Proc. of 3rd KSV Conference
SNU, Seoul, Korea, Apr. 23, 2004

탄화수소/산소 혼합기체가 채워진 관 내부를 전파하는 데토네이션 파의 해석과 가시화

최정열 교수

부산대학교 항공우주공학과

A numerical study is carried out on the detonation wave propagation through a T-shaped flame tube, which represents a crucial part of the combustion wave ignition (CWI) system aimed for simultaneous ignition of multiple combustion chambers by delivering detonation waves. The formulation includes the Euler equations and an induction-parameter model. The reaction rate is treated based on a chemical kinetics database obtained from a detailed chemistry mechanism. A second-order implicit time integration and a third-order TVD algorithm are implemented to solve the theoretical model numerically. A total of more than two-million grid points are used to provide direct insight into the dynamics of the detonation wave. Several important phenomena including detonation wave propagation, degeneration, and re-initiation are carefully examined. Information obtained can be effectively used to facilitate the design and optimization of the flame tubes of CWI systems.

강연자 전자메일
aerochoi@pusan.ac.kr

Numerical analysis and visualization of a detonation wave propagating through a Hydrocarbon/Oxygen mixture

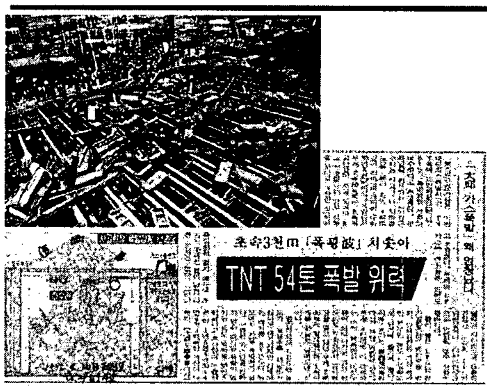
Jeong-Yeol Choi
Pusan National University

Contents

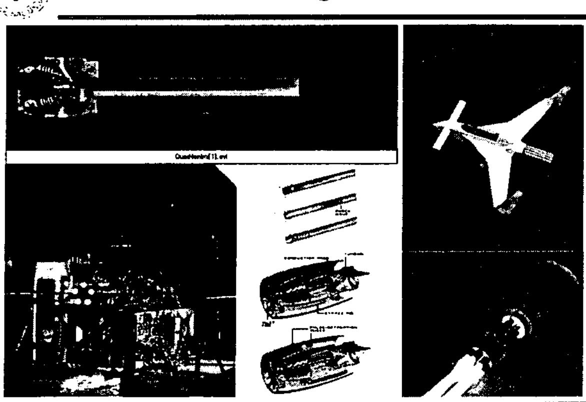
What is Detonation ?

- **Detonation** [1]An explosion or sudden report made by the instantaneous decomposition or combustion of unstable substances' as, the detonation of gun cotton.(Webster) [2] a violent release of energy caused by a chemical or nuclear reaction [syn: explosion] (WordNet)
- Detonation Wave = Coupled shock and combustion wave
- Examples
  - Bomb Explosion
  - Explosion in coal mine and granary
  - Daegu subway disaster (Equivalent to TNT 54t, 1995.4.28)
  - Aerospace propulsion systems (Pulse Detonation Engine, Ram Accelerator, Combustion Wave Igniter)

Daegu subway disaster

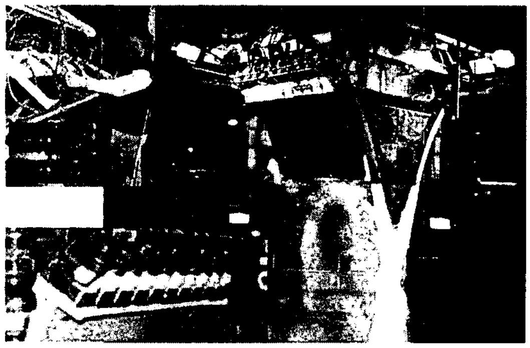


Pulse Detonation Engine



CWI system for X-33 Aerospike Engine

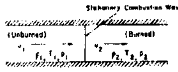
- Hydrogen/Oxygen CWI system



Combustion Phenomena

Combustion Phenomena	Diffusive	Premixed
Wave Stationary	Candle Flame	Gas-Range
Geo-Stationary	Diesel Engine	Gasoline Engine

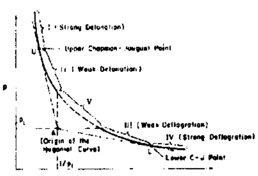
- Premixed Combustion : Detonation Wave & Deflagration Wave(flame)



$\rho_1 u_1 = \rho_2 u_2$

$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2$

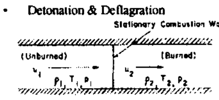
$h_1 + q + \frac{1}{2}u_1^2 = h_2 + \frac{1}{2}u_2^2$



⇨ Rayleigh Line
⇨ Rankin-Hugoniot Relation
⇨ C-J (Chapmann-Jouguet) Condition : $u_2 = c_2$

