RECENT DEVELOPMENTS IN DETONATION MODELING – CONDENSED PHASE MEDIA

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Gas Phase vs Condensed Phase Detonations

- simple thermodynamics
- cell structure can be measured
- role of turbulence
- no mass transfer control
- near CJ conditions

- supercritical fluids
- heterogeneity, hot spot control
- VOD < VOD_{CJ}
- limited characterization
- pronounced shock front curvature

Condensed Phase Detonations

- mining, quarrying, seismic applications
- demolition, tunneling
- safety eg FCMO, transport
- defence
- security & improvised devices

Modeling of the Detonation (and Rarefaction) Processes for Commercial (Non-Ideal, heterogeneous) Explosives in Rock

- Simple Theoretical Approach
- Validation using AMR Finite Volume code

Pressure History at Detonation Product – Rock Interface for Shock, Detonation (and Rarefaction)

Ammonium Nitrate Based Bulk Explosives – ANFO, Emulsions

- Heterogeneous, gas sensitized

  eg separate oil and oxidiser phases
  porous prill, chemical gassing

- Large critical diameter (detonation) & VOD < Ideal VOD

  ex critical diameter > 30 mms
  reaction zone (DDZ) > 10 mms

- Limited characterization studies for most explosives

Typically, unconfined VOD vs charge diameter
Density and thermodynamic parameters
Limited Shock Front Curvature data (unconfined)
Particle, droplet size distributions

Confinement – Rock

Compression, crack propagation,fragmentation and muckpile formation

- Non-isotropic
- Variable properties – strength, composition, density
- Acoustic velocity < VOD – This study

Detonation

- Steady state , axisymmetric
- Homogeneous media
- Simple EoS, thermodynamics and rate law for both the explosive, detonation products and confinement
- Detonation Velocity greater than sound speed of confining media

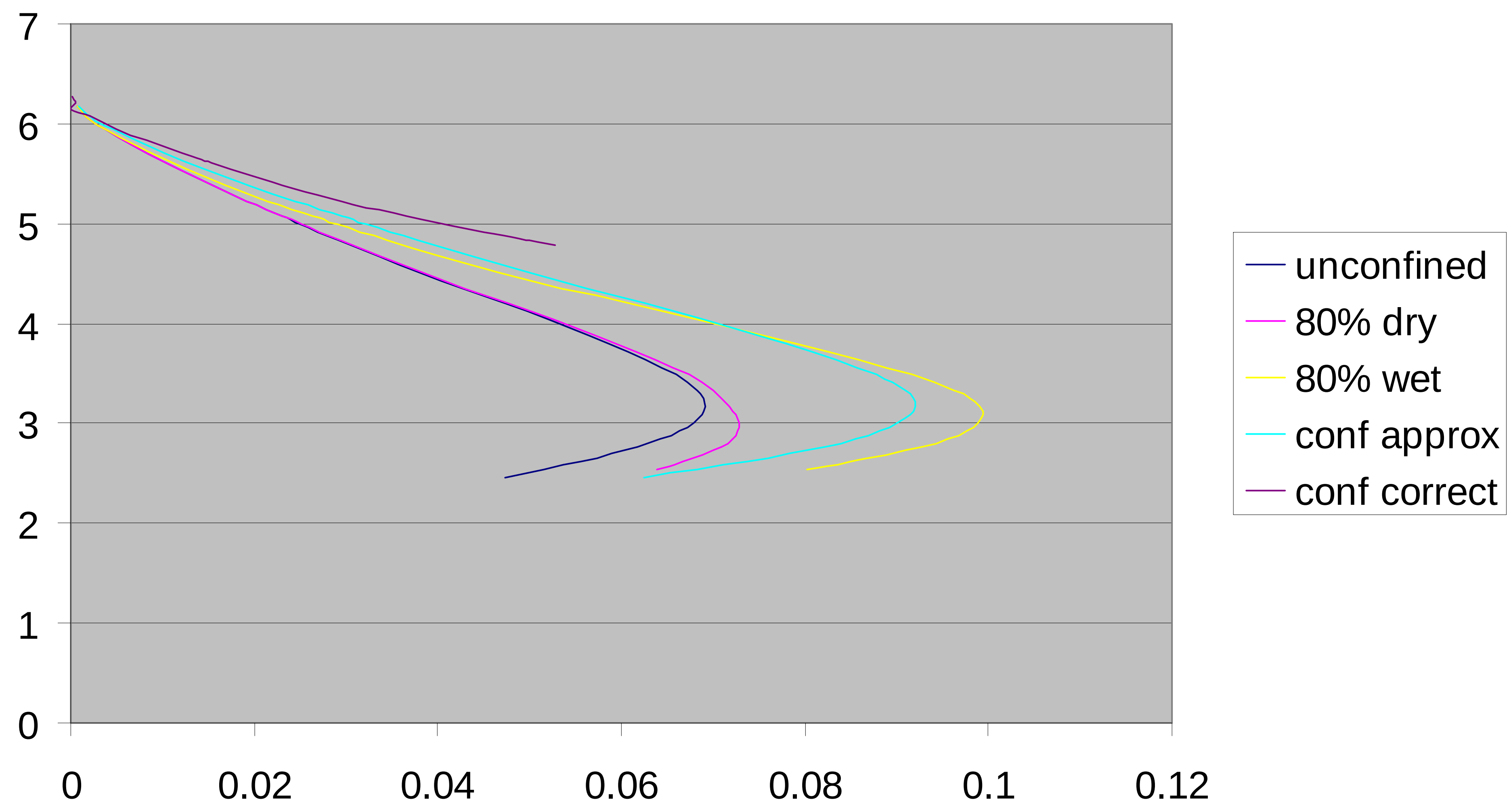
nb major aim of this work is to ascertain where fluid mechanics approximations in quasi-1-D theories are valid – therefore not a test for EoS or thermodynamics

