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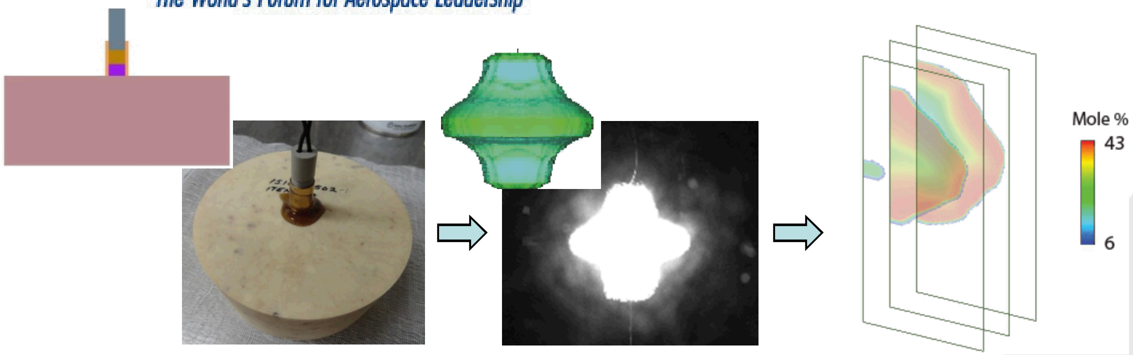

Prediction of Spatial Distributions of Equilibrium Product Species from High Explosive Blasts in Air

Aaron L. Brundage, S. Attaway, M. Hobbs, M. Kaneshige, L. Boye

Sandia National Laboratories

50th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, July 28-30, 2014, Cleveland, OH

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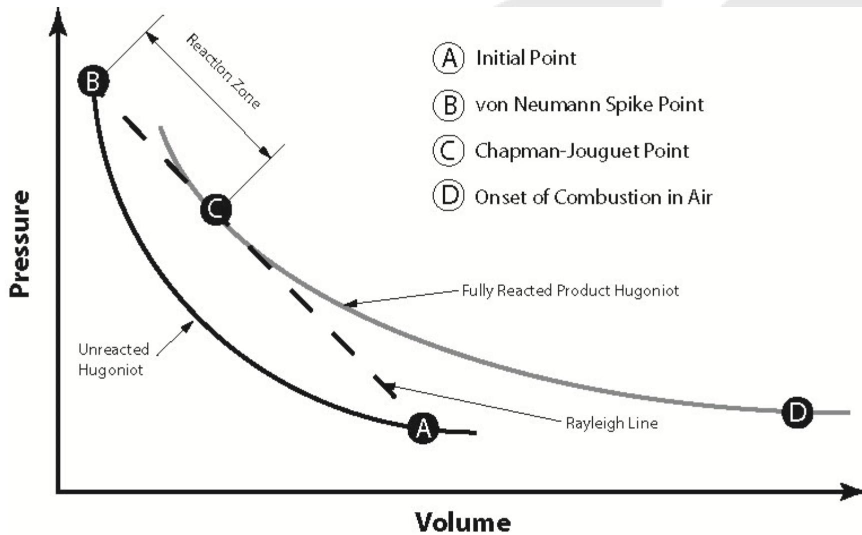
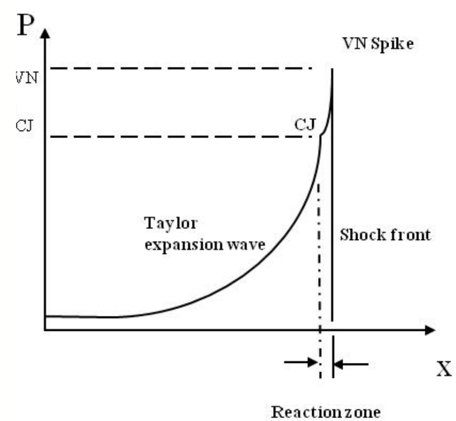
Applications

- Explosives safety
- DDT in Pulse Detonator Engines
- Shock impingement heating of re-entry vehicles and meteriods
- Afterburning in exhaust gases of jet engines, rockets, guided missiles

Process of Detonation on a *P-v* diagram

- Shock to detonation transition at early times
- Secondary combustion at late times



