Spherical Combustion Layer in a TNT Explosion

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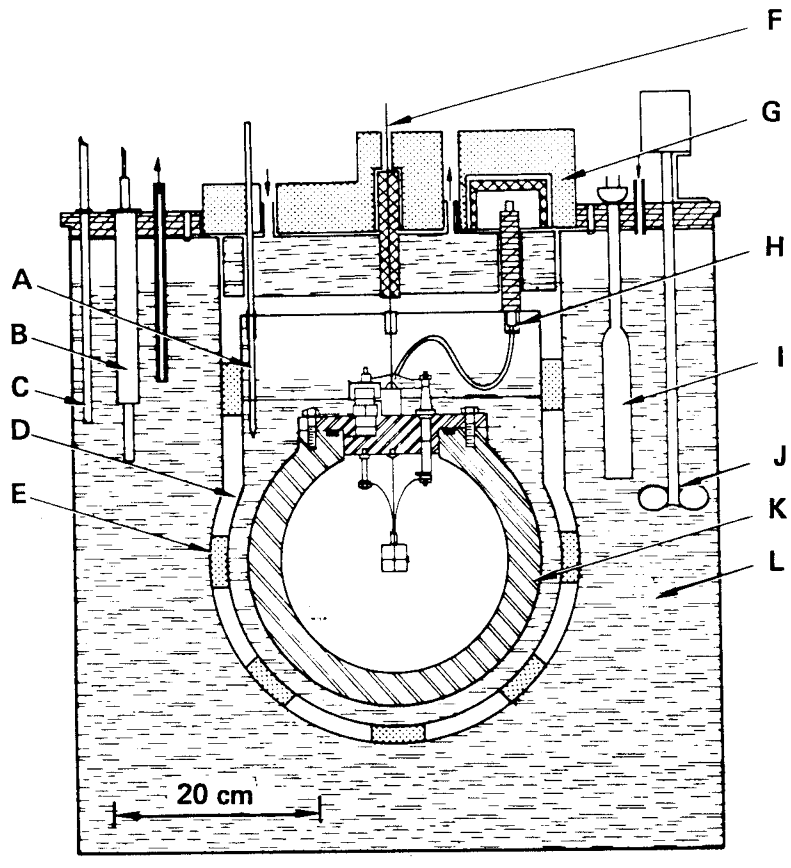
Background: mixing at HE-air interface

1977: S. I. Anisimov & Ya. B. Zel'dovich, "Rayleigh-Taylor instabilitiy of the boundary between deotnation products and gas in a spherical explosion", *Pis'ma Zh. Eksp. Teor. Fiz*, **3**, pp. 1081-1084.

1983: S. I. Anisimov, Ya. B. Zel'dovich, M. A. Inogamov & M. F. Ivanov, " "Taylor instability of contact boundary between expanding detonation products and a surrounding gas", Shock Waves, Explosions & Detonations" *Prog. Astronautics & Astronautics Series,* **87**, AIAA, Wash., DC, pp 218-227.

1996: A. L. Kuhl, "Spherical Mixing Layers in Explosions", *Dynamics of Exothermicity*, Ed. J. R. Bowen, Gordon & Breach, Amsterdam, pp. 291-320.

LLNL Bomb Calorimeter (V=5.28 l)



Composition: *TNT products in O_2 & vacuum*

Experimental conditions		Atmosphere		
		Vacuum, detonation	Carbon dioxide, detonation	Oxygen, detonation
Balance level attempted		-	CO and H_2O	CO_2 and H_2O
Pressure, atm (absolute)		-	1.66	2.46
$-\Delta H$ detonation[c]				
Experimental		1093 ± 11	1116 ± 11	3575 ± 35
Calculated from products		1133 ± 15	1105 ± 15	3594 ± 60
Products, mol/mol TNT	N_2	1.32	1.22	1.54
	H_2O	1.60	1.55	2.65
	CO_2	1.25	1.19[c]	6.82
	CO	1.98	2.05	0.38
	C(s)	3.65	3.65	Not detected
	H_2	0.46	0.45	0.050
	NH_3	0.16	0.19	0.0050
	CH_4	0.099	0.099	0.0011
	HCN	0.020	0.009	0.0005
	NO	Not detected	Not detected	0.0011
	C_2H_6	0.004	0.003	Not detected
Material recovery, mol%	C	47.9	48.2	103
	H	100	99.9	109
	N	94.1	88.1	103
	O	101	99.7	101