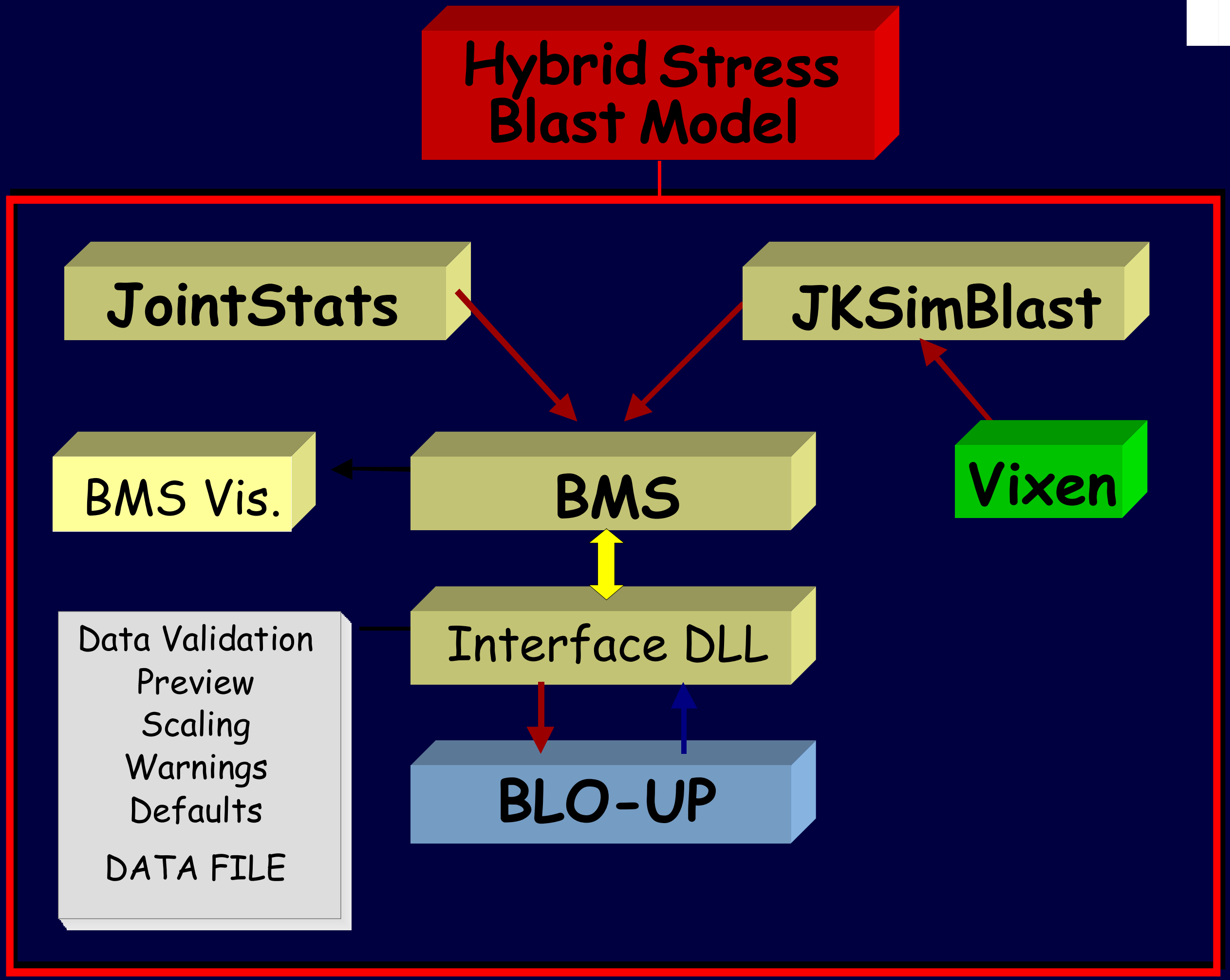
(i) Are the fluid dynamics in a quasi-one dimensional theory adequate to approximately describe the detonation process for central axis and product-confinement interface in the context of rock blasting ?

(ii) What resolution is required in a finite volume computer simulation study such that the DDZ predictions are invariant with grid size ?

(iii) Is some order of DSD theory as opposed to Wood Kirkwood slightly divergent flow appropriate to the rock blasting problem ?

Plot of VOD (km/s) vs inverse diameter (1/mm)





Hybrid Stress Blast Model

JointStats

JKSimBlast

BMS Vis.

