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Modeling Shock-Driven Reaction in Low Density PMDI Foam

Aaron Brundage, Scott Alexander, Bill Reinhart, David Peterson

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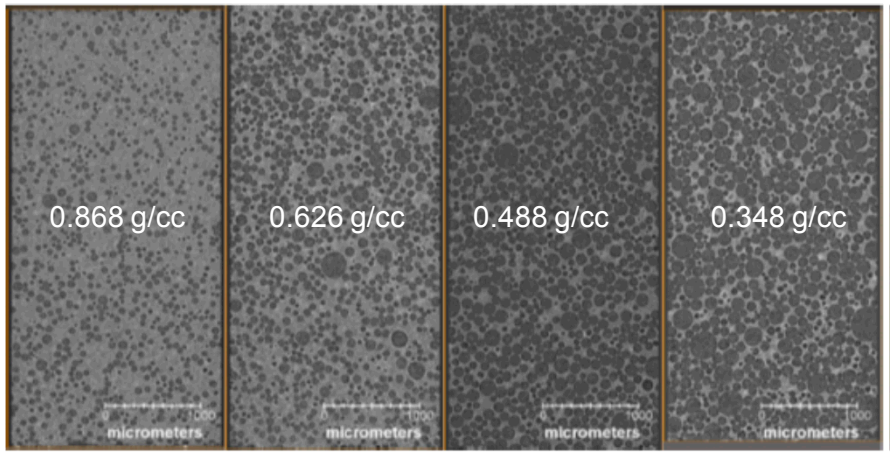
Introduction

- Polymeric foams ubiquitous in society and used in almost everything including packaging, insulation, cushioning
- Although a well-known engineering material, response is poorly understood under shock loading (aircraft, vehicles, sports equipment, etc.)
- Under impact pressures at or below 1 GPa, low-density foams (<0.1 g/cc or 6 pcf) can react and decompose
- Gap in literature on behavior of very low-density foams under shock impact (<0.1 g/cc or 6 pcf)

Foams have complex 3D morphologies

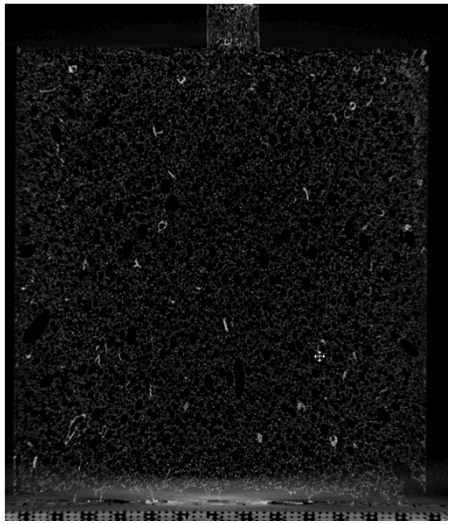
- Large foam samples rarely have uniform density
- Morphology changes considerably across wide density ranges
- Foams inherently multiphase—polymer matrix + gas (CO2,air?)

Closed cell?



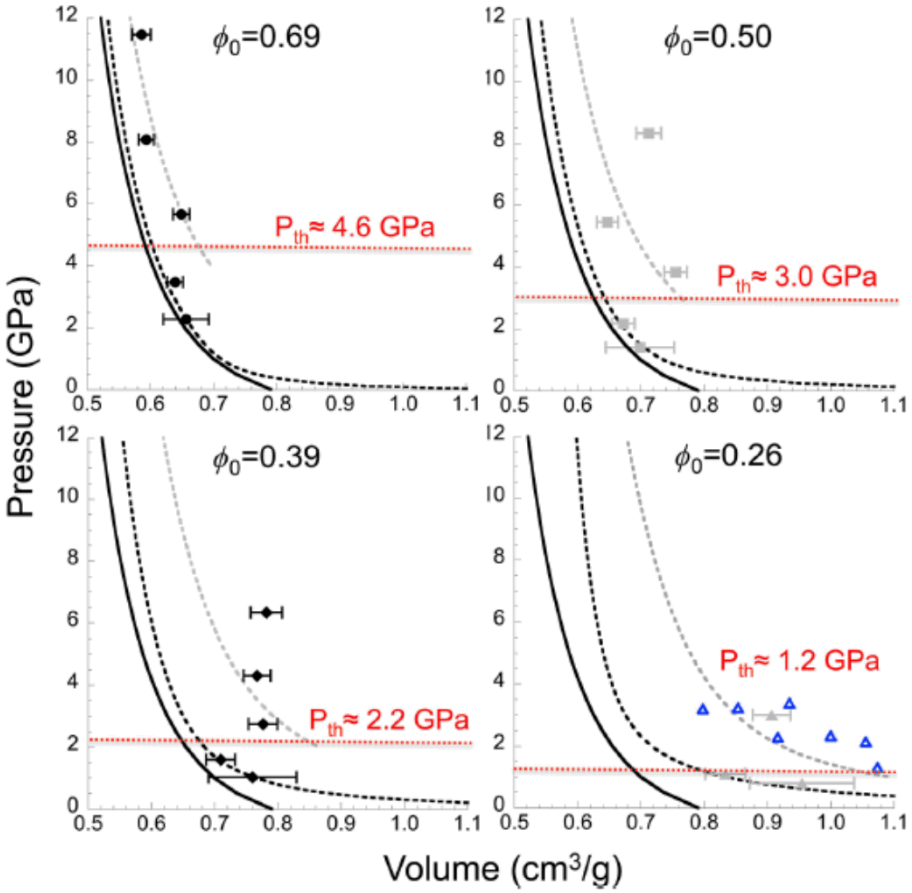
Dattelbaum *et al.*, JAP (2014)

