium was treated as reactive), and gave the best correlation of any product library for the experimental composition ARX-2010. However BKWC substantially overestimated the detonation velocity of PBXW-115, regardless of the treatment for aluminium. The NEWC1 product library is renormalised to include a three-phase carbon EOS, used with the more reliable Murnaghan EOS for solids [Howard et al (1998)]. Use of this product library gives good correlation for PBXW-115, particularly if the aluminium is treated as reactive, but it substantially underestimates the detonation velocity for each of the other explosive compositions.

3.2 Kinetic detonation

The new chemical kinetics model implemented in CHEETAH is based on the Wood-Kirkwood detonation theory, which considers detonation in composite explosives with large reaction zones, and the interplay between the energy produced by kinetically controlled reactions and the energy lost due to radial expansion of the product gases. Wood-Kirkwood theory thus allows prediction of the dependence of detonation parameters on charge diameters, and estimation of the length of the detonation zone, identified as the region behind the detonation wave for which the local velocity of sound is equal to or greater than the detonation velocity [Howard et al.1998].

Kinetic CHEETAH assumes the concentrations of individual reactants are controlled by the rate of the kinetic reactions, while the products are assumed to be in thermochemical equilibrium. The reaction kinetics are pressure-dependent rate laws describing surface controlled reactions and have the following form:

$$\frac{d\lambda}{dt} = (1 - \lambda) R P^2 \quad (2)$$

where P is the pressure, R is the rate constant and λ represents the amount of unburned reactant normalised to vary between zero (all unburned) and one (all burned). The rate constants R for the reactants used in this study are listed in Table 6, and are the updated values defined by Howard et al. [1998], rather than those initially recorded in the CHEETAH 2.0 User's Manual.

Table 6. Rate constant R used in pressure-dependent rate laws

Reactant	R ($\mu\text{s}^{-1}\text{GPa}^{-2}$)
Al	0.0075
AP	0.0075
HTPB	0.001
RDX	0.2
TNT	0.1

WK theory also requires the specification of the rate of radial expansion, ω_r , as a function of radius. In this study, the simple pressure model with the following time rate of change of ω_r is used:

$$\frac{d\omega_r}{dt} = \frac{2SP}{R_o^2 \rho_o} - S\omega_r^2 \quad (3)$$

where

$$\omega_r(t=0) = (D - u)/R_c \quad (4)$$

Here, R_0 is the charge radius and S is an empirical scaling factor. If this model is used with $S = 0$, ω is a constant with the initial value determined by the radius of curvature R_c , the detonation velocity D , and the particle velocity u at the detonation front. The radius of curvature is obtained from Souer's detonation front curvature and size effect data (Souers 1998).

To assess the capability of predicting the detonation characteristics with this new kinetic version of CHEETAH, three non-ideal explosive examples are analysed, i.e. "mildly non-ideal" PBXN-109, "moderately non-ideal" Tritonal and a "strongly non-ideal" PBXW-115. Both the detonation velocity and the detonation zone length at varying charge diameters are predicted.

For PBXN-109, the calculated detonation velocity and the detonation zone length at the charge radius of 65 mm are 7365 m/s and 0.304 mm respectively. The detonation velocity as a function of charge radius was also calculated, and these data are plotted in Figure 1. The sharp decrease in detonation velocity at charge radius less than 20 mm is consistent with the reported critical diameter of 12.9 mm [Hall and Holden, 1988], while it is seen that the detonation velocity asymptotically approaches a constant value as the radius becomes larger. According to Cooper [1996], when these data are plotted in the form of detonation velocity versus reciprocal radius, $1/r$, the relationship becomes linear in $1/r$ as radius increases. Hence, the detonation velocity for an infinite diameter charge of PBXN-109 of 7372 m/s can be estimated by extrapolating the linear portion of the relationship to $1/r=0$ (see Figure 2). This value falls between the experimental value of 7630 m/s obtained at the charge diameter of 102 mm [Hall and Holden 1988], and the value predicted using the BKWS product library. The discrepancy shown in the figure indicates that the CHEETAH predictions using its intrinsic parameters are not the final answer and the measurement is still necessary in order to derive feasible parameters for reproducing experimental observations.

