TWO-PHASE STEADY DETONATION ANALYSIS

with applications for

DEFLAGRATION-TO-DETONATION TRANSITION (DDT)

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Publications in Progress

Powers, J. M., Stewart, D. S., and Krier, H., "Two-Phase Steady Detonation Analysis," presented at 11th ICDERS, Warsaw, 1987, to appear in AIAA Progress Series.

Powers, J. M., Stewart, D. S., and Krier, H., "Analysis of Steady Compaction Waves in Porous Materials, submitted to *Journal of Applied Mechanics*, 1987.

Powers, J. M., "Analysis of Two-Phase Steady Detonation Structure," PhD Dissertation, University of Illinois at Urbana-Champaign, to be published, May 1988.

papers from dissertation to be submitted to either

International Journal of Multiphase Flow

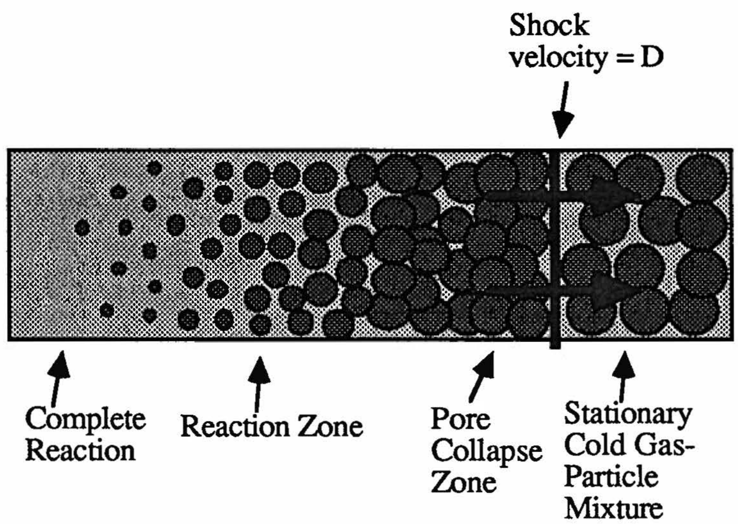
Combustion and Flame

Journal of Fluid Mechanics

Review of Two-Phase Unsteady Detonation Deflagration to Detonation Transition (DDT)

Bernecker and Price	1974	Combust. Flame
Butler, Lembeck, and Krier	1982	Combust. Flame
Butler and Krier	1986	Combust. Flame
Baer and Nunziato	1986	Int. J. Multiphase Flow

Envisioned Two-Phase Detonation



Scope of Discussion

TWO-PHASE REACTIVE FLOW MODEL

-granulated solid propellant

-similar to models of Butler-Krier and Baer-Nunziato

-one phase reactive solid, the other inert gas

-concerned with *steady, one-dimensional* solutions

-two-phase strong, weak, and CJ solutions are predicted

Motivation

-to establish if a two-phase model admits steady detonation solutions

-to study the fundamental influence of two phases on detonation properties

-to classify all possible two-phase steady detonation states

-to determine the relevant length scales

-to provide a base for further study:

1. time-dependent one-dimensional theory
2. one-dimensional stability theory
3. multidimensional theory
4. effective one-phase properties

Unsteady Model Features

-presented at 11th ICDERS, Warsaw, 1987

-representative of a larger class of two-phase models

-each phase obeys a mass, momentum, and energy evolution equation

-gas and solid mass, momentum, and energy equations add to form homogeneous mixture mass, momentum, and energy equations

-volume fraction ($\phi \equiv$ phase volume / total volume) utilized

-PDE's are hyperbolic

-characteristic wave speeds: $u_1, u_2, u_1 \pm c_1, u_2 \pm c_2$

-dynamic compaction equation employed for closure

-number of particles conserved

-compressible spherical reactive particles

-simplified drag and heat transfer relations

-virial gas equation of state for inert gas

-Tait equation of state for reactive particles

Unsteady Model Equations

$$\frac{\partial}{\partial t}\left[\rho_1\phi_1\right] + \frac{\partial}{\partial x}\left[\rho_1\phi_1 u_1\right] = \left(\frac{3}{r}\right)\rho_2\phi_2 a P_1^m \qquad \text{gas mass}$$

$$\frac{\partial}{\partial t}\left[\rho_2\phi_2\right] + \frac{\partial}{\partial x}\left[\rho_2\phi_2 u_2\right] = -\left(\frac{3}{r}\right)\rho_2\phi_2 a P_1^m \qquad \text{solid mass}$$

$$\frac{\partial}{\partial t}\left[\rho_1\phi_1 u_1\right] + \frac{\partial}{\partial x}\left[P_1\phi_1 + \rho_1\phi_1 u_1^2\right] = u_2\left(\frac{3}{r}\right)\rho_2\phi_2 a P_1^m - \beta\frac{\phi_1\phi_2}{r}(u_1-u_2) \qquad \text{gas momentum}$$

$$\frac{\partial}{\partial t}\left[\rho_2\phi_2 u_2\right] + \frac{\partial}{\partial x}\left[P_2\phi_2 + \rho_2\phi_2 u_2^2\right] = -u_2\left(\frac{3}{r}\right)\rho_2\phi_2 a P_1^m + \beta\frac{\phi_1\phi_2}{r}(u_1-u_2) \qquad \text{solid momentum}$$

$$\frac{\partial}{\partial t}\left[\rho_1\phi_1\left(e_1 + u_1^2/2\right)\right] + \frac{\partial}{\partial x}\left[\rho_1\phi_1 u_1\left(e_1 + u_1^2/2 + P_1/\rho_1\right)\right] =$$

$$\left(e_2 + u_2^2/2\right)\left(\frac{3}{r}\right)\rho_2\phi_2 a P_1^m - \beta\frac{\phi_1\phi_2}{r}u_2(u_1-u_2) - h\frac{\phi_1\phi_2}{r^{1/3}}(T_1-T_2) \qquad \text{gas energy}$$

$$\frac{\partial}{\partial t}\left[\rho_2\phi_2\left(e_2 + u_2^2/2\right)\right] + \frac{\partial}{\partial x}\left[\rho_2\phi_2 u_2\left(e_2 + u_2^2/2 + P_2/\rho_2\right)\right] =$$

$$-\left(e_2 + u_2^2/2\right)\left(\frac{3}{r}\right)\rho_2\phi_2 a P_1^m + \beta\frac{\phi_1\phi_2}{r}u_2(u_1-u_2) + h\frac{\phi_1\phi_2}{r^{1/3}}(T_1-T_2) \qquad \text{solid energy}$$

$$\frac{\partial}{\partial t}\left[\phi_2/r^3\right] + \frac{\partial}{\partial x}\left[u_2\phi_2/r^3\right] = 0 \qquad \text{number conservation}$$

$$\frac{\partial\phi_2}{\partial t} + u_2\frac{\partial\phi_2}{\partial x} = \frac{\phi_1\phi_2}{\mu_c}\left[P_2 - P_1 - G\phi_2\right] - \left(\frac{3}{r}\right)\phi_2 a P_1^m \qquad \text{compaction}$$

$$P_1 = \rho_1 R T_1\left(1 + b\rho_1\right) \qquad e_1 = c_{v1}T_1 \qquad \text{gas state equations}$$

$$P_2 = \left(\gamma_2 - 1\right)c_{v2}\rho_2 T_2 - \frac{\rho_{20}c_{20}^2}{\gamma_2} \qquad e_2 = \frac{P_2 + \rho_{20}c_{20}^2}{(\gamma_2 - 1)\,\rho_2} + q \qquad \text{solid state equations}$$

$$\phi_1 + \phi_2 = 1 \qquad \text{porosity equation}$$

Number Conservation

-number density of particles conserved; no splitting or agglomeration

-provides functional relationship for particle diameter

-not in common usage in DDT modeling

$$\phi_2 = \frac{\text{solid volume}}{\text{total volume}} = \frac{\text{number particles x volume particle}}{\text{total volume}} = n\frac{4}{3}\pi r^3$$

$$n = \frac{3\phi_2}{4\pi r^3}$$

From control volume analysis--number conservation:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}\left[u_2 n\right] = 0 \qquad \text{(a)}$$

or with definition of n

$$\frac{\partial}{\partial t}\left[\phi_2 / r^3\right] + \frac{\partial}{\partial x}\left[u_2\phi_2 / r^3\right] = 0 \qquad \text{(b)}$$

With solid mass (c)

$$\frac{\partial}{\partial t}\left[\rho_2\phi_2\right] + \frac{\partial}{\partial x}\left[\rho_2\phi_2 u_2\right] = -\left(\frac{3}{r}\right)\rho_2\phi_2 a P_1^m \qquad \text{(c)}$$

Combine (b) and (c):

$$\frac{\partial r}{\partial t} + u_2\frac{\partial r}{\partial x} = -a P_1^m - \frac{r}{3\rho_2}\left(\frac{\partial \rho_2}{\partial t} + u_2\frac{\partial \rho_2}{\partial x}\right) \qquad \text{(d)}$$

radius change   chemical reaction   density change

Dynamic Pore Collapse and Compaction Viscosity

$$\frac{\partial \phi_2}{\partial t} + u_2 \frac{\partial \phi_2}{\partial x} = \frac{\phi_1 \phi_2}{\mu_c}\left[P_2 - P_1 - G\phi_2\right] - \left(\frac{3}{r}\right)\phi_2 a P_1^m$$

-Models time-dependent collapse of pores (Carroll and Holt, 1974); based on static experiments

-volume fraction changes from pore collapse and chemical reaction

-compaction viscosity controls pore collapse time

μ_c assumed constant

Nunziato's equation $\mu_c = r\, c_2\, \rho_2$ only an estimate

solid sound speed c_2 variable

-insures hyperbolic system

Dimensional Input Parameters

a	[m / (s Pa)]	2.90×10^{-9}
ρ_{10}	[kg / m³]	1.
m		1.
β	[kg / (s m²)]	3.5×10^{5}
ρ_{20}	[kg / m³]	1900.
h	[J / (s K m²)] 8/3	1.0×10^{7}
c_{v1}	[J / (kg K)]	2400.
c_{v2}	[J / (kg K)]	1500.
R	[J / (kg K)]	850.
c_{20}	[m / s]	2996.
q	[J / kg]	5.84×10^{6}
ϕ_{10}		0.30
r_0	[m]	0.0001
b	[m³ / kg]	0.0011
γ_2		5.
α		1.
μ_c	[kg / (m s)]	1.0×10^{6}
T_0	[K]	300.

