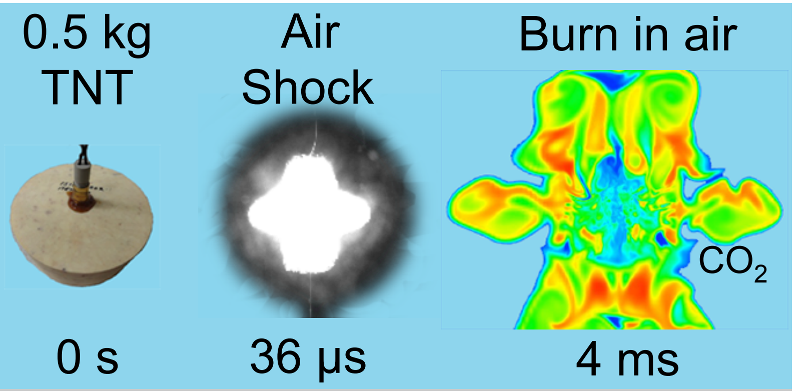
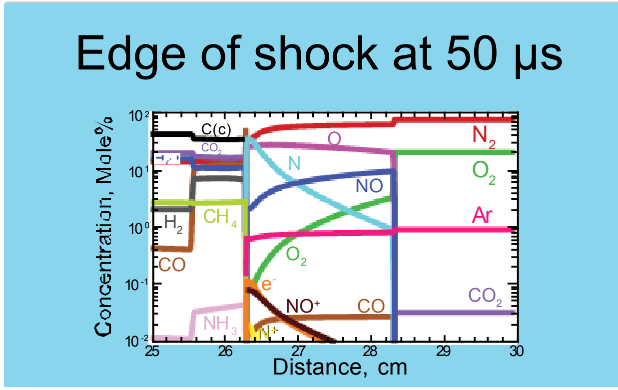
Exceptional service in the national interest

SAND2014-19288PE





JCZS2i: An improved JCZ database for EOS calculations at high temperatures and pressures

Michael L. Hobbs, Aaron L. Brundage, Cole D. Yarrington

Sandia National Laboratory, USA

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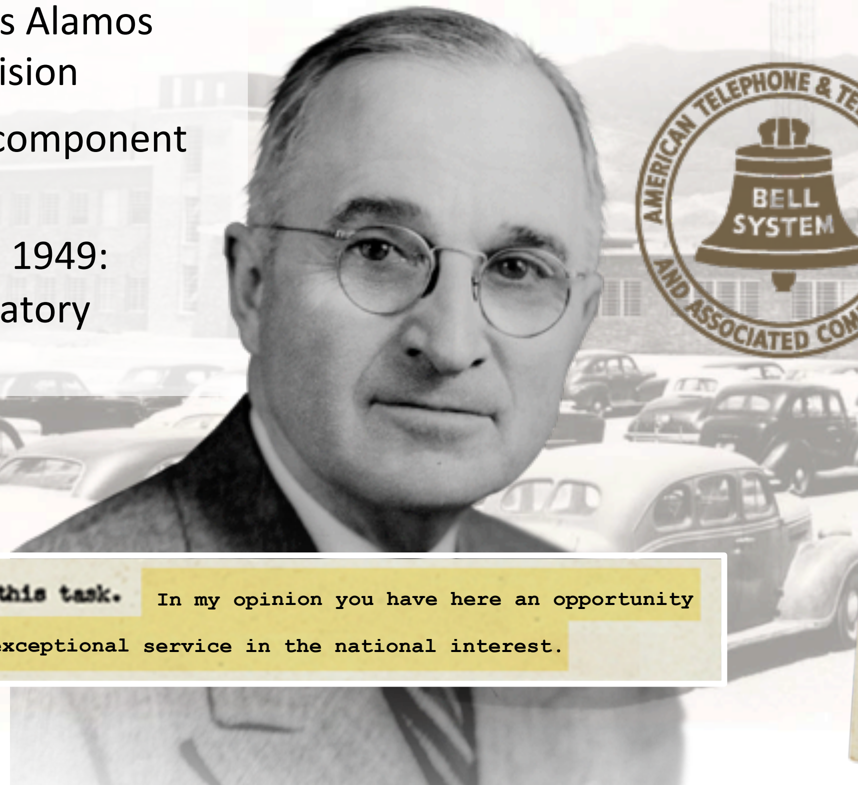
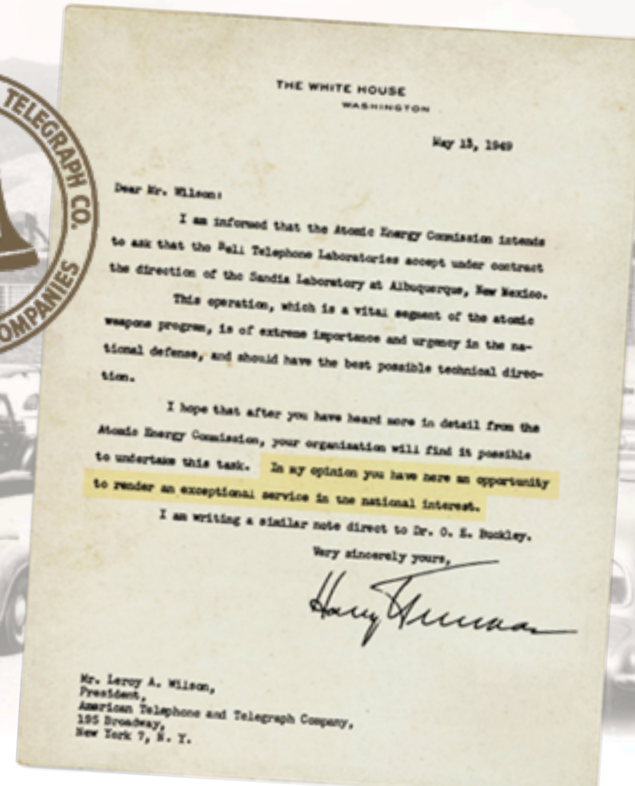
Sandia's History