Open-cell (ρ_0<6pcf)



- Present an approach that captures the response of these extremely heterogeneous samples to shock loading
- Includes response of composite behavior + polymer itself

Polyurethane foams decompose at low transition pressures under shock

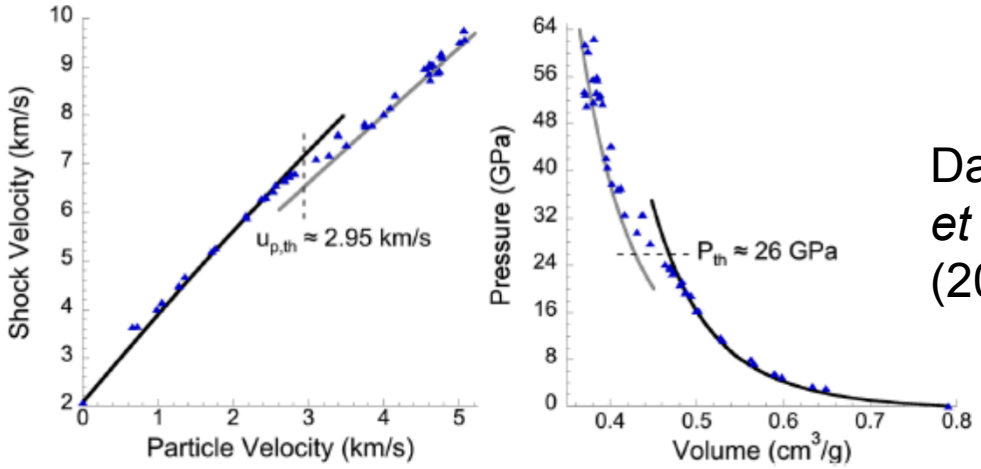


Dattelbaum *et al.*, JAP (2014)

- According to Dattelbaum et al., 2014, transition pressure scales with solid volume fraction
- Used different models to capture the inert response and compression of products (graphite or diamond)

Polymer decomposition at high pressures

- Polyurethane decomposes at high pressure
- According to Dattelbaum et al., 2014 transition occurs at 26 Gpa
- Used separate models to capture inert response and decomposition at high pressures



Dattelbaum *et al*., JAP (2014)

Single composite modeling approach developed for low density foams

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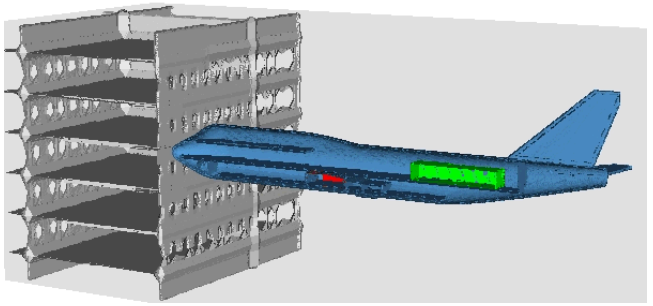
- Two-state Arrhenius Reactive Burn model adapted to foams
  - Inert: Mie-Gruneisen EOS with P-alpha model for foam compaction
  - Transition: Single-step Arrhenius kinetics with Distributed Activation Energy (new to CTH)
  - Decomposition: JCZS EOS in TIGER using same tabular EOS developed for solid PU high-pressure response
- Evidence of foam decomposition for in both legacy Marsh data and recent LANL data (Dattelbaum et al., 2014)
- Fill in gaps at low densities (<0.1 g/cc) by using recent STAR experiments for model validation
- Composite modeling approach needed to capture the complex response of three-dimensional structural materials having a PU matrix

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: A Thermochemical Equilibrium Code