Multi-Fluid Model

FORMULATION: *turbulent combustion in un-mixed gases*

- **Three Fluids:** Fuel-*F*, Air-*A* & Products-*P* defined by: $\{\rho_K, u_K\}$ where $K = F, A, P$
- **Asymptotic Limit:** $Re = Pe = Da \to \infty$
- **Compressible Flow:** $M > 0$

CONSERVATION EQUATIONS: *mixture*

- **Mass:** $\partial_t \rho_m + \nabla \cdot \rho_m \mathbf{u} = 0$
- **Momentum:** $\partial_t \rho_m \mathbf{u} + \nabla \cdot \rho_m \mathbf{uu} = -\nabla p_m$
- **Energy:** $\partial_t \rho_m U_T + \nabla \cdot \rho_m U_T \mathbf{u} = -\nabla \cdot (p_m \mathbf{u})$ where $U_T = u_m + \mathbf{u} \cdot \mathbf{u} / 2$

THERMODYANMIC FIELDS: *fluids*

- **Fuel:** $\partial_t \rho_F + \nabla \cdot \rho_F \mathbf{u} = -\rho_s$ & $\partial_t \rho_F u_F + \nabla \cdot \rho_F u_F \mathbf{u} = -p_F \nabla \cdot \mathbf{u} - \rho_s u_F$
- **Air:** $\partial_t \rho_A + \nabla \cdot \rho_A \mathbf{u} = -\sigma \rho_s$ & $\partial_t \rho_A u_A + \nabla \cdot \rho_A u_A \mathbf{u} = -p_A \nabla \cdot \mathbf{u} - \sigma \rho_s u_A$
- **Products:** $\partial_t \rho_P + \nabla \cdot \rho_P \mathbf{u} = (1+\sigma) \dot{\rho}_s$ & $\partial_t \rho_P u_P + \nabla \cdot \rho_P u_P \mathbf{u} = -p_P \nabla \cdot \mathbf{u} + (1+\sigma) \dot{\rho}_s u_P$
- **Stoichiometric Source:** $\dot{\rho}_s = \begin{cases} \rho_F(\mathbf{x}_s, t_s)\delta(t - t_s) & \text{for } \lambda_e \geq 1 \\ \rho_A(\mathbf{x}_s, t_s)\delta(t - t_s)/\sigma & \text{for } \lambda_e < 1 \end{cases}$
- **Adiabatic Constraint:** $\sum_K \dot{\rho}_K u_K = 0$

SOLUTION: *high-order Godunov scheme & AMR to follow turbulent mixing*

Thermodynamic Model

Equations of State: *fluid K (=F, A & P)*

- Perfect Gas Equation: $p_K v_K \equiv w_K \equiv R_K T_K$

- Caloric Equation: $u_K = F_K(w_K) \cong -|q_K| + C_K w_K \Leftrightarrow w_K = F_K^{-1}(u_K) \cong [u_K + |q_K|]/C_K$