BMS

Vixen

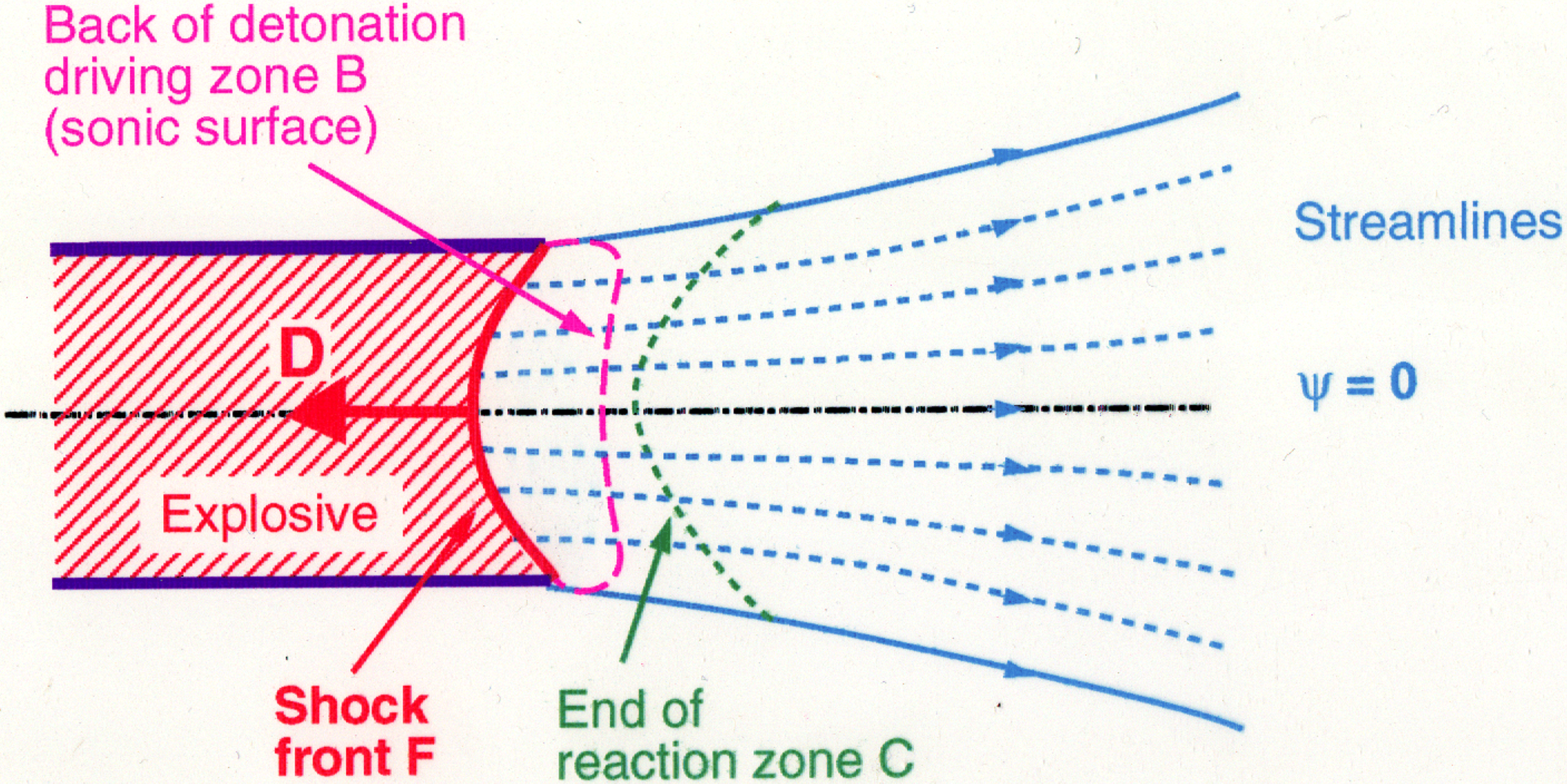
Interface DLL

BLO-UP

Data Validation
Preview
Scaling
Warnings
Defaults

DATA FILE

TWO–DIMENSIONAL DETONATION



Condensed Phase Detonations - Model

- Conservation relations (Euler equations)
  - Mass
  - Momentum
  - Energy
- Thermodynamic EoS – all phases
  - P, V, T, E relations
  - Mixing rules (finite reaction zones)
- Rate Expression – lumped
- Initial and Boundary Conditions

Cobra solution of 2-D Reactive Euler Equations

Cobra Analysis of ANFO Rate Stick

- simplified rate expression
- same EoS – explosive, detonation products and confinement
- open tube (rear boundary condition)
- run to steady state detonation

(all simplifications (rate and EoS) necessary to reduce run times to > 2 weeks on Linux based PCs)

Cobra Analysis Approach
ANFO Rate Stick

- simple pseudo-polytropic EoS – explosive, products and confinement

$$e=\frac{P}{(\gamma-1)\rho}+Q(1-\lambda):\quad \gamma=\gamma_0+\gamma_1\frac{\rho}{\rho_0}+\gamma_2\frac{\rho^2}{\rho_0{}^2}$$

- simplified rate expression

$$w=\frac{1}{\tau}\left(\frac{P}{P_{\mathrm{ref}}}\right)^{\frac{3}{2}}(1-\lambda)$$

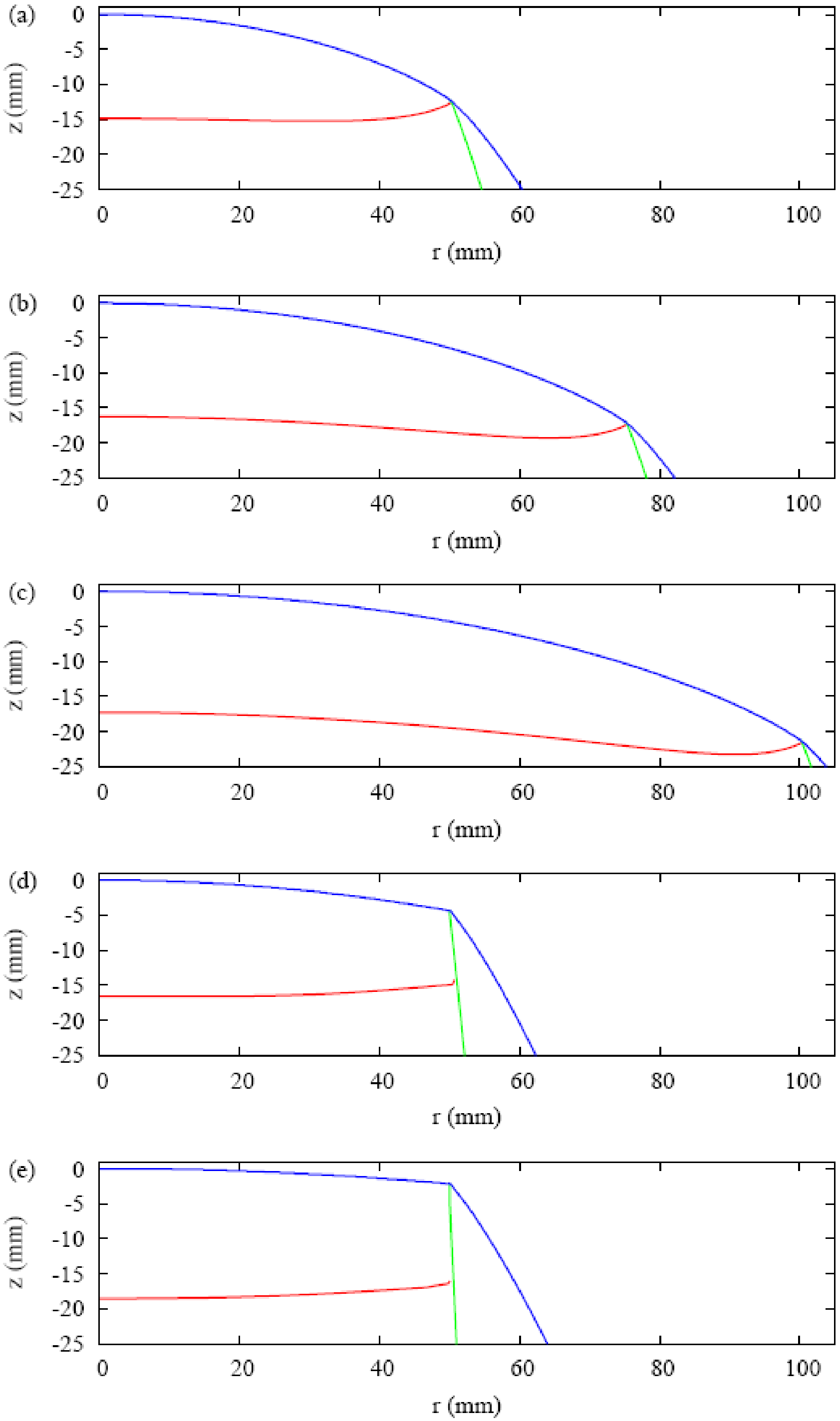
Δ(mm)	Points/l_{DDZ}	VOD (km/s)	Pshock GPa	Lambda$_{shk}$
0.1	149	3.13	4.32	0.05
0.2	74.5	3.12	4.24	0.09
0.4	37.3	3.10	4.11	0.12
0.8	18.7	3.05	3.88	0.15
1.6	9.3	3.01	3.67	0.21
3.2	4.7	2.93	3.25	0.52

Effect of grid spacing/ no of points in DDZ on predicted VOD, shock pressure and extent of reaction at the shock front

Cobra Analysis Comparison - ANFO Rate Stick

Case	Diameter (mm)	Confinement Density g/cc	D/D_{CJ}
A	100	0.8	0.652
B	150	0.8	0.778
C	200	0.8	0.837
D	100	4	0.829
E	100	8	0.901
F	100	0.0013 - air	0.648
G	100	2	0.746
H	100	6	0.873