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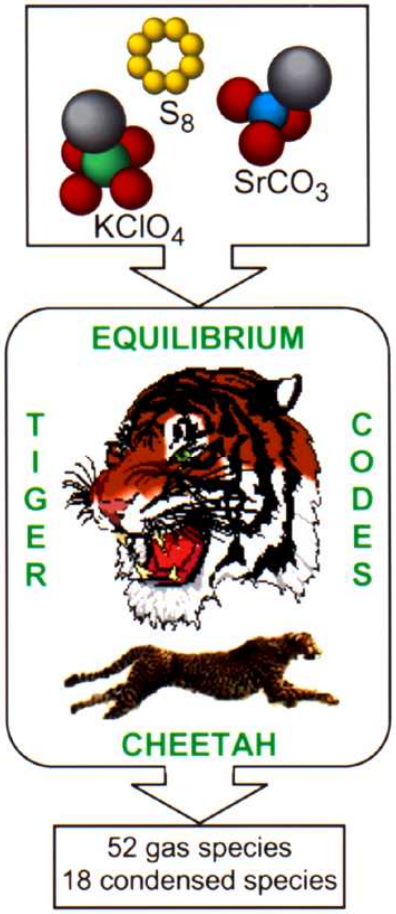
Exotic reactants

- 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

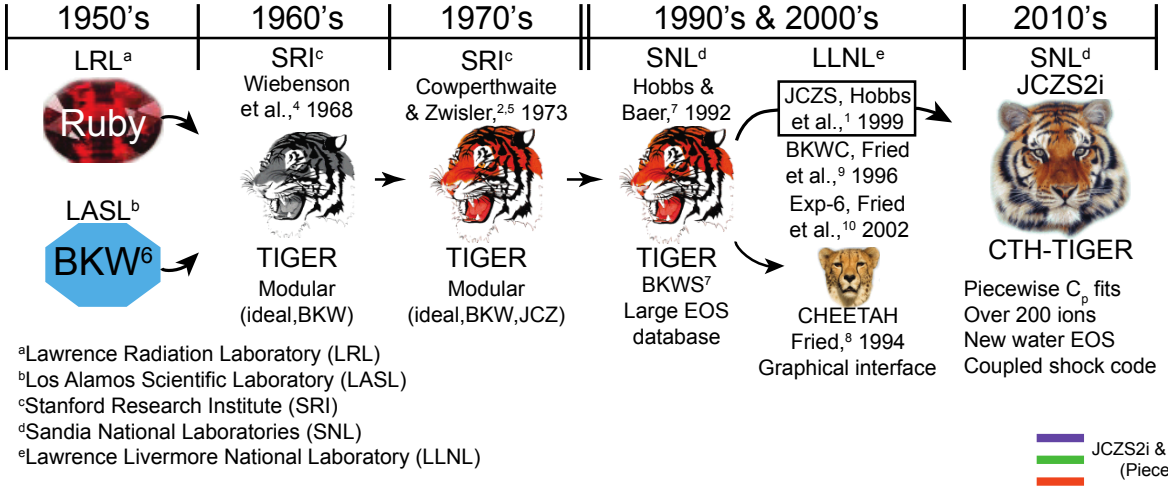
State-of-the-art predictions

- 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*

TIGER: History of Development



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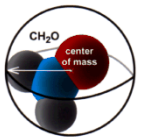
JCZS2i has 1757 species: 490 condensed & 1267 gases with 189 ions.

- 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

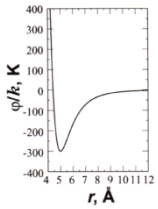
$$P = \frac{nRT}{V}(1 + Xe^{\beta X}), \quad X = \frac{\kappa \sum n_i k_i}{V(T+\theta)^{\alpha}}$$

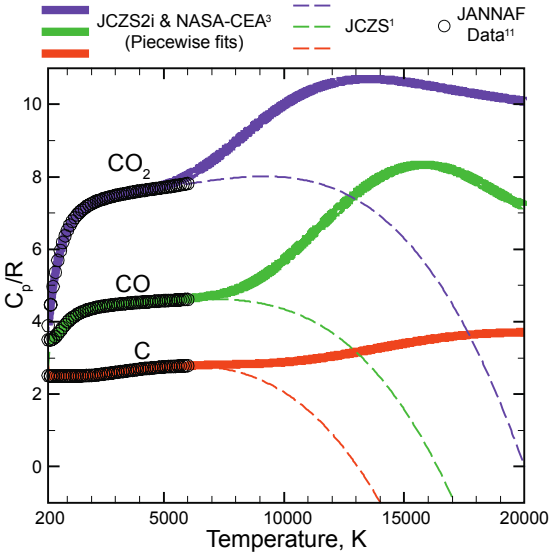


BKWS covolume based on rotation about center of mass

JCZS - intermolecular potential based EOS

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





Gas Gun Data Reduction to Find Experimental Properties of Solid Matrix

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Known: *Bulk properties from gas gun experiments [ρ, P, u, ϕ_{s0}, ρ_{s0}]*

