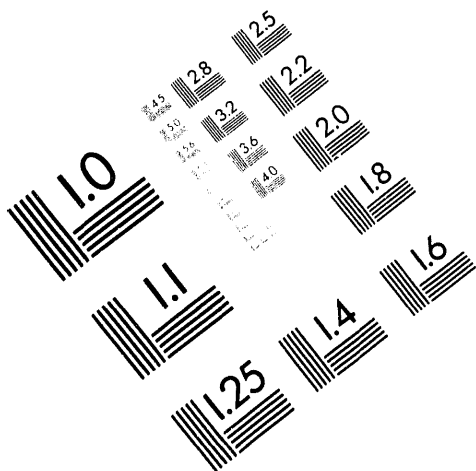


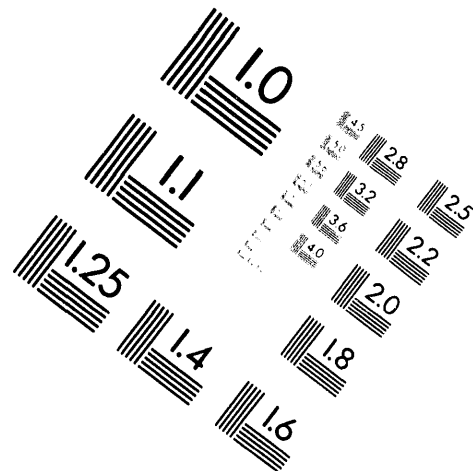


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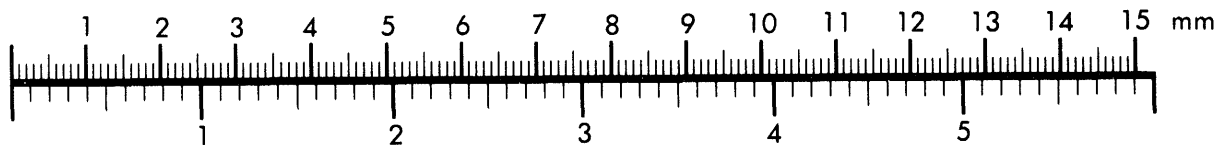
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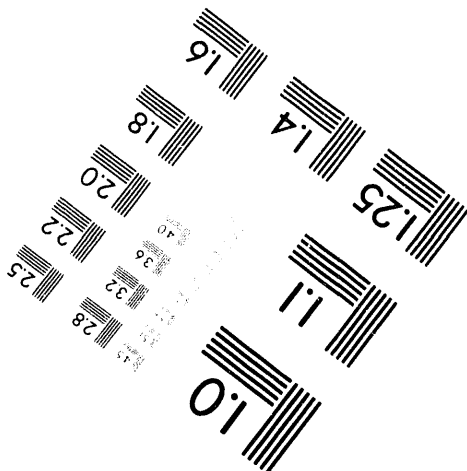
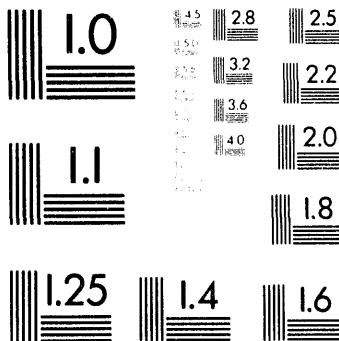
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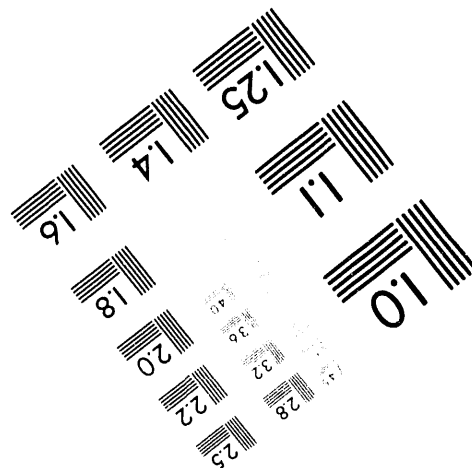
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Submitted to the
1994 Joint USA-Russia Energetic Material Technology Symposium
Livermore, California (May 18-25, 1994)

**EQUATIONS OF STATE FOR EXPLOSIVE
DETONATION PRODUCTS: THE PANDA MODEL**

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(PRESENTATION ABSTRACT)

This paper discusses a thermochemical model for calculating equations of state (EOS) for the detonation products of explosives. This model, which was first presented at the Eighth Detonation Symposium [1], is available in the PANDA code [2] and is referred to here as "the PANDA model."

Overview: The basic features of the PANDA model are summarized below.