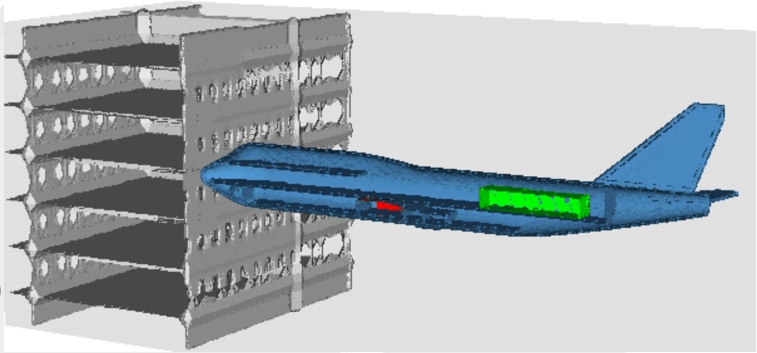


Detonation wave structure according to ZND theory

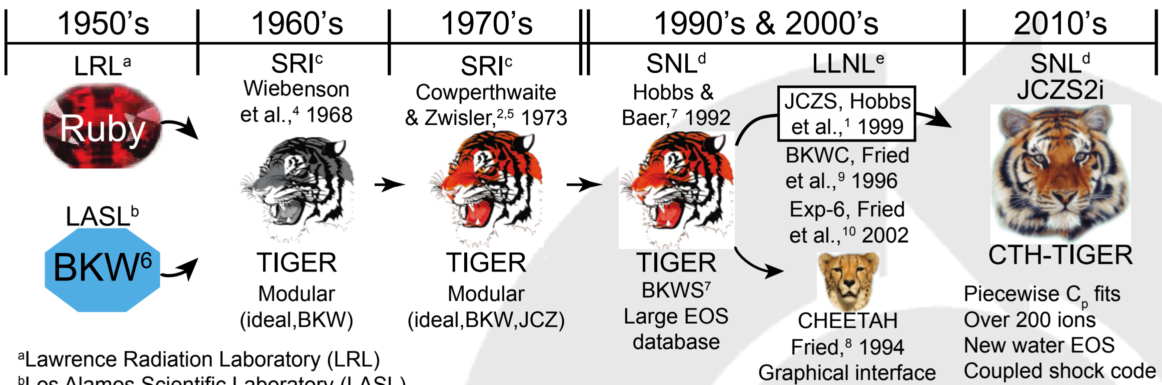
Unique methodology needed to transition from a detonation to a blast wave to a fireball

CTH: A Shock Physics Analysis Package

- Eulerian shock wave physics computer code solving *conservation equations* of mass, momentum, & energy for multimaterials (up to 98) including gases, fluids, solids, & reactive mixtures; *constitutive equations* (material behavior in elastic, plastic, and shock regimes); and *failure models*
  - Analytic & Tabular Equation-of-State representations
  - Advanced Strength & Fracture models
  - Adaptive Mesh Refinement
  - High Explosive models
  - Parallel and Serial platforms
- Applications (CTH licensed to many organizations)
  - large strain and/or high strain rate dynamics
  - multiphase interactions
  - examples include: high speed impact, blast-structural loads and deformations, armor/anti-armor, explosive detonation



TIGER: History of Development



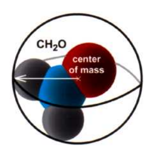
[a]Lawrence Radiation Laboratory (LRL)
[b]Los Alamos Scientific Laboratory (LASL)
[c]Stanford Research Institute (SRI)
[d]Sandia National Laboratories (SNL)
[e]Lawrence Livermore National Laboratory (LLNL)

JCZS2i has 1757 species: 490 condensed & 1267 gases with 189 ions.

- Thermochemical equilibrium codes are commonly used to compute EOS of explosive products, liquids or gases
- Solves thermodynamic equations between product species to find chemical equilibrium for a given pressure and temperature

BKWS - covolume based EOS

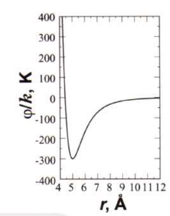
$$P = \frac{nRT}{V}\left(1 + Xe^{\beta X}\right), \quad X = \frac{\kappa \sum n_i k_i}{V(T+\theta)^{\alpha}}$$