Find: *Properties of solid matrix using conservation equations [p_s, ϕ_s, ρ_s]*

Hugoniot Jump Conditions: Cons. of Mass and Momentum across a shock in PU ***foam***

$$\rho_s \phi_s \left(U_c - u\right) = \rho_{s0} \phi_{s0} U_c$$

$$P = \rho_{s0} \phi_{s0} u U_c$$

Crystalline density from P-ρ **Hugoniot** for ***PU at TMD***

$$p_s = \rho_{s0} \varepsilon C_s^2 \left/ \left[1 - s\varepsilon\right]^2 \right. \quad \varepsilon = 1 - \rho_{s0} / \rho_s$$

Density and pressure in the solid matrix

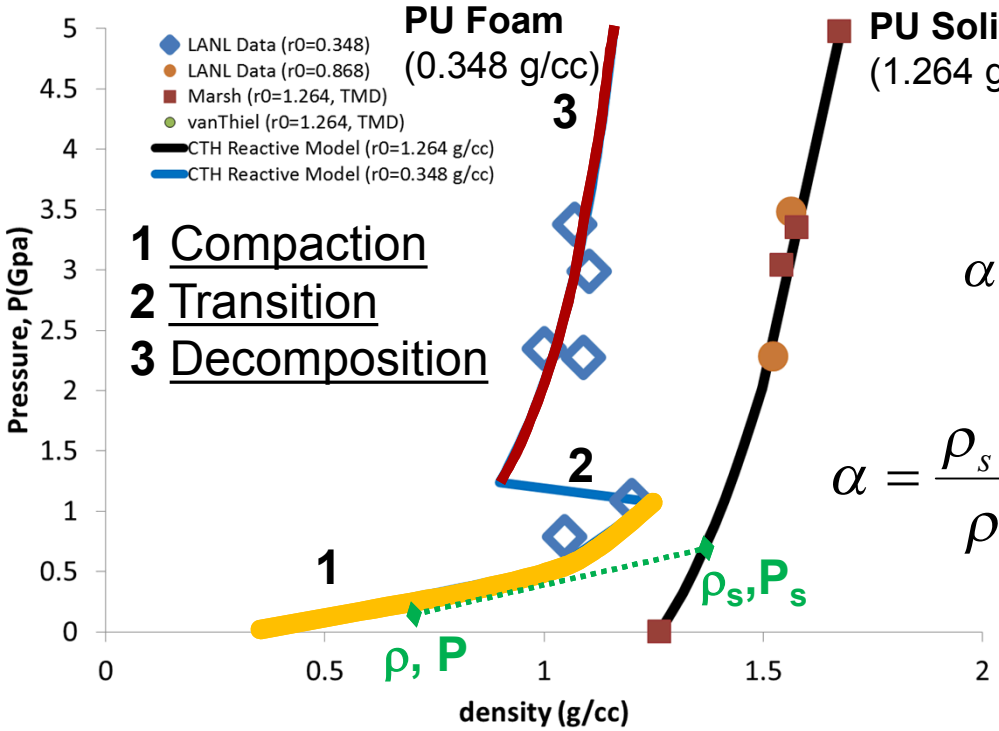
$$p_s = P / \phi_s \quad \rho_s = \rho / \phi_s$$