- Statistical-mechanical theories are used to construct EOS tables for each of the chemical species that are to be allowed in the detonation products. For CHNO compositions, the principal species are: CO₂, N₂, H₂O, CO, NO, NH₃, CH₄, H₂, O₂, HCOOH (formic acid), atomic N, O, and H, and three forms of condensed carbon - graphite, diamond, and liquid carbon. (This data base is being extended to include aluminum compounds.)
- The ideal mixing model is used to compute the thermodynamic functions for a mixture of these species, and the composition of the system is determined from assumption of chemical equilibrium. Since the same library of EOS tables for the chemical species is used for all explosive compositions, the only input parameters required by PANDA are the chemical formula and the heat of formation for the unreacted explosive.
- For hydrocode calculations, the detonation product EOS are used in tabular form, together with a reactive burn model that allows description of shock-induced initiation and growth or failure as well as ideal detonation wave propagation. This model has been implemented in the three-dimensional Eulerian code, CTH [3].

Results: The principal conclusions of work to date are as follows.

- The PANDA model gives accurate *a priori* predictions of the detonation properties, including the dependence on loading density, for all explosives that have been considered (about 30 CHNO compositions) [1] [4] [5].
- It gives accurate predictions of the Hugoniot for explosives in the overdriven shock region and other CHNO compounds at pressures high enough to dissociate them (>20 GPa) [4].

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- Hydrocode calculations using the PANDA EOS give accurate predictions of the wall motion in cylinder tests [5].
- Formic acid is a very important reaction product for explosives having a negative oxygen balance, especially for HMX and RDX [1] [4].
- The atomic forms of nitrogen and oxygen are important in some cases, especially in the overdriven shock regime [4].
- A three-phase model of condensed carbon (graphite, diamond, and liquid) is necessary for explaining variations in detonation properties with changes in composition and loading density [1] [4]. In particular, the first observation of the effect of the graphite-diamond transition on the detonation velocity curve of TNT was given in Ref. [1].
- The ideal mixing approximation gives surprisingly accurate results, not only for detonation products, but also when compared with Monte Carlo simulations of mixtures [4] [6]. As a result, more realistic EOS can be used for complicated chemical species than would be possible with mixture theories based upon simple intermolecular pair potentials.
- The accuracy of the model in predicting detonation properties, overdriven Hugoniot, and cylinder test wall motion is comparable to experimental error for all but nonideal CHNO explosives, such as TATB [5]. This fact suggests that time-dependent effects are only important in isolated cases.

References

- [1] G. I. Kerley, "Theoretical Equations of State for the Detonation Properties of Explosives," in Proceedings of the Eighth Symposium (International) on Detonation, edited by J. M. Short, NSWL MP 86-194 (Naval Surface Weapons Center, White Oak, MD, 1986), pp. 540-547.
- [2] G. I. Kerley, "User's Manual for PANDA II: A Computer Code for Calculating Equations of State," Sandia National Laboratories report SAND88-2291, 1991.
- [3] J. M. McGlaun, et al., poster session to be presented at this conference.
- [4] G. I. Kerley, "Theoretical Model of Explosive Detonation Products: Tests and Sensitivity Studies," in Proceedings of the Ninth Symposium (International) on Detonation, edited by W. J. Morat, OCNR 113291-7 (Office of the Chief of Naval Research, 1990), pp. 443-451.
- [5] G. I. Kerley and T. L. Christian-Frear, "Prediction of Explosive Cylinder Tests Using Equations of State from the PANDA Code," Sandia National Laboratories report SAND93-2131, 1993.
- [6] G. I. Kerley, "Equations of State and Gas-Gas Phase Separation in Soft Sphere Mixtures," J. Chem. Phys. **91**, 1204-1210 (1989).



Equations of State for Explosive Detonation Products: the PANDA Model

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**U.S./Russia Energetic Materials
Technology Symposium
Pleasanton, CA, May 18-25, 1994**

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Detonation Product EOS - Review



Analytic fits to experiment (JWL)

- lack predictive capability
- inaccurate outside region of calibration

Theoretical (chemical) methods (BKW, JCZ, CHEQ, ETARC, ...)

- offer predictive capability
- often lack accuracy and reliability

Criteria for a satisfactory model

- ability to predict detonation properties
 - including dependence on initial density (porosity)
- ability to predict detonation product expansion
 - cylinder tests and other hydrodynamic experiments
- ability to predict response in other regimes
 - overdriven detonations, reshocked detonation products
- usable in hydrocode environment

Sandia Capabilities - EOS



TIGER/BKW (Hobbs & Baer)

- Mader (1960's), Cowperthwaite & Zwisler (1970's)
- Sandia version has widely extended and recalibrated data base
- can handle a broad range of chemical compositions

PANDA (Kerley)

- more sophisticated "statistical mechanical" models
- accurate a priori predictions
- certain features quite different from JWL and TIGER
- CHNO compositions - working on CHNO-Al

Tabular EOS package for hydrocodes

- presently implemented in 3-D Eulerian code (CTH)
- includes History Variable Reactive Burn (HVRB) model
- efficient for numerical calculations