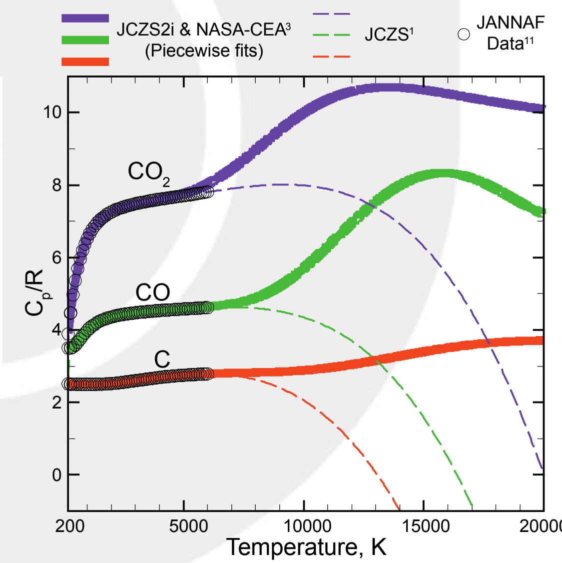


BKWS covolume based on rotation about center of mass

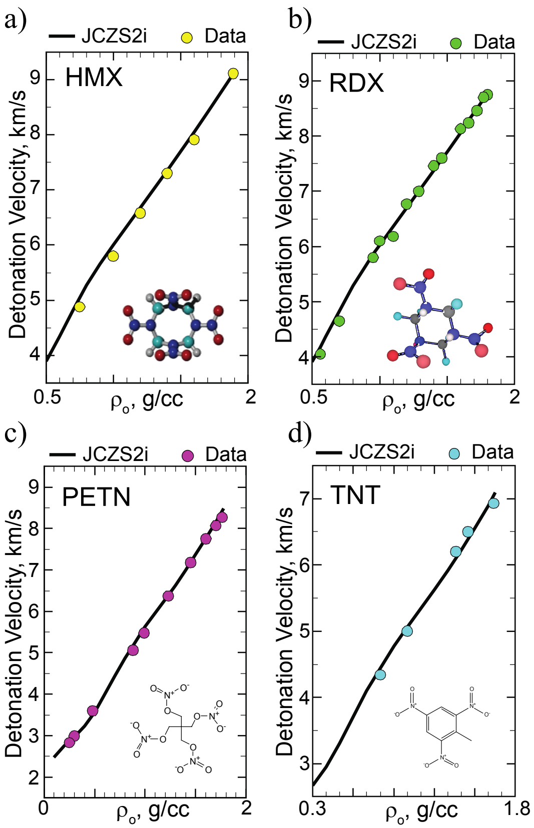
JCZS - intermolecular potential based EOS