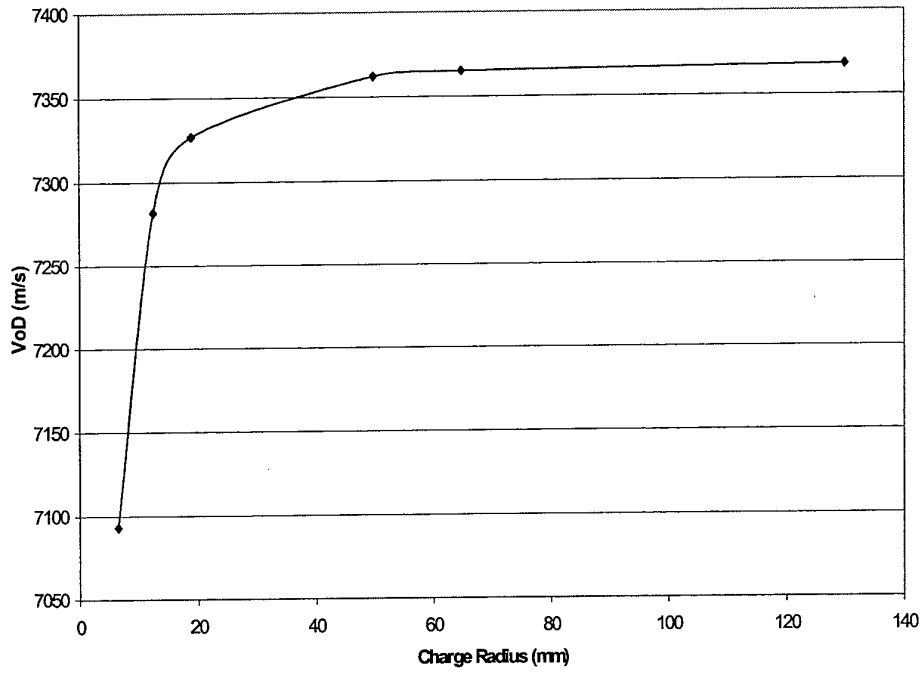


Figure 1. Detonation velocity versus charge radius of PBXN109

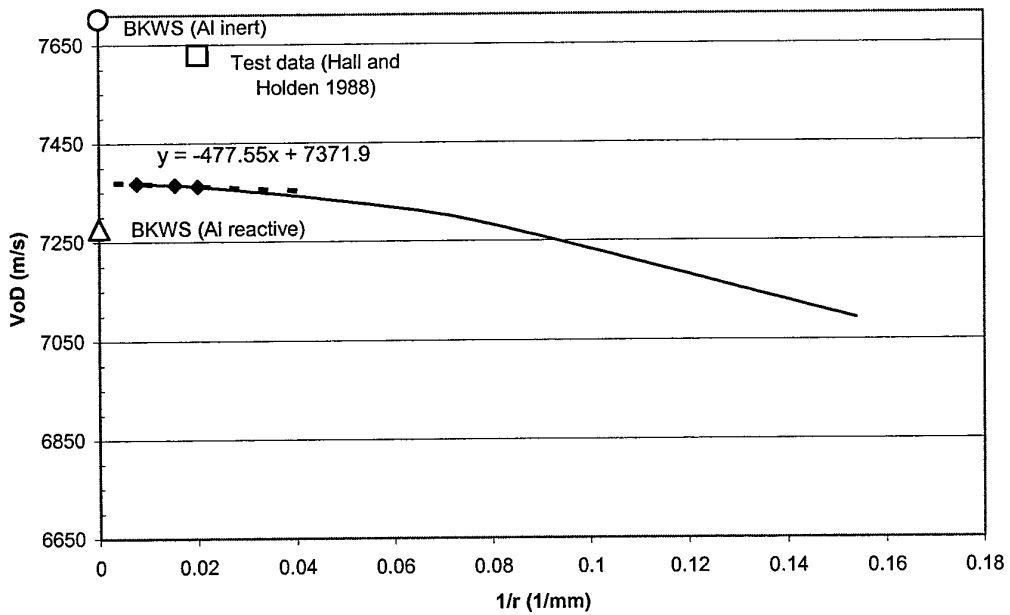


Figure 2. Detonation velocity versus reciprocal radius of PBXN109

For Tritonal, the detonation velocity and the detonation zone length at the charge radius of 45.75mm are calculated as 6122m/s and 0.951mm respectively. The detonation velocity versus charge radius is shown in Figure 3 and the detonation velocity versus the reciprocal of charge radius in Figure 4. The extrapolated detonation velocity at infinite diameter, 6152m/s, compares reasonably well with the experimental data of 6475m/s [Mader 1979], and with the value predicted using BKWS. The decrease in detonation velocity at charge radius less than 20mm is consistent with the critical diameter of 18.3mm reported for Tritonal [Hall and Holden, 1988]. Again further measurement is necessary for determining parameters that can reproduce the experimental results more accurately.

