Simulation of Detonations in Mining Applications

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Intro

Bulk mining applications/ pumpable AN based explosives – open cast
Optimization of blasting operations – vibration, fines, downstream & costs
Modest cpu, laptop simulation

Detonation in heterogeneous media

Scales – mass. length, diameter , density, pressure etc
Ideal and non-ideal steady detonations – 2-D, inviscid media
Work & relevant zone in the detonation-rarefaction process

Mining Practice

Characterization data available – explosive and rock
Stochastic effects & precision
Confiner acoustic velocity and VOD

Modeling (Reactive Euler equations)

- Conservation relations
- Thermodynamic EoS
- Rate expression & approximation to homogenous fluid explosive
- Boundary conditions

Approaches

- Classical thermodynamic analysis
- Quasi 1-D and WK
- DSD
- DNS – validation studies/ course refinement
- Link to geo-mechanical models (rock movement - fragmentation, heave)
- VOD < acoustic velocity

Questions

- Where are the points of diminishing returns –
  - accuracy and sophistication of detonation model ?
  - parameterisation of rate expression ?

Ammonium Nitrate Based Bulk Explosives – ANFO, Emulsions

- Heterogeneous, gas sensitized

eg separate oil and oxidiser phases
porous prill, chemical gassing

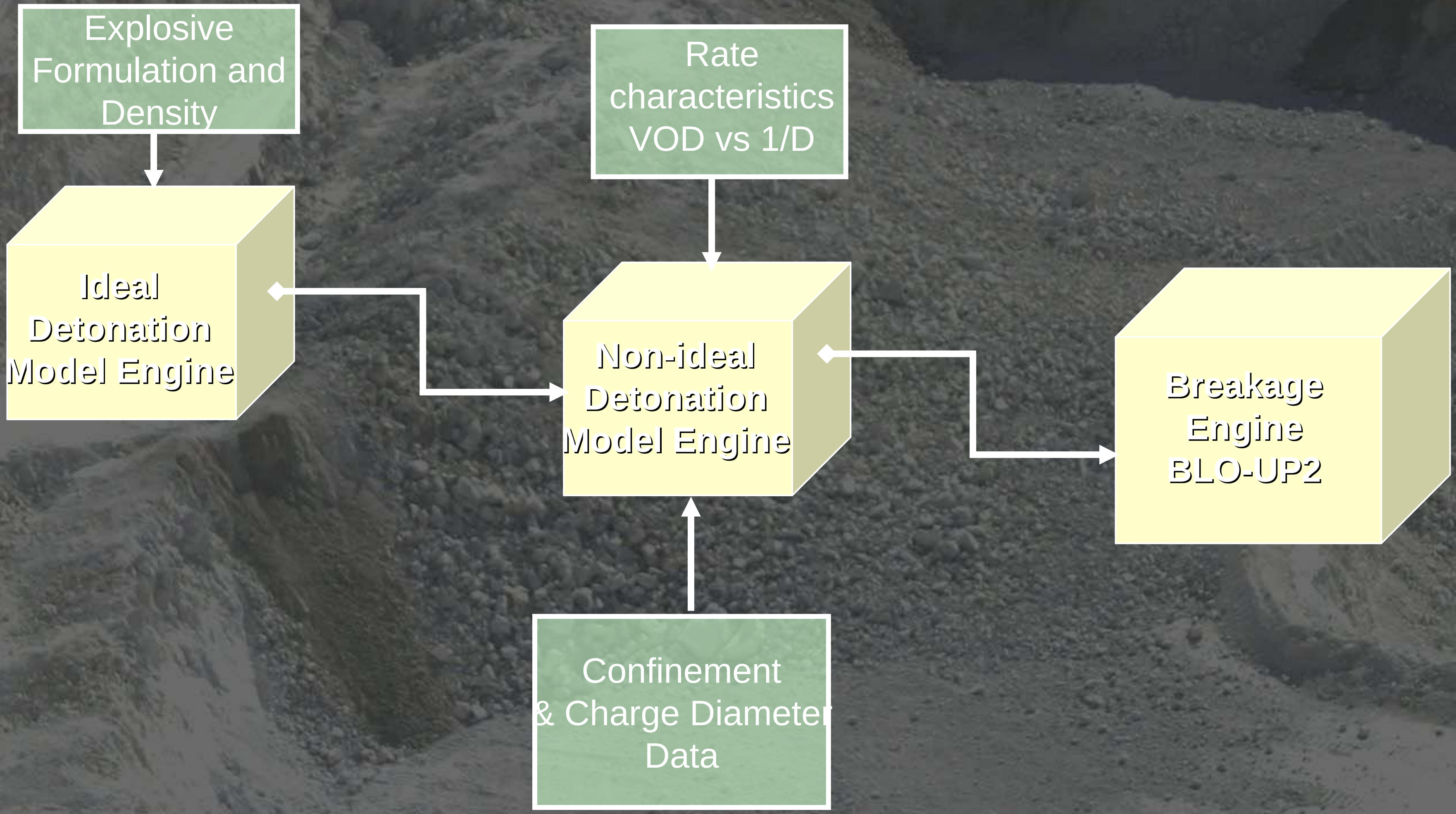
- Large critical diameter (detonation) & VOD < Ideal VOD