Dimensionless Parameters

Assume a steady wave propagates through the two-phase mixture with speed D.

Examine the solution in the steady wave frame; let $\xi = x - Dt$

$\xi_* = \xi / L$ $\quad v_{*i} = v_i / D$ $\quad P_{*i} = P_i / (\rho_{i0} D^2)$ $\quad i = 1, 2$

$\rho_{*i} = \rho_i / \rho_{i0}$ $\quad e_{*i} = e_i / D^2$ $\quad T_{*i} = c_{vi} T_i / D^2$ $\quad r_* = r / L$

π_1	$3a\rho_{10}{}^m D^{2m-1}$	Damkohler Number for Particle Burning
π_2	$\beta / \rho_{20} D$	Drag Coefficient
π_3	$h\, L^{2/3} / (\rho_{20} c_{v1} D)$	Heat Transfer Parameter
π_4	m	Burning Exponent
π_5	ρ_{10} / ρ_{20}	Gas/Solid Density Ratio
π_6	c_{v1} / c_{v2}	Gas/Solid Specific Heat Ratio
π_7	$R / c_{v1} + 1$	Gas Gruneisen Ratio + 1
π_8	$c_{20}{}^2 / (D^2 \gamma_2)$	Non-Ideal Solid Parameter
π_9	$\rho_{20}\, D\, L / \mu_c$	Compaction Reynolds Number
π_{10}	q / D^2	Dimensionless Heat Release
π_{11}	ϕ_{10}	Initial Porosity
π_{12}	r_0 / L	Initial Particle Radius
π_{13}	$b\, \rho_{10}$	Non-Ideal Gas Parameter
π_{14}	$c_{v2} T_0 / D^2$	$1 / [\gamma_2(\gamma_2 - 1)$Solid Mach Number$]^2$
π_{17}	γ_2	~~Gas~~ Solid Gruneisen Ratio + 1

Dependent Dimensionless Parameters

$$\pi_{15} = \frac{\pi_{21} - \pi_5\pi_{19}}{1 - \pi_{11}}$$ pore collapse parameter

$$\pi_{18} = \pi_{11} + \frac{1 - \pi_{11}}{\pi_5}$$ mixture density

$$\pi_{19} = \left[\pi_7 - 1\right]\pi_6\,\pi_{14}\left[1 + \pi_{13}\right]$$ initial gas pressure

$$\pi_{20} = 1 - \pi_{11}$$ initial solid volume fraction

$$\pi_{21} = \left[\pi_{17} - 1\right]\pi_{14} - \pi_8$$ initial solid pressure

$$\pi_{22} = \pi_{11}\left[\pi_6\,\pi_{14} + \frac{1}{2} + \pi_{19}\right] + \frac{1 - \pi_{11}}{\pi_5}\left[\pi_{14} + \pi_8 + \pi_{10} + \frac{1}{2} + \pi_{21}\right]$$

mixture energy

$$\pi_{23} = \pi_{11}\,\pi_{19} + \frac{1 - \pi_{11}}{\pi_5}\pi_{21}$$ mixture pressure

Dimensionless Steady Equations

$$\frac{d}{d\xi}\left[\rho_2\phi_2 v_2\right] = -\pi_1 \frac{\rho_2\phi_2 P_1^{\pi_4}}{r}$$ solid mass

$$\rho_2\phi_2 v_2\frac{dv_2}{d\xi} + \frac{d}{d\xi}\left[P_2\phi_2\right] = -\pi_2\left[v_2 - v_1\right]\frac{\phi_1\phi_2}{r}$$ solid momentum

$$\rho_2 v_2\frac{de_2}{d\xi} + P_2\frac{dv_2}{d\xi} = -\pi_3\left[\pi_6 T_2 - T_1\right]\frac{\phi_1}{r^{1/3}}$$ solid energy

$$v_2\frac{d\phi_2}{d\xi} = \pi_9\phi_1\phi_2\left[P_2 - \pi_5 P_1 - \pi_{15}\phi_2\right] - \pi_1\frac{\phi_2 P_1^{\pi_4}}{r}$$ compaction

$$\rho_1\phi_1 v_1 + \frac{1}{\pi_5}\rho_2\phi_2 v_2 = -\pi_{18}$$ mixture mass

$$\rho_1\phi_1 v_1^2 + P_1\phi_1 + \frac{1}{\pi_5}\left[\rho_2\phi_2 v_2^2 + P_2\phi_2\right] = \pi_{18} + \pi_{23}$$ mixture momentum

$$\rho_1\phi_1 v_1\left[e_1 + \frac{v_1^2}{2} + \frac{P_1}{\rho_1}\right] + \frac{1}{\pi_5}\rho_2\phi_2 v_2\left[e_2 + \frac{v_2^2}{2} + \frac{P_2}{\rho_2}\right] = -\pi_{22}$$ mixture energy

$$r = \pi_{12}\sqrt[3]{\frac{-v_2\phi_2}{1-\pi_{11}}}$$ number conservation

$$P_1 = \left[\pi_7 - 1\right]\rho_1 T_1\left[1 + \pi_{13}\rho_1\right] \qquad e_1 = T_1$$ gas state equations

$$P_2 = \left[\pi_{17} - 1\right]\rho_2 T_2 - \pi_8 \qquad e_2 = \frac{P_2 + \pi_{17}\pi_8}{(\pi_{17}-1)\,\rho_2} + \pi_{10}$$ solid state equations

$$\phi_1 + \phi_2 = 1$$ porosity equation

$$\rho_2 = 1 \qquad v_2 = -1 \qquad \phi_2 = \pi_{20} \qquad T_2 = \pi_{14}$$ undisturbed conditions

Inert Shock Jump Conditions

$$\left[\rho_2 \phi_2 v_2 \right]_0^s = 0$$ solid mass

$$\left[P_2 \phi_2 + \rho_2 \phi_2 v_2^2 \right]_0^s = 0$$ solid momentum

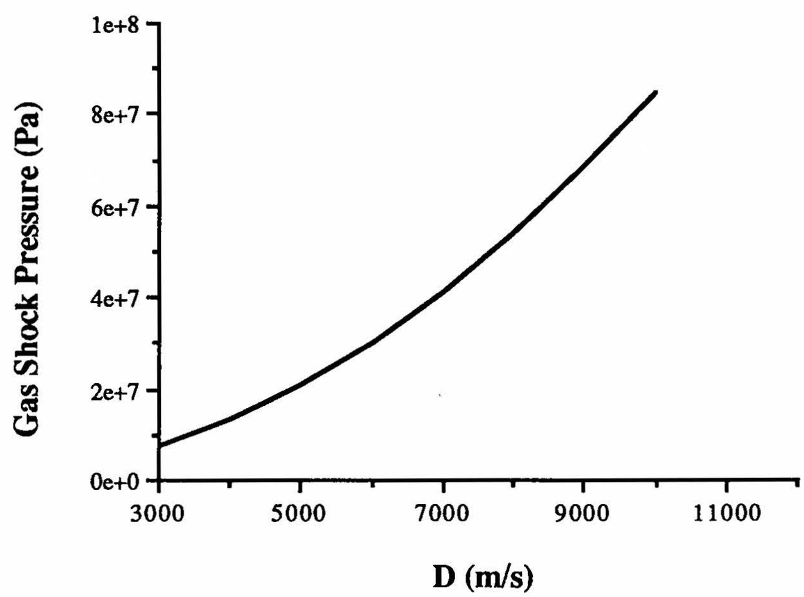
$$\left[\rho_2 \phi_2 v_2 \left(e_2 + v_2^2/2 + P_2/\rho_2 \right) \right]_0^s = 0$$ solid energy

$$\left[\phi_2 \right]_0^s = 0$$ porosity

Mixture equations define gas shock jumps--four possibilities

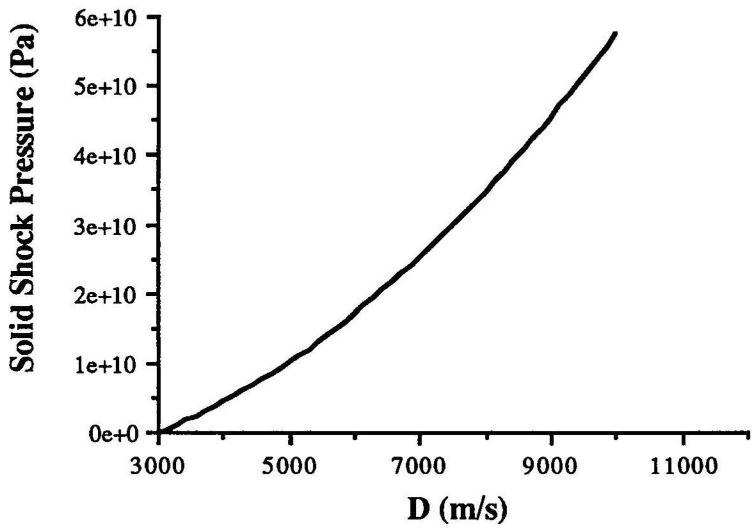
1. Unshocked gas, unshocked solid
2. Shocked gas, shocked solid
3. Unshocked gas, shocked solid
4. *Shocked gas, unshocked solid (analog with ZND theory)*