Pressures & Temperatures

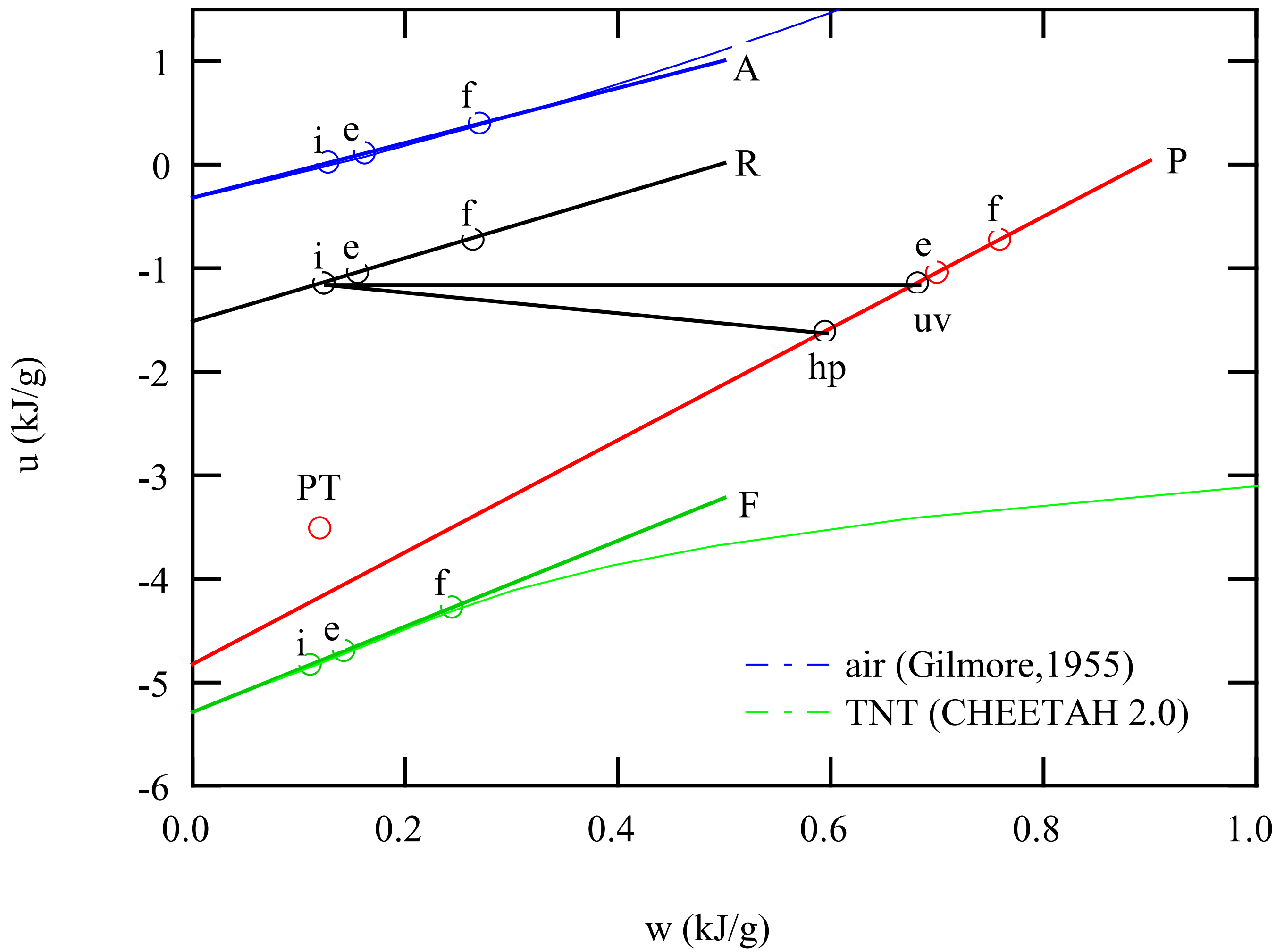
- *fluid K*: $p_K \equiv \rho_K w_K = \rho_K [u_K + |q_K|]/C_K \quad \& \quad T_K = w_K / R_K$

- *mixture m:* $p_m \equiv \rho_m w_m = \rho_m [u_m + |q_m|]/C_m \quad \& \quad T_m = w_m / R_m$

where

$$\rho_m \equiv \sum_K \rho_K \; ; \; Y_K \equiv \rho_K / \rho_m \; ; \; u_m \equiv \sum_K Y_K u_K \; ; \; w_m \equiv \sum_K Y_K w_K \; ; \; q_m \equiv \sum_K Y_K q_K \; ; \; C_m = \sum_K Y_K C_K w_K / w_m$$