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

HSBM II



Explosive Formulation and Density

Rate characteristics VOD vs 1/D

Ideal Detonation Model Engine

Non-ideal Detonation Model Engine

Breakage Engine BLO-UP2

Confinement & Charge Diameter Data

Typical Scales

- Pressures ➔ 20 GPa

- Temperatures ➔ 4000 K

- Densities ➔ 2000 kg/m^3

- Velocities (Mach No) ➔ 7000 m/s (< 5)
- Reaction zone lengths > 20 mm

- Energy release < 5MJ/kg

- Detonation products – small (diatomic, triatomic) molecules

Note that VOD can be < acoustic velocity in confining rock

Detonation Physics

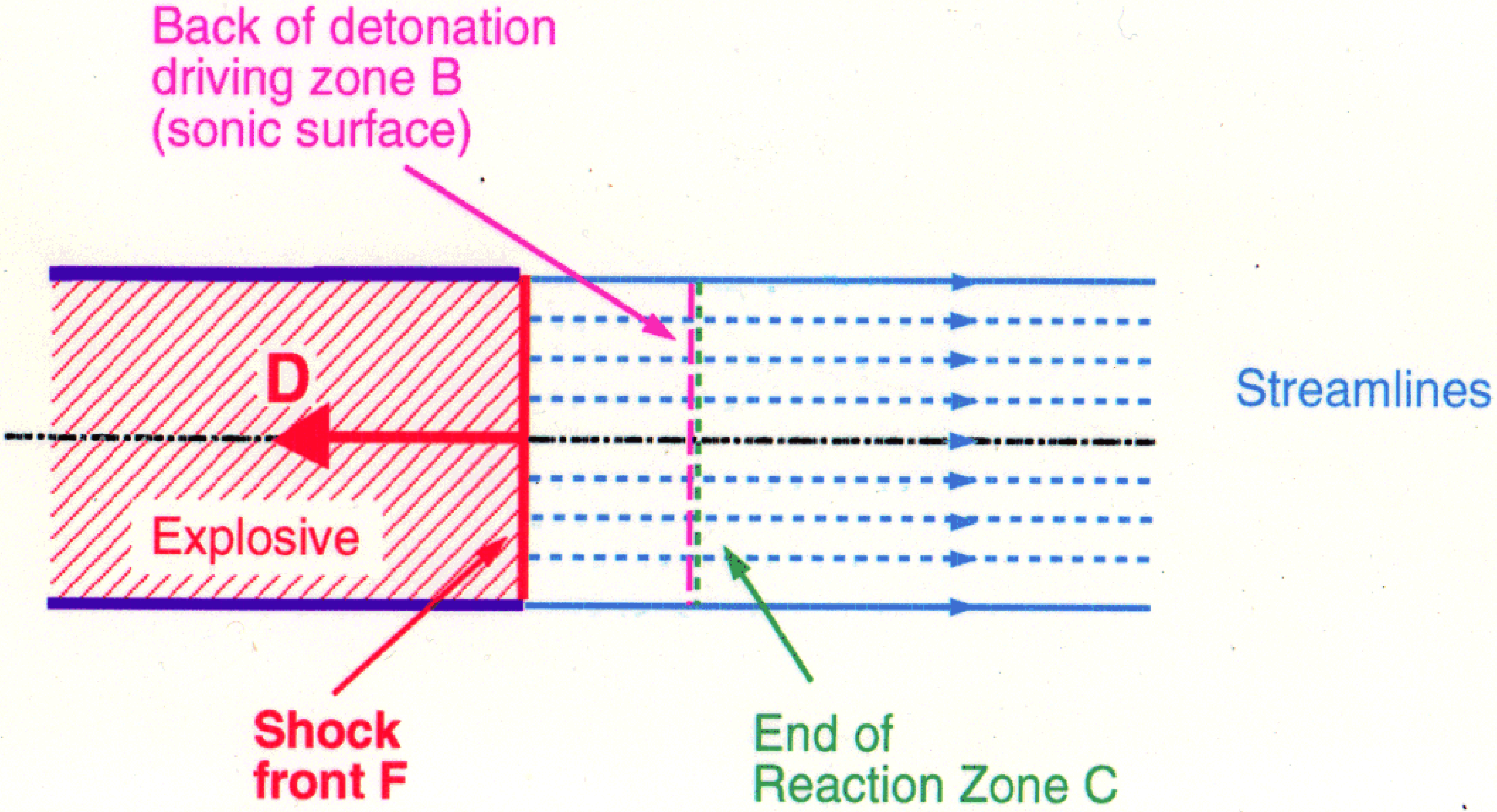
- Assumptions

  Homogeneous Fluid - equivalence
  Inviscid Fluid
  Adiabatic Process

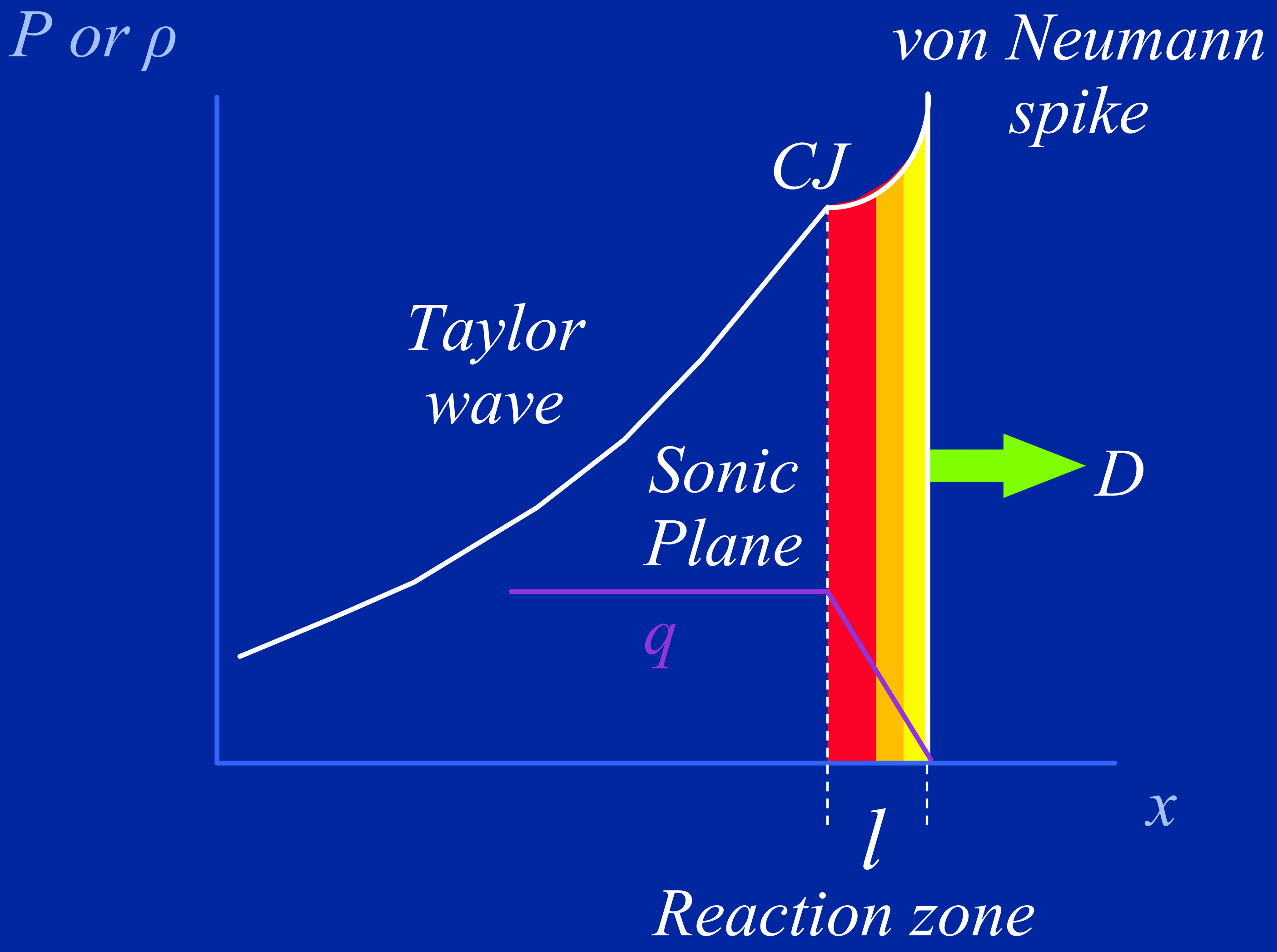
  Equilibria – mechanical, thermal (or isolation)

  Dimensionality
    0 – Chapman Jouguet
    1 – ZND
    2 – Rate-stick
    3 – Complex 3-D flow