Gas Shock Pressure



$$P_{1s} \cong \underbrace{\left[\frac{2 - \pi_{14}\pi_6 \left(\pi_7 - 1\right)^2}{\pi_7 + 1} \right]}_{\text{ideal}} - \underbrace{\left[\frac{2 + \pi_{14}\pi_6 \left(\pi_7 - 1\right)^2}{\pi_7 + 1} \right] \pi_{13}}_{\text{non-ideal correction}}$$ Gas Shock Pressure

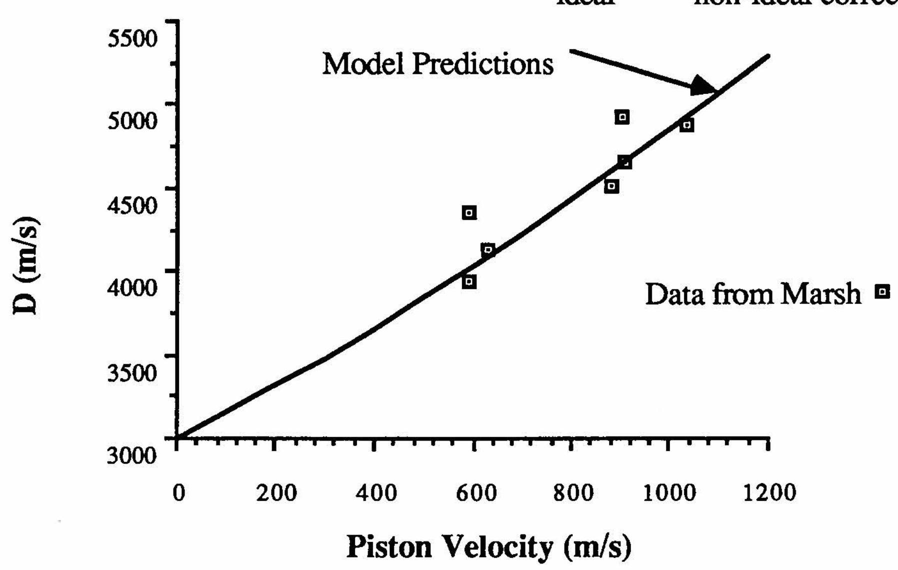
Solid Shock Properties



$$P_{2s} = \frac{2 - \pi_{14}\left(\pi_{17} - 1\right)^2}{\pi_{17} + 1} - \pi_8$$

solid shock pressure

ideal non-ideal correction



$$D = \frac{1+\gamma_2}{4} u_p + \sqrt{\left(\frac{1+\gamma_2}{4} u_p\right)^2 + \gamma_2(\gamma_2 - 1)\, c_{v2}\, T_{20}}$$

(ambient sound speed)^2

End States

-Setting inhomogenities to zero determines the end state

- -complete reaction state
- -drag balances chemical reaction

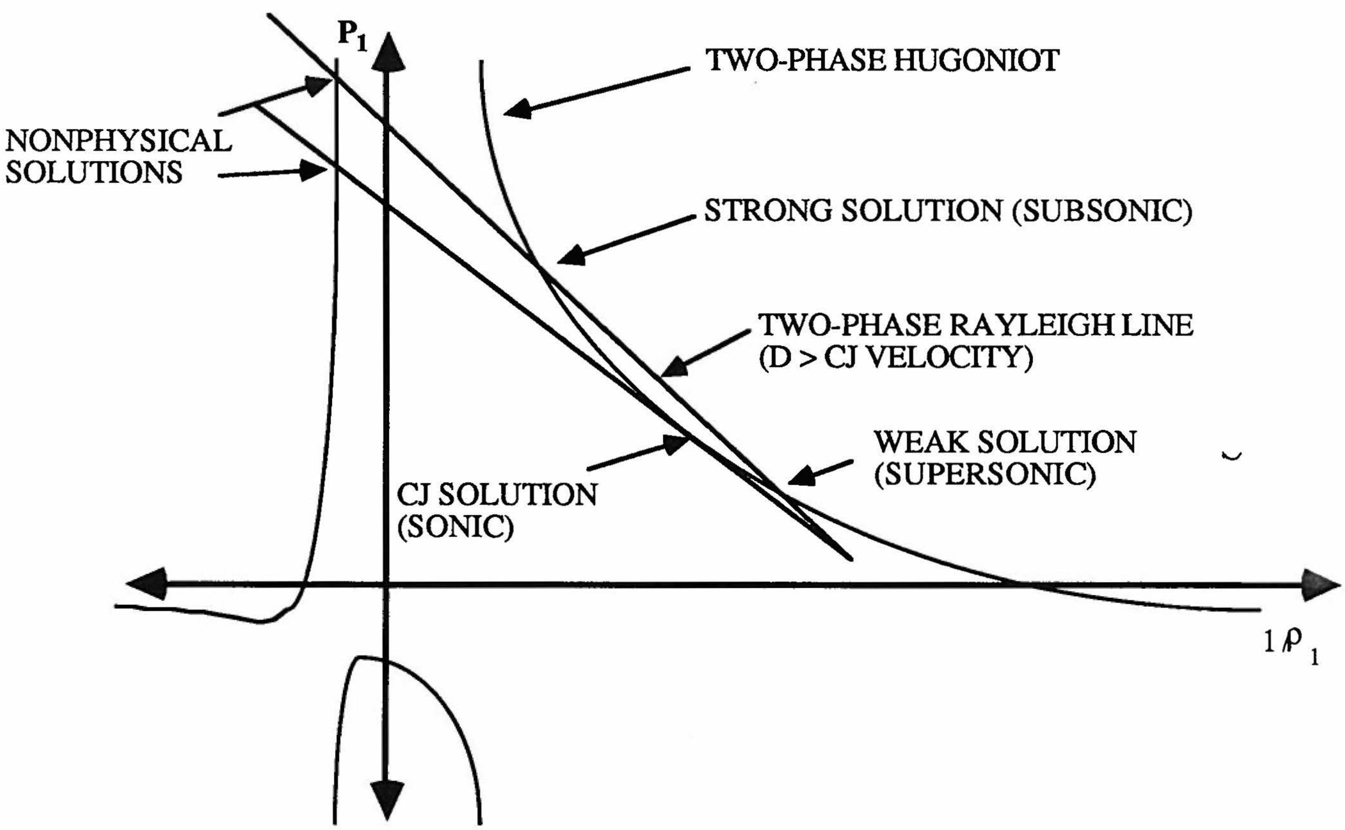
-Leading shock in gas, unshocked solid--CJ wave speed is the speed of an unsupported two-phase detonation

- -gas velocity at complete reaction state is sonic
- -unsteady rarefactions cannot catch steady reaction zone structure
- -analogous to one-phase ZND model