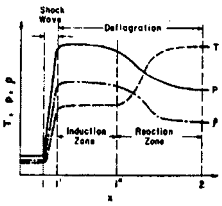
Detonation Wave Structure

- Detonation & Deflagration



	Detonation	Deflagration
u_1/c_1	5~10	0.0001~0.03
u_2/u_1	0.4~0.7(decel.)	4~6 (acc.)
p_2/p_1	13~55 (comp.)	~0.98(expan.)
T_2/T_1	8~21	4~16
ρ_2/ρ_1	1.7~2.6	0.06~0.25

- ZND Structure
  - Zel'dovich-Neumann-Döring
  - Thin Combustion zone behind a Shock Wave
  - Coupled Shock and Reaction Wave

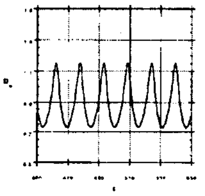


Propagating Detonation Wave

- Unsteadiness
  - Instability Characteristics by Chemical Kinetic
  - Exponential Growth or Decay of Reaction Rate

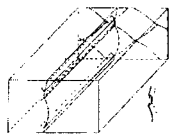
$$w_k = M_k \sum_{r=1}^{Nr} \left(\nu''_{k,r} - \nu'_{k,r}\right) \left(k_{fr} \prod_{k=1}^{N} \left(\frac{\rho_k}{M_k}\right)^{\nu'_{k,r}} - k_{br} \prod_{k=1}^{N} \left(\frac{\rho_k}{M_k}\right)^{\nu''_{k,r}} \right), \quad k_{fr} = A_{fr} T^{B_{fr}} e^{-E_{fr}/T}$$

- 1-D Characteristics
  - Oscillating Characteristics around C-J Condition
  - Galloping Detonation Wave (Pulsating Detonation Wave)

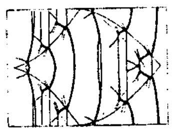


Multi-Dimensional Structure

- Cellular Structure

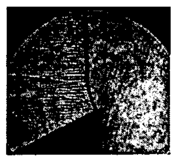


- Unsteady Wave Structure



- Smoked Foil Record

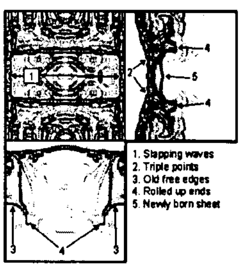
- Large Scale Image

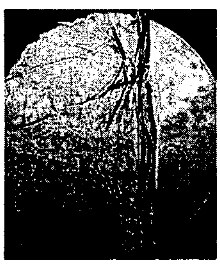


- Cell Width (Cell Size)

Detailed Wave Front

- Fully 3-Dimensional Structure
- Vortex Structure behind the Wave Front





Background of IPM

- Detonation Wave = Coupled shock and combustion wave
  - Explosion analysis and Propulsion applications
- Themo-chemical properties that characterize the detonation wave
  - Detonation cell-size, Pressure ratio, temperature ratio
  - Amount of heat addition
  - Chemical characteristic time (induction time)
    - changes exponentially
    - Very high grid resolution to capture the broad range of induction region.
  - Also true for many combustion dynamics problems
  - IPM : modeling of heat and induction time with reaction progress variable
- Class of Chemical kinetics Model for HC fuel combustion
  - Detailed Chemistry : ~50 species, ~300 reaction steps
  - Reduce Chemistry : ~20 species, ~30 reaction steps
  - Global Chemistry : 5 species, 1~4 steps
  - Reaction progress variable modeling : 1~2 variables, 1 step

Computational Costs for Kinetics

- Computational Cost for CFD/chemical kinetics calculations at P!!! 650MHz

Fluid dynamics/ Kinetics Model	μs/iter/node
Non-Reacting flow	9.60
Non-Reacting flow + 1 more conservation equation	12.73
Reaction Progress variable modeling : Non-Reacting flow + 1 more conservation equation with exponential source term	16.01
Global Chemistry : 5 species and 1 step kinetics for CH4/Air	30.53
Detailed Chemistry : 9 Species and 19 steps kinetics for H2/Air	80.40
Reduced Chemistry : 22 species and 34 steps kinetics for CH4/Air	233.06
Detailed Chemistry for HC	N/A

- Motivation ! – Accurate Induction Parameter (reaction progress variable) Modeling based on induction time database calculated by detailed kinetics mechanisms.