ONE–DIMENSIONAL NORMAL DETONATION



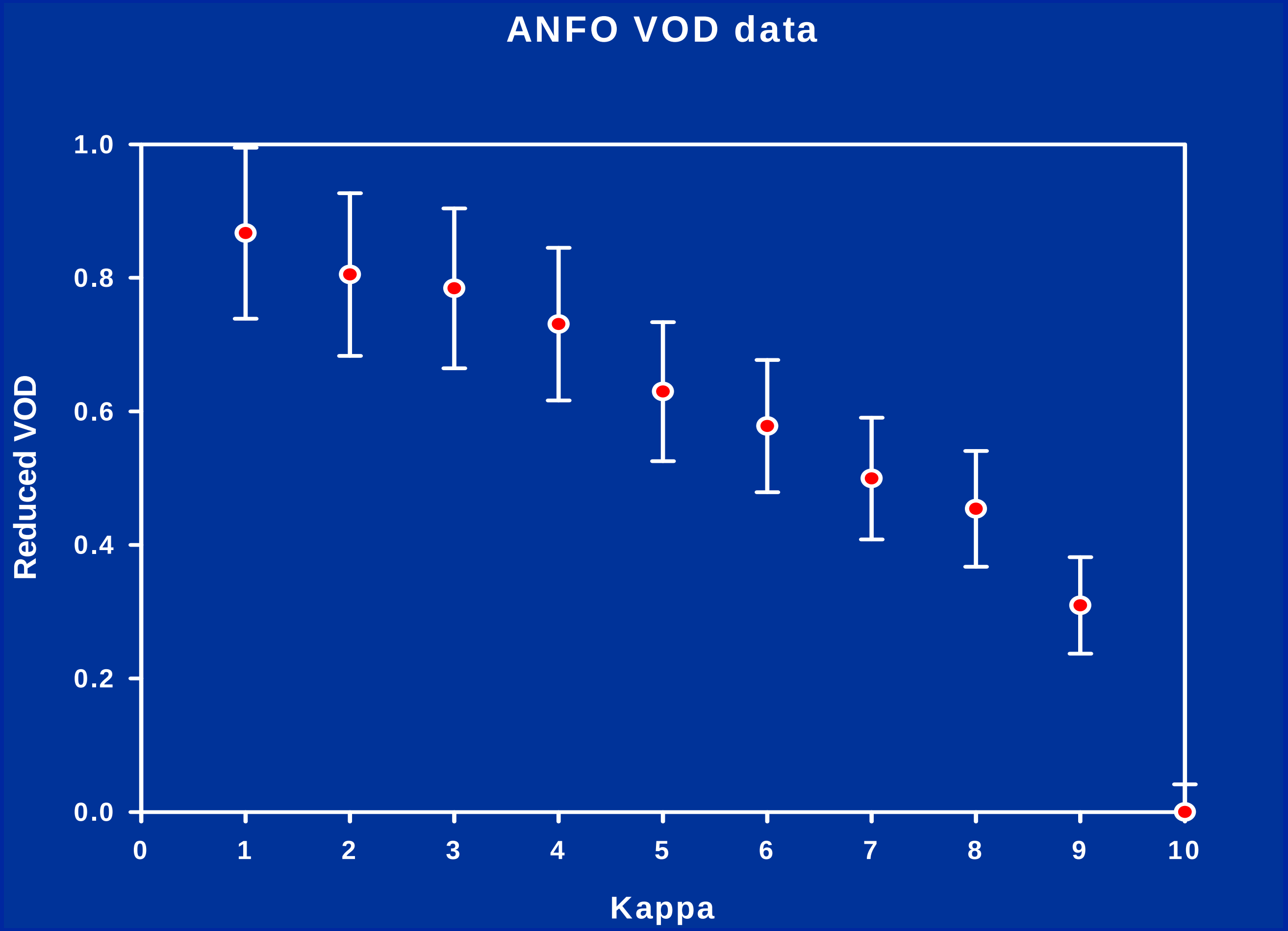
ZND Detonation and Rarefaction



Characteristics of steady two-dimensional non-ideal detonation

- Shock front curved
- Flow diverges
- Detonation driving zone (DDZ) terminates at sonic locus where relative particle speed equals local sound speed
- Reaction is always incomplete in DDZ
- Velocity of detonation decreases with diameter
- If diameter of cylindrical charge is too small detonation fails

Rate expression, data for parameters & fitting



How many parameters required to fit above unconfined data ?
How accurate are these data ?
Should the infinite diameter (theoretical) point and those data
near the critical diameter be included ?

Errors in measured VOD – diameter data for heterogeneous explosives

- departures in density & explosive formulation
- changes if void/ prill/ droplet size and size distributions
- incomplete filling
- unsteady VOD
- partial crystallization
- miscellaneous damage
- ill defined/ variable confinement “nominally unconfined”
- differences between laboratory and field

Note – it is extremely difficult to make an acceptable gassed emulsion explosives on a laboratory scale – and replacement of gas voids by microspheres or microballoons yields an explosive of different properties

Detonation Simulation

- Equations of State – Explosive, Products

  Multi-phase, multi-component
  High density & pressure
  Practical – computational and no. of parameters

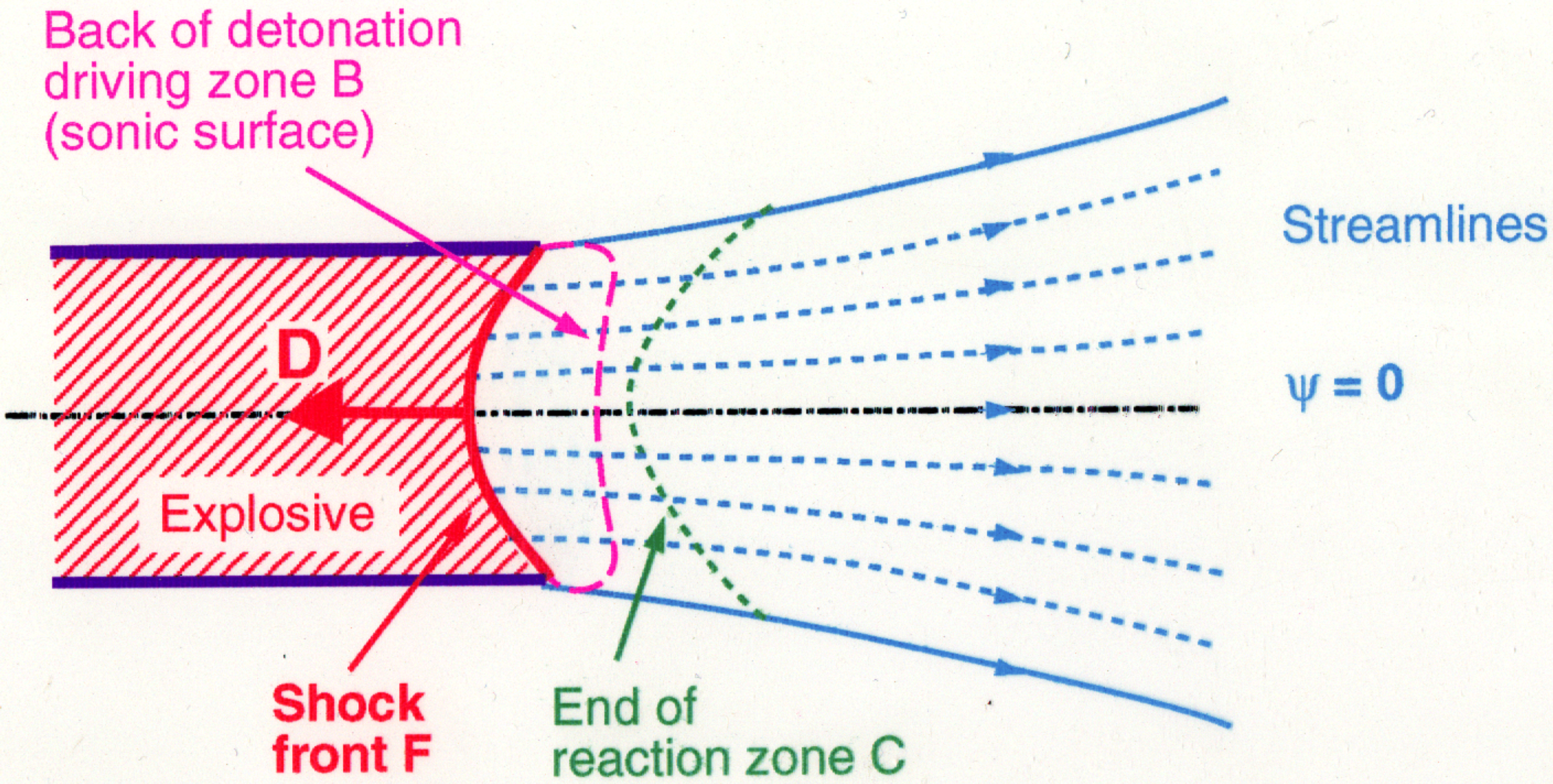
- Rate expression

  Lumped – mass, momentum and energy transfer, chemical reaction
  Chemistry implicit eg I & G, Vieille form
  Practical – computational and no. of parameters

- Initial/ Boundary conditions

  Shocked unreacted explosive/ end of detonation zone
  BC's at radius – confinement/ explosive interaction

TWO–DIMENSIONAL DETONATION



Condensed Phase Detonation Modelling

- Reactive Euler Equations

$$W_t + F(W)_x + G(W)_y = S(W)$$

$$W = \begin{bmatrix} \rho \\ \rho u \\ \rho w \\ E \\ \rho\lambda \\ \rho Q \end{bmatrix}, \qquad F = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho uw \\ uE + uP \\ \rho u\lambda \\ \rho uQ \end{bmatrix}$$

$$G = \begin{bmatrix} \rho w \\ \rho uw \\ \rho w^2 + P \\ wE + wP \\ \rho w\lambda \\ \rho wQ \end{bmatrix}, \qquad S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho r \\ 0 \end{bmatrix}$$