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

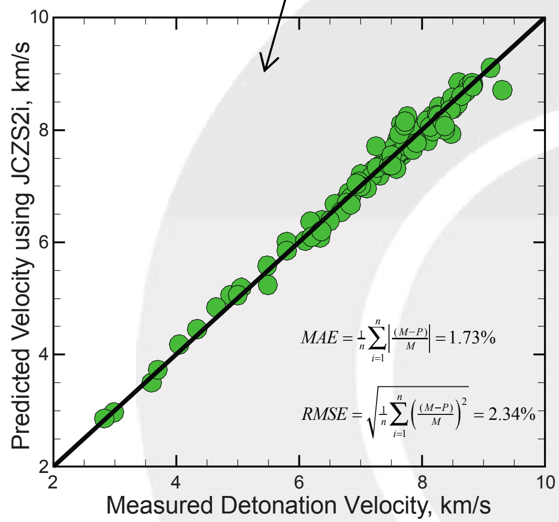




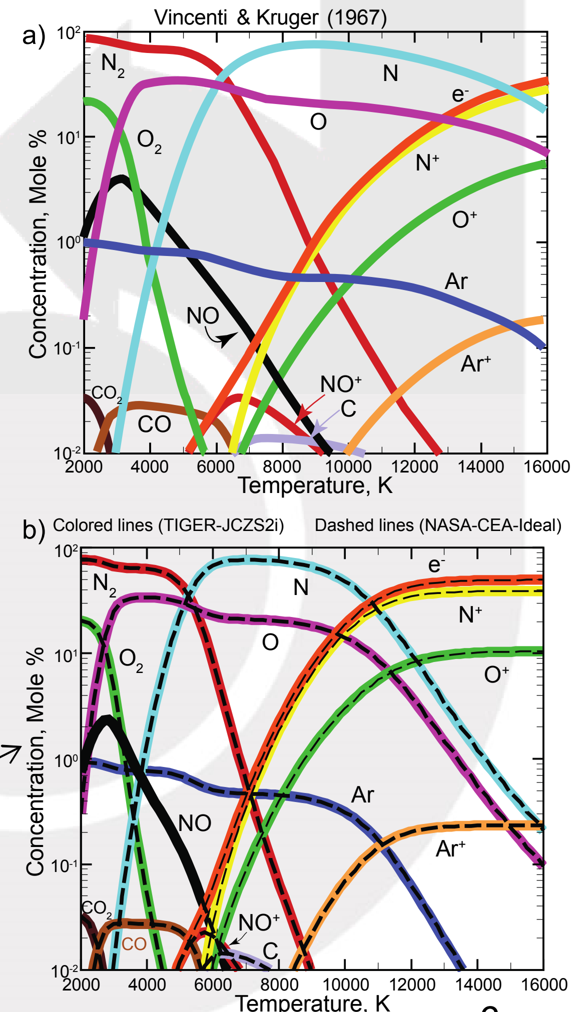
TIGER: Validation Studies



Predicted detonation velocities within 1.73% of data



JCZS2i and NASA-CEA nearly identical for composition of rarefied air at 0.01 atm, 2,000-16,000 K



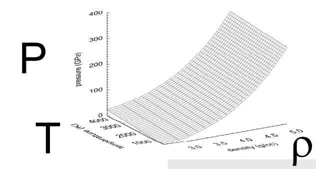
Hobbs, Brundage, Yarrington, 15th International Detonation Symposium, 2014

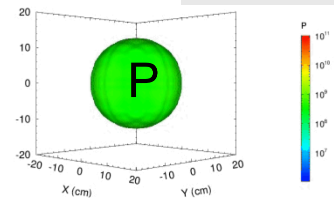
CTH-TIGER: Detonation to Deflagration Coupling

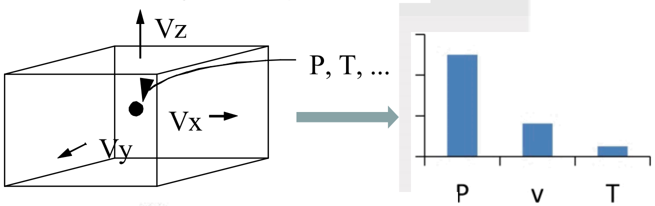
TIGER

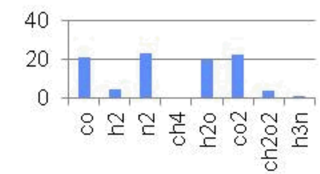
TIGER	1	Define EOS surface using SESAME format
CTH	2	Solve for flow field from detonation calculation
Tecplot 360™	3	Export field data at the center of each computational cell
TIGER	4	Compute equilibrium species concentration for each cell
Tecplot 360	5	Append species field data to previous Tecplot file
CFD	6	Initialize combustion fluid dynamics (CFD) code with species distribution at given thermodynamic state for each cell volume