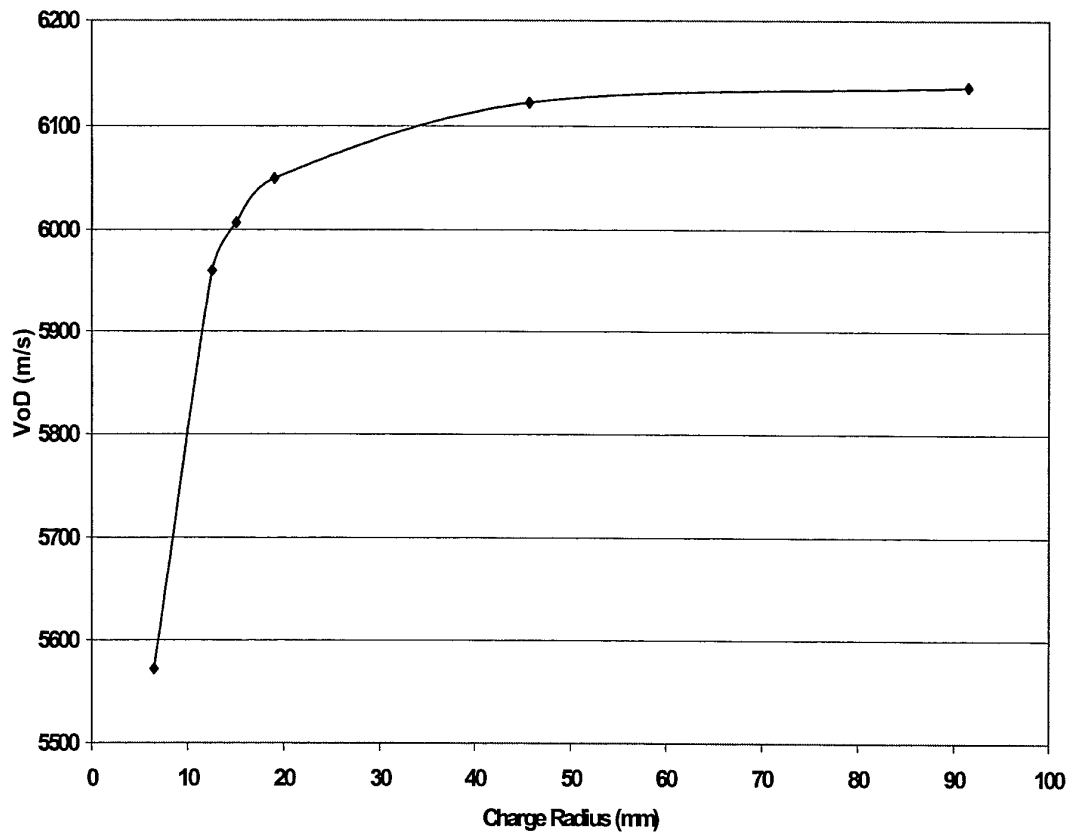


Figure 3. Detonation velocity versus charge radius of Tritonal

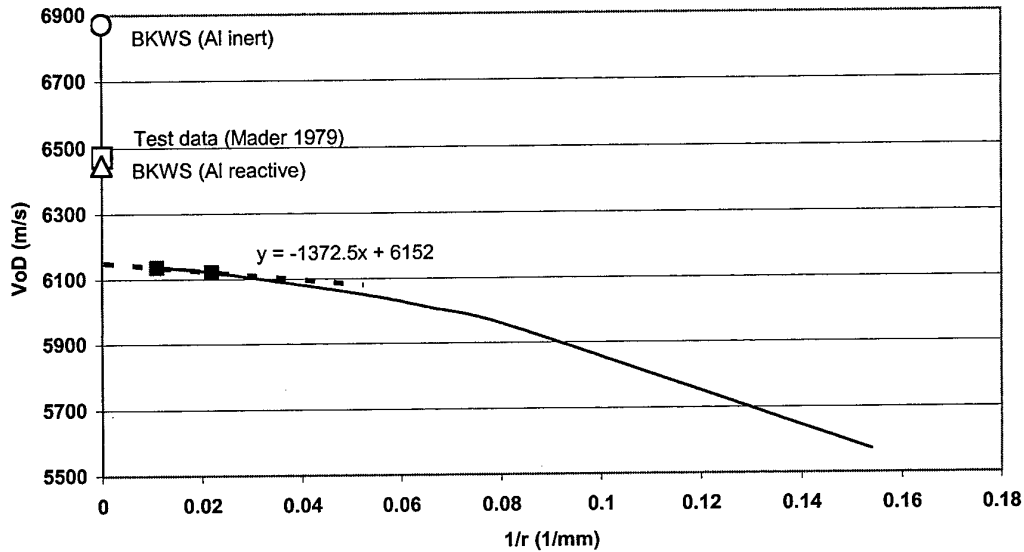


Figure 4. Detonation velocity versus reciprocal radius of Tritonal

In attempting to apply CHEETAH 2.0 to PBXW-115(Aust) using the estimated radius of curvature for the detonation front built into the code, difficulties were initially encountered in achieving convergence to a self-propagating detonation velocity. However, if an experimentally determined radius of curvature is used, good results are achieved from "Kinetic" CHEETAH, reflecting non-ideal features such as detonation velocities dependent on charge radius.

Figure 5 summarises the Kinetic CHEETAH predictions of detonation velocity using the NEWC1 product library, compared with the experimental data listed in Souer's database (1998). Although CHEETAH cannot reproduce exactly the experimental results, it follows a similar trend which demonstrates the diameter effect. The agreement could be improved with further parameter adjustment. Work on improving the fit to the detonation velocities by decreasing the pressure exponent in the rate law from 2.0 to 0.5 is currently in progress.

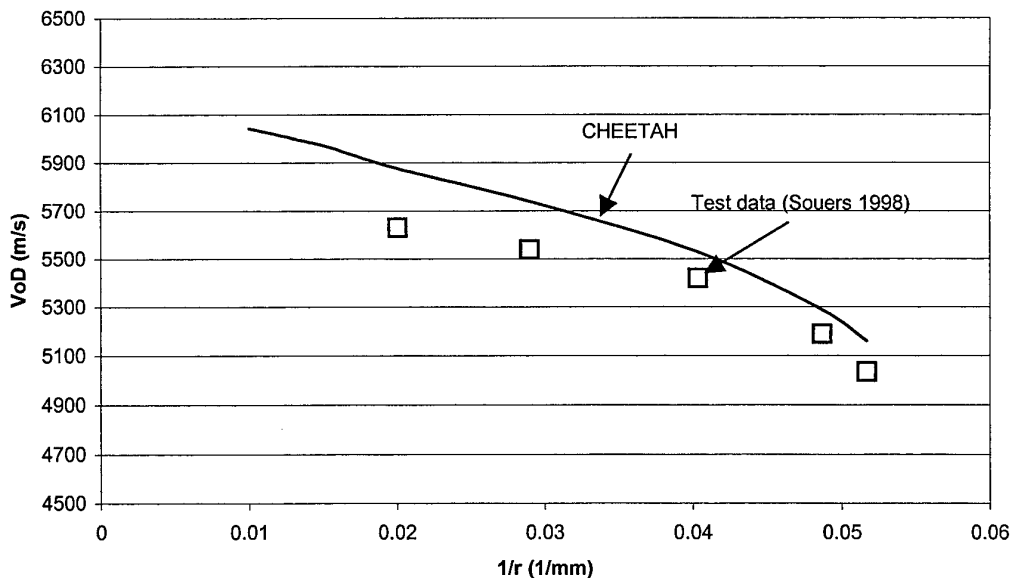


Figure 5 Detonation velocity versus reciprocal radius of PBXW-115

3.3 New and proposed explosives

From the evaluations in Section 3.1, it is seen that the CHEETAH 2.0 program using the traditional Chapman-Jouget thermodynamic detonation theory can accurately model and predict performance for most ideal explosives and mildly non-ideal explosives. This gives us confidence in applying CHEETAH to evaluation of newly developed and proposed explosives.