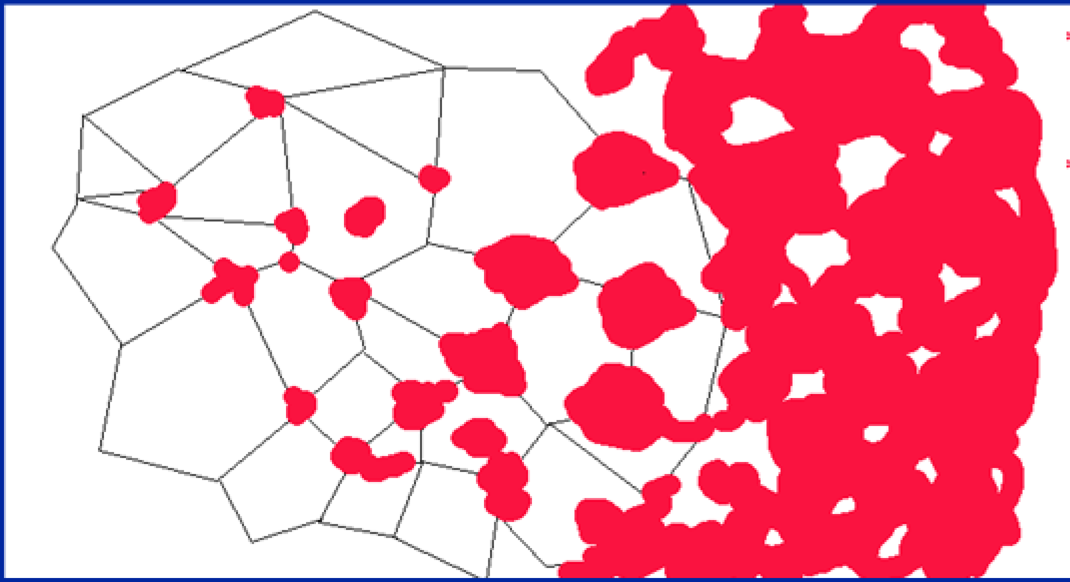
Clarke et al 1990

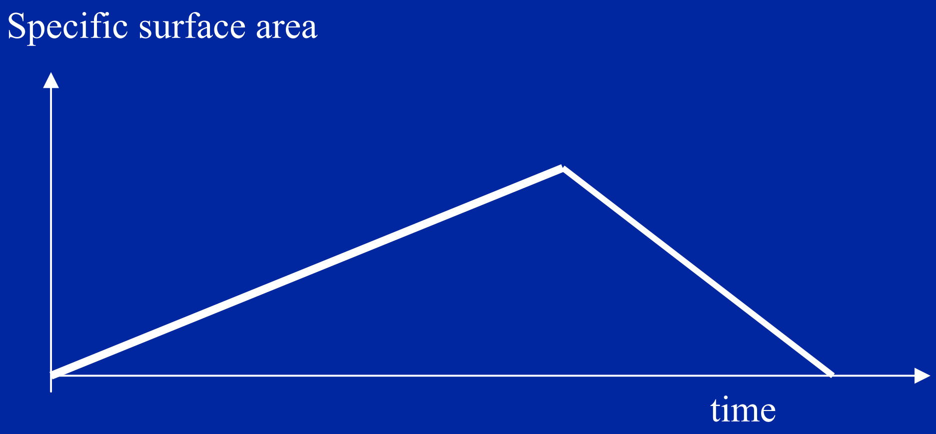
$$P = (\gamma - 1)(E - \frac{1}{2}\rho(U^2 + w^2) + \rho\lambda Q)$$

$$r = \frac{2}{T_R}(1-\lambda)^{\frac{1}{2}}$$

Grain Burning and Hotspots
Geometry based kinetics

- Initial reactions start in hotspots.
- Grow by burning neighbouring material.
- Cool by conduction, expansion and radiation.
- Once enough hotspots grow they coalesce.
- Burn rate thus goes from progressive to regressive.





Pressure Dependent Kinetics

The burning rate is

$$\partial F/\partial t=\partial F/\partial t\big|_1+\partial F/\partial t\big|_2+\partial F/\partial t\big|_3.$$

where the burning process moves through terms 1, 2 and 3 in order and F is fraction reacted.
The initiation term is

$$\partial F/\partial t\big|_1=F_q\left(1-F\right)^{F_r}\left[\frac{1}{V_e}-1-C_{crit}\right]^{\eta}$$

where V_e is the relative volume of the solid explosive and F_q, F_r, C_{crit}, and η are constants. The term is needed to start an explosive burn with a low-level trigger such that initiation may fail or take some time to get started.
The G_1 growth term in DYNA2D is the only such term when two terms (the other being initiation) are used. When three terms are used, it is the fast-growth kinetics term. This term is

$$\partial F/\partial t\big|_2=G_1\left(1-F\right)^{s_1}F^{a_1}P_s^m,$$

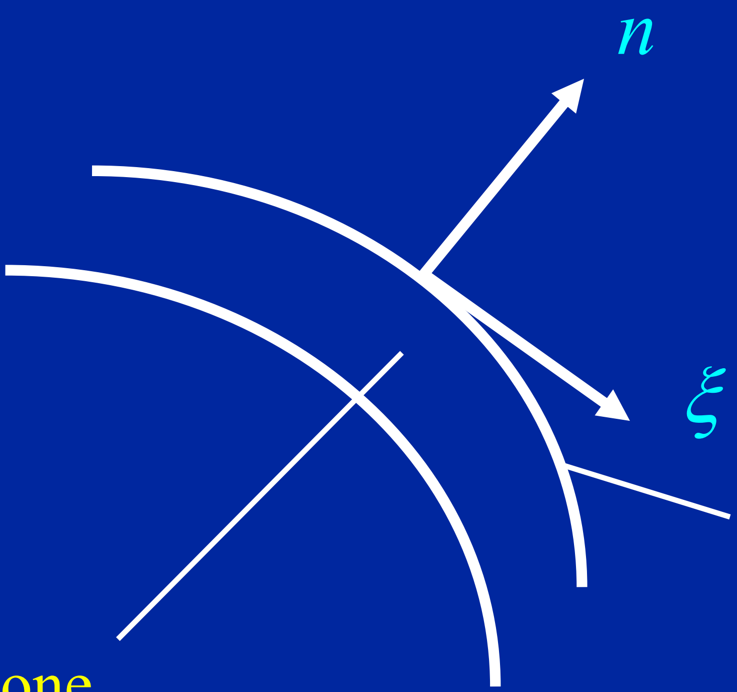
where G_1, s_1, and a_1 are constants.
It is the G_1 growth term, with its pressure dependence, that creates the curved detonation front in a cylinder. At steady state, the curvature is much less than in the early stages.
The G_2 growth term represents slow kinetics when three terms are used. It is not included for the two-term model. It is

$$\partial F/\partial t\big|_3=G_2\left(1-F\right)^{s_2}F^{a_2}P_s^n,$$

where G_2, s_2, and a_2 are constants.

In the ignition model the three terms, in order, aim to relate to (1) hot-spot creation, (2) hot-spot spreading, and (3) hot-spot coalescing.

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



n

ξ

shock

Reaction Zone

Note for axial solution

n is z direction

ξ is r direction

Steady Euler Equations in curvilinear coordinates

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

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

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

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

where ξ terms involve $\dfrac{\partial}{\partial \xi}$ derivatives and u_ξ: Reaction rate and EoS, are given by W=W$(\rho,\mathrm{P},\lambda)$ & $e = e(\rho, P, \lambda)$. 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.