Exceptional service in the national interest

- July 1945: Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949: Sandia Laboratory established



to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely yours,

Harry Truman

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

Governance of Sandia Laboratories

Sandia Corporation

- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–present
- Existing contract expires: April 30, 2016, with a one-year contract extension option
- Government owned, contractor operated

Federally funded research and development center

Sandia Sites

Sandia National Laboratories


Albuquerque, New Mexico


Livermore, California


Kauai, Hawaii

Waste Isolation Pilot Plant, Carlsbad, New Mexico


Pantex Plant, Amarillo, Texas


Tonopah, Nevada

Sandia Addresses National Security Challenges

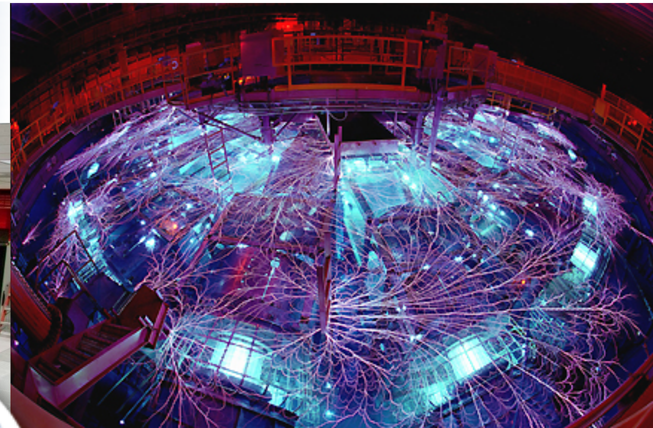
Sandia National Laboratories

1950s	1960s	1970s	1980s	1990s	2000s	2010s
Nuclear weapons	Development engineering	Multiprogram laboratory	Missile defense work	Post–Cold War transition	START Post 9/11	LEPs Cyber, biosecurity proliferation
Production and manufacturing engineering	Vietnam conflict	Energy crisis	Cold War	Stockpile stewardship	National security	Evolving national security challenges

Our Research Framework

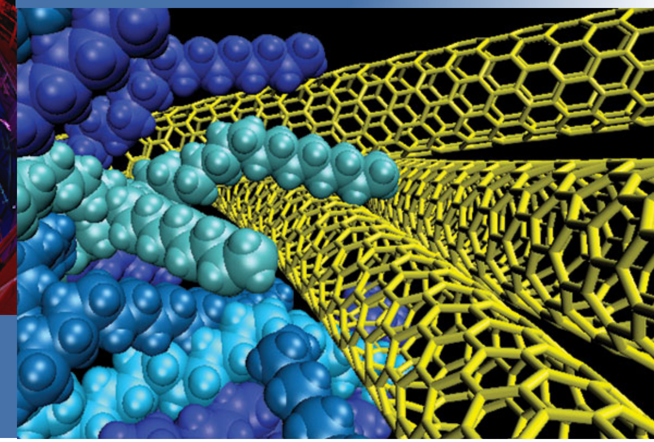
Strong research foundations play a differentiating role in our mission delivery

Computing & Information Sciences

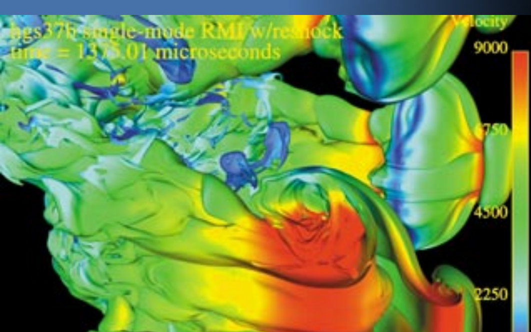


Radiation Effects & High Energy Density Science

Materials Sciences

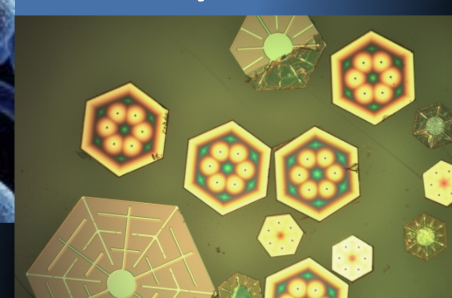


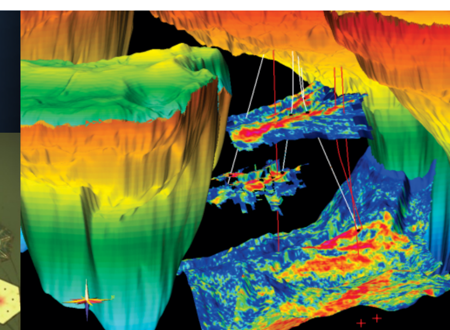
Engineering Sciences



Bioscience

Nanodevices & Microsystems





Geoscience

History of Equation of State at Sandia

1950's

LRL[a]

LASL[b]

BKW[6]

1960's

SRI[c]

Wiebenson et al.,[4] 1968

TIGER

Modular (ideal,BKW)

1970's

SRI[c]

Cowperthwaite & Zwisler,[2,5] 1973

TIGER

Modular (ideal,BKW,JCZ)

1990's & 2000's

SNL[d]

Hobbs & Baer,[7] 1992

TIGER

BKWS[7]

Large EOS database

Tanaka, K., 'Detonation Properties of High Explosives Calculated by Revised Kihara-Hikita Equation of State," *8th Detonation Symposium*, 548-557 (1985).