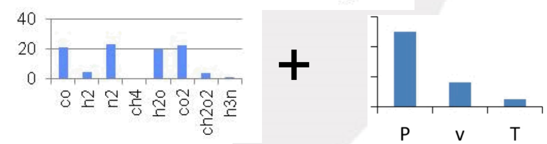
TIGER







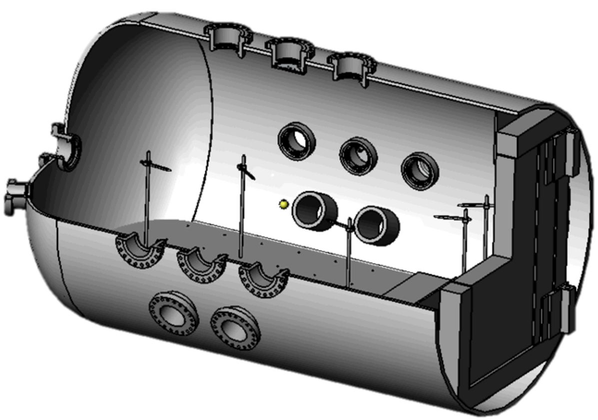


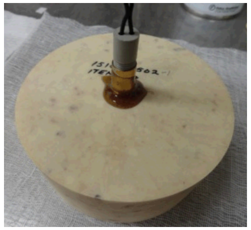


Blast Chamber Experiments and Results

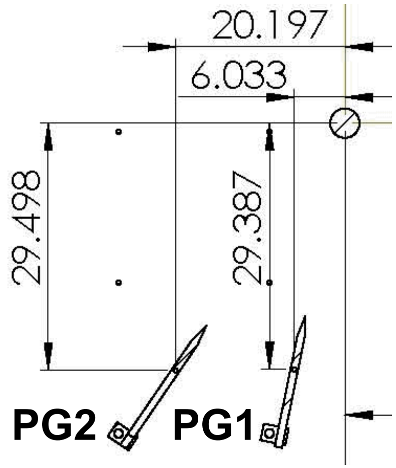
Explosive Components Facility
Test Chamber

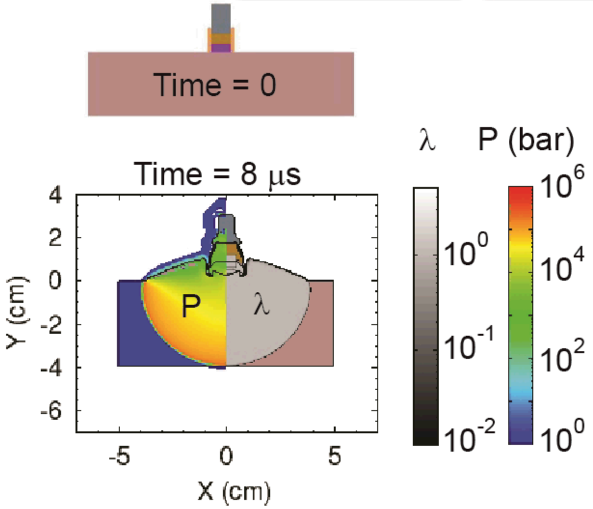
CTH Calculations and Experimental Results