Blue – shock
Red – sonic locus
Green - contact



100 mm 0.8 g/cc

150 mm 0.8 g/cc

200 mm 0.8 g/cc

100 mm 4 g/cc

100 mm 8 g/cc

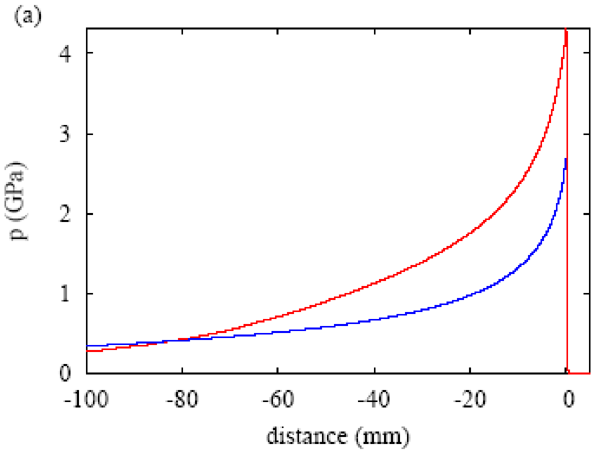
100 mm 0.8 g/cc

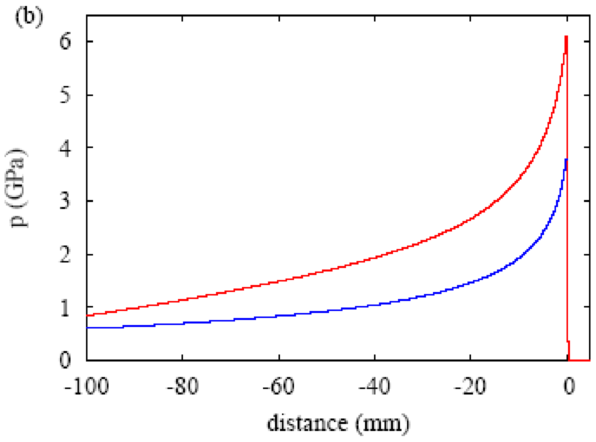
150 mm 0.8 g/cc