LLNL[e]

JCZS, Hobbs et al.,[1] 1999

BKWC, Fried et al.,[9] 1996

Exp-6, Fried et al.,[10] 2002

CHEETAH

Fried,[8] 1994

Graphical interface

Hobbs, M. L. Tanaka, K., Iida, M. and Matsunaga, T., "Equilibrium Calculations of Firework Mixtures," *3rd (Beijing) International Symposium on Pyrotechnics and Explosives*, Beijing, China (1995).

2010's

SNL[d]

JCZS2i

CTH-TIGER

Piecewise C_p fits

Over 200 ions

New water EOS

Coupled shock code

[a]Lawrence Radiation Laboratory (LRL)

[b]Los Alamos Scientific Laboratory (LASL)

[c]Stanford Research Institute (SRI)

[d]Sandia National Laboratories (SNL)

[e]Lawrence Livermore National Laboratory (LLNL)

どこからきたのか？

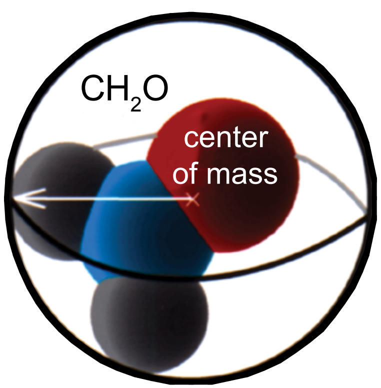
どこえいくのか？

High pressure, temperature EOS basics

BKW, covolume based

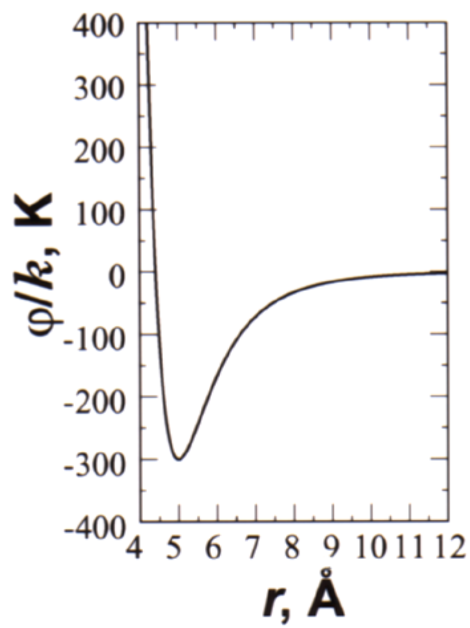
$$\frac{PV}{RT} = 1 + X\exp(\beta X)$$

$$X = \frac{\mathrm{K}\sum n_i k_i}{V\left(T+\theta\right)^{\alpha}}$$



JCZ, intermolecular potential based

$$P = \frac{G\left(V,T,\varphi\right)nRT}{V} + P_o\left(V,\varphi\right)$$

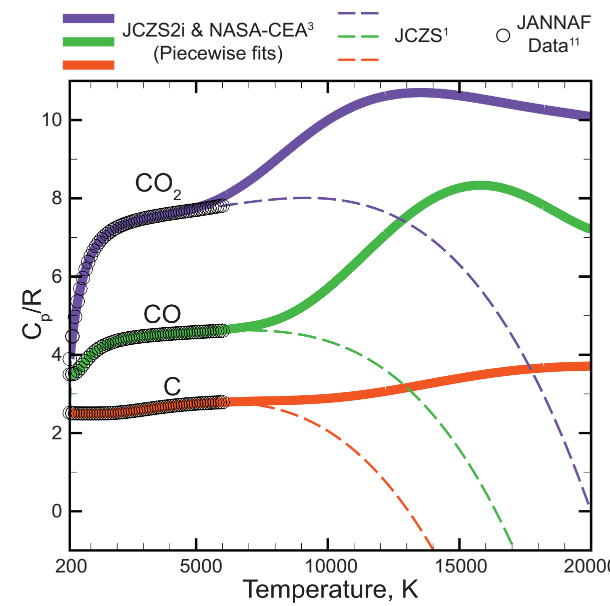


Thermodynamics

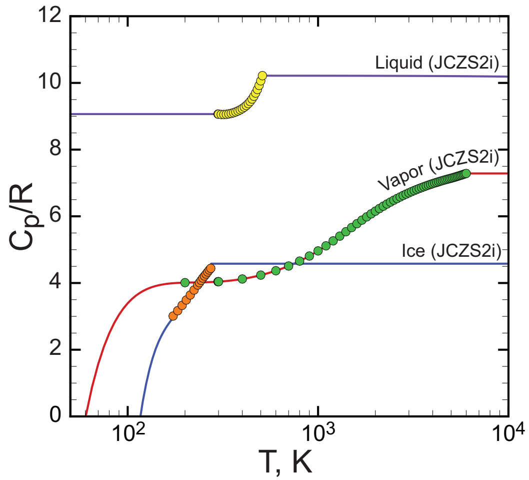
$$C_p/R = \sum_{i=1}^{7} a_i T^{i-3} \qquad \left(\partial S/\partial T\right) = C_p/T$$

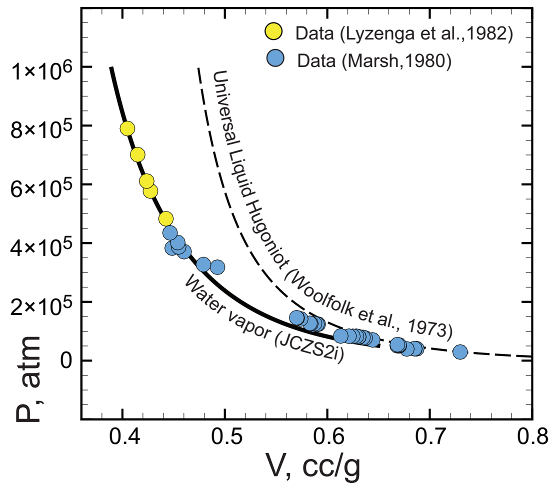
$$C_p = \left(\partial H/\partial T\right)_P \qquad S = \int \tfrac{C_p}{T}\,dT$$