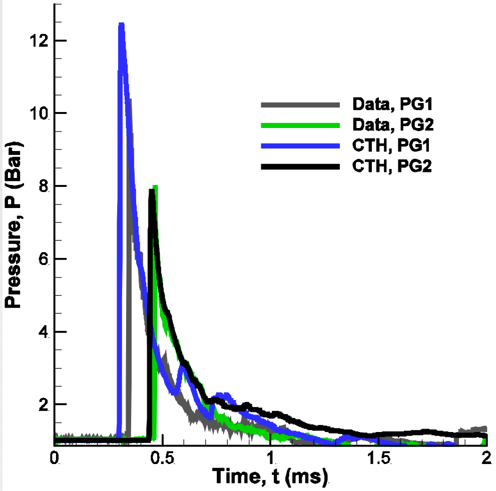


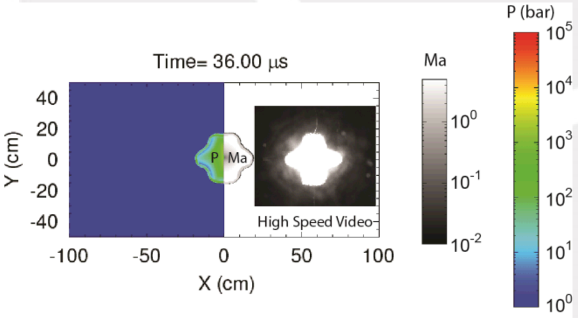


511 g TNT charge, 1.60-1.63 g/cc



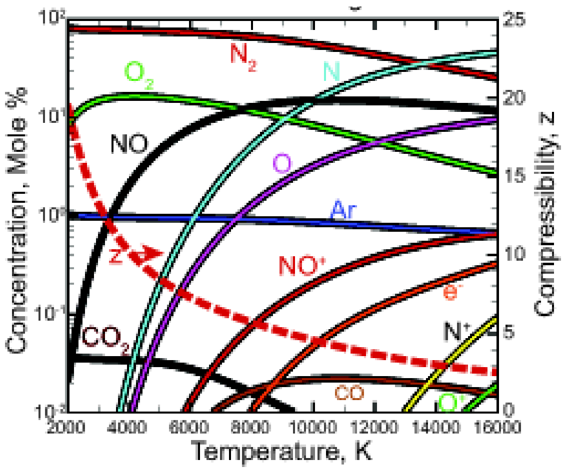






Good agreement between primary pressure pulse and gage data

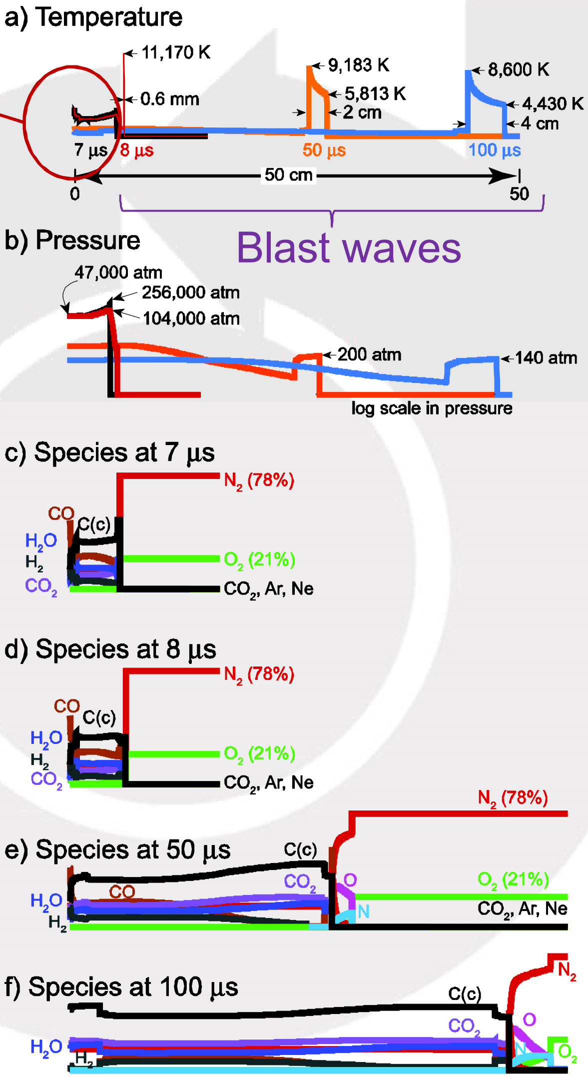
1D CTH-TIGER Predictions



Air composition at 250,000 atm as calculated with the JCZS2i-EOS

Detonation Wave

Detonation wave, air shock, and species concentrations up to 100 μs

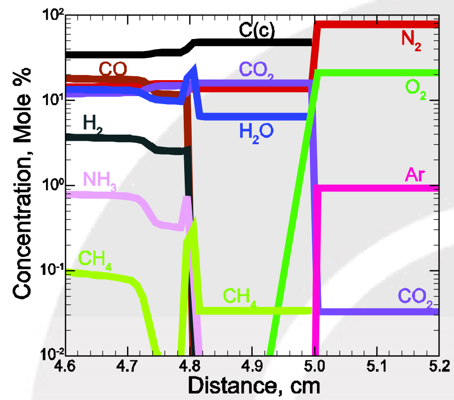


Species Profiles within Shock (1D CTH-TIGER)