Distension parameter

$$\alpha = 1 / \phi_s$$

Equilibrium stress calculations solved algebraically

P-α Compaction Model to Describe Removal of Void in CTH for Foam



P-α Compaction Relationship

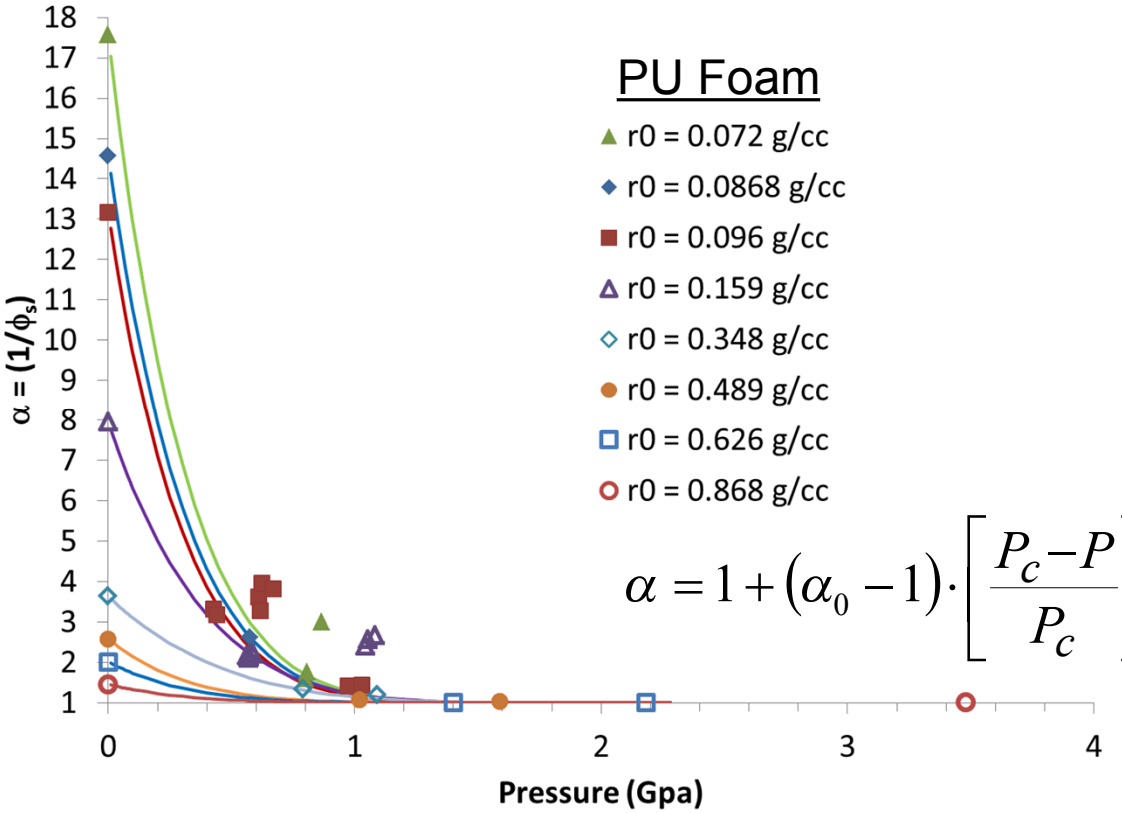
$$\alpha = 1 + (\alpha_0 - 1)\cdot\left[\frac{P_c - P}{P_c}\right]^n \quad for\ P < P_c$$

$$\alpha = \frac{\rho_s(P_s, E_s)}{\rho(P, E)} = \frac{\rho_s(P\alpha, E)}{\rho(P, E)}$$

Solid computed from Mie-Gruneisen EOS

- Compaction relationship modified in CTH with general power law for applicability beyond metal foams
- Low-density PU foams react under shock loading before achieving full compaction

Distension (α) determined from experimental data



$$\alpha = 1 + (\alpha_0 - 1) \cdot \left[\frac{P_c - P}{P_c} \right]^n \quad for\ P < P_c$$

- Distension parameter calculated experimentally from shock Hugoniot data (Marsh, Dattelbaum, Alexander, Reinhart)
- An exponent of 7.3 generally required to fit most of this data

Transition from unreacted to reacted state with modified Arrhenius kinetics

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Two-state model with Arrhenius kinetics

$$P(\rho,T,\lambda) = (1-\lambda)P_i(\rho,T) + \lambda P_f(\rho,T)$$

$$E(\rho,T,\lambda) = (1-\lambda)E_i(\rho,T) + \lambda E_f(\rho,T)$$

$$\frac{d\lambda}{dt} = (A + z\sigma)(1-\lambda)e^{-\theta/T}$$

Nomenclature

λ	extent of reaction
i,f	initial/final states
A	frequency factor
θ	activation temperature
σ	standard deviation
z	ordinate of CDF

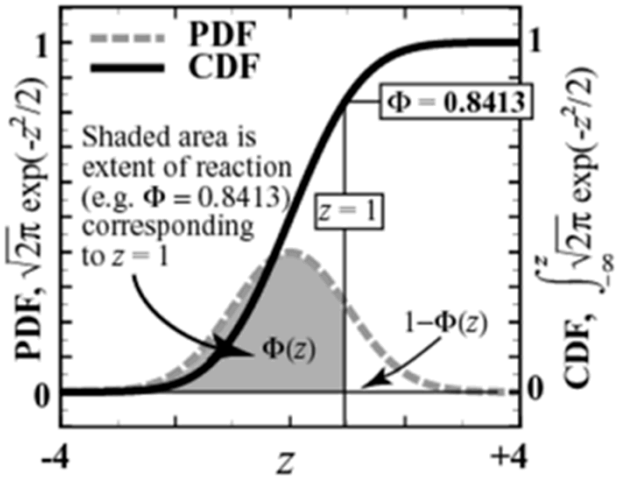
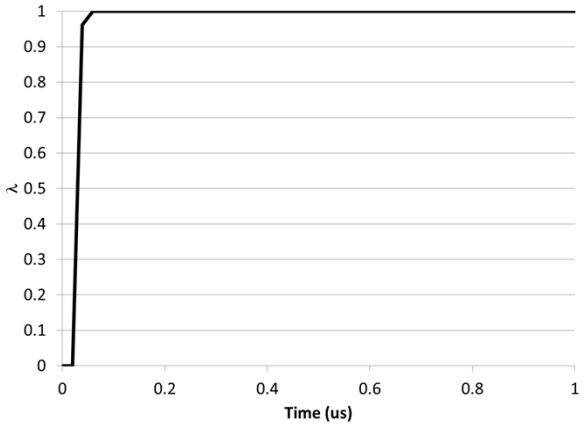