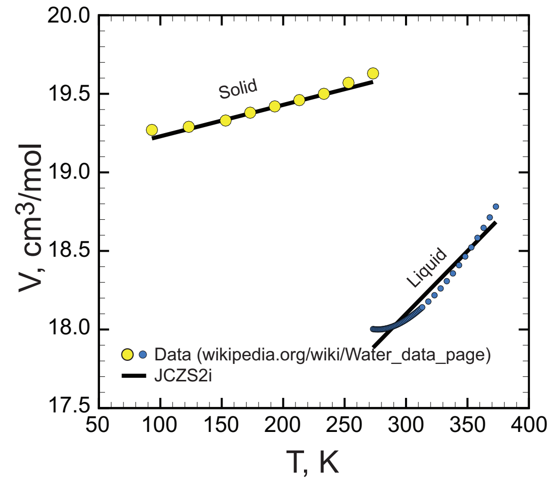
$$h = \int C_p\,dT \qquad \mu/RT = H/RT - S/R$$

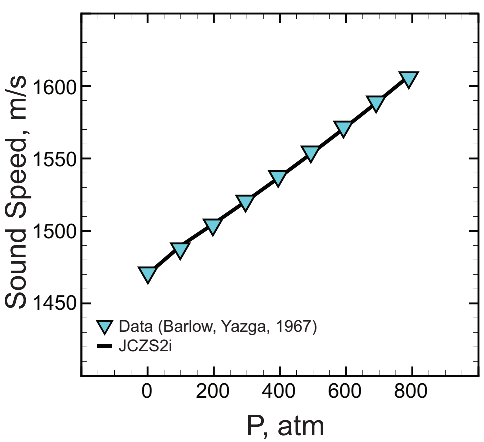


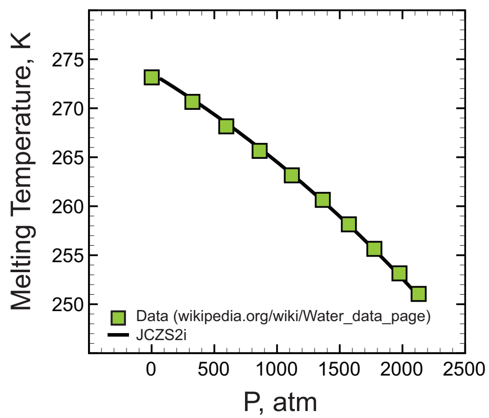
Water EOS

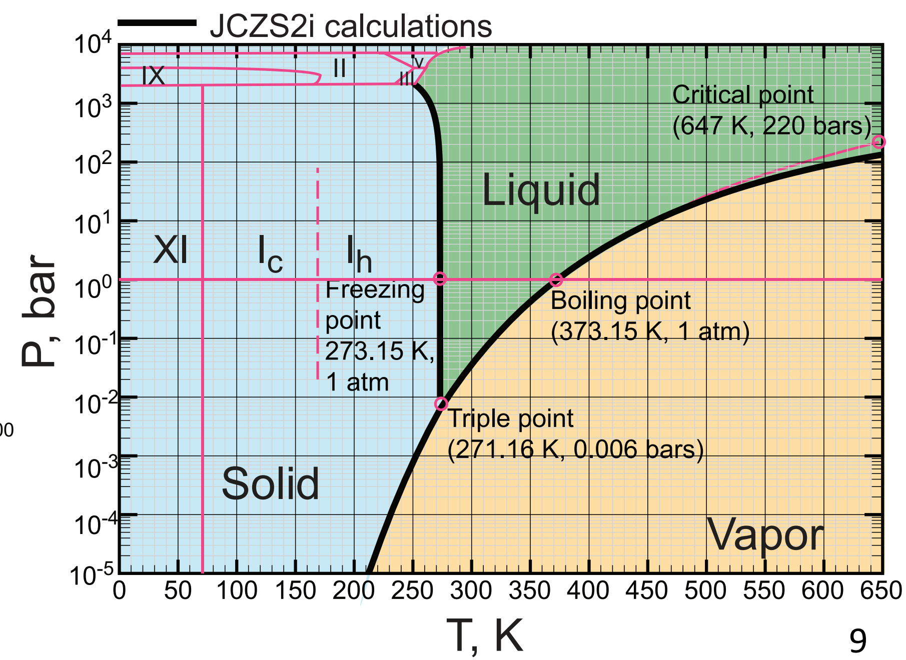






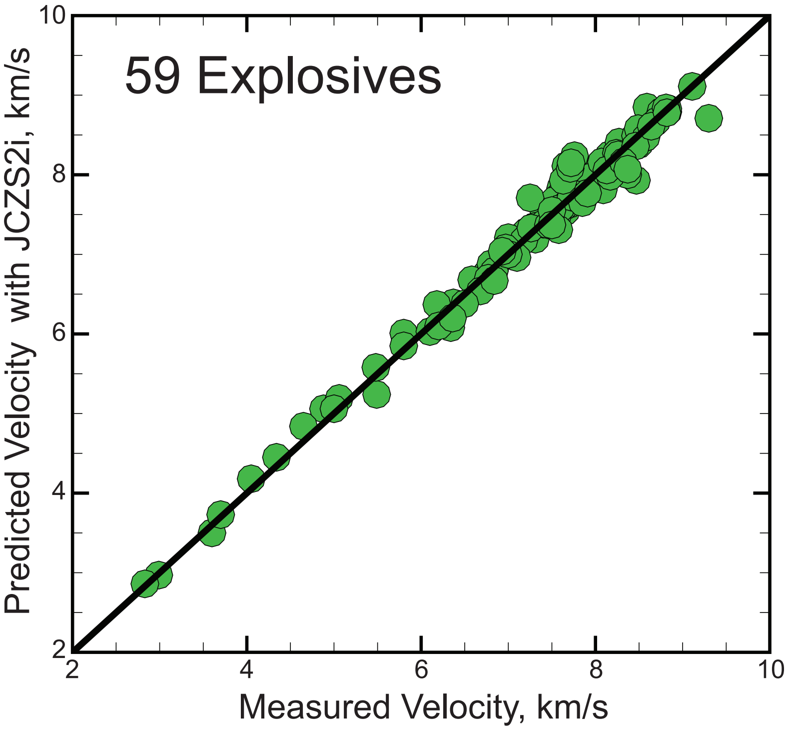


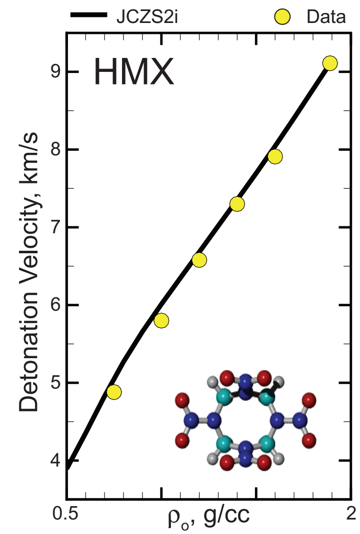