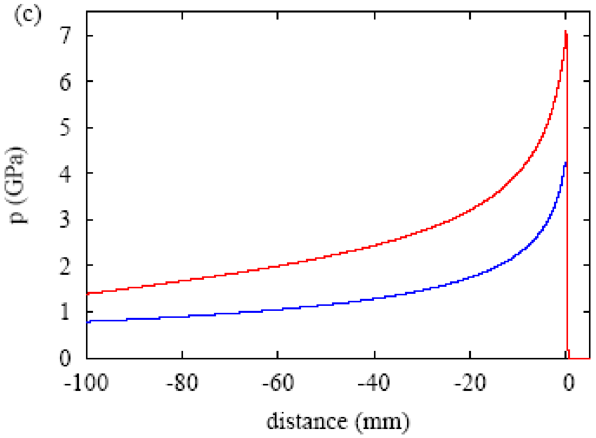
200 mm 0.8 g/cc

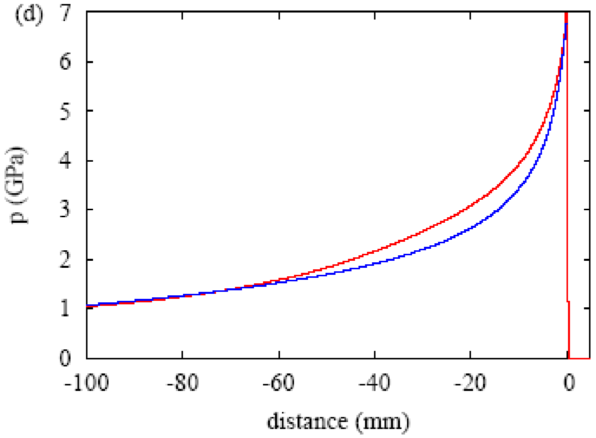
100 mm 4.0 g/cc

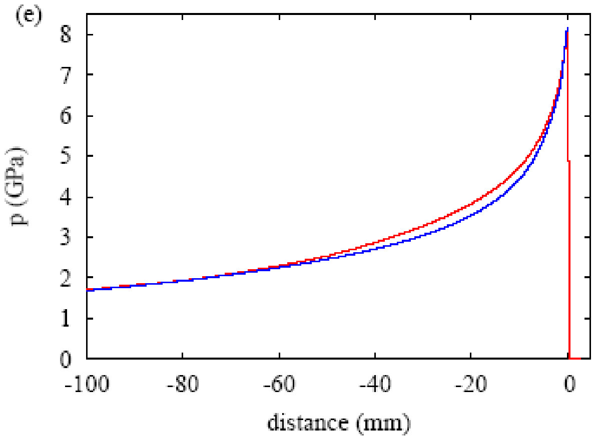
100 mm 8.0 g/cc



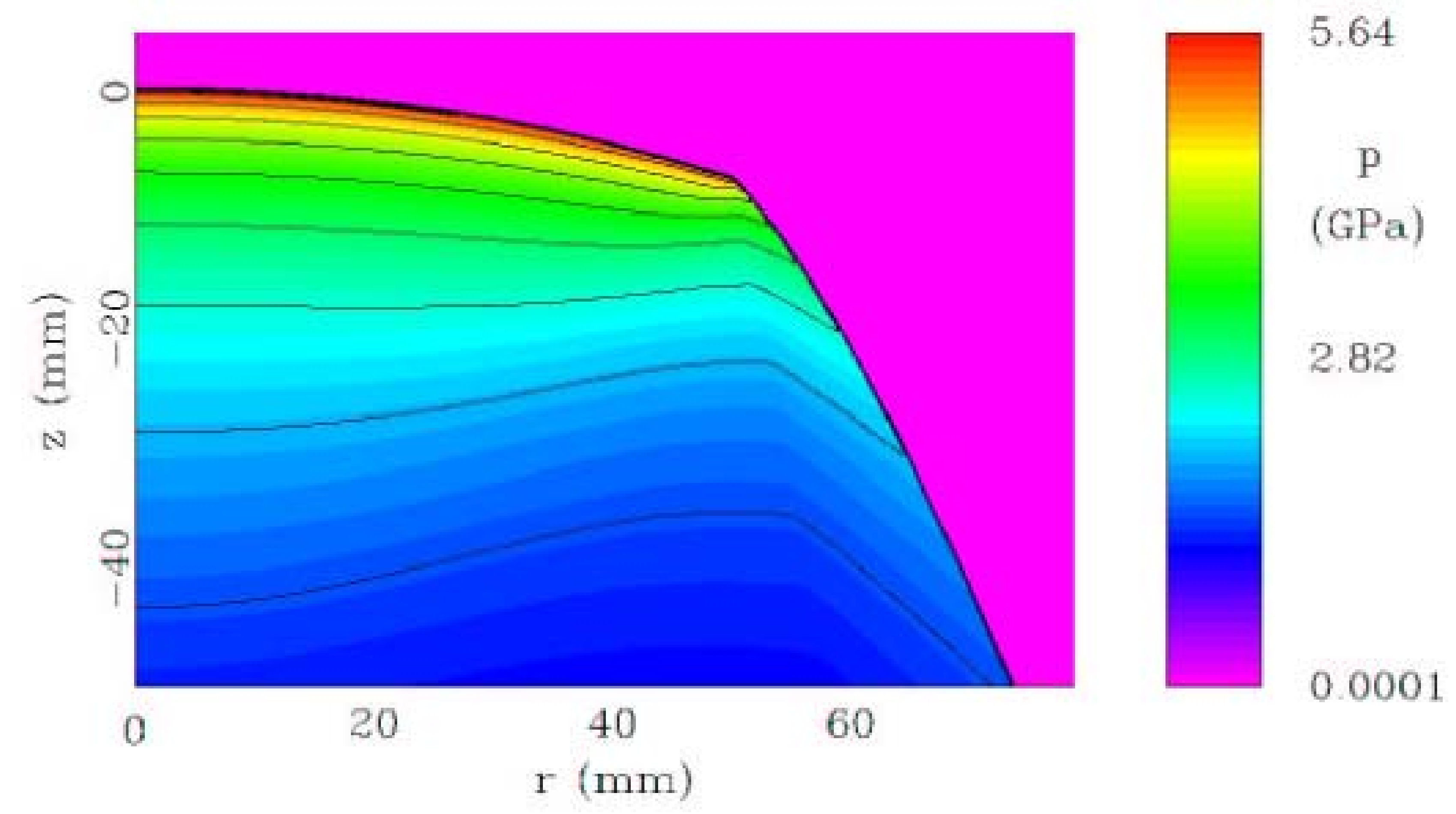