References to PANDA Model



1. G. I. Kerley, "User's Manual for PANDA II: A Computer Code for Calculating Equations of State," *Sandia National Laboratories report SAND88-2291*, 1991.
2. G. I. Kerley, "Theoretical Equations of State for the Detonation Properties of Explosives," in *Proceedings of the Eighth Symposium (International) on Detonation*, edited by J. M. Short, NSWL MP 86-194 (Naval Surface Weapons Center, White Oak, MD, 1986), pp. 540-547.
3. G. I. Kerley, "Theoretical Model of Explosive Detonation Products: Tests and Sensitivity Studies," in *Proceedings of the Ninth Symposium (International) on Detonation*, edited by W. J. Morat, OCNR 113291-7 (Office of the Chief of Naval Research, 1990), pp. 443-451.
4. G. I. Kerley and T. L. Christian-Frear, "Prediction of Explosive Cylinder Tests Using Equations of State from the PANDA Code," *Sandia National Laboratories report SAND93-2131*, 1993.
5. G. I. Kerley, "Equations of State and Gas-Gas Phase Separation in Soft Sphere Mixtures," *J. Chem. Phys.* 91, 1204-1210 (1989).
6. J. M. McGlaun, E. S. Hertel, G. I. Kerley, and M. R. Baer, "Energetic Material Performance Modelling," *poster session, this conference*.

Basic Problems in Modeling



Any thermochemical model must address the following problems:

- Identify chemical species that can be formed in explosive detonation products.
- Determine thermodynamic functions and model parameters for all species.
 - best not to introduce explosive data in this step
- Devise model for properties of detonation product mixture as functions of density, temperature, and chemical composition.
- Determine chemical composition as function of density and temperature, subject to chemical constraints.
 - will assume chemical equilibrium except as indicated
- Energy of unreactive explosive relative to detonation products (heat of formation).

Treatment of Individual Chemical Species



16 CHNO species included in the PANDA model:

- CO_2 , N_2 , H_2O , CO , NO , NH_3 , CH_4 , O_2 , H_2 , C , HCOOH , N , O , H
- three phases of carbon (graphite, diamond, liquid) - necessary to explain variations with loading density and composition
- HCOOH (formic acid) - important for negative oxygen balance
- atomic nitrogen and oxygen - important for overdriven shocks
- database being expanded to include Al compounds

Tabular EOS constructed for all species

- statistical-mechanical models, PANDA code
- liquid perturbation theory for all phases (except solid carbon)
- parameters were not adjusted to fit explosive data
- exception - formic acid (estimates from CO_2 with adjustments to RDX/HMX)
- same library of EOS tables for all explosives

PANDA Mixture Model



The PANDA model assumes ideal mixing, chemical equilibrium.

- phases have equal pressures and temperatures
- ideal entropy of mixing within homogeneous phase, zero entropy for separate phases
- composition determined by minimizing free energy, subject to chemical constraints

How valid is ideal mixing?

- a posteriori - surprisingly good results for most cases
- Monte Carlo calculations for soft-sphere and $\text{H}_2\text{O}/\text{N}_2$ mixtures
- nothing better presently available
- problem - does not predict phase separation (liq. C, N, O)

How valid is chemical equilibrium?

- a posteriori - agreement with predictions for most cases
- exceptions - TATB, NQ may be nonideal explosives

Prediction of Detonation Properties



Detonation properties have been computed for ~30 CHNO explosive compositions.

- PANDA input - composition $C_wH_xN_yO_z$, heat of formation for unreacted explosive. Same tables used for all compositions.

Deviations between predictions and measurements are on the order of experimental uncertainty.

- D_{CJ} - -0.1% (average difference), $\pm 1.4\%$ (standard deviation)
- P_{CJ} - -4%, $\pm 8\%$ T_{CJ} - -6%, $\pm 16\%$
- Trends with loading density are explained.

Some problems remain.

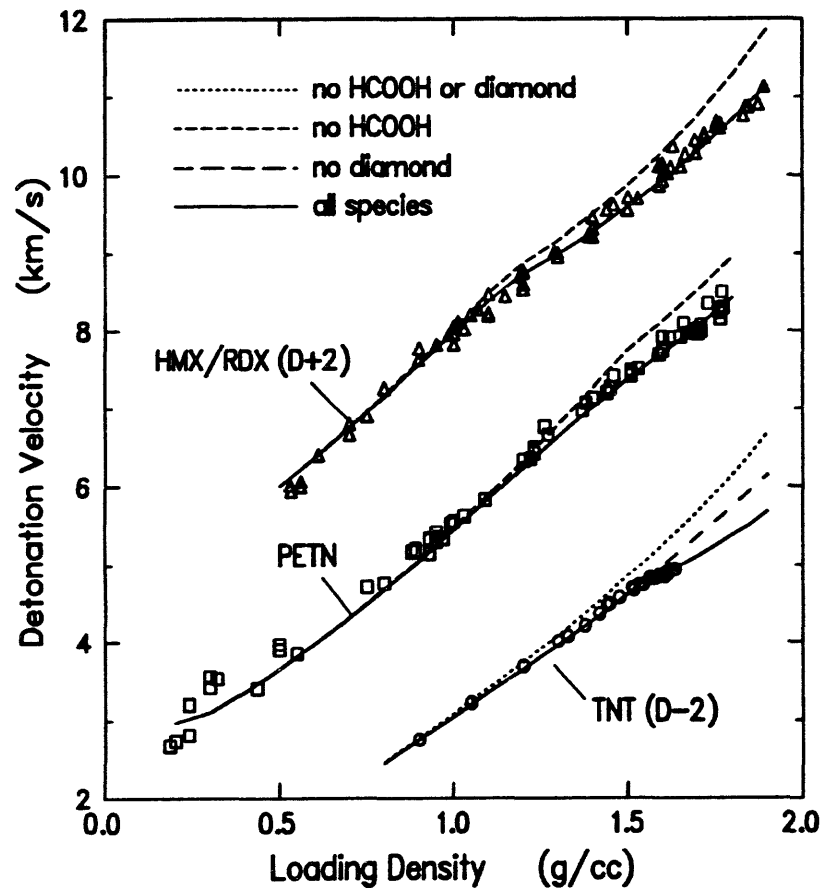
- TATB, NQ are worse than other explosives - ~5% error in D_{CJ} .
- Carbon EOS is inadequate near graphite-liquid melting line.
- Reaction zone and structure of expansion wave affect measured detonation pressure.