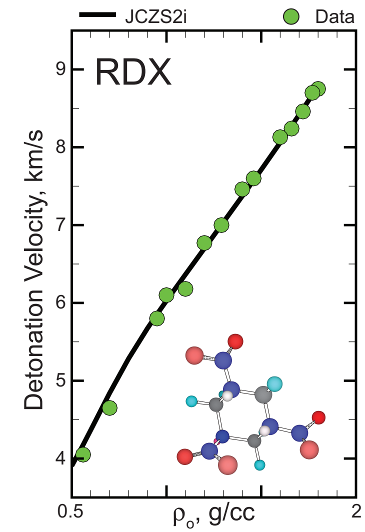


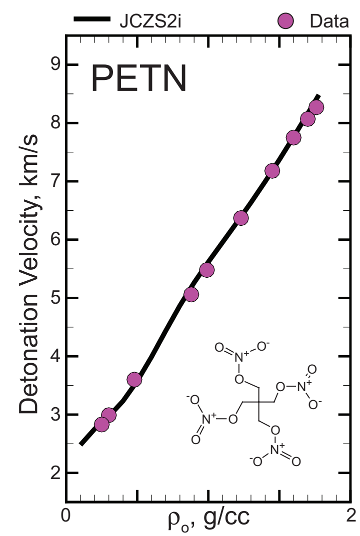
$$V = A + BT + CP\exp\left(1 - P / D\right)$$

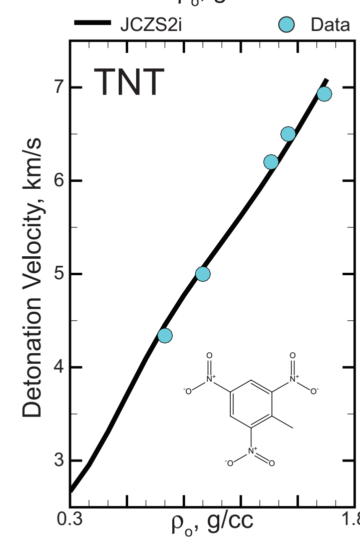
Detonation predictions











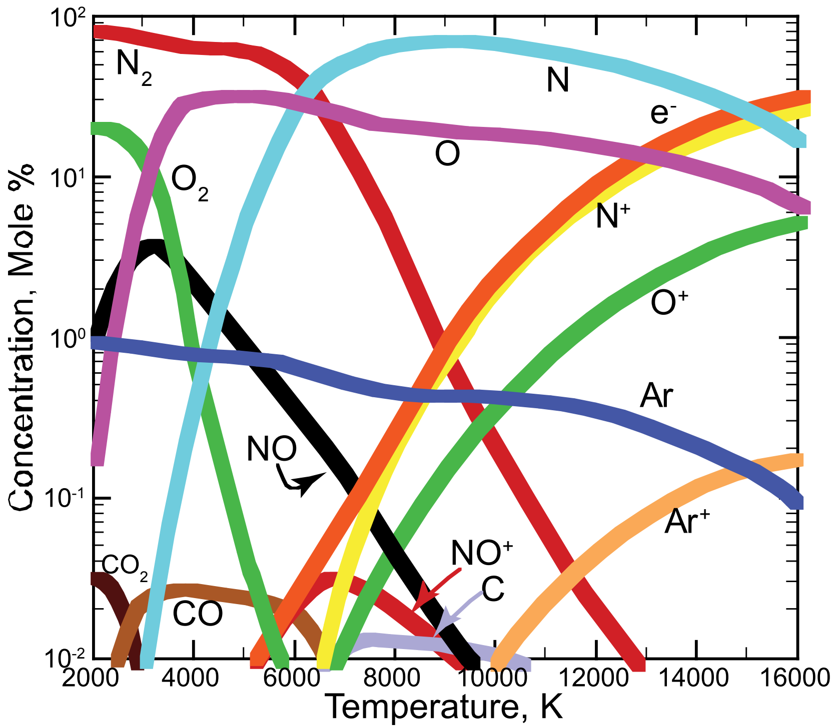
	Mean Absolute Error		RMS Error
JCZS[a]	1.76%		2.37%
Exp-6[b]	1.90%		2.51%
JCZS2i	1.73%	Awesome!	2.34%