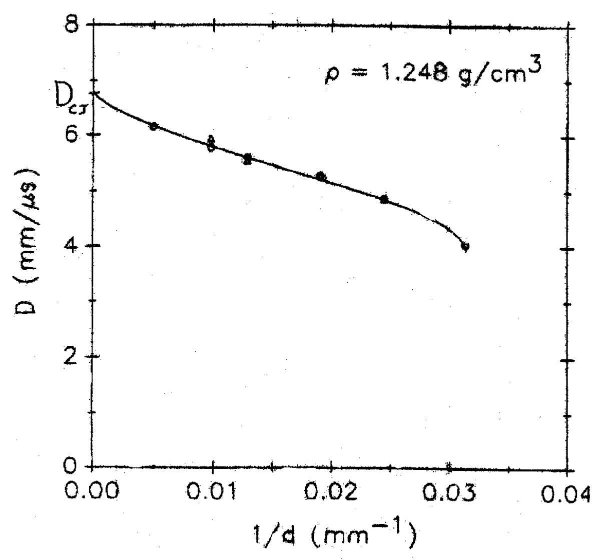
Quasi-1-D approximation

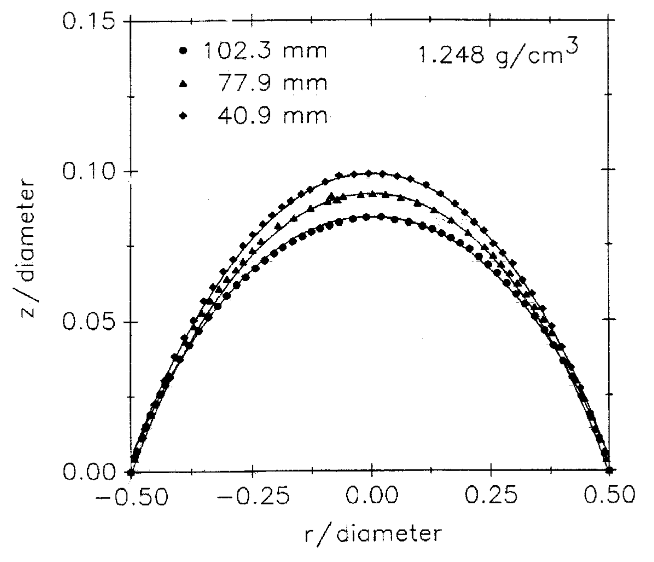
- radial derivative and velocity terms are assumed negligible
- remaining partial derivatives become full
- D_n normal velocity becomes VOD

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

Key features of steady non-ideal detonation

(plots from J.Lee PhD thesis, Socorro, 1990)





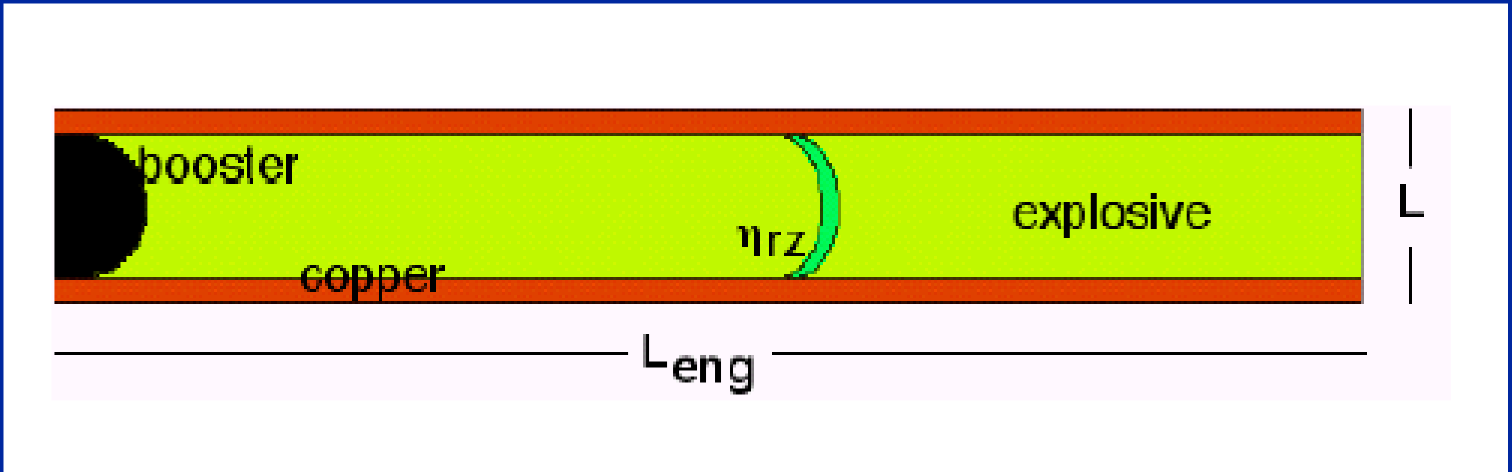
- Experimental plots for ANFO emulsion of:

a) VoD versus reciprocal diameter (1/d) showing critical point (last);

b) Scaled axial coordinate z_F/d versus scaled radial coordinate r/d for 3 diameters.

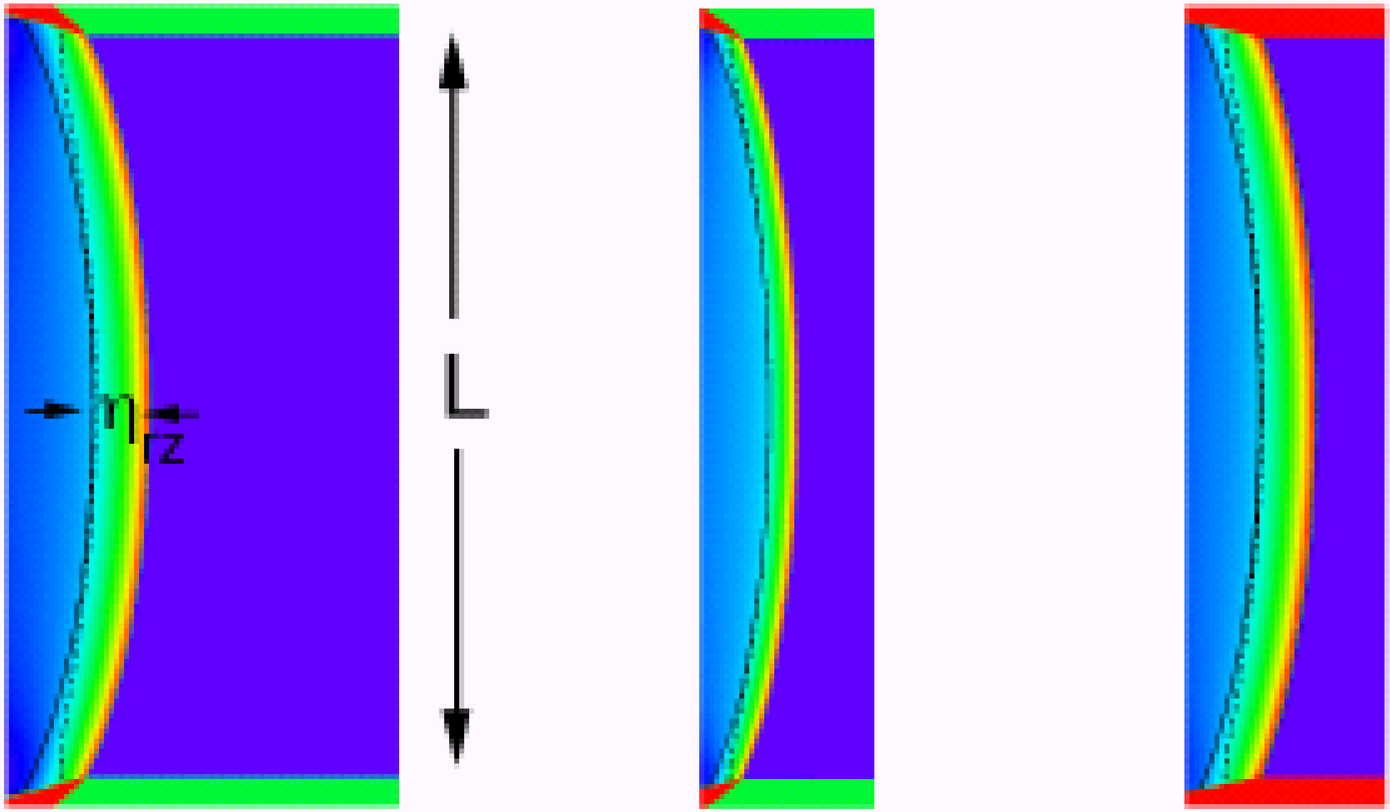
- Curves are fits to forms suggested by DSD theory