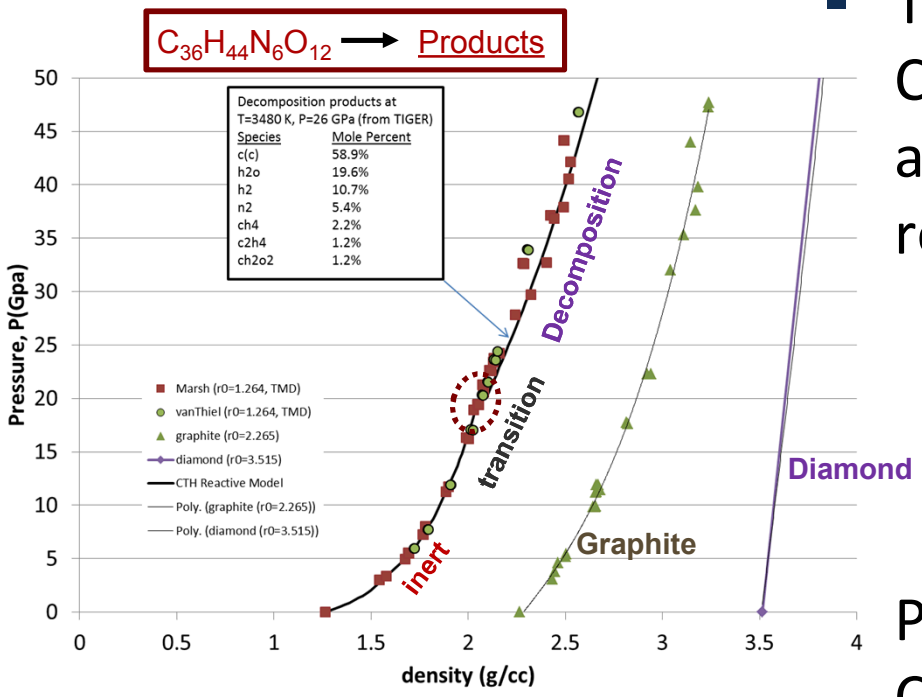
Fig. 3.3. Cumulative distribution function of a standardized normal random variable.

Hobbs & Lemmon, 2004



- One step reaction kinetics using Arrhenius Reactive Burn model in CTH
- Coalescence of hot spots in shock-heated foams initiate reaction
- To represent complex reaction mechanisms in foam, modified activation energy by applying a normal distribution of states