[a]Hobbs, M. L., Baer, M. R., McGee, B. C., Propellants, Explosives, Pyrotechnics, 24, 269-279 (1999).
[b]Fried, L. E., Howard, W. M., Souers, P. C. 12th International Detonation Symposium, San Diego, CA p. 567 (2002)

Air at low pressure, high temperature (reentry)

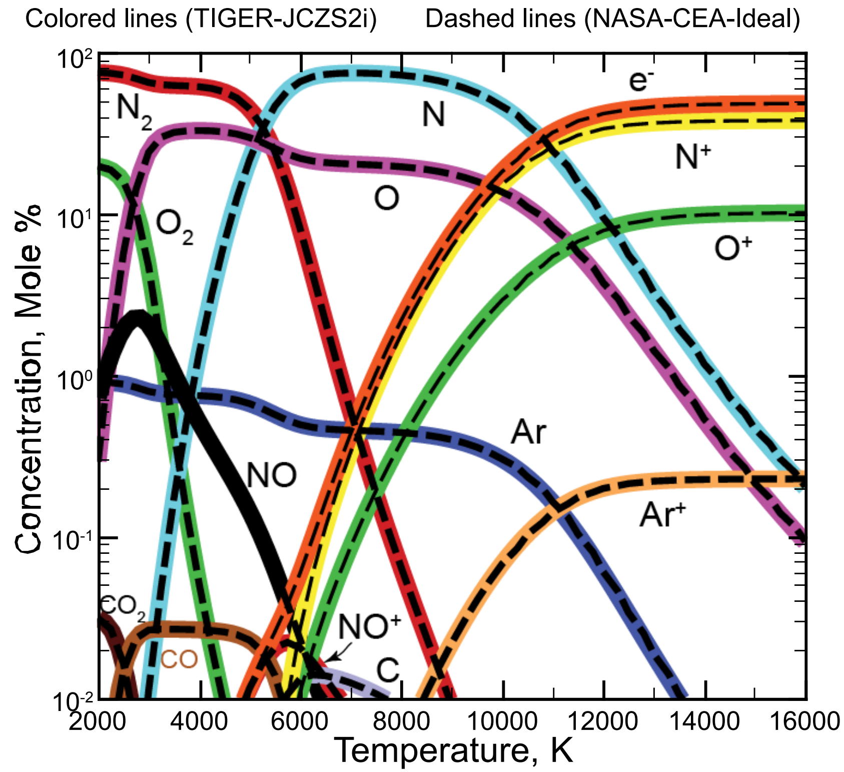
1950's

P = 0.01 atm, (Vincenti, Kruger, 1967)



Air at 0.01 atm

P = 0.01 atm, improved C_p

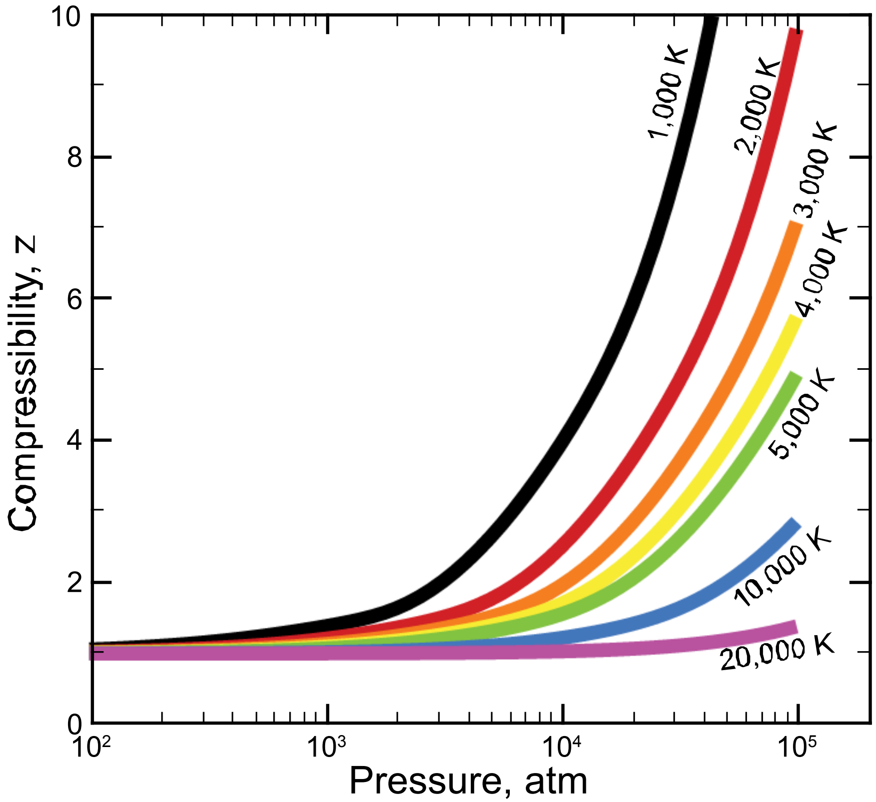


NASA-CEC and CTH-TIGER give same results at low pressure.