Detonation in a Cylinder



Disparate length scales

L_{eng} >> L >> Reaction zone



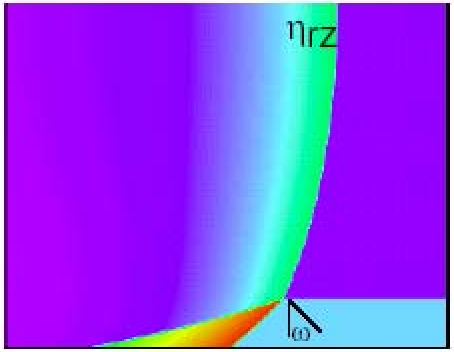
base case

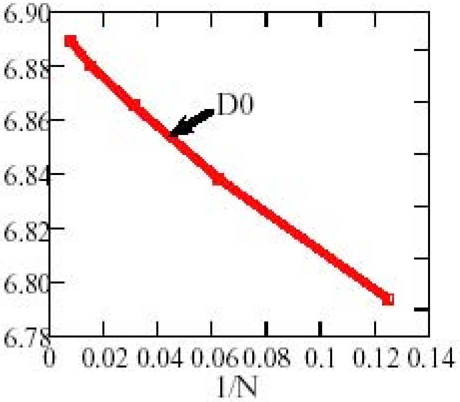
shorter η_{rz}

heavier confinement

DNS of Detonation

- given a well calibrated “reactive Euler model,” these effects can be calculated via direct numerical simulation (DNS)
- resolved DNS requires fine zoning





- O(50 pts) are needed in the reaction zone to get D_0 converged to O(0.02 mm/us) using modern, hi-res methods. Multistep reaction models require more resolution. Maximum error of 1% in computed η_{rz}

DNS Cost Estimates

- instantaneous volume of 3D reaction zone, V_{rz}, is $V_{rz} \sim (L_{eng})^2 \eta_{rz}$. For $L_{eng} \sim 300$mm, $\eta_{rz} \sim 1$mm and 50 points in the η_{rz} direction, $O(10^{10})$ cells in the reaction zone at any instant
- with $\Delta t = 4 \mathrm{x} 10^{-3}$ μs and a problem time of 50 μs gives $1.25 \mathrm{x} 10^{4}$ time steps
- grind time of 10^{-4} s/cell/cycle
- computation time for the reaction zone only

  $$T_{cpu3D} \sim (10^{-4})(10^{10})(1.25 \mathrm{x} 10^{4}) = 1.45 \mathrm{x} 10^{5} \text{ days}$$
- 1,000 cpu perfect parallelization, $T_{cpu3D||} = 145$ days
- with AMR, 2D calculations may be feasible
- a subscale model of detonation propagation is indicated

Cobra Analysis Comparison ANFO Rate Stick

- Cobra (Leeds)

  AMR Hydrocode – 2nd order Godunov
  Run from initial impulse to a steady state condition
  Examine effect of confinement and charge diameter

- Simple Non-ideal detonation model

  Wood Kirkwood pseudo 1-D model
  Eos and rate expression as Cobra

- ZND (1-D) calculation

  Set up parameters and scaling for Cobra

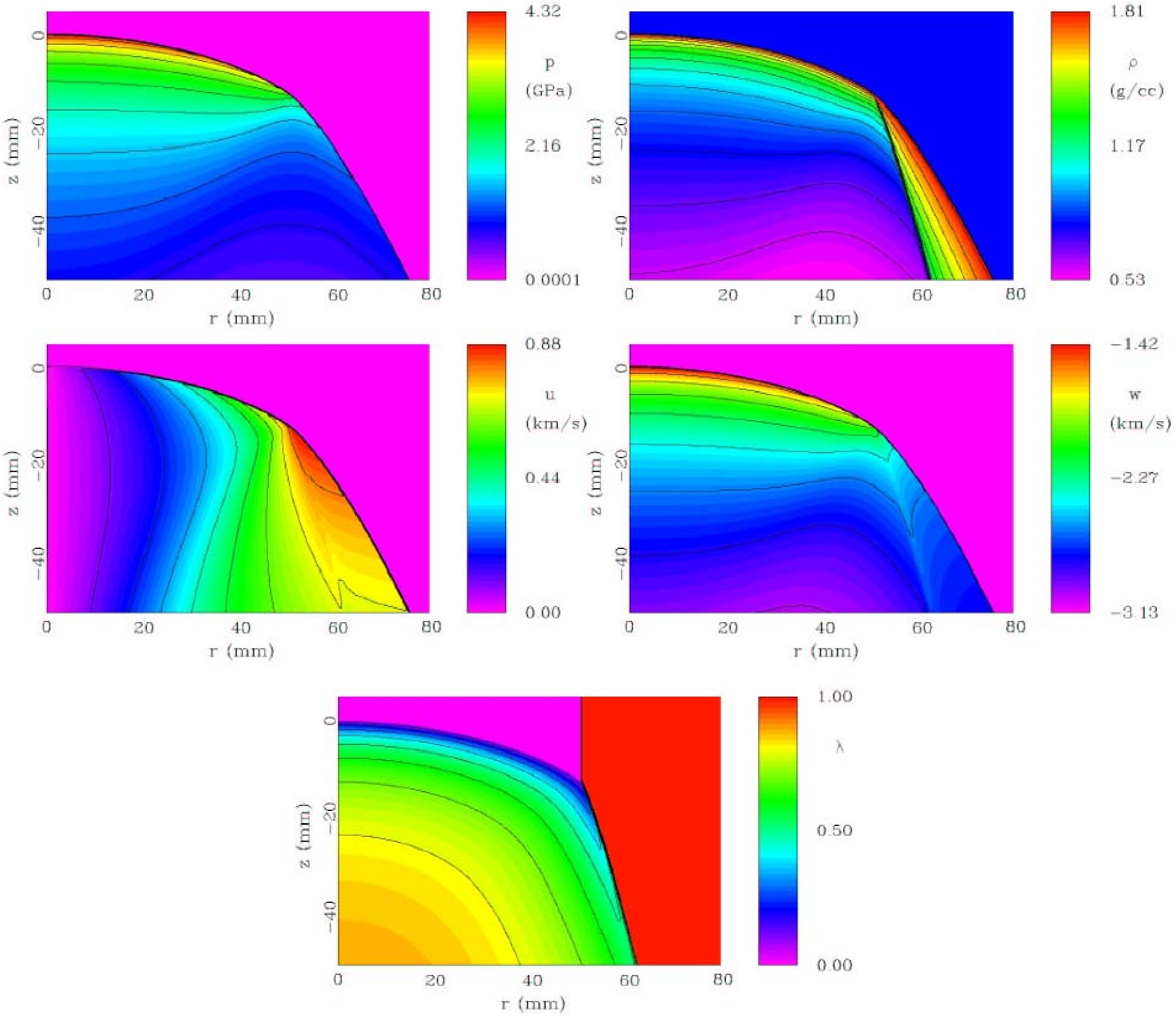
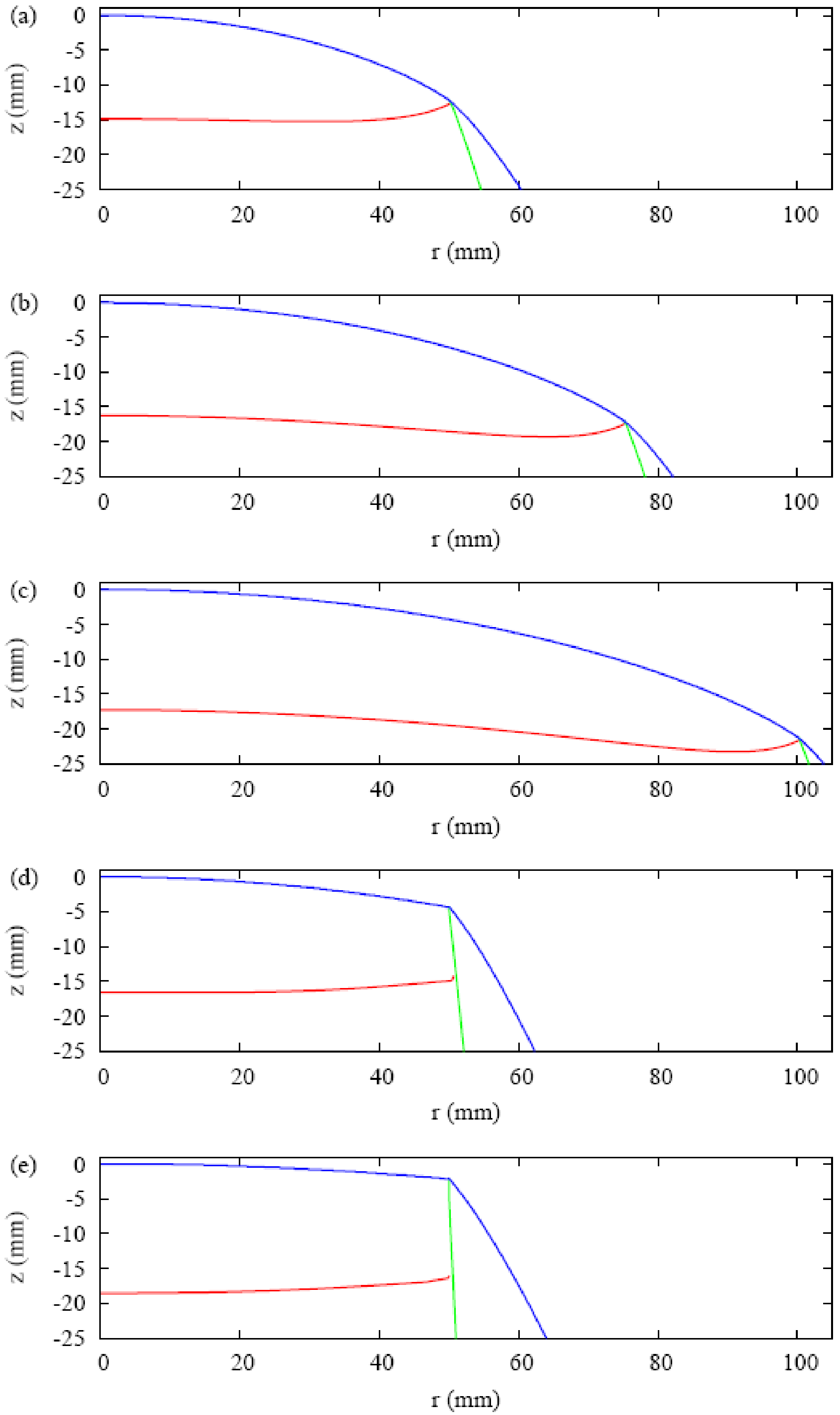