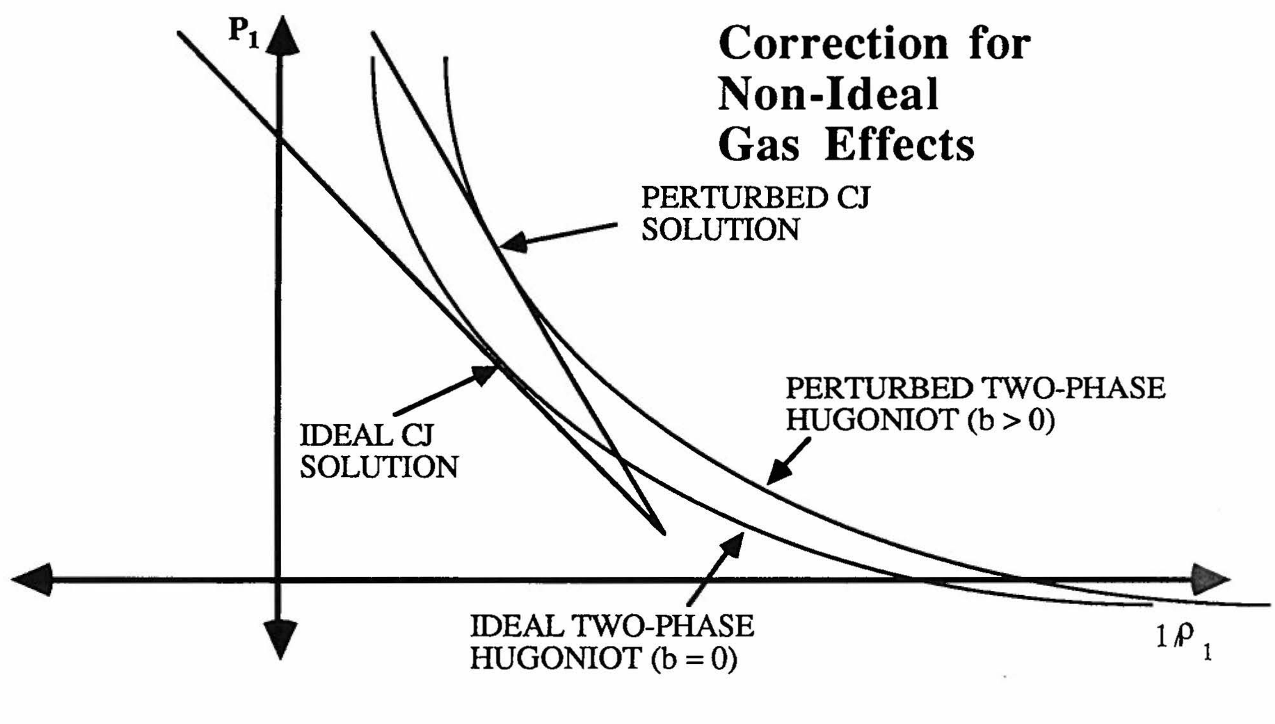
-Other types of detonations possible

- -leading shock in gas, unshocked solid, $D>D_{cj}$--analogous to strong solution of ZND model
- -unshocked solid and gas--weak solutions available for continuum of wave speeds for $D>D_{cj}$
- -shocked gas and solid--eigenvalue solution available
- -unshocked gas and shocked solid--potential for LVD (low-velocity detonation)-not found yet

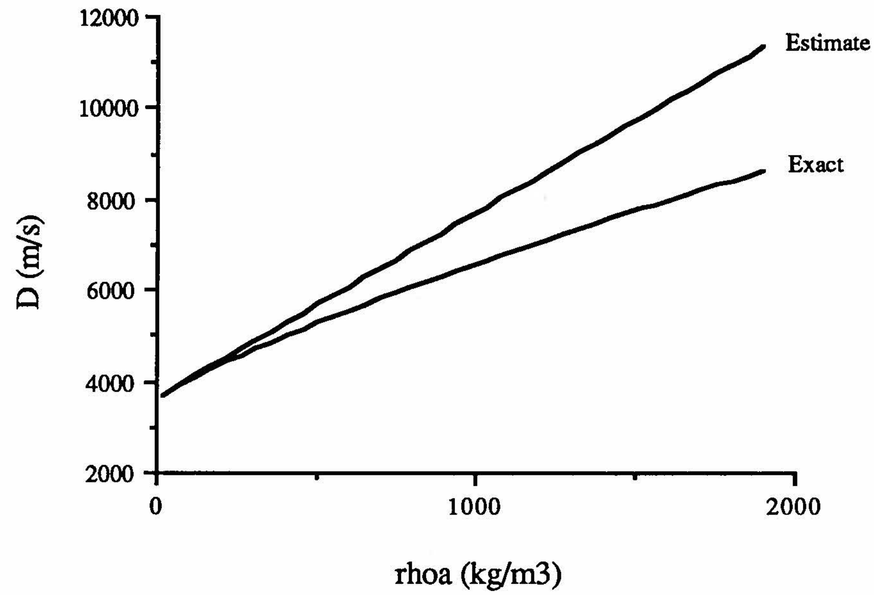
Two-Phase End States



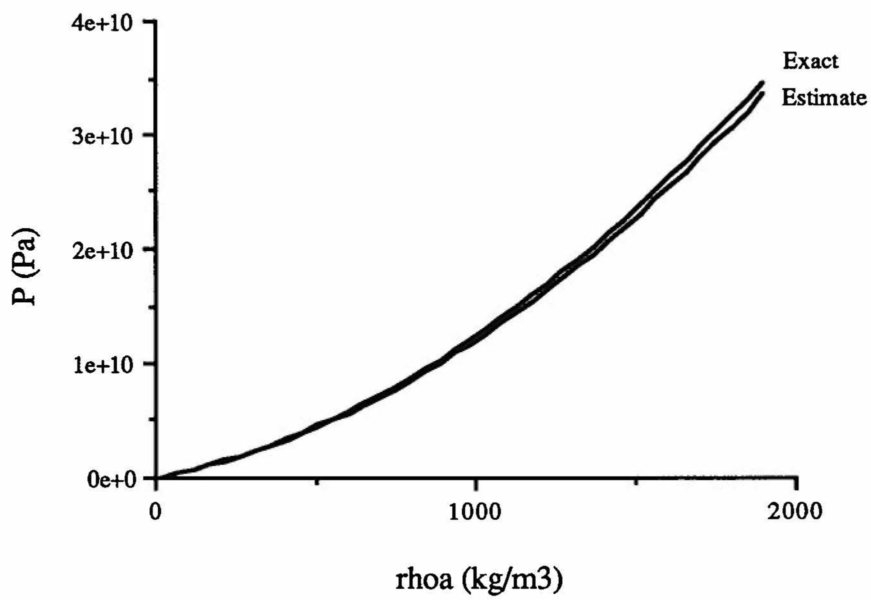
Correction for Non-Ideal Gas Effects



CJ Properties

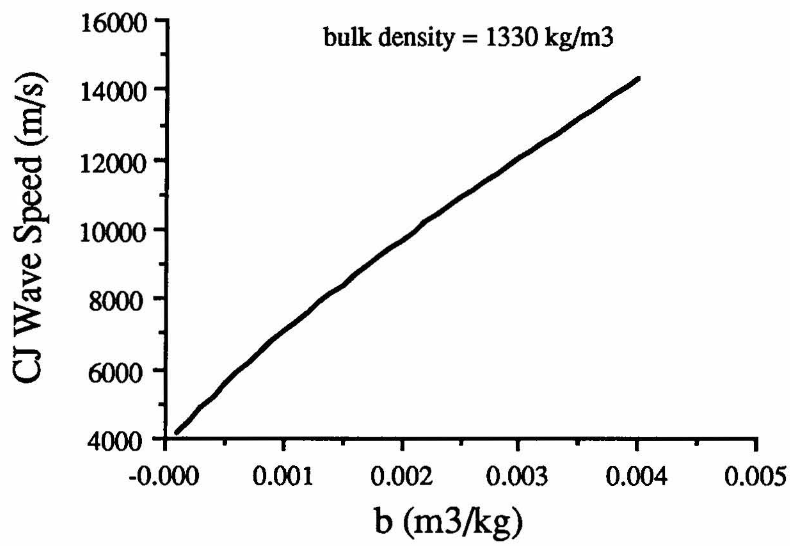


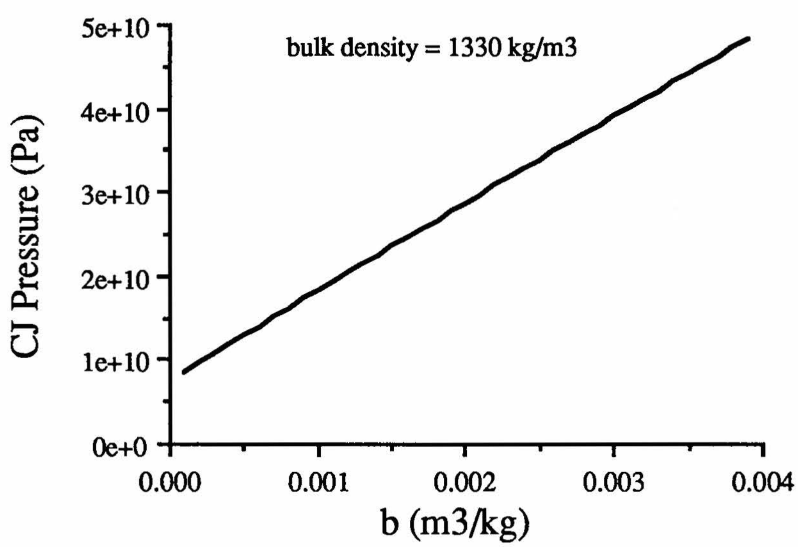
$$D_{CJ} \cong \frac{\sqrt{2e_a R(R+2c_{v1})}}{c_{v1}} \left(1 + b\rho_a - \frac{c_{v1}^2}{2R(R+2c_{v1})} \frac{P_a}{\rho_a e_a} \right)$$



$$P_{CJ} \cong \frac{2e_a R}{c_{v1}} \rho_a \left(1 + b\rho_a - \frac{c_{v1}^2}{2R(R+2c_{v1})} \frac{P_a}{\rho_a e_a} \right)$$