Trends With Loading Density

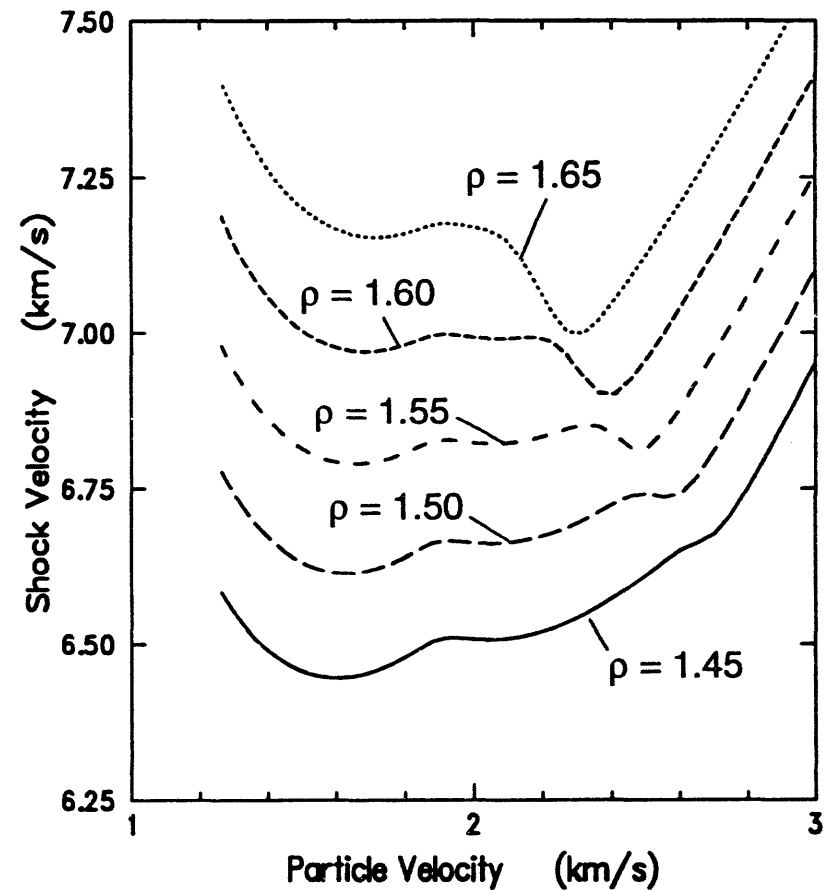


Shifts in product composition affect detonation velocity

Detonation Velocity vs. Loading Density



TNT Hugoniot Near CJ Point

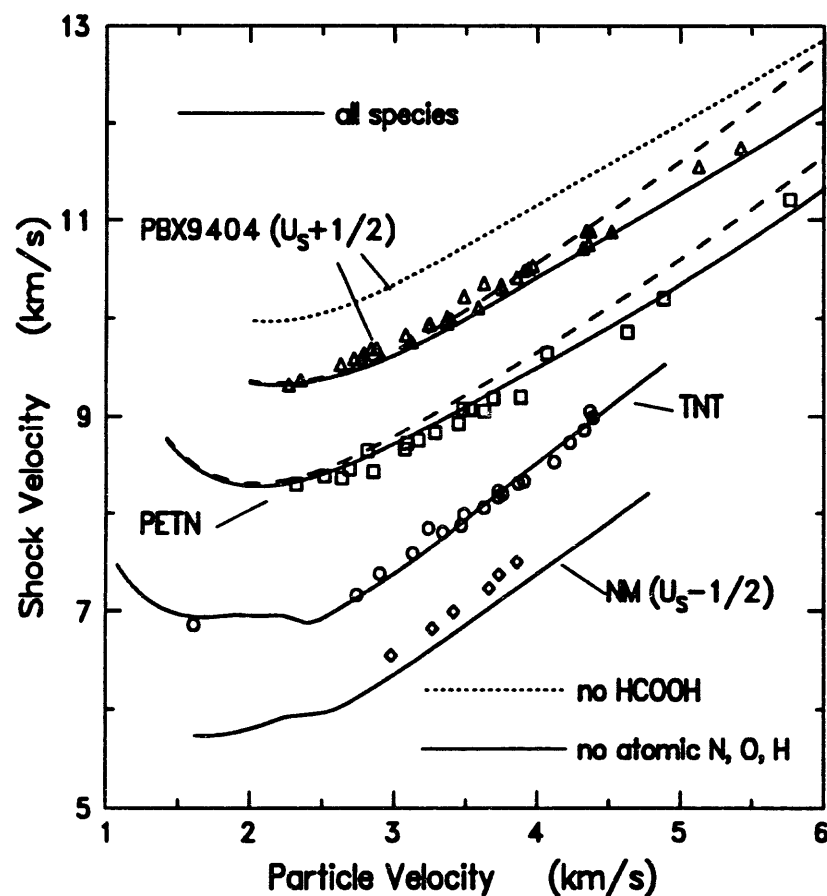


Panda Predictions - Overdriven Hugoniots

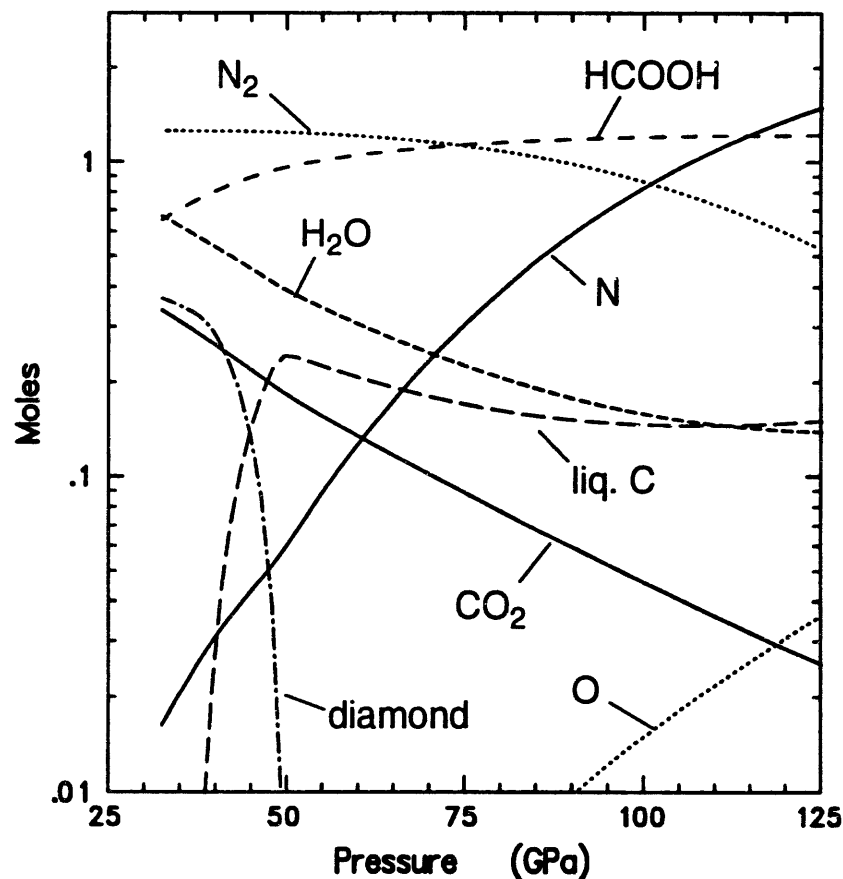


Formic acid, liquid carbon, atomic N & O
are important in overdriven shock regime

Overdriven Hugoniots



Overdriven Hugoniot for PBX-9404



Cylinder Test Calculations



Cylinder tests have been computed for ~30 variations of CHNO explosive composition and loading density

- 2-D calculations using CTH code.
- PANDA EOS for detonation products, HVRB model for detonation wave propagation.
- Plate acceleration tests for LX-14 (HMX) also studied.

Good agreement between predicted and measured expansion velocities

- 0.3% (ave. diff.), $\pm 2.6\%$ (std. dev.) at 5-fold expansion
- Reproduced takeoff velocity, early time history.
- Reproduced trends with loading density and composition.