The input parameters required by CHEETAH for evaluating a new material in CHEETAH are its elemental composition, density and heat of formation. Elemental composition of new or proposed explosives will be known. Density of a *new* ingredient can be measured non-destructively and on relatively small quantities by gas pycnometry or from single crystal X-ray structures, while densities of *proposed* molecules can be estimated by group additivity methods [Cichra et al., 1980] or by crystal packing approaches [Cromer et al., 1987]. Heats of formation are typically measured experimentally by burning several grams of material in a bomb calorimeter. Alternatively they may be estimated by group additivity methods [Benson, 1958], which unfortunately are not well suited to nitroaromatics.

The CHEETAH code was used to screen FOX-7 and NTO-based explosive formulations currently under investigation in WSD, using experimentally measured values for densities and heats of formation. FOX-7 (1,1-diamino-2,2-dinitroethylene) is a novel

explosive with high performance and low sensitivity. The study by Ostmark et al [1998] has shown that FOX-7 is much less sensitive than RDX, while the predicted performance of FOX-7 is comparable to that of RDX. It appears that no experimental data have yet been published. The unpublished WSD experimental results by Lochert [2000] on FOX-7 coated with 5% EVA binder are the only data available to date, and they are used herein to confirm CHEETAH predictions.

NTO (3-nitro-1,2,4-triazol-5-one) is another new explosive with powerful performance and low sensitivity, which shows promise for application in Insensitive Munitions (IM) formulations [Smith and Cliff, 1999]. Melt-castable NTO/TNT compositions, which could be processed using Australia industrial plant, have been identified as possible candidates to meet IM criteria in certain munitions [Cliff and Smith 2000]. A baseline 50:50 NTO/TNT formulation (ARX-4002) has been developed, which can be processed using conventional melt-cast techniques and which exhibits reduced sensitiveness in comparison to Composition B and H-6. The updated experimental data by Cliff [2000] are used herein for validating CHEETAH predictions.

Tables 7 and 8 present performance properties predicted using the traditional Chapman-Jouget thermodynamic detonation theory for explosive formulations based on FOX-7 and NTO respectively. For comparison, WSD experimental data are also included where available. It can be seen that very good agreement has been achieved between the experimental results and those predicted from CHEETAH for all the new explosive formulations. This gives us great confidence in applying CHEETAH to predict performance properties for new and proposed explosives.

Table 7. Detonation properties for compositions based on FOX-7

Name	Density (g/cm ³)	P (GPa)	VoD (m/s)		
		Cal.	Cal.	Exp.#	Err. %
FOX-7	1.885	37.08	9126		
FOX-7/EVA 95/5	1.646	25.27	7955	7730	2.9
RDX/EVA 95/5	1.563	22.99	7731	7630	1.3
FOX-7/TNT 60/40	1.785	29.04	8120		

Data obtained at charge diameter of 12.7mm from [Lochert, 2000]

Table 8. Detonation properties for compositions based on NTO

Name	Density (g/cm ³)	P (GPa)			VoD (m/s)		
		Cal.	Exp.*	Err. %	Cal.	Exp.*	Err. %
RDX/TNT 60/40	1.72	27.23	28.7	-5.1	7974	7840	1.71
NTO/TNT 50/50	1.71	22.5	22.6	-0.4	7418	7370	0.65
NTO/TNT 60/40	1.78	25.18	25.6	-1.6	7734	7840	-1.35
NTO/RDX/TNT 50/12/38	1.792	25.76	26.5	-2.8	7810	7660	1.96
NTO/RDX/TNT 40/20/40	1.779	26.67			7887		
NTO/RDX/TNT 50/10/40	1.789	26.28			7843		
NTO/RDX/TNT 50/15/35	1.797	27.09			7952		
NTO/RDX/TNT 50/20/30	1.805	27.92			8063		
NTO/RDX/TNT 55/10/35	1.802	26.9			7930		
NTO/RDX/TNT/Paraffin 50/14/35/1	1.774	25.82			7812		
NTO/RDX/TNT/Paraffin 50/12/35/3	1.729	23.44			7540		
NTO/RDX/TNT/Paraffin 50/10/35/5	1.686	21.25			7279		

* Data obtained at charge diameter of 38mm from [Cliff, 2000]