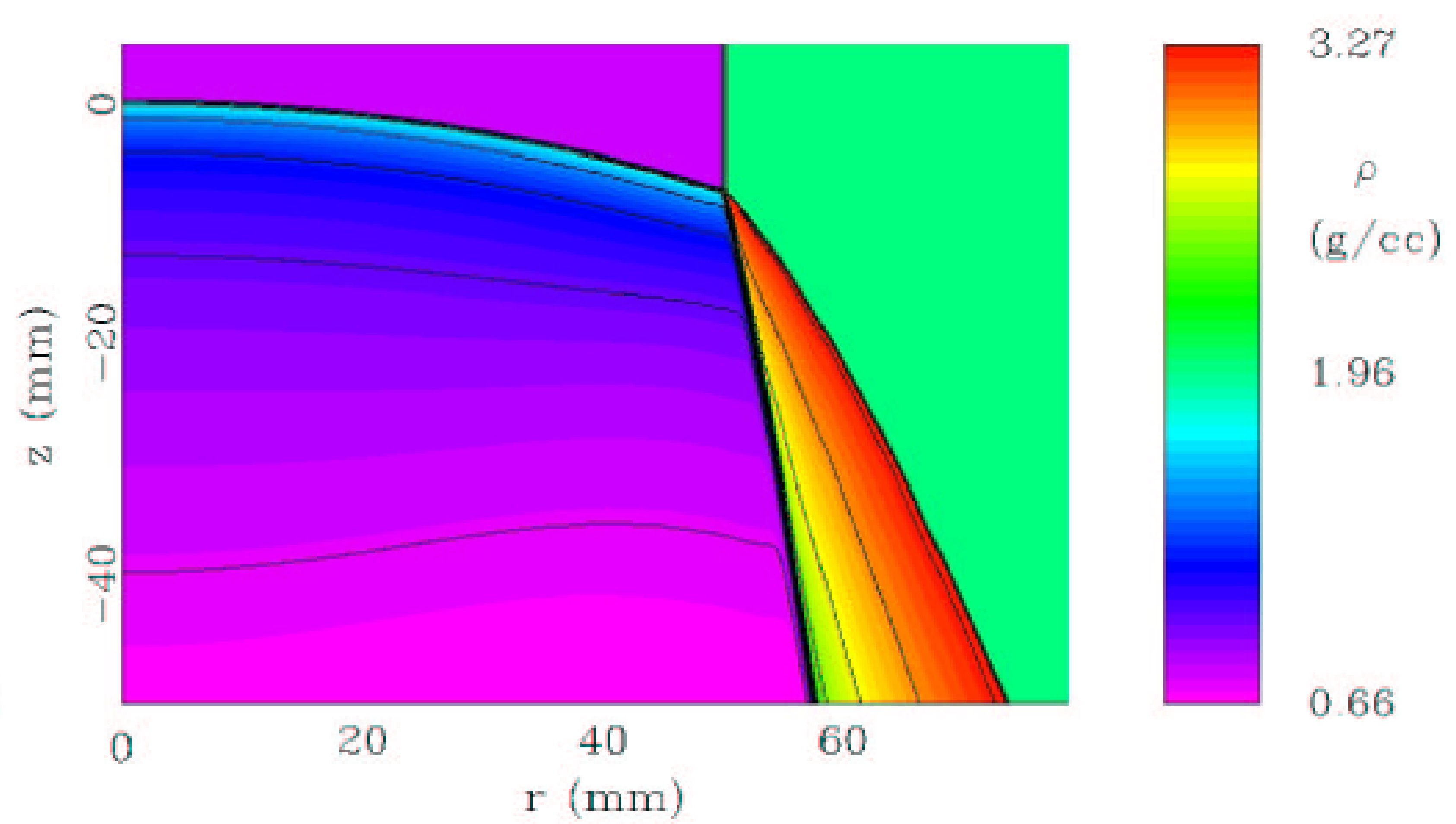




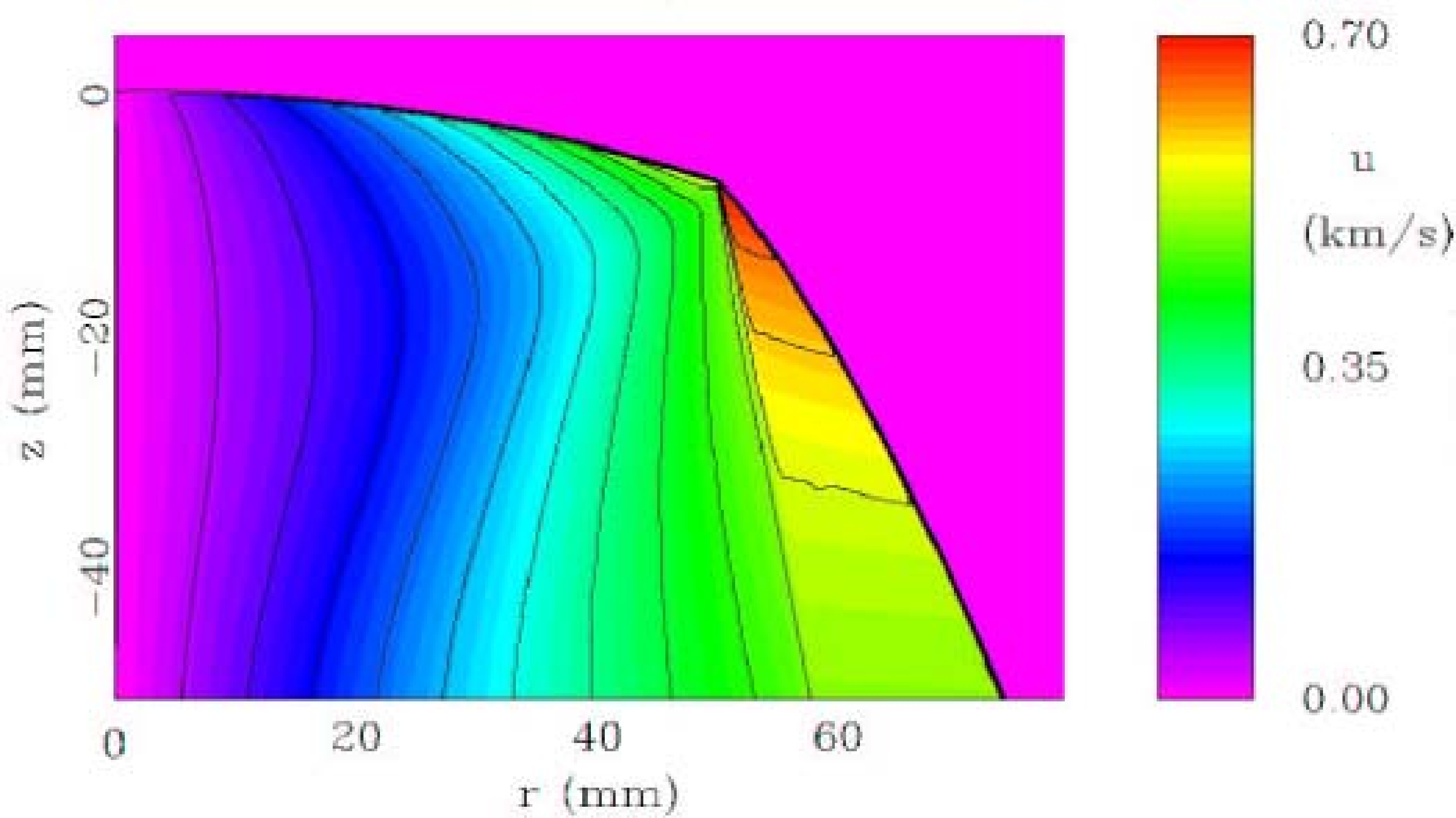
100 mm ANFO charge in 2 g/cc confinement – Pressure profile



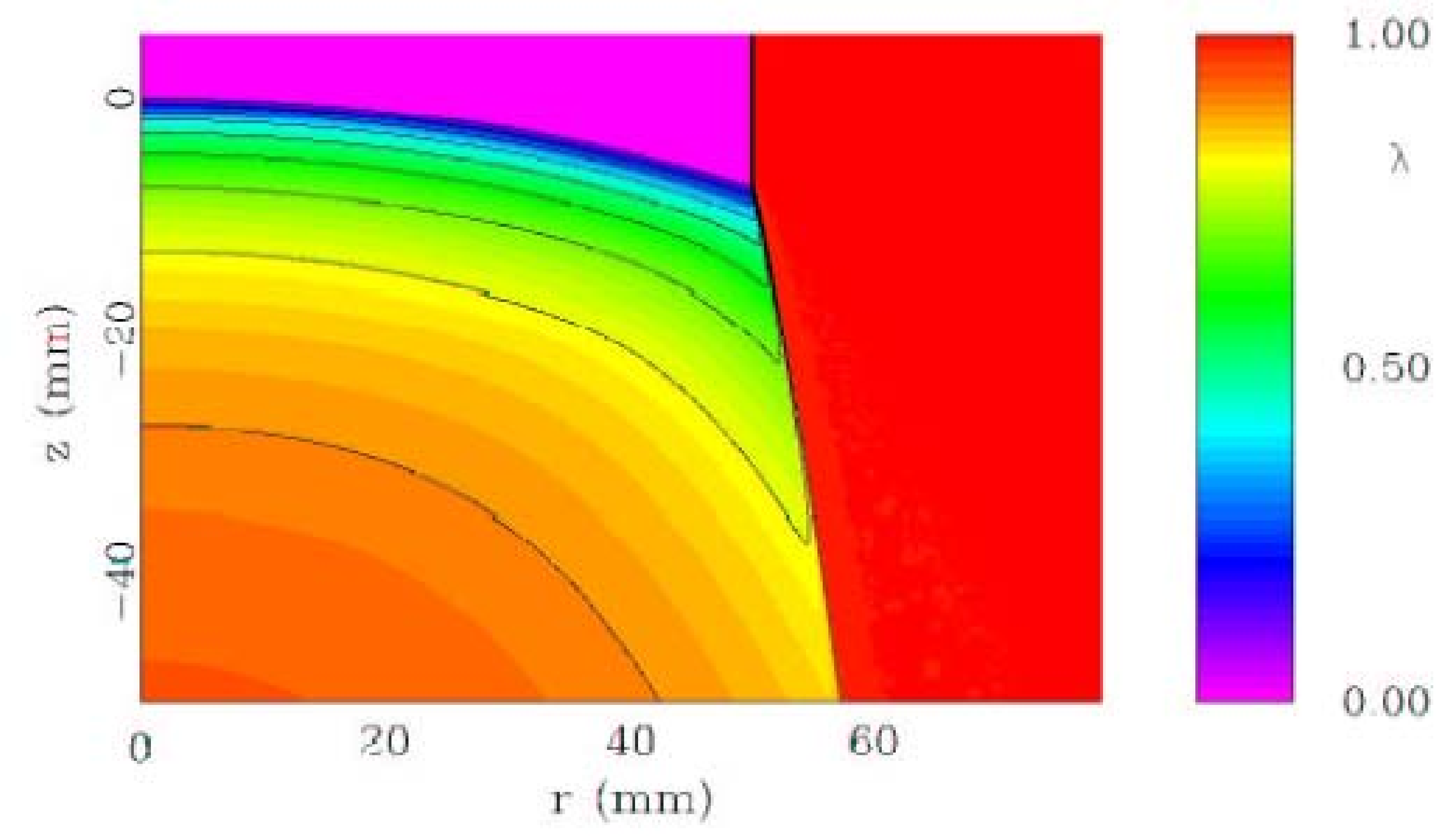
100 mm ANFO charge in 2 g/cc confinement - Density Profile