Problems - consistent with results for detonation properties

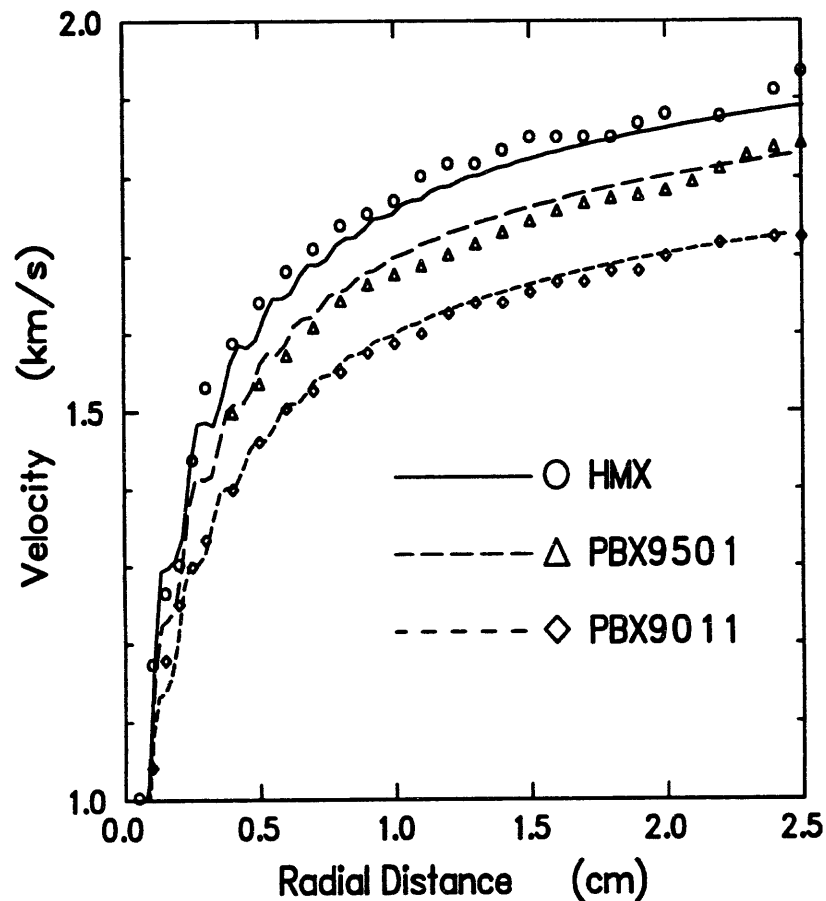
- TATB worse than other explosives - expansion velocities ~5% high.
- Reactive burn effects important for early time history.

PANDA Predictions - Cylinder Tests

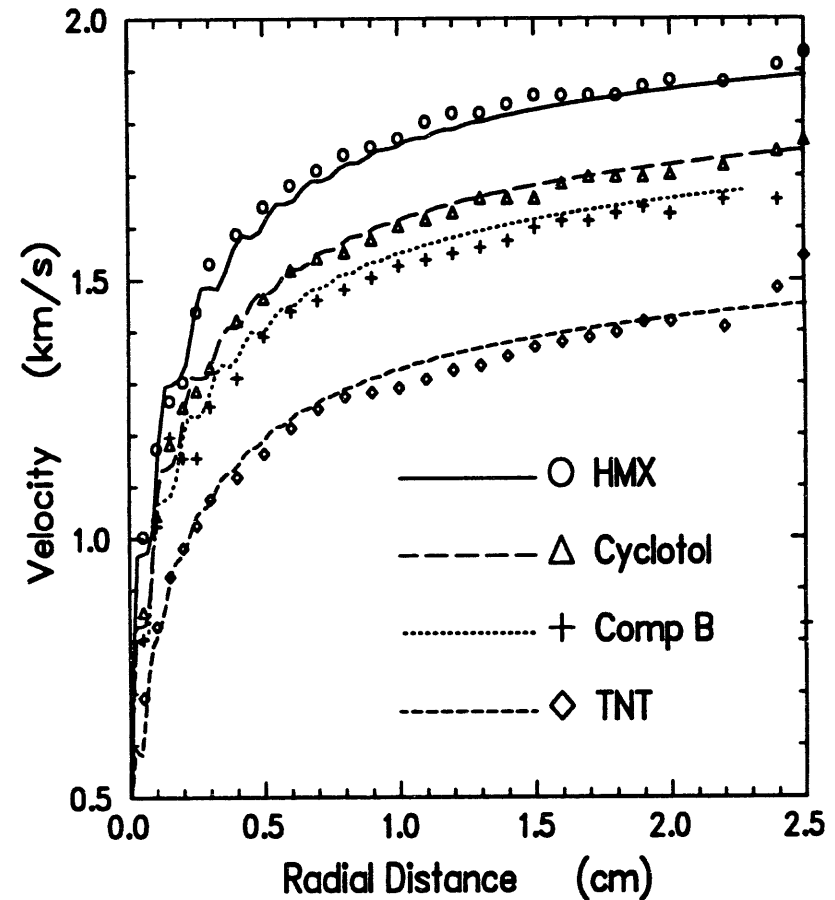


Correct predictions of trends with chemical composition.