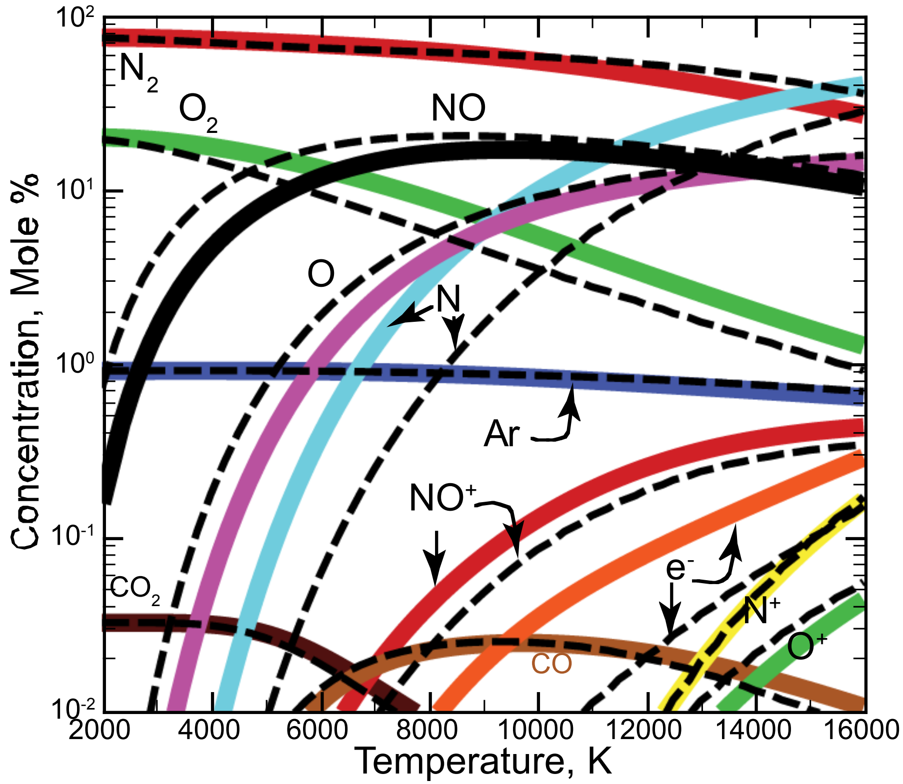
Air at high temperature and pressure

Sandia National Laboratories

Air Compressibility



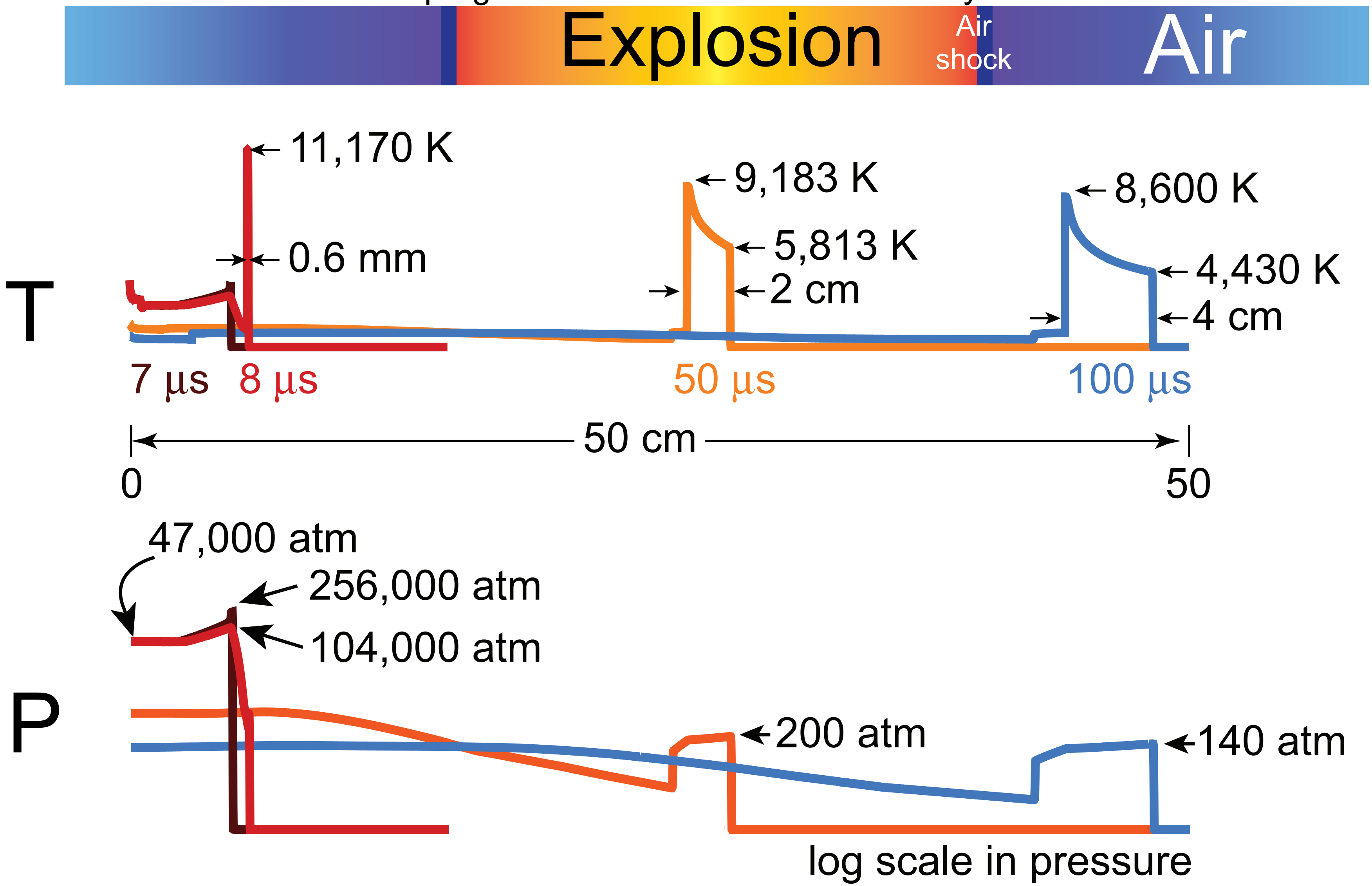
Air at 100,000 atm



*Debye-Hückel effect is negligible on air compressibility. Calculation from Hilsenrath J. and Klein M., National Bureau of Standards, Washington, D.C. (1965).