Sensitivity to Non-Ideal Parameter b





Special Case

Mass and energy equations may be integrated analytically in the following limits:

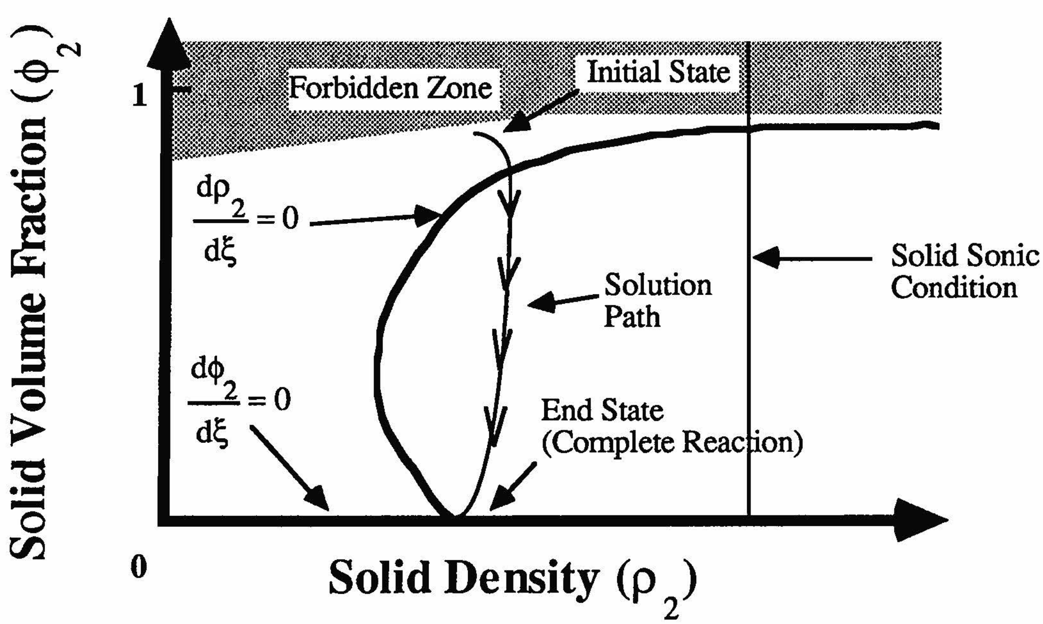
- -chemical reaction dominates compaction ($\pi_1 >> \pi_9$)
- -negligible heat transfer ($\pi_3 \rightarrow 0$)

Take limit of ideal gas to reduce algebraic complexity

Resulting equations can be expressed as two differential equations in two unknowns, solid density and solid volume fraction.

Phase space is the ρ_2-ϕ_2 plane--easy to understand

$\rho_2 - \phi_2$ Phase Plane



Canonical Equations

$$\frac{d\rho_2}{d\xi} = \frac{\pi_2(v_1-v_2)\rho_2^2\phi_1 - \pi_1\left[(\pi_{21}+\pi_8)\rho_2^{\pi_{17}} - \pi_8\right]\rho_2^3 P_1^{\pi_4}}{r\left[\pi_{17}(\pi_{21}+\pi_8)\rho_2^{\pi_{17}+1} - 1\right]} \qquad \frac{d\phi_2}{d\xi} = \frac{\pi_1\rho_2\phi_2 P_1^{\pi_4}}{r}$$

$$\phi_1 = 1 - \phi_2$$

$$v_2 = -\frac{1}{\rho_2} \qquad P_2 = (\pi_{21} + \pi_8)\,\rho_2^{\pi_{17}} - \pi_8$$

$$\rho_1 = \Theta\left[\Omega \pm \sqrt{\Omega^2 - \Lambda}\right] \qquad P_1 = \Delta - \frac{\Theta}{\Omega \pm \sqrt{\Omega^2 - \Lambda}}$$

$$v_1 = \frac{-1}{\Omega \pm \sqrt{\Omega^2 - \Lambda}} \qquad r = \pi_{12}\sqrt[3]{\frac{-v_2\,\phi_2}{1 - \pi_{11}}}$$

$$T_1 = \frac{1}{\pi_7 - 1}\frac{P_1}{\rho_1} \qquad e_1 = \frac{1}{\pi_7 - 1}\frac{P_1}{\rho_1}$$

$$T_2 = \frac{1}{\pi_{17} - 1}\frac{P_2 + \pi_8}{\rho_2} \qquad e_2 = \frac{P_2 + \pi_{17}\pi_8}{(\pi_{17} - 1)\rho_2} + \pi_{10}$$

$$\Omega = \frac{\pi_7}{\pi_7 - 1}\frac{\pi_{18} + \pi_{23} - \frac{1}{\pi_5}\left(\rho_2\phi_2 v_2^2 + P_2\phi_2\right)}{2\left[\pi_{22} + \frac{1}{\pi_5}\rho_2\phi_2 v_2\left(e_2 + \frac{v_2^2}{2} + \frac{P_2}{\rho_2}\right)\right]} \qquad \Lambda = \frac{\pi_7 + 1}{\pi_7 - 1}\frac{\pi_{18} + \frac{1}{\pi_5}\rho_2\phi_2 v_2}{2\left[\pi_{22} + \frac{1}{\pi_5}\rho_2\phi_2 v_2\left(e_2 + \frac{v_2^2}{2} + \frac{P_2}{\rho_2}\right)\right]}$$

$$\Delta = \frac{\pi_{18} + \pi_{23} - \frac{1}{\pi_5}\left(\rho_2\phi_2 v_2^2 + P_2\phi_2\right)}{1 - \phi_2} \qquad \Theta = \frac{\pi_{18} + \frac{1}{\pi_5}\rho_2\phi_2 v_2}{1 - \phi_2}$$