Le Chatelier Diagram: *combustion of TNT in air*



Combustion Model

1. Reactants Formation: *stoichiometric sub-grid mass mixing*:

$$u_R = (u_F + \sigma u_A)/(1+\sigma) \quad \& \quad w_R = (w_F + \sigma w_A)/(1+\sigma)$$

2. Combustion ≡ *material transformations in the Le Chatelier plane*

- at *uv = constant* (closed systems): $u_P = u_R$

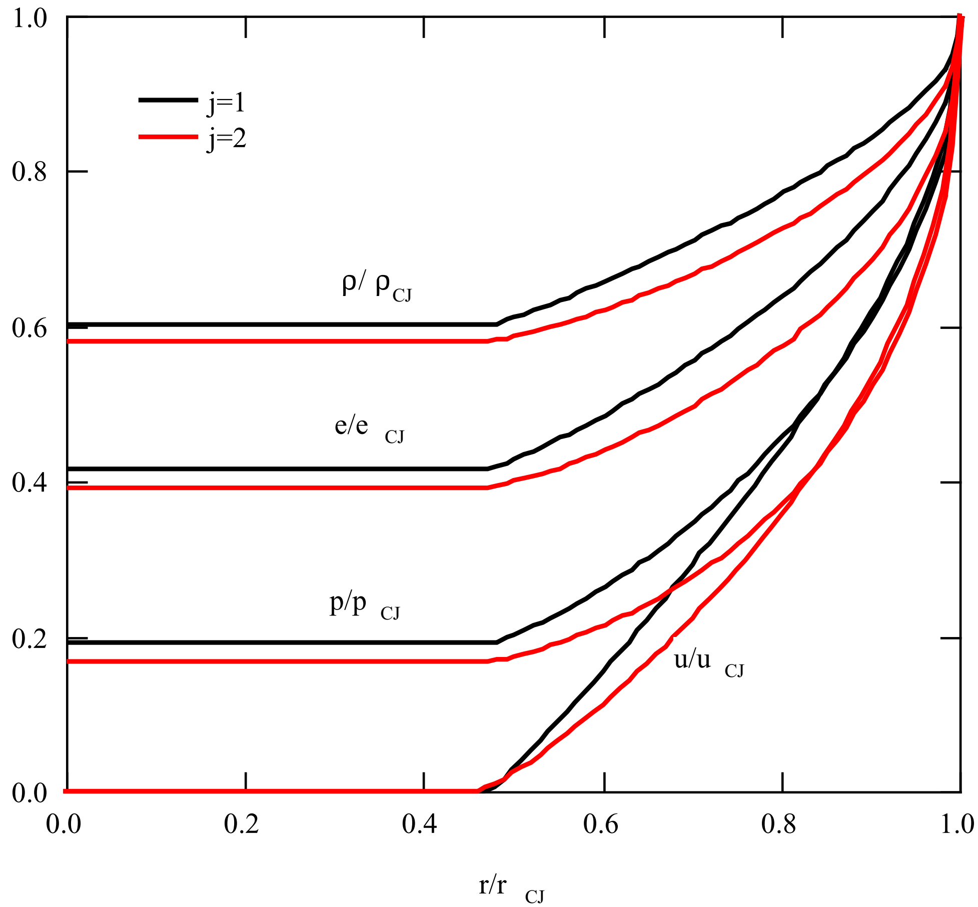
- at *hp = constant* (deflagrations): $u_P = u_R - \dfrac{\Delta Q - (C_P - C_R) w_R}{C_P + 1}$