Both dissociation and ionization predicted within thin air shock structures

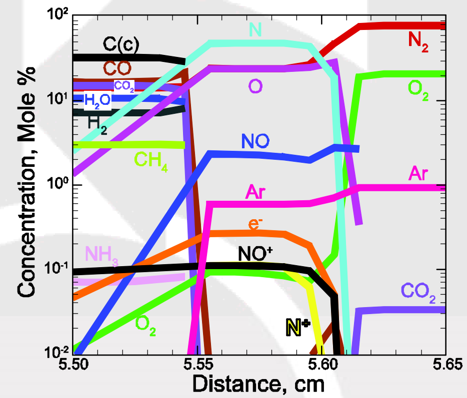
Detonation Wave

a) Edge of shock at 7 µs



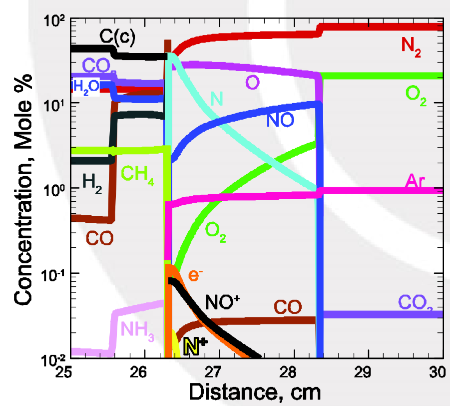
Blast wave

b) Edge of shock at 8 µs



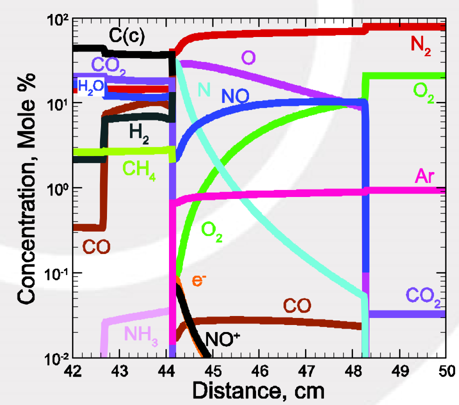
Blast wave

d) Edge of shock at 50 µs



Blast wave

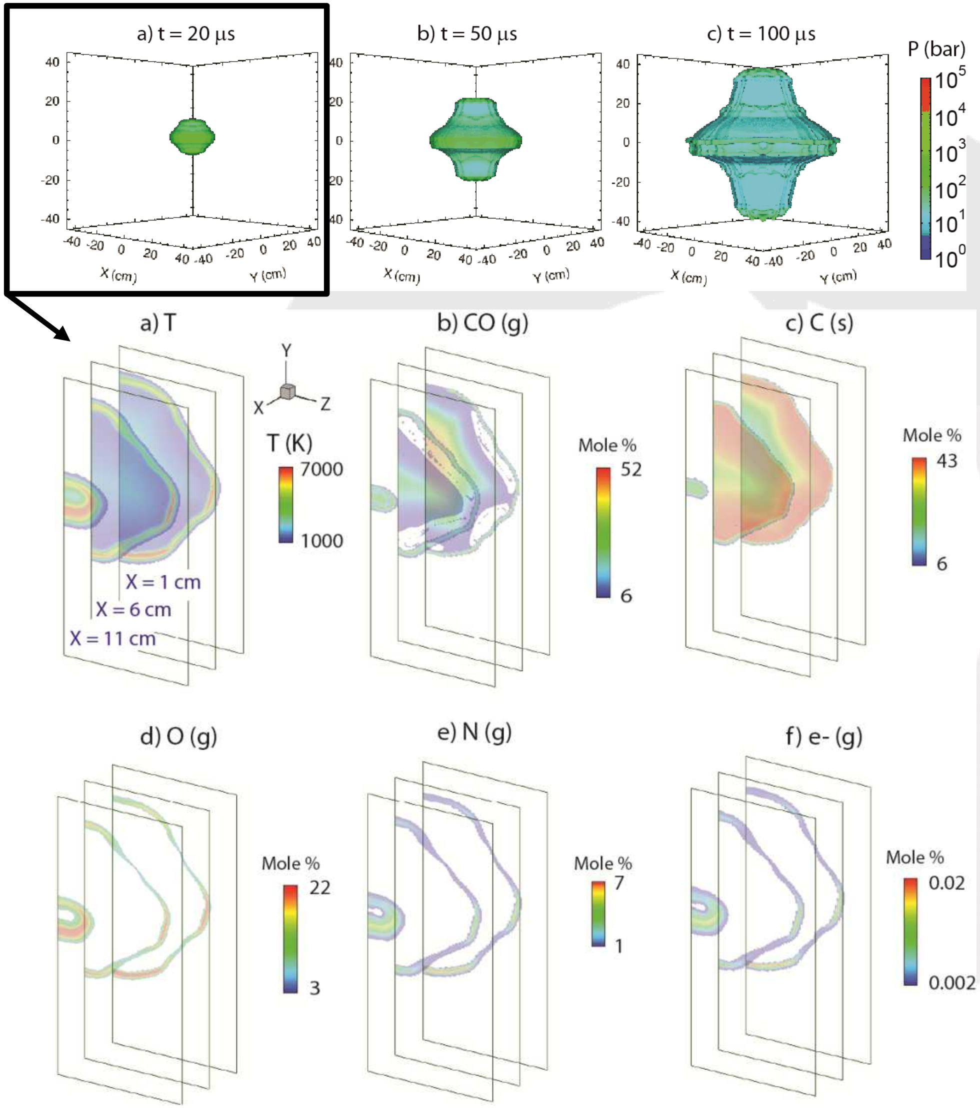
e) Edge of shock at 100 µs



3D CTH & CTH-TIGER Predictions

Complex blast wave structure predicted by CTH

Since CTH-TIGER does not model mixing within cells, appropriate time for handoff to be determined