Conditions for Existence of CJ Detonation

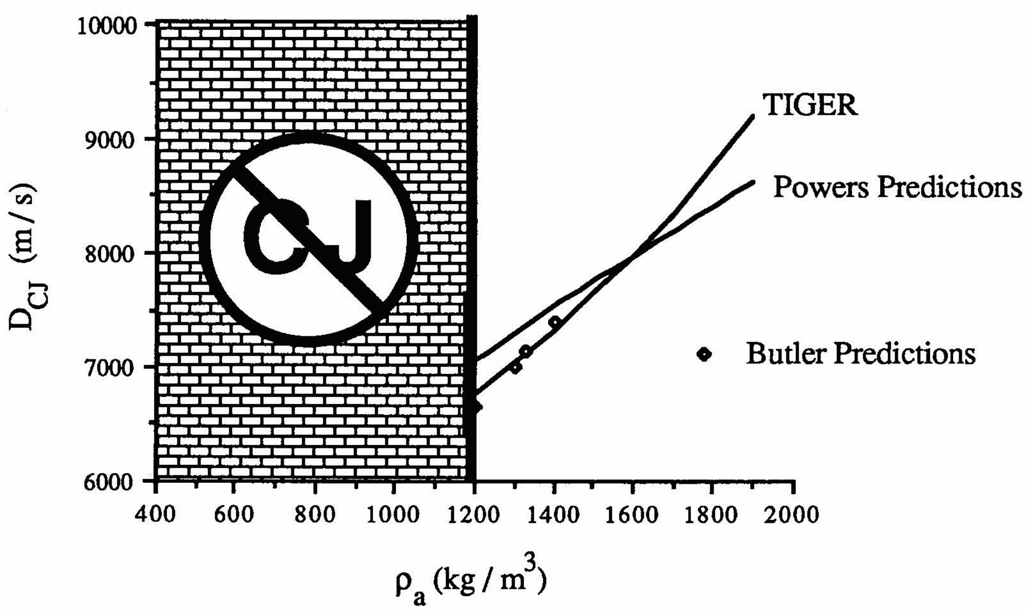
-CJ conditions predicted algebraically

-Reaction zone structure must be acceptable

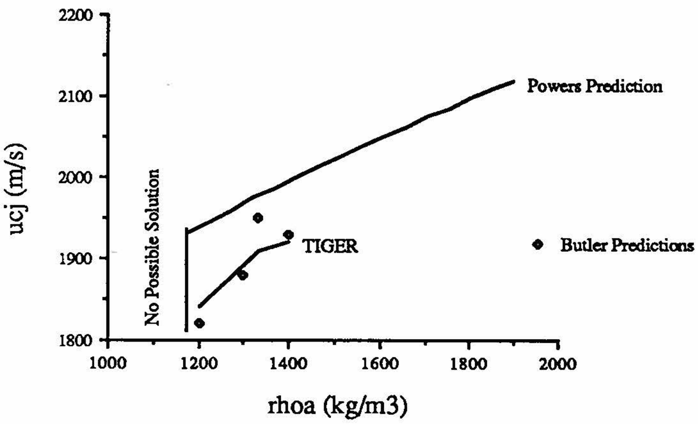
density, pressure, temperature > 0

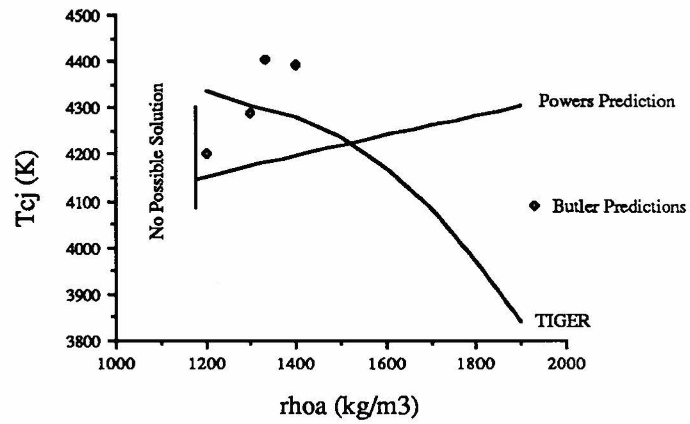
in general $M_1, M_2 \neq 1$

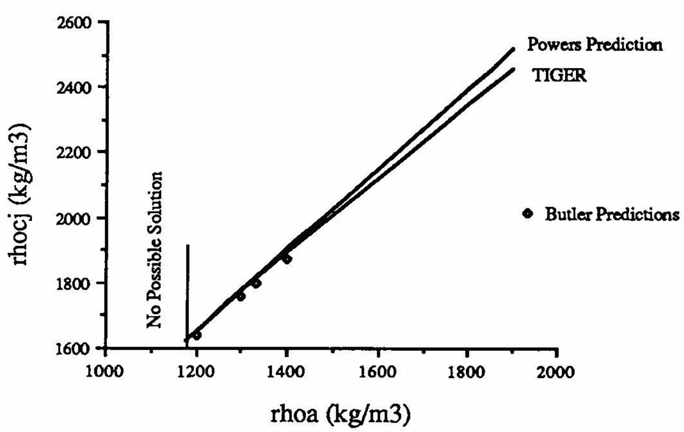
for $\phi_{20} < 0.6$ solid sonic condition reached