Figure 1: Pressure, density, radial velocity, axial velocity and reaction progress variable for case A ($d = 100$ mm, $\rho_I = 0.8$ g/cm^3).

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

Cobra results – analysis

- Engineering model appears OK for confined charges
- DDZ contact finite at boundary for confined media
- Scaling laws for isobars & shock front curvature promising
- Small radial gradients in confined media
- Spherical (confined) shock front → ellipse (unconfined)

Raises questions about whether unconfined tests are appropriate
Confinement model and rate law development likely priorities

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

Non-ideal detonation – steady, 2D axisymmetric – VOD > c

Unconfined – empirical shock front curvature form based on experiment
used to fit unconfined data (VOD vs 1/diameter)

Q1D – quasi one dimensional – applies central stream tube
general solution for detonation zone carried out once for specific
explosive, but all diameters and confinements

DSD – Detonation Shock Dynamics – 2-D/ shock polar match
carried out within BLO-UP to characterise shock front for specific
charge diameter and confinement

Rate Expression and associated parameters

- Describe chemical kinetics and transport dynamics in complex multi-component heterogeneous (multi-phase) media

- Simple form commensurate with experimental data

- Orthogonal parameters where possible

- Ability to efficiently auto-fit

$$d\lambda \big/ dt = \frac{(1-\lambda)^{\alpha}}{\tau}\left(\frac{P}{P_{\mathrm{ref}}}\right)^{\beta}$$