Cylinder Expansion Data for HMX-Based Explosives



Cylinder Expansion Data for RDX-TNT Mixtures

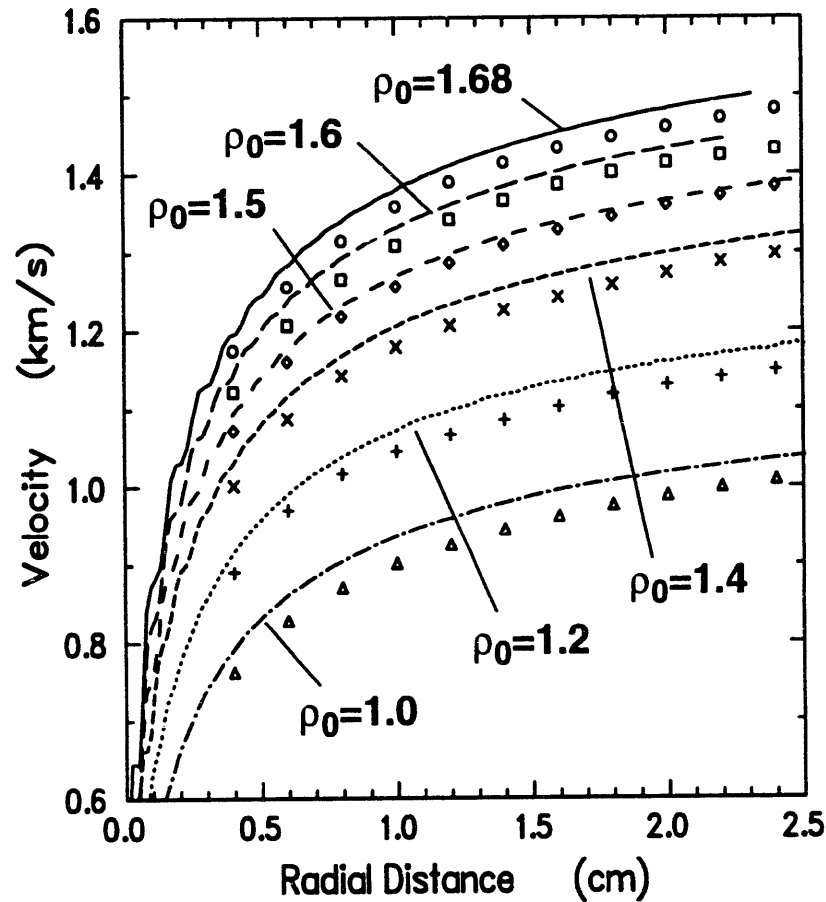


PANDA Predictions - Cylinder Tests

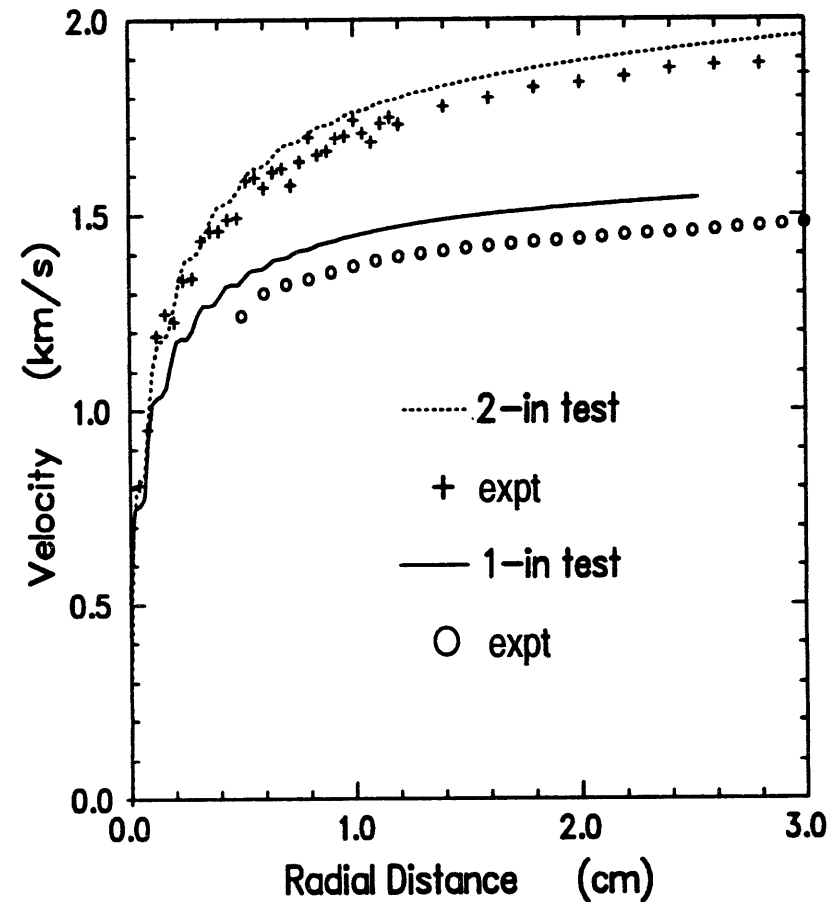


Predicts trends in loading density. TATB may be a non-ideal explosive.