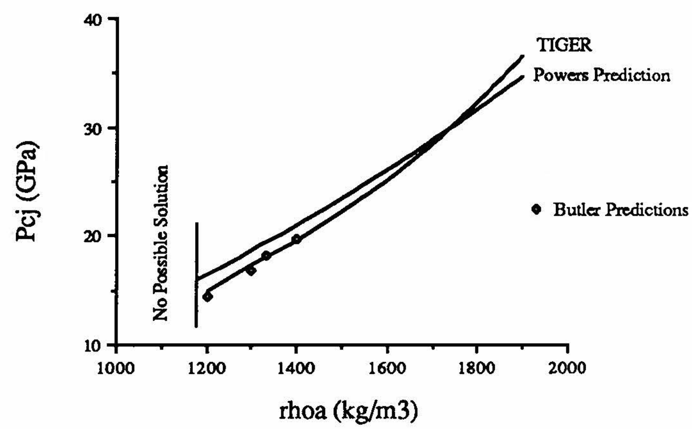


CJ Properties vs. Initial Bulk Density

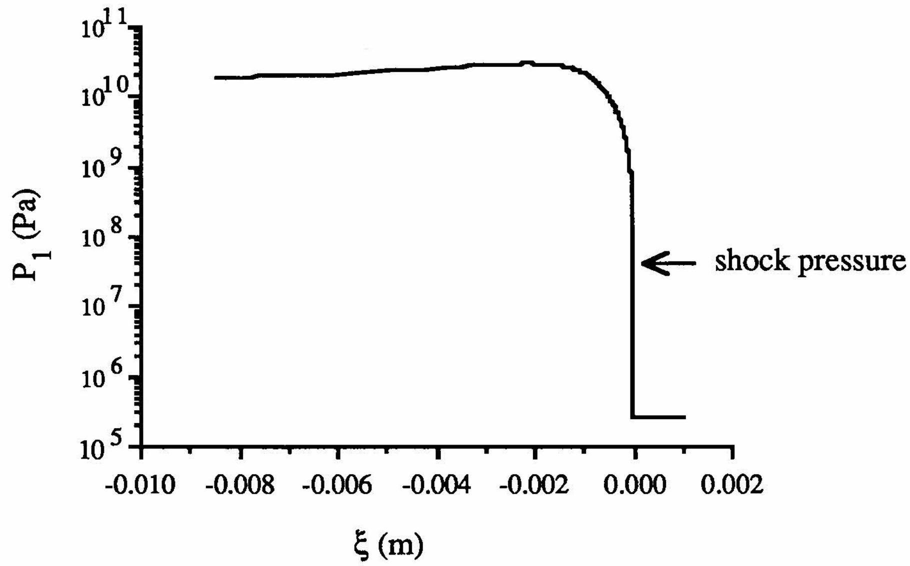


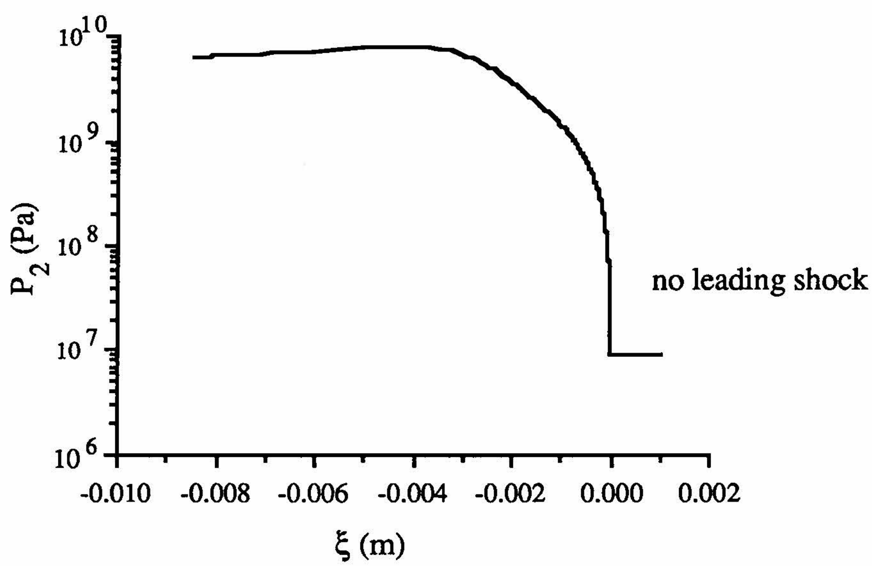




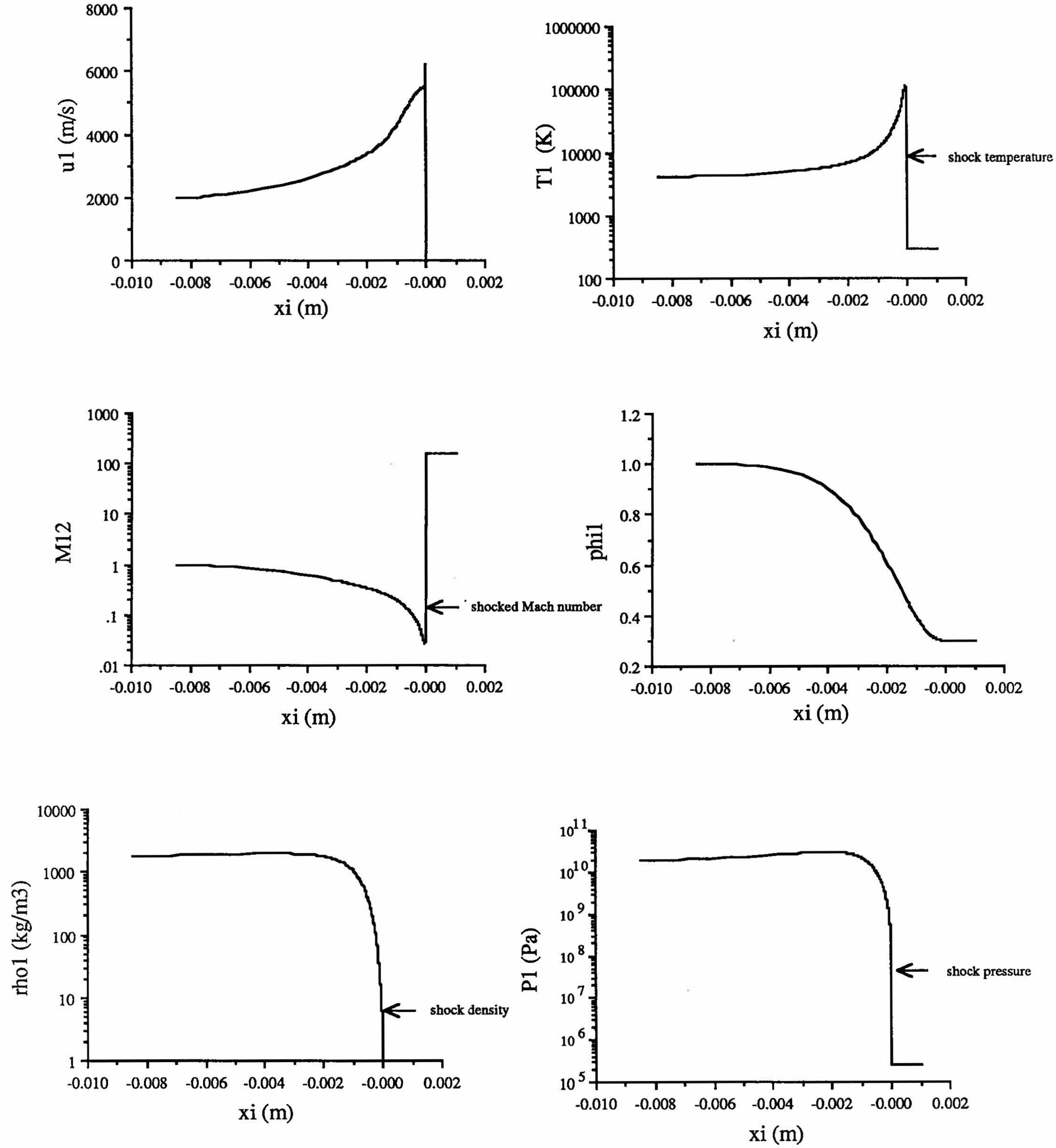


Reaction Zone Structure

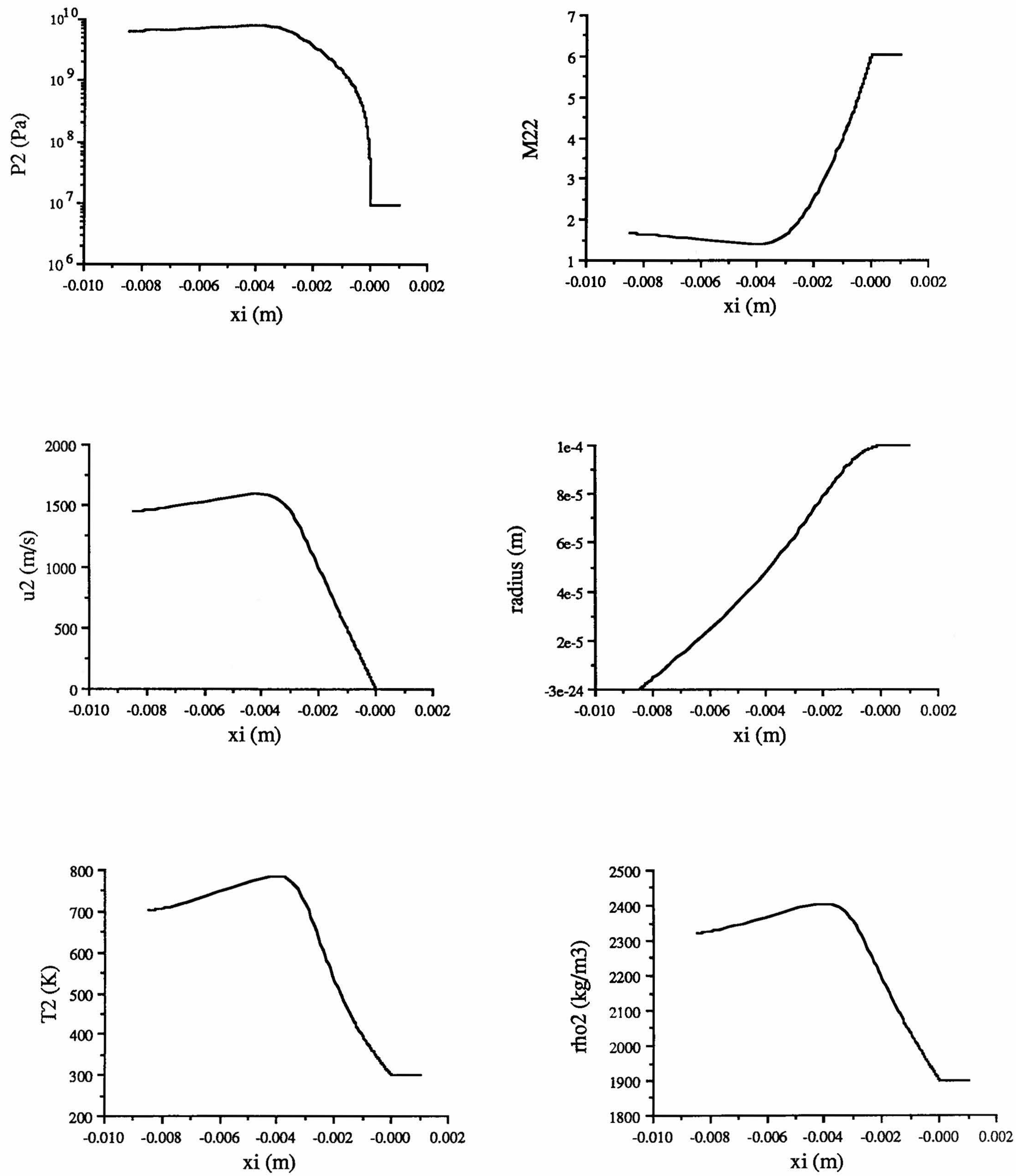




Gas Phase Reaction Zone Structure



Solid Phase Reaction Zone Structure



Compaction Zone Structure

-thin layer (thickness ~ 10 μm) near wave head

-adjustments in gas phase only

-cell size of ~0.1 μm necessary to capture this layer

-Butler-Krier, Nunziato-Baer miss this (cell size ~ 1.0 mm)