Composite modeling approach developed to capture PU reaction

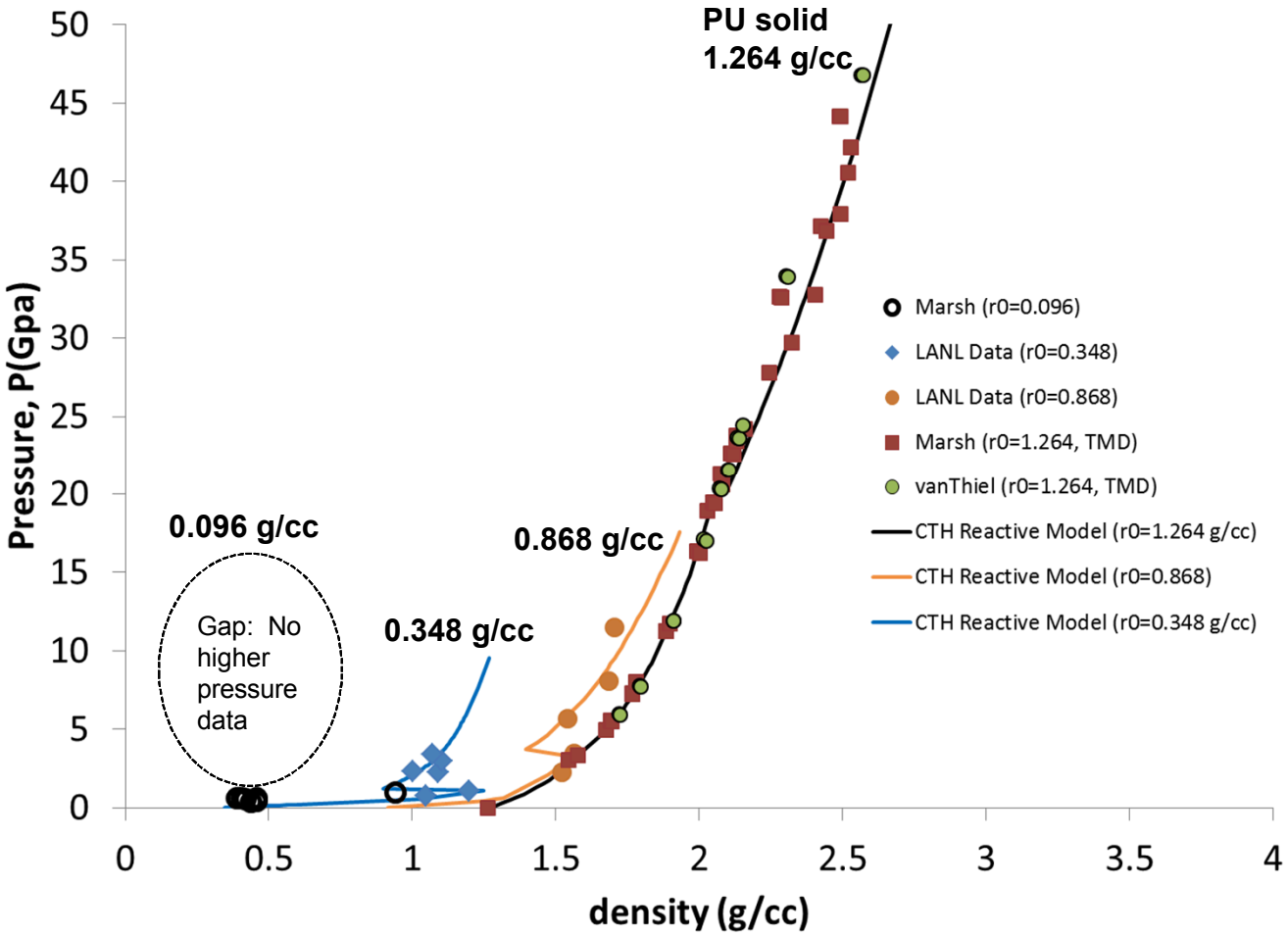


- Two-state reactive burn model in CTH using Arrhenius kinetics adapted for PU captures three regimes:
  - Inert: Mie-Gruneisen EOS
  - Transition: Single Step Arrhenius kinetics
  - Decomposition: JCZS2 EOS in TIGER

Product species mostly solid Carbon (60%) and gas

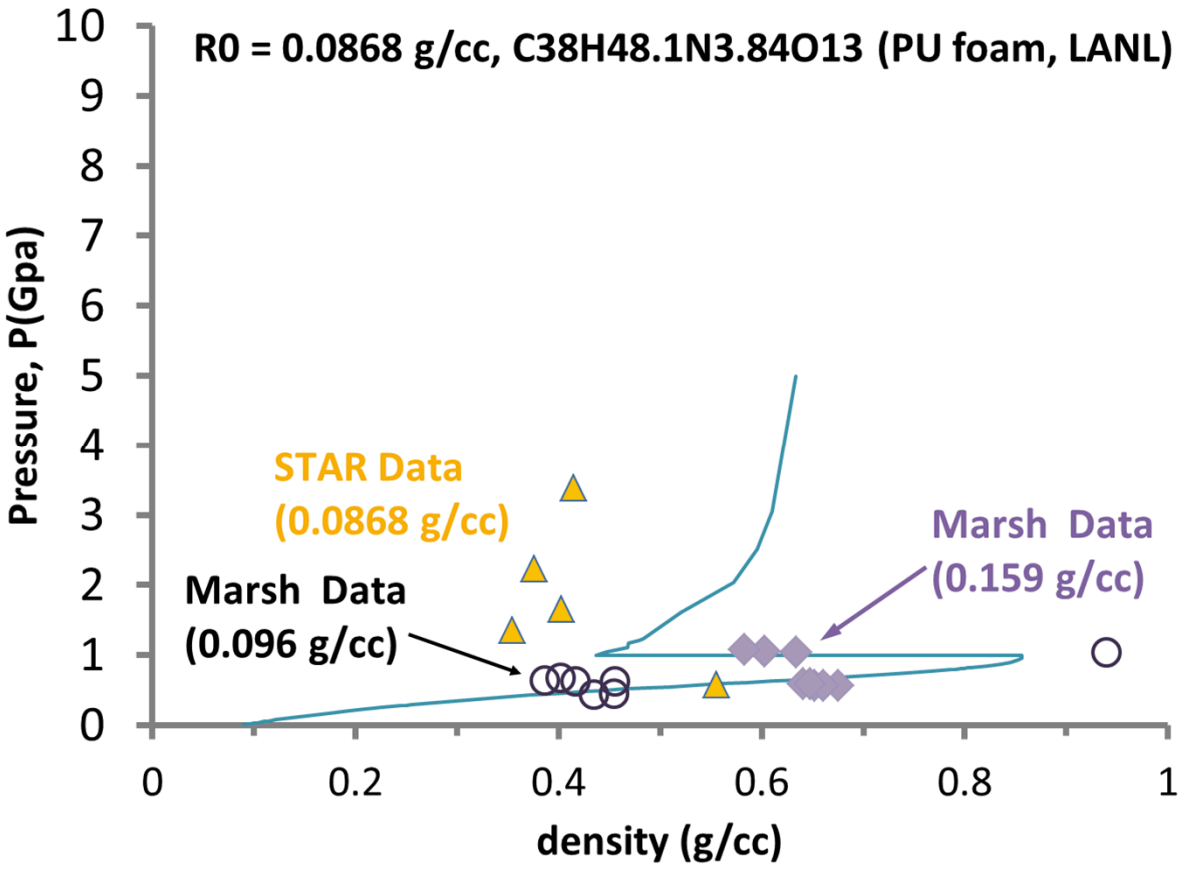
- Amount of carbon predicted compares well with LANL, although form of carbon not specified by JCZS EOS