3.4 Influence of heats of formation

Elemental composition of new or proposed explosive ingredients is known precisely. Densities can be measured very accurately by gas pycnometry or X-ray crystallography, or they can be predicted (generally within 1%) by empirical methods. There are greater errors in experimental measurement of heats of formation by bomb calorimetry, but explosive performance has a relatively weak dependence on this parameter. Thus, Fried et al. [1998] concluded that the uncertainties in *measured* heats of formation are not large enough to influence the predicted performance of an explosive by more than 1%. *Estimation* of heats of formation of proposed explosive molecules by group additivity methods, however, introduces greater uncertainties. One problem with the Benson method is that it does not handle well nitro groups, almost ubiquitous in energetic materials. More important, however, is that the method predicts heats of formation for the gaseous state. Calculation of heats of formation in the solid state requires estimation of the heat of sublimation.

In order to assess the influence of the uncertainties of calculated heats of formation on the predicted performance of explosives, two ideal explosives FOX-7 and RDX are analysed with seven different hypothetical heats of formation. These values, -300 kJ/mol, -100, 0, 100, 200, 300 and 400 kJ/mol, were selected to encompass the range of heats of formation found for energetic ingredients in the CHEETAH library. The detonation velocities are plotted against heats of formation in Figure 6. The maximum

changes in detonation velocities for the range of heats of formation studied (-300 kJ/mol to 400 kJ/mol) are 10% for RDX and 14% for FOX-7; adoption of a default heat of formation of zero generally gives an error of less than 5%, and usually less than 2%.

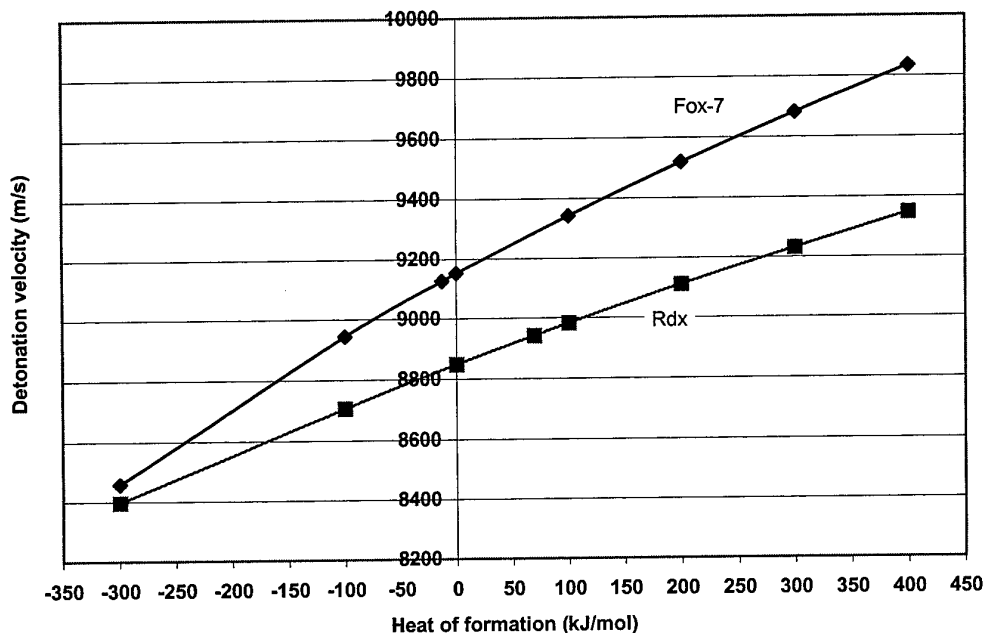


Figure 6. Detonation velocity versus heat of formation

3.5 Influence of binders

The CHEETAH code provides a convenient means to illustrate the influence of the binder system in the development of new explosive compositions. A series of RDX/Binder (90/10) formulations was considered with a range of binder systems, and their explosive performance was calculated using CHEETAH 2.0. Figure 7 illustrates the dependence of detonation velocity on the binder material. It is seen that oxygen deficient hydrocarbons such as paraffins, HTPB, Kraton and polystyrene generally lead to more modest performance, while oxygen-rich binders such as cellulose acetate and the energetic polyGLYN lead to significantly enhanced performance.