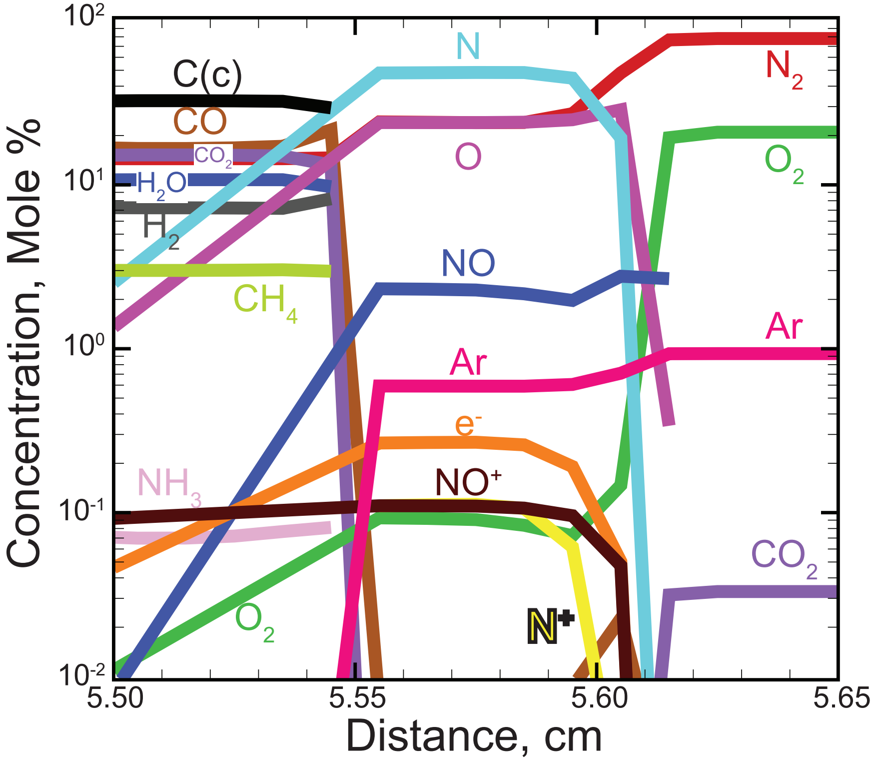
Air shock from TNT detonation

CTH programmed burn of a 5 cm radius cylinder.

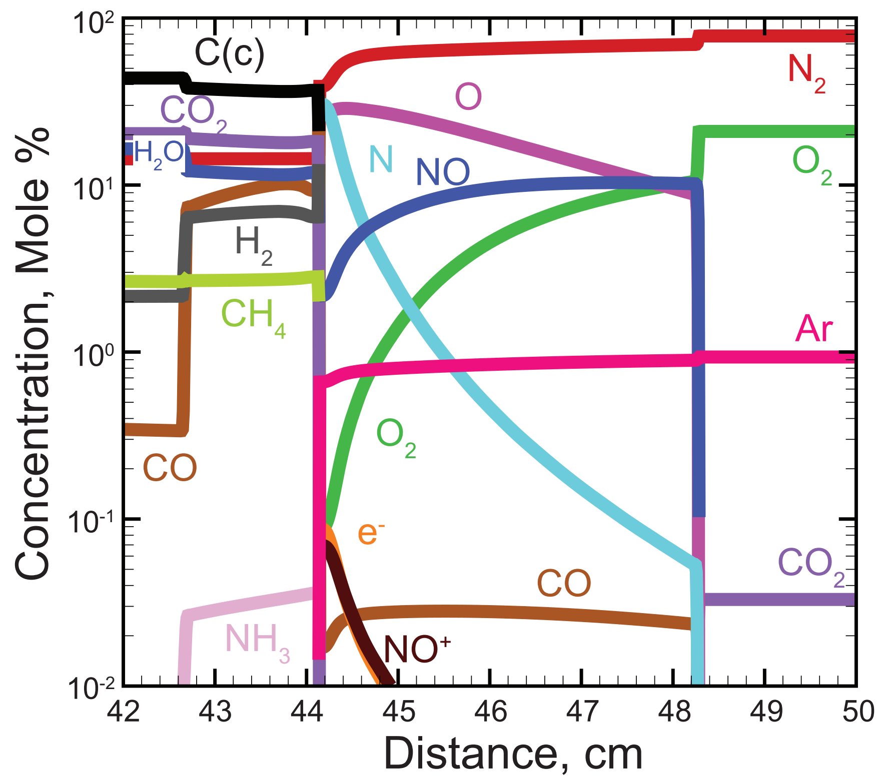


Edge of shock at 8 μs and 100 μs

8 μs



100 μs



CTH programmed burn with JCZS-EOS fit with CTH TIGER JWL fitter. Initial geometry is a 5 cm radius cylinder. Profiles plotted at 8 and 100 μs.

reflected wave | air shock | quiescent air

Summary and Conclusions

- New JCZS database was improved by incorporating piecewise specific heat fits of NASA's latest specific heat parameters.
- The new JCZS2i database considers over 200 ionic species, as well as a new condensed water equation of state.
- JCZS2i database gives accurate expansions to low pressure when liquid water is formed.
- JCZS2i database was used to calculate detonation velocity for 59 explosives are various densities with an mean absolute error of 1.76%.
- Air composition calculated at rarefied and high pressure conditions.
- Air shock created by detonation of TNT had temperatures as high as 11,000 K and contained ions and dissociated molecules.