Cylinder Expansion Data for HNS



Cylinder test calculations for PBX9502

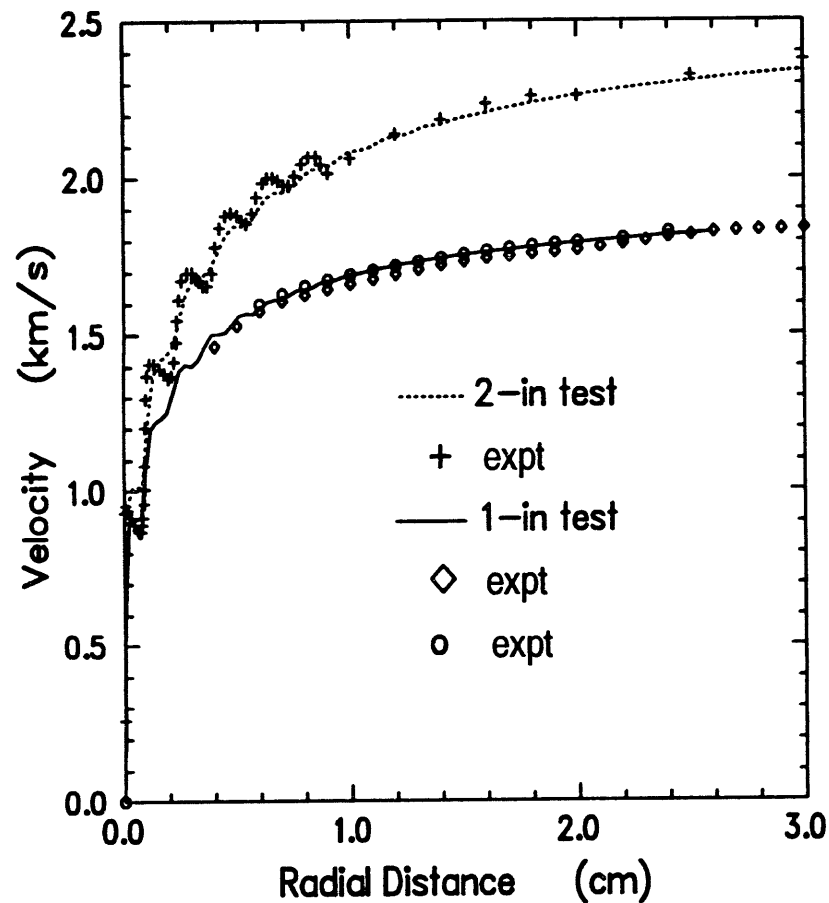


Cylinder vs. Plate Acceleration Tests

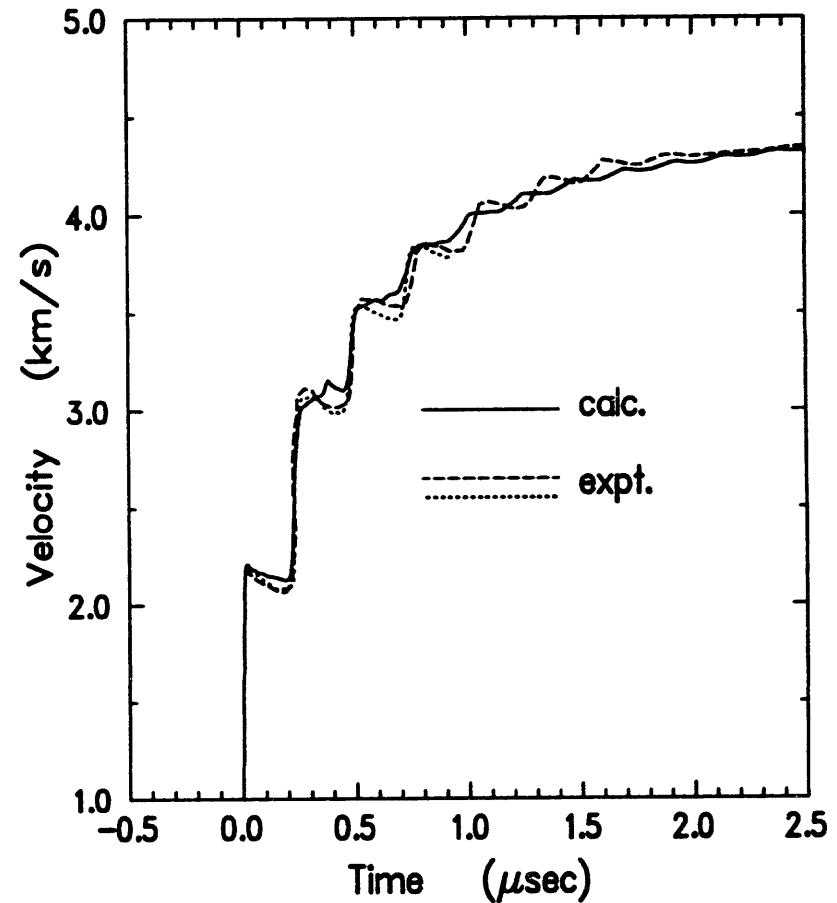


PANDA model gives equally good results in both geometries

Cylinder test calculations for LX14



LX14 Plate Test #9634



Current and Future Interests



Aluminized explosives and propellants

- extend EOS data base, examine reaction rate effects

Improvements to carbon EOS

- region of graphite-liquid melting line

Nonideal explosives

- TATB, ANFO

Plastics and other reactive materials

- application of EOS and reactive burn models

Reactive burn models

- improved calibration and evaluation of HVRB model
- explosive shock desensitization
- Arrhenius burn - slapper detonators

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