3. Thermal Equilibration ⇔ *sub-grid energy mixing*: $T_K^e = T_m$

$$w_K^e = R_K T_m$$

$$u_K^e = -|q_K| + C_K w_K^e$$

Initial Conditions: *Self-Similar CJ Detonation*



Evolution: Material & Vorticity Fields

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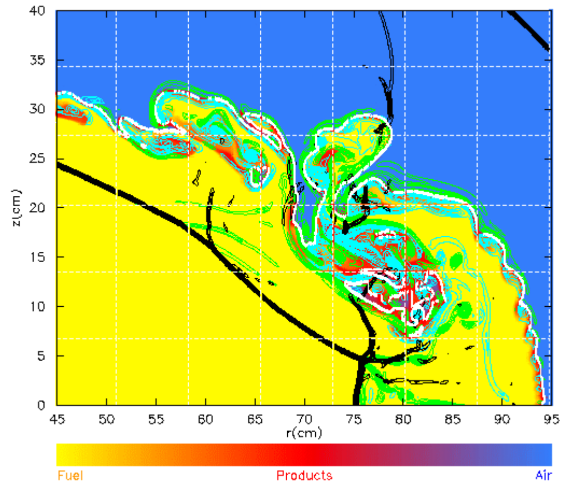
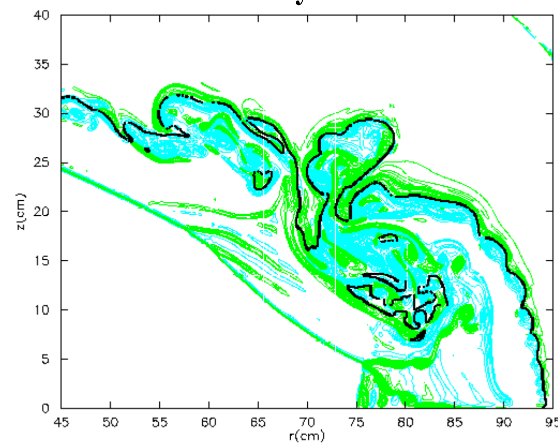
Visualization of Exothermic Fields