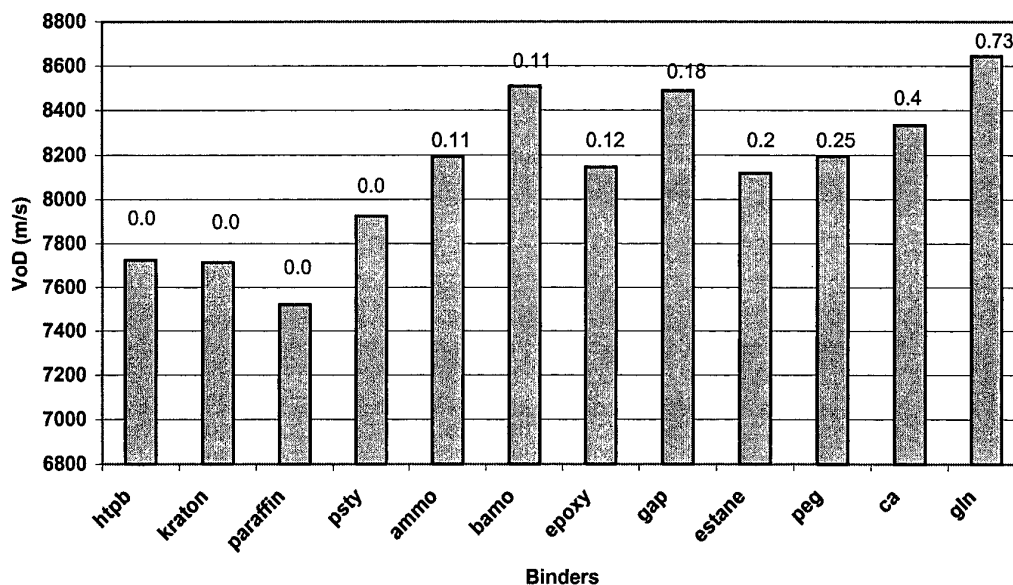


Figure 7. Detonation velocity versus types of binders (the value above each bar is the oxygen balance)

Cliff [1999] investigated PBX's based on HMX and energetic binders for use in air-launched weapons, and studied cure of the pre-polymer and plasticisation as means to tailor and optimise the binder system in a current HMX-based PBX composition. In order to further evaluate CHEETAH's application to such HMX-based PBX compositions with energetic binders, formulations used in Cliff's research have been analysed and the results are given in Table 9. In general, the agreement between the CHEETAH calculations and the experimental results is good, although in each case the experimentally determined detonation velocity is seen to be less than that predicted. The most probable reason for this discrepancy is that the density of the castings is unlikely to match the theoretical maximum density (TMD); unfortunately, the actual density was not measured. In addition, experimental VoD measurements were carried out at a single charge diameter (25mm), whereas CHEETAH predictions are based on infinite charge diameters.

Table 9 Detonation properties for HMX-based explosives with binders

Name	Density (TMD) (g/cm ³)	P (GPa)	VoD (m/s)		
		Cal.	Cal.	Exp.*	Err. %
RF-02-32 (HMX/K10/polyNIMMO 82.2/9.33/8.47) CPX-471	1.77	31.4	8437	8420	0.2
(HMX/K10/polyNIMMO 77/11.5/11.5) CPX-472	1.73	29.4	8224	7930	3.7
(HMX/K10/polyGLYN 77/11.5/11.5) CPX-473	1.76	30.0	8320	7990	4.1
(HMX/BDNPAF/polyGLYN 77/11.5/11.5)	1.77	30.9	8476	8260	2.6

* Data from [Cliff, 1999]

Based on a review of recent advances on energetic polymers and plasticisers for explosive formulation by Provatas [2000], polyGLYN is currently the most energetic polymer available. He indicates that the most effective use of energetic polymers will be achieved by inclusion of energetic plasticisers to modify the mechanical properties. According to his recommendations, DSTO research into high performance explosive compositions is currently based on PBX's composed of solid nitramines, suspended in a matrix of polyNIMMO and polyGLYN polymers combined with the nitroaromatic plasticiser K10. Two examples of RDX/Polymer/Plasticiser of this type have been analysed and the predicted performance is given in Table 10; experimental results are not yet available.