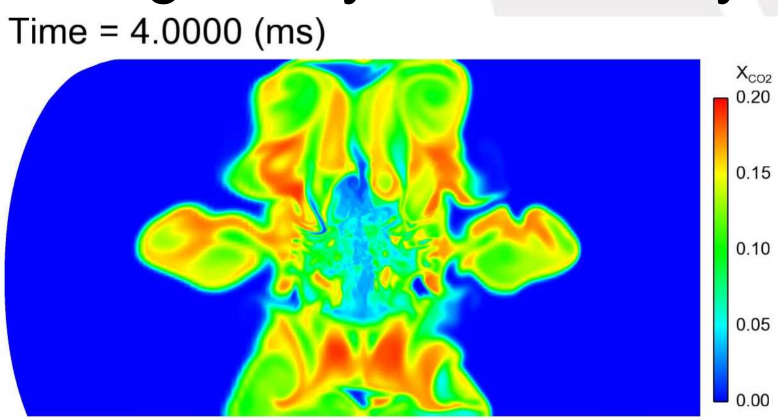
3D species profiles at 20 μs

Conclusions

- CTH-TIGER developed to transition from a detonation wave to an air shock
- Unburned species concentrations within a cell predicted at high temperature and pressure states
- Distribution molecules, atoms, and electrons predicted within thin shocks at early times
- Provides initial conditions for secondary combustion

Acknowledgements

- Gratefully acknowledge research collaboration with Combustion Research and Flow Technology, Inc. (CRAFT-Tech) –helped shape methodology and was end-user of these input files to predict afterburn
- Funding of 3 year effort by LDRD office



Combustion Research and Flow Technology, Inc.

Predicted afterburn at 4 ms

The World's Forum for Aerospace Leadership

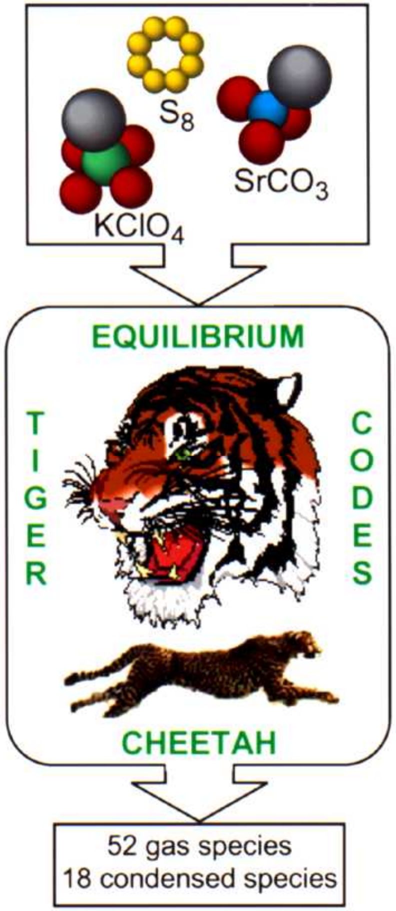
TIGER: A Thermochemical Equilibrium Code

Exotic reactants

- Composite explosives
- Pyrotechnics
- Balloechnics

Nonideal thermoequilibrium

- Point/Grid/Isoline
- Explosion/C-J/Hugoniot
- Thermal-elastic EOS
- Semi-empirical BKWS
- Intermolecular potential JCZ-3



Importance

- Many high energy reactants are composed of diverse compositions
- Predicting high and low pressure states requires a large number of species with an intermolecular potential based EOS models

State-of-the-art predictions

- Pure liquid shock Hugoniot
- Det. velocities for gas mixtures at high initial pressures (low to intermediate pressure regime)
- Det. velocities and pressures for condensed-phase explosives within 2% and 8% of measured values, respectively (high pressure regime)

Publications

- *Eleventh (International) Detonation Symp.*
- *Propellants, Explosives, and Pyrotechnics*