CTH Reactive foam models predict legacy Marsh data for PU foam



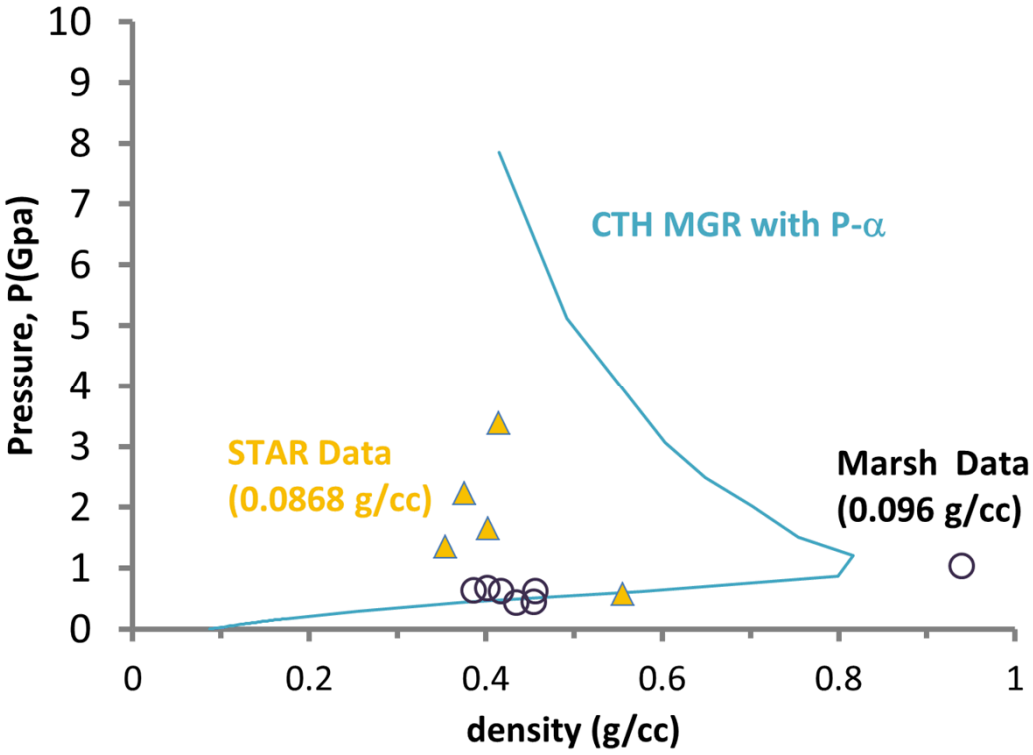
- Approach works well for available foam data with high pressure decomposition response (> 0.3 g/cc)
- No high pressure data available at very low densities below 0.1 g/cc

Reactive foam models for 0.0868 g/cc PU foam with Distributed Activation E.



- Foam decomposition model predicts compaction in all foams, and reaction at higher densities, but more work needed to predict highly distended foams at 0.0868 g/cc
- Originally used product stoichiometry from **solid** PU
- Stoichiometry of PU **foam** different than PU **solid**, as obtained from KCP measurements reported by LANL

Mie-Gruneisen w/P-alpha model traditional approach in CTH for modeling porous crush



- P-α compaction model captures inert response of foam
- Shock heating causes significant volume expansion
- Traditional MGR/P-α approach assumes material remains a solid and insufficient for predicting foam decomposition to gaseous products
- Traditional method inadequate for predicting response of highly distended foams