Table 10. Detonation properties for explosives with energetic binders comprising polymer and plasticiser

Name	Density (g/cm ³)	P (GPa)	VoD (m/s)
		Cal.	Cal.
RDX/polyGLYN/K10 (75/12.5/12.5)	1.69	26.92	8036
RDX/polyNIMMO/K10 (75/12.5/12.5)	1.654	26.37	7951

3.6 Current developments

Anderson and Katsabanis [2000] have recently studied the effect of aluminium particle size on the behaviour of Composition B containing 10% by weight aluminium, and of TNT containing 30% by weight aluminium and measured heats of detonation using a detonation bomb calorimeter. They indicated that CHEETAH 2.0 using the NEWC1 library appeared to be the most appropriate code for this investigation. Better agreement was achieved by assuming an isentropic expansion to a moderate specific volume, rather than assuming the products are "frozen" at the explosion state. It was also found that only two-thirds of the Al appeared to be consumed in detonation of TNT/Al, and CHEETAH could be forced to reproduce this result by limiting the amount of aluminium reacting. The findings of Anderson and Katsabanis no doubt further widen CHEETAH's applicability. Nevertheless, given the nature of thermodynamic codes, CHEETAH is limited to prediction only of the performance parameters of explosives. Although it can provide insight into the detonation process, it cannot model the whole process including such facets as corner-turning ability, air-blast, and so on. Reactive hydrocodes must be used, together with appropriate reaction rate models, to simulate the whole propagation process.

Personal communication by D.A. Jones [October, 2000] indicated that the new Kinetic CHEETAH based on the Wood-Kirkwood detonation theory can also be used to replace the analytical non-ideal detonation model CPeX developed to describe the detonics of non-ideal explosives by Kirby and Leiper [1985]. This observation has added a further dimension to CHEETAH's potential.

4. Conclusions and Future Directions

The Lawrence Livermore National Laboratory CHEETAH 2.0 program has been used to analyse a number of cases with reference to conventional ideal explosive ingredients, ideal explosive compositions, non-ideal explosive compositions, and new and proposed explosives. It has also been used to study the effect of heats of formation and different types of binders on the predicted performance of explosive formulations. From the evaluations outlined previously, the following conclusions have been reached.

- a. The CHEETAH 2.0 program using the traditional Chapman-Jouget thermodynamic detonation theory can accurately model and predict performance of new explosive materials such as FOX-7 and NTO-based formulations, and of ideal explosives such as Composition B and Pentolite. It can also predict reasonably accurately experimental results for mildly non-ideal explosives such as AFX-645, PBXN-109 and Tritonal.

- b. The CHEETAH 2.0 program based on the Wood-Kirkwood detonation theory can successfully model both mildly non-ideal explosives and moderately non-ideal explosives. The kinetic CHEETAH predicts more detailed information than can that based solely on CJ theory. Although not attempted in this study, it could be used to replicate the experimentally observed variation of detonation velocity with charge diameter by calibrating the kinetic parameters that describe the decomposition of its ingredients. This would lead to a more detailed understanding of the sonic detonation zone lengths, the pressure histories and the energy release rates during non-ideal detonation.
- c. In attempting to apply CHEETAH 2.0 to strongly non-ideal explosives such as PBXW-115 using the estimated radius of curvature for the detonation front built into the code, difficulties were initially encountered in achieving convergence to a self-propagating detonation velocity. However, if an experimentally determined radius of curvature is used, good results are achieved from "Kinetic" CHEETAH, reflecting non-ideal features such as detonation velocities dependent on charge radius.

In view of the strengths and limitations of CHEETAH, it is recommended that the following areas be considered for the future work.

- a. Combined with experimental results, use CHEETAH based on the traditional Chapman-Jouget thermodynamic detonation theory to calculate CJ states of Tritonal with different amounts of the aluminium "frozen", in order to estimate the amount of aluminium that supports the propagation of detonation. Repeated with Tritonal utilising various particle sizes of aluminium, this should provide insight into the size-dependent rates of aluminium combustion in non-ideal explosives.
- b. Refine the kinetic parameters used in "kinetic" CHEETAH (based on the Wood-Kirkwood detonation theory), to match more closely available experimental data on Tritonal and PBXN-109.
- c. Model strongly non-ideal explosives such as PBXW-115 with further parameter adjustment to improve the fit to the detonation velocities by decreasing the pressure exponent in the rate law from 2.0 to 0.5.

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