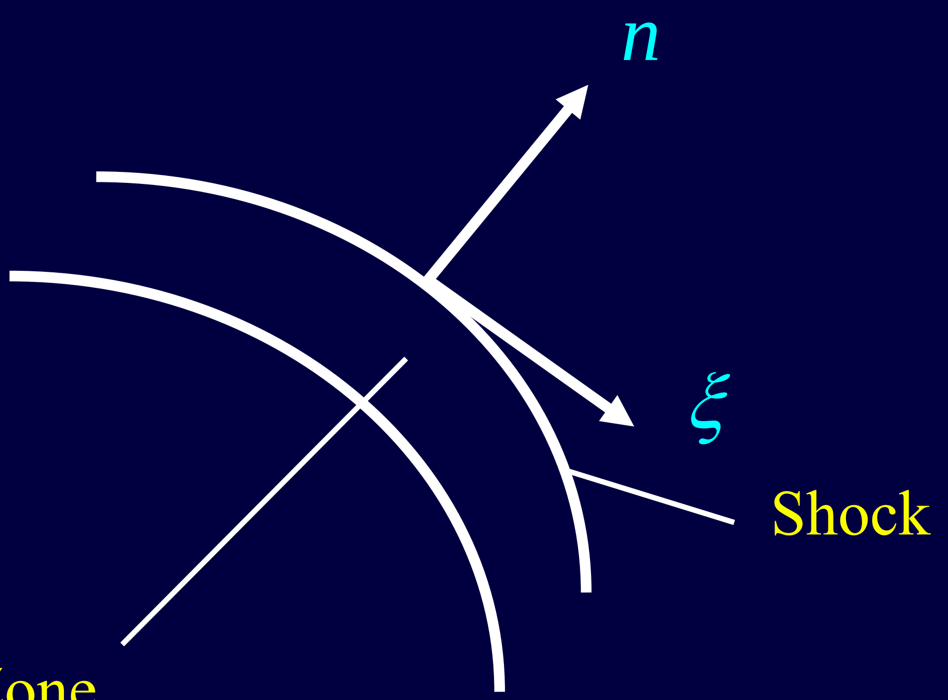
100 mm ANFO charge in 2 g/cc confinement – Radial Velocity Profile



100 mm ANFO charge in 2 g/cc confinement – Reaction Extent Profile



Quasi- 1-D – Analysis for General EoS and Rate Law



n is normal direction to shock

ξ is tangential direction to shock

u_n & u_ξ are fluid velocities normal and perpendicular to shock

Steady Euler Equations in curvilinear coordinates

$$\rho\frac{\partial u_n}{\partial n}+u_n\frac{\partial \rho}{\partial n}=-\frac{\mathrm{K}\rho\left(u_n+D_n\right)}{\left(1+nK\right)}+\xi \text{ terms}$$

$$u_n\frac{\partial u_n}{\partial n}=-\frac{1}{\rho}\frac{\partial P}{\partial n}+\xi \text{ terms}$$

$$\frac{\partial e}{\partial n}-\frac{P}{\rho^2}\frac{\partial \rho}{\partial n}=\xi \text{ terms}$$

$$u_n\frac{\partial u_n}{\partial n}=W+\xi \text{ terms}$$

where ξ terms involve $\frac{\partial}{\partial \xi}$ derivatives and u_ξ: Reaction rate and EoS, are given by W=W $(\rho,\mathrm{P},\lambda)$ & $e=e\left(\rho,P,\lambda\right)$. K and D_n are the local total curvature and normal component of detonation speed. P,ρ and λ correspond to pressure, density and extent of reaction respectively.

Quasi-1-D approximation

- radial derivative and velocity terms are assumed negligible
- remaining partial derivatives become full
- D_n normal velocity becomes VOD

Analogous to WK central stream-tube but without unknown divergence term

Q1D Equations in curvilinear coordinates final

$$\frac{d\rho}{dn} = -\frac{\dfrac{\sigma W}{u_n} - \dfrac{\mathrm{K}\rho u_n (u_n + D_n)}{(1 + n\mathrm{K})}}{c^2 - u_n}$$

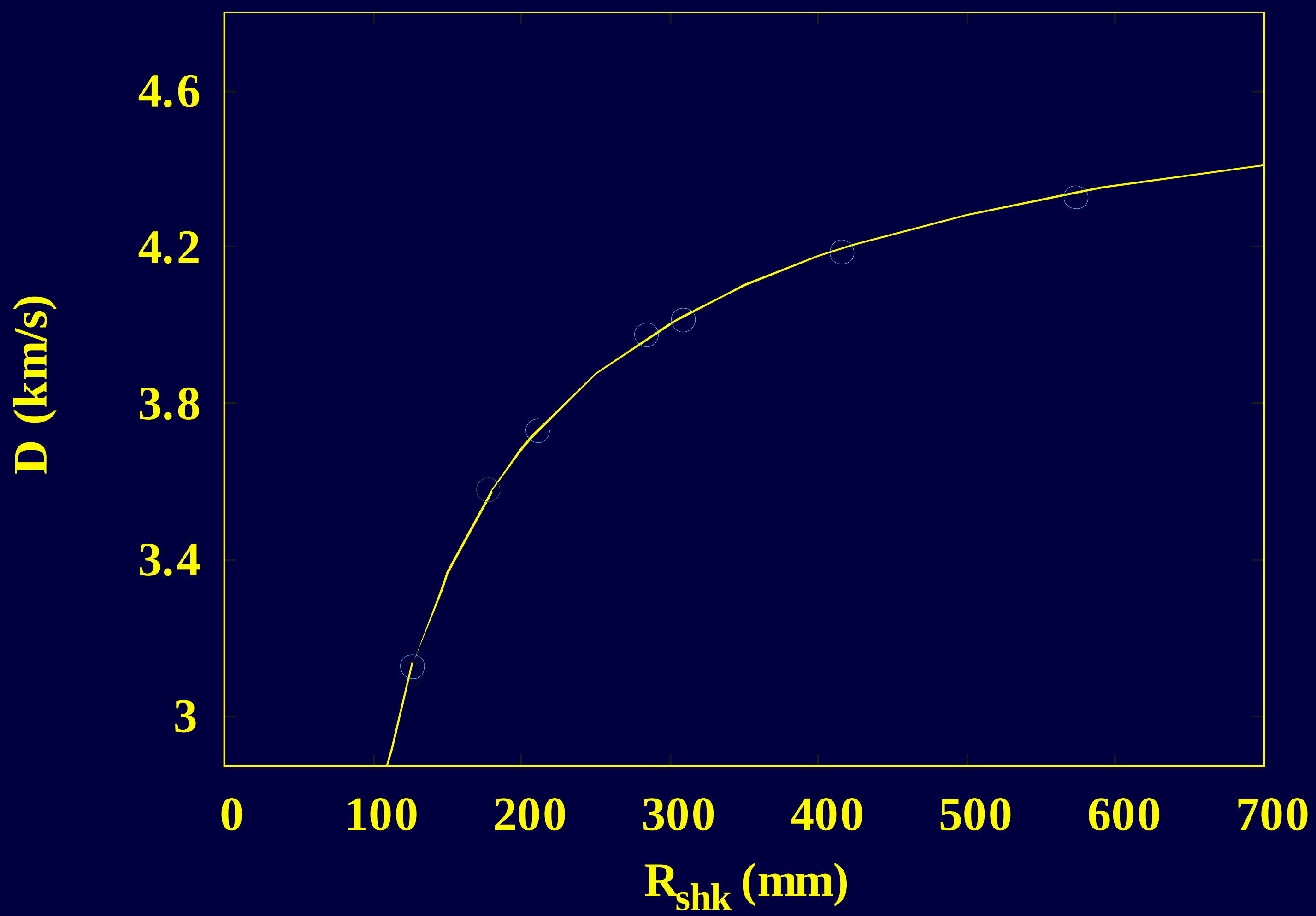
$$\frac{du_n}{dn} = \frac{\sigma W - \dfrac{\mathrm{K}\rho u_n (u_n + D_n)}{(1 + n\mathrm{K})}}{c^2 - u_n{}^2}$$