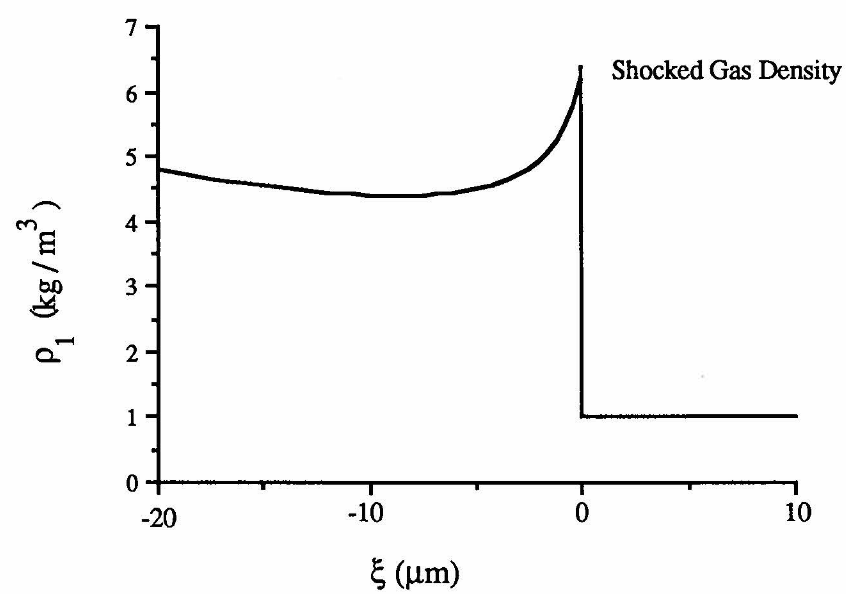
-Dilemma

Equations predict changes on the order of 1 μm

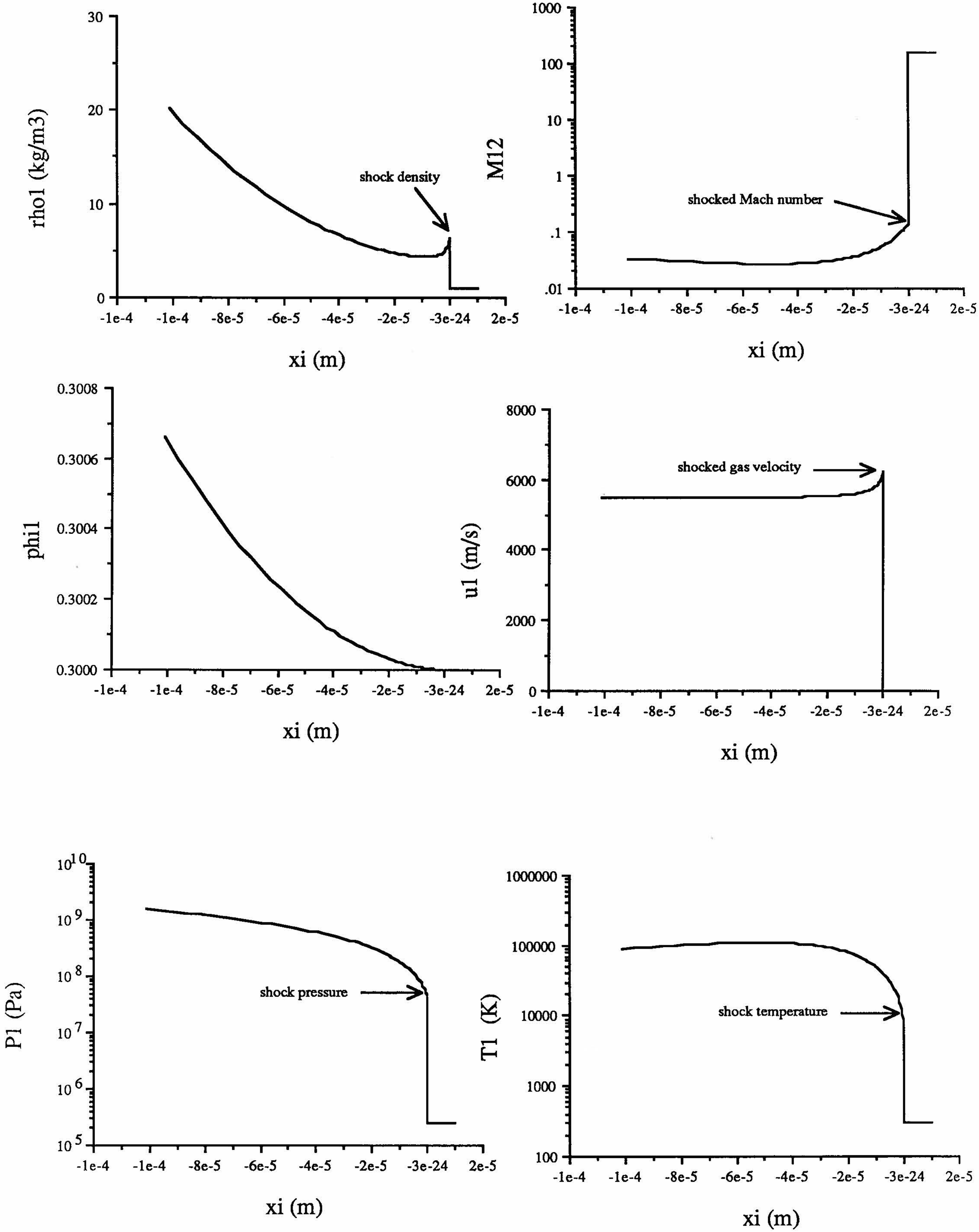
Particle Size ~ 100 μm

Proper averaging volumes require cell size ~ 1 mm

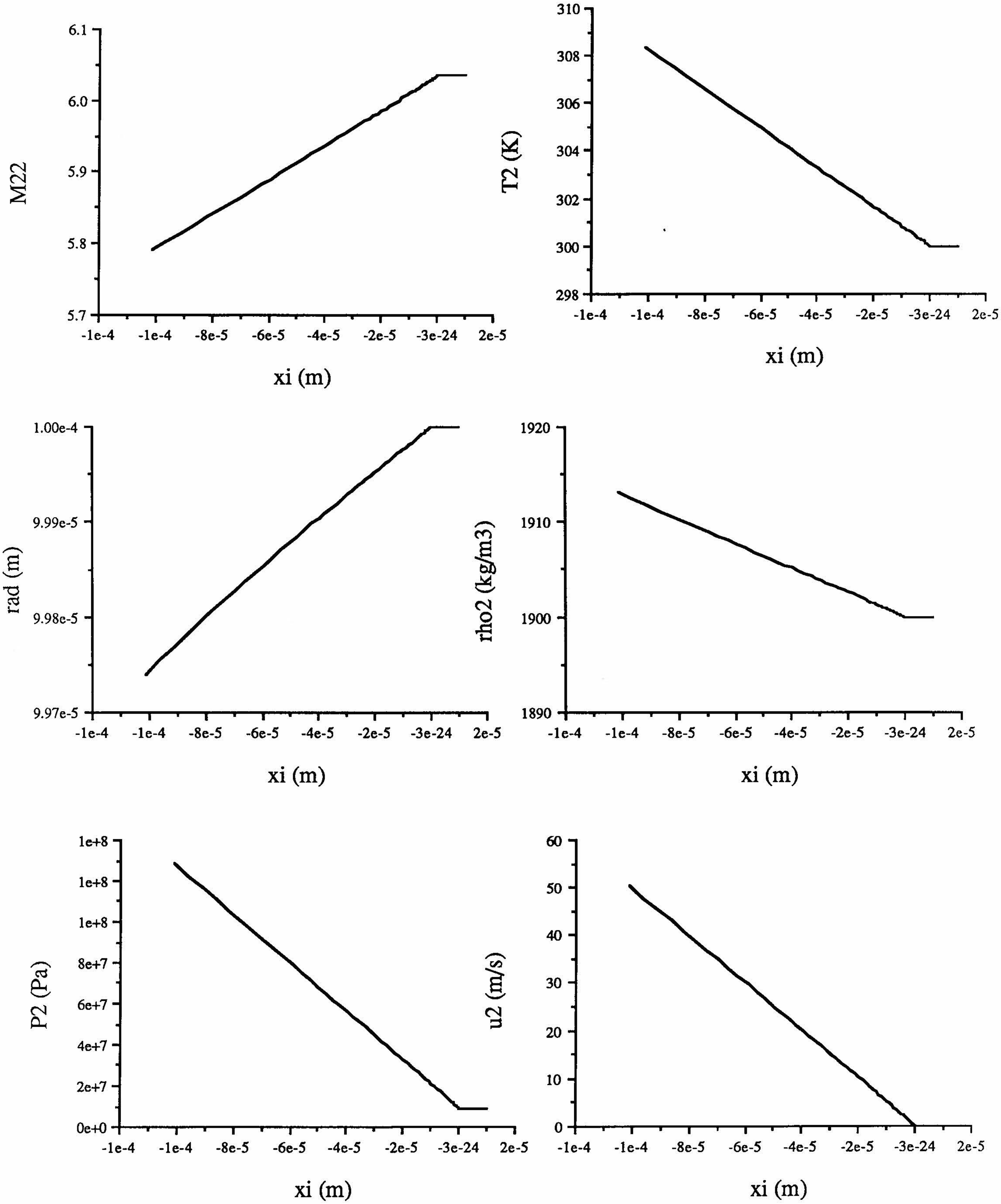
-Compaction zone discussed in paper submitted to *Journal of Applied Mechanics*



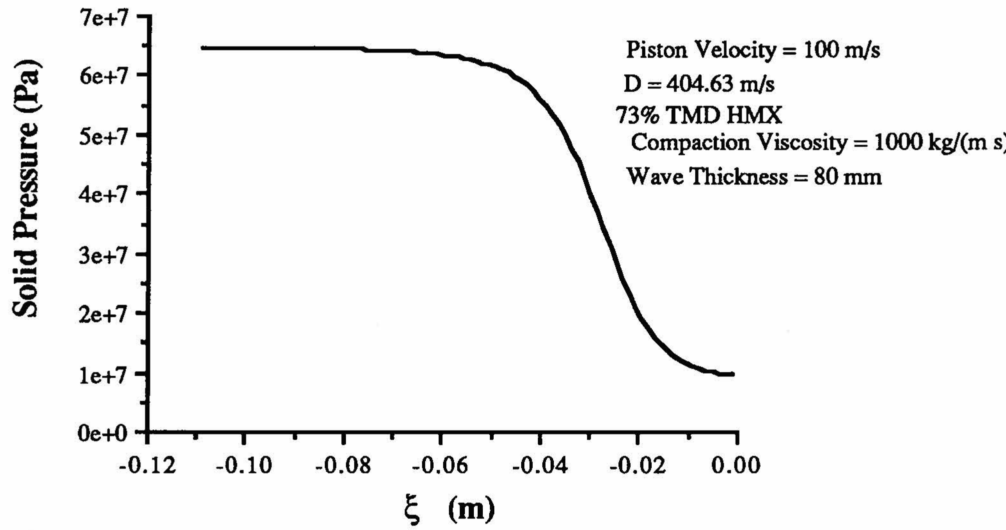
Gas Phase Compaction Zone Structure



Solid Phase Compaction Zone Structure



Compaction Wave Structure



-By considering only solid equations with no reaction, compaction waves are predicted.

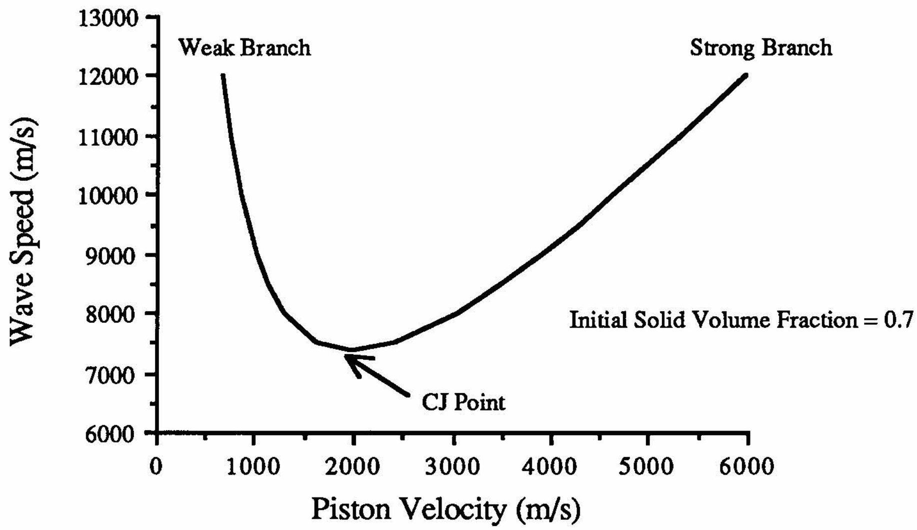
-compaction wave may initiate chemical reaction

-documented in article submitted to Journal of Applied Mechanics

Non-CJ Two-Phase Detonations

Leading shock in gas

Unshocked solid



-CJ wave propagates without piston support

-Strong wave requires piston support

-Weak wave propagates without piston support--reasons to discard weak wave ?

-Other classes of waves may exist for special conditions