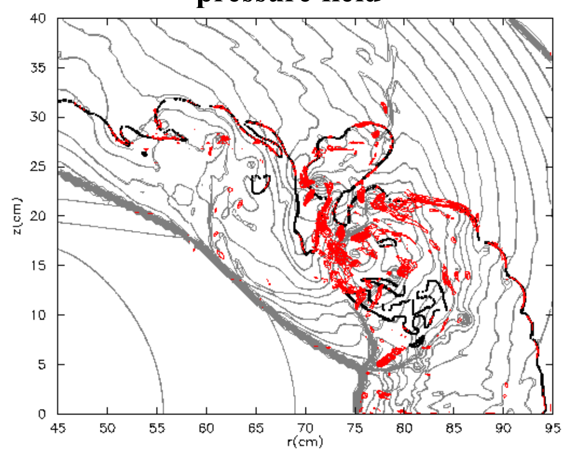
material fields



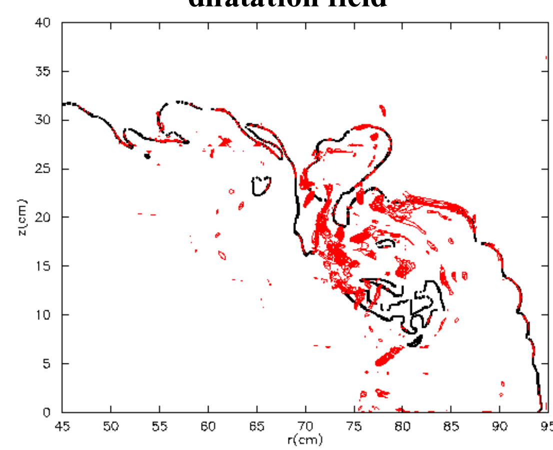
vorticity field



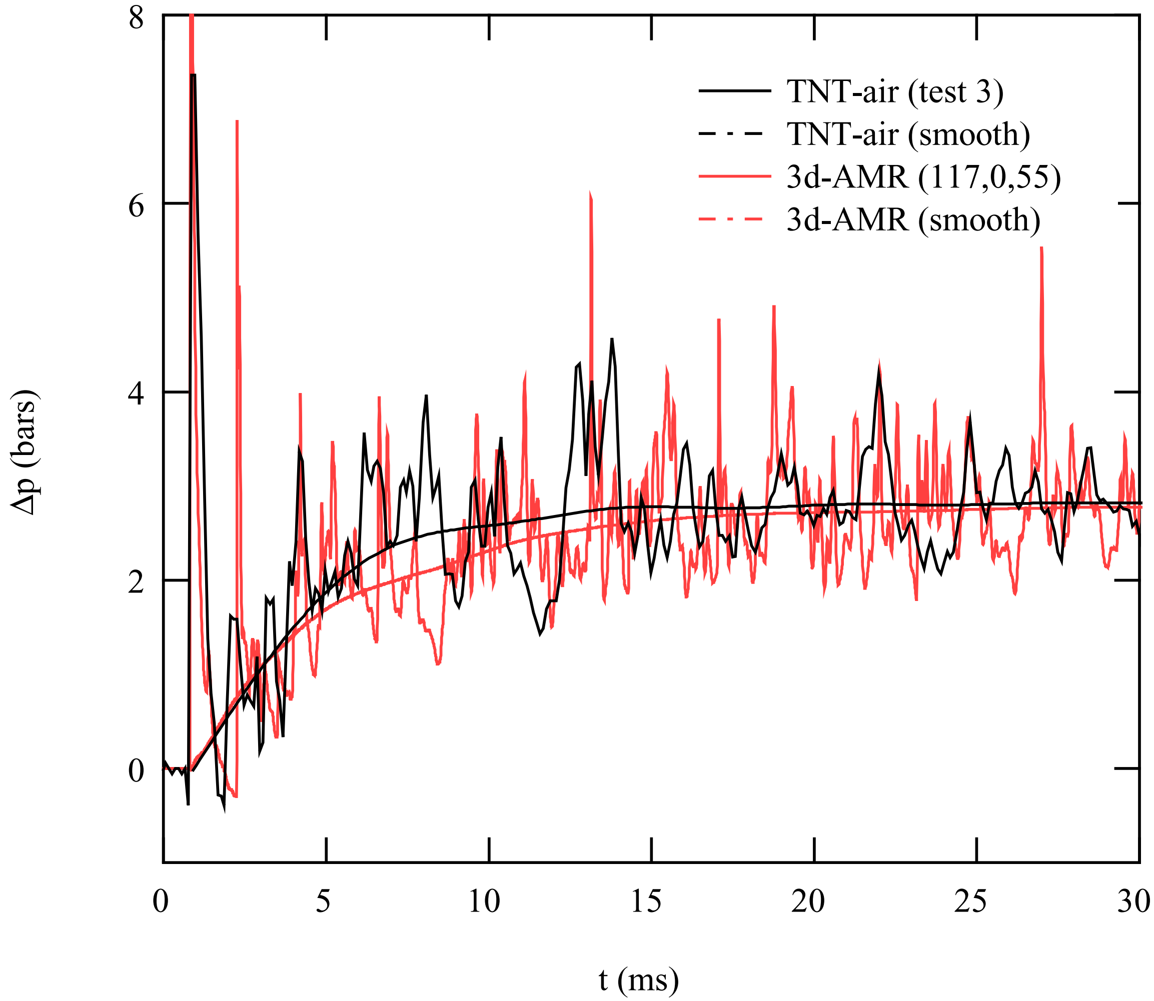
pressure field



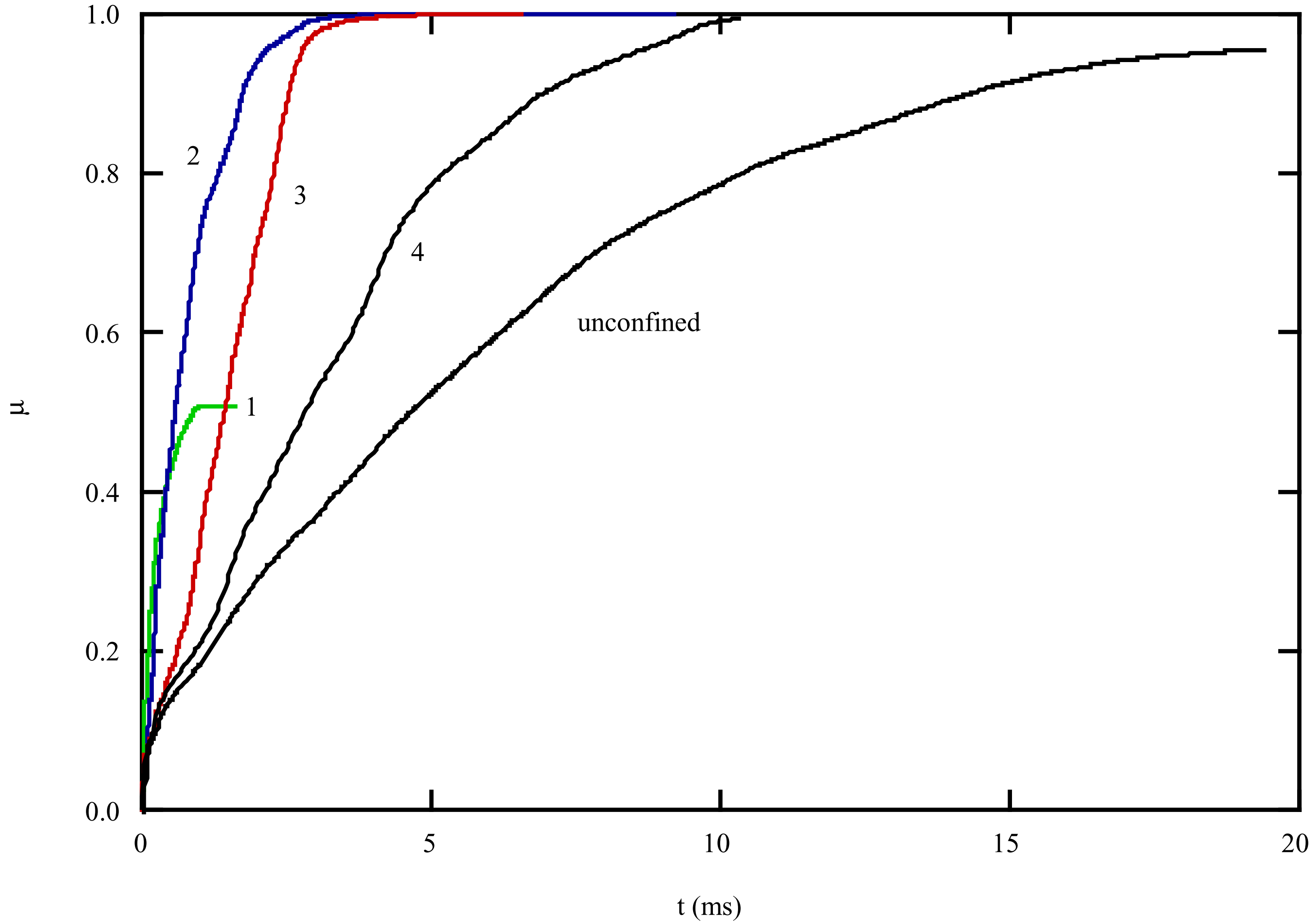
dilatation field



Post-Explosion Combustion of HE in Chamber



Fuel Consumption



Résumé

Multi-fluid Model

- Gas-dynamic Conservation Equations for the mixture
- Mass & Energy Conservation Equations for each fluid, with source/sink terms

Thermodynamic Model

- *Equations of State*: for each fluid
- *Thermodynamic-Equilibrium Relations*: for mixed cells

Combustion Model

- combustion occurs at thin exothermic sheets: $\mathbf{x}_s(t_s)$ (stoichiometric surface)
- **sink** for *Fuel & Air* mass and energy
- **source** for *Products* mass and energy
- Combustion ≡ material transformations in the Le Chatelier plane:

$$u_R(w_R) \Rightarrow u_P(w_P)$$

Conclusions

- This **Model** elucidates the link between **turbulence** (≡ **vorticity**) and **exothermicity** (≡ **dilatation**) in the limit of fast chemistry.

- It thus illustrates the dynamics of turbulent combustion where **exothermic effects** are controlled by mixing — rather than by the reaction-diffusion mechanism of Zel'dovich & Frank-Kamenetzkii (1938)