$$\frac{d\lambda}{dn} = \frac{W}{u_n}$$

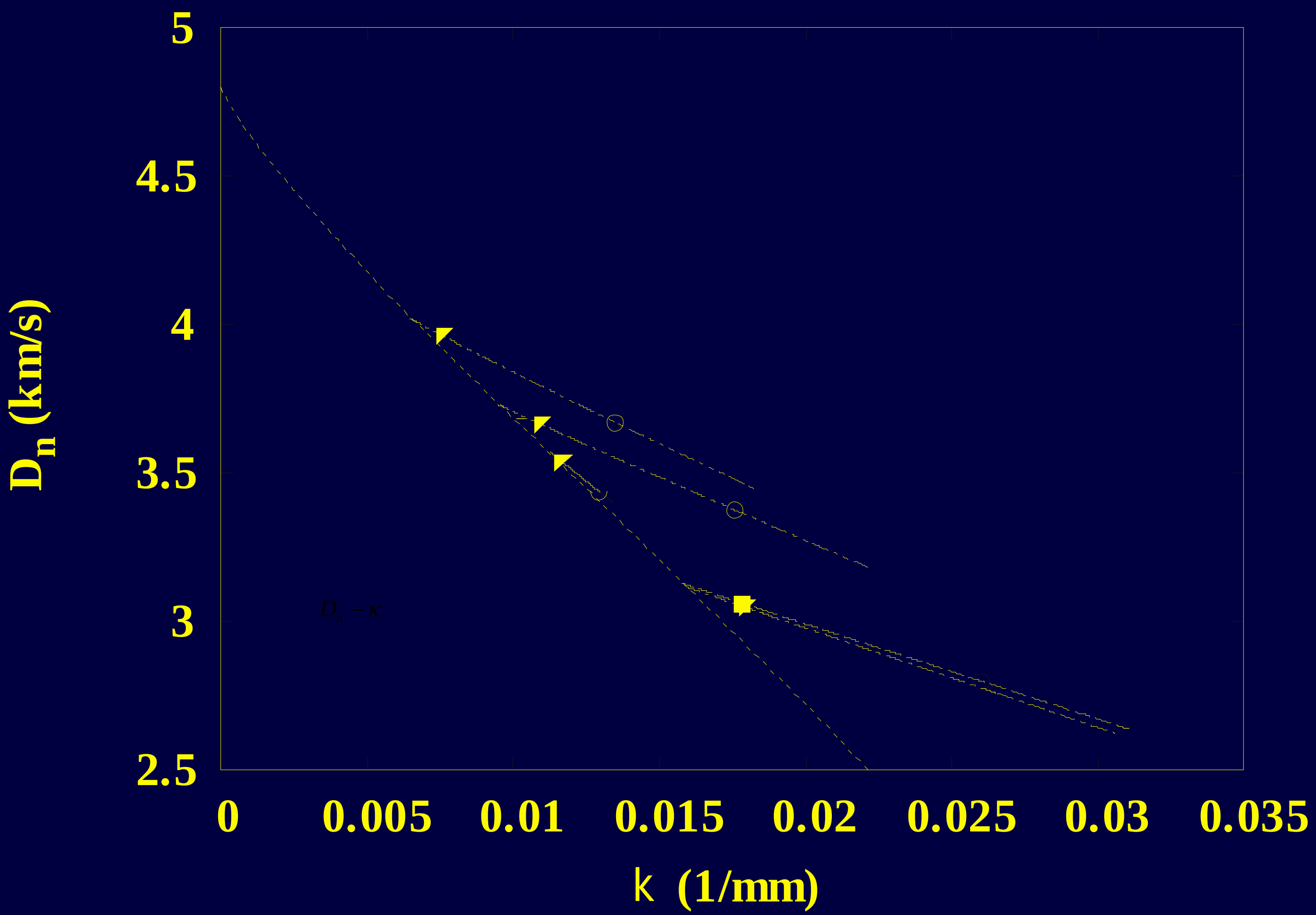
$$e\left(\rho, P, \lambda\right) + \frac{P}{\rho} + \frac{1}{2} u_n{}^2 = e_0 + \frac{P_0}{\rho_0} + \frac{1}{2} D_n{}^2$$

$$c^2 = \left[\frac{P}{\rho^2} - \left(\frac{\partial e}{\partial \rho}\right)\right] \Big/ \left(\frac{\partial e}{\partial P}\right)$$

$$\sigma = \left(\frac{\partial e}{\partial \lambda}\right) \Big/ \left(\frac{\partial e}{\partial P}\right)$$



Axial Detonation velocity vs axial radius of curvature,
Q1D predictions are given as a solid line
and the data from COBRA runs as circles



**Normal Detonation Speed vs curvature (ex COBRA)
for a range of charge diameter and confinement density
cf Q1D theory (dotted line)**

Conclusions

High resolution AMR simulations required ~ 0.1 mm

Reasonable to good agreement – Q1D and COBRA for central axis

Disadvantage of Wood Kirkwood – unknown axial divergence parameter

DSD for non-ideal explosives in heavy confinement eg rock ?

Limited "impact" of DDZ directly on rock

Acknowledgements

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