λ - extent of reaction

P - pressure

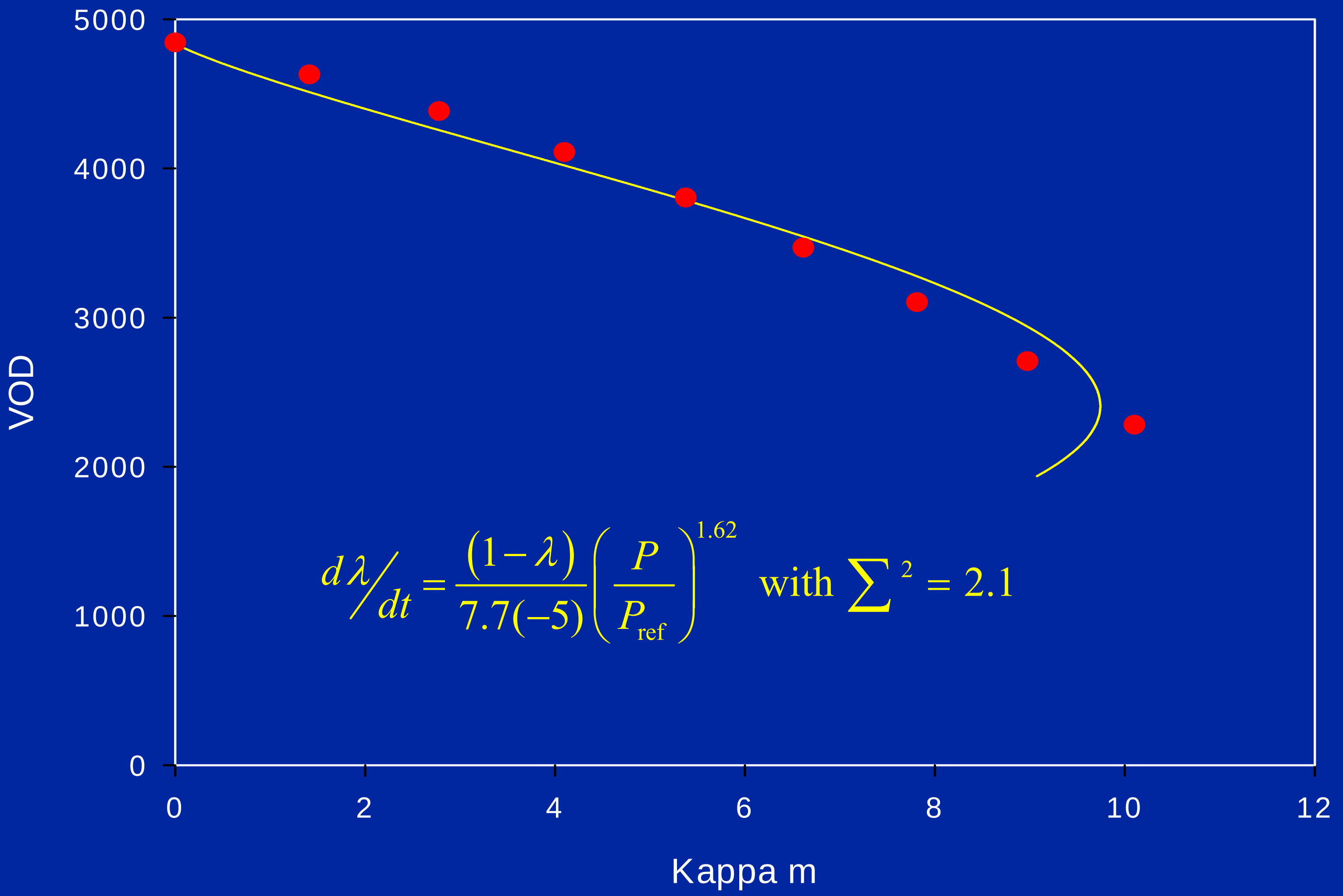
α - reaction exponent - not used

t - time

τ - inverse rate constant

β - pressure exponent

ANFO – 800 kg/m³ – 94 % w/w AN (dry) & 6 % w/w oil



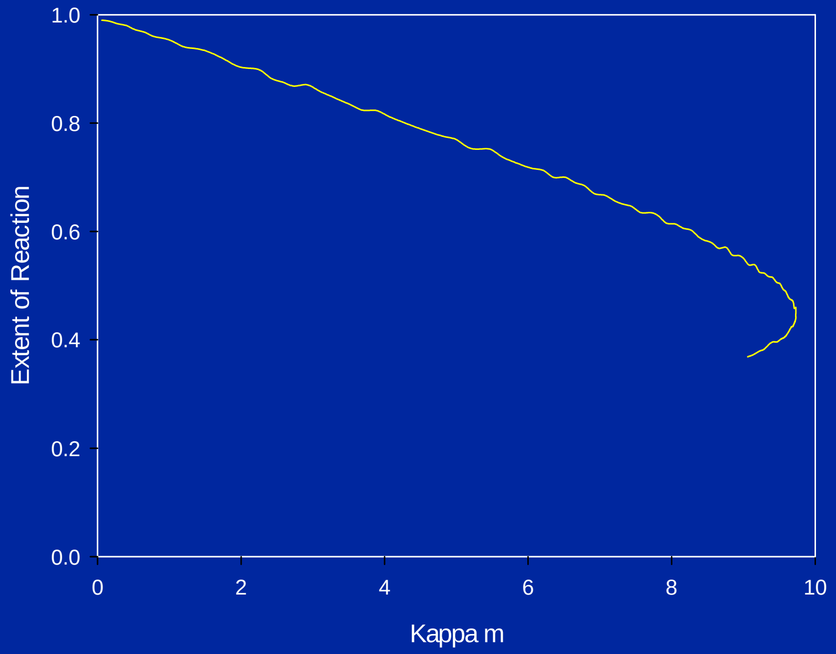
$$\left.d\lambda\middle/dt\right. = \frac{(1-\lambda)}{7.7(-5)}\left(\frac{P}{P_{\mathrm{ref}}}\right)^{1.62} \quad \text{with } \sum{}^{2} = 2.1$$

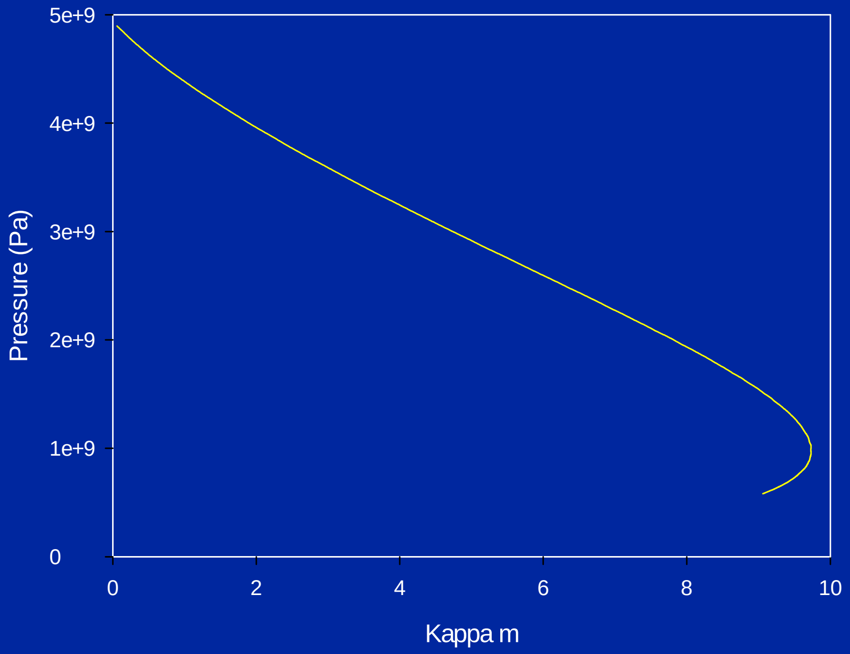
Smoothed data with a VOD=1500 m/s removed

Some doubt on use of next low velocity point – VOD/VOD_ideal > 0.5

ANFO Example

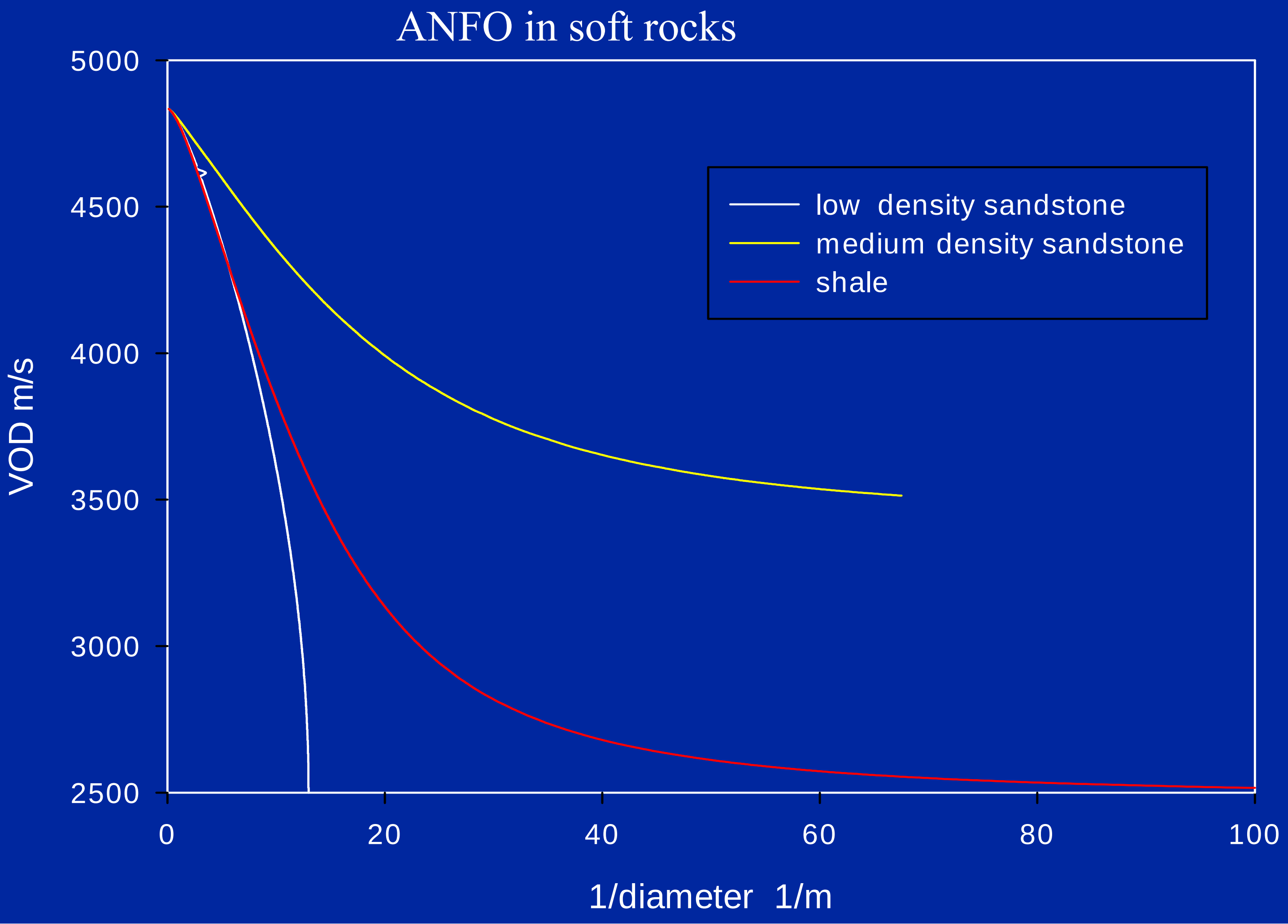
Extent of Reaction & Pressure Profiles as function of Kappa





Q1D determines a general 1-D solution for central stream tube for all diameters and confinements

DSD uses these data and rock and unreacted explosive properties to predict nature of shock front



Questions

Where are the points of diminishing returns –

(i) accuracy and sophistication of detonation model ?

fluid mechanics and resolution of detonation zone
constitutive relations for rock and explosive:
EoS products
Rate expression

(ii) parameterisation of rate expression ?

experimental data & associated errors

(iii) Where VOD < acoustic velocity in rock ?