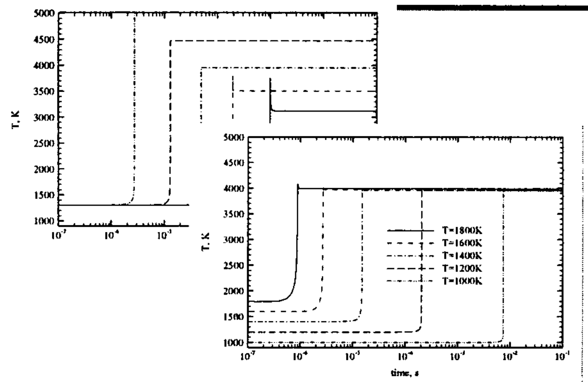
Construction of Induction Time Database

- Selected fuel : Cracked JP-7 in catalytic reactor
  - $C_{1.39}H_{4.31} = x_{H2}H_2 + x_{CH4}CH_4 + x_{C2H6}C_2H_6 + x_{C2H4}C_2H_4$
  - Mw=21.066 kg/kmole, $(O/F)_{stoi}$ = 3.75

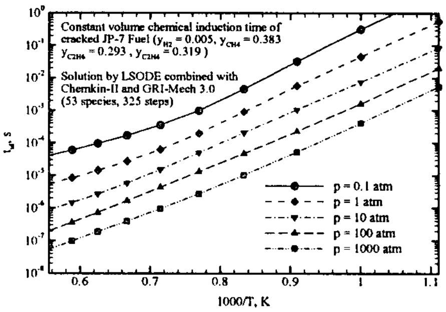
Component	H_2	CH_4	C_2H_6	C_2H_4
mass fraction, y_i	0.005	0.383	0.293	0.319
mole fraction, x_i	0.052	0.503	0.205	0.240

- Detonation Characteristics : NASA CEA
  - Temperature : 250~500 K, Pressure : 0.1~100 bar, Equivalence ratio : 0.6~1.8
- Induction time calculation with Chemkin-II and GRI-Mech. 3.0
  - Shocked temperature : 900 ~1,800 K
  - Shocked pressure : 0.1~1000 bar

Examples of Induction Time Calculation



Induction Time Summary



* Equivalence ratio = 1.23 (O/F=3.04)

Induction Parameter Model

- Curve-fit of induction time database
  - Two-dimensional Least-square methods

$$\tau^*(T,p) = \exp\left(A^*(p) + \frac{E^*(p)}{T - T^*(p)}\right)$$

where, $A^*(p)$, $T^*(p)$ and

$$E^*(p) = a_0 + a_1 \log p + a_2 (\log p)^2 + a_3 (\log p)^3$$

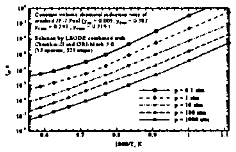
- Induction parameter modeling

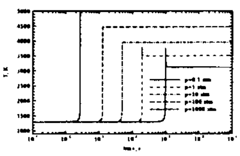
$$\frac{dZ}{dt} = w(Z) = \frac{1}{\tau(T,p)} \qquad w_{max} = \frac{1}{\tau^*(T,p)}$$

- Assumption : locally quadratic approximation

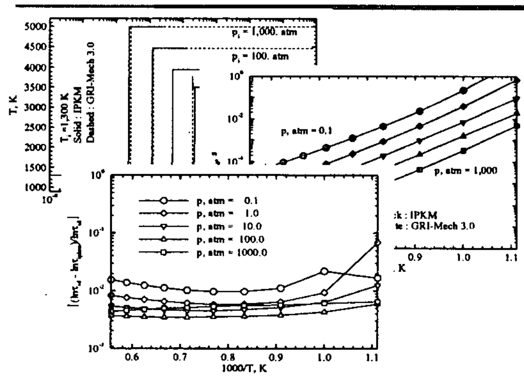
$$w(Z) = \frac{C}{f'(Z)} \exp(-f(Z))$$

$$\frac{dZ}{dt} = w(Z) = C\frac{(T - T^*(p))}{E^*(p)T_1}\exp\left(-A^*(p) - \frac{E^*(p)}{T - T^*(p)}\right), \quad C = -\frac{4T_1}{E^*} \text{ or } C = 1$$





IPM Validation



One-D Formulation

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho u\\ \rho e\\ \rho Z\end{bmatrix}+\frac{\partial}{\partial x}\begin{bmatrix}\rho u\\ \rho u^2+p\\ (\rho e+p)u\\ \rho Z u\end{bmatrix}+\frac{\alpha}{x}\begin{bmatrix}\rho u\\ \rho u\\ (\rho e+p)u\\ \rho Z u\end{bmatrix}=\begin{bmatrix}0\\ 0\\ 0\\ \rho w\end{bmatrix}$$

$$e=\frac{R(Z)}{\gamma(Z)-1}T+\frac{1}{2}u^2-Zq \qquad p=\rho R(Z)T$$

$$R(Z)=R_u(1-Z)+R_bZ \qquad \gamma(Z)=\frac{\gamma_u(\gamma_b-1)(1-Z)+\gamma_b(\gamma_u-1)Z}{(\gamma_b-1)(1-Z)+(\gamma_u-1)Z}$$

$$w=\frac{(T-T^*(p))}{E^*(p)T_1}\exp\left(-A^*(p)-\frac{E^*(p)}{T-T^*(p)}\right)$$

- TVD upwind discretization – AUSM+/Roe, MUSCL
- 4th order Runge-Kutta time stepping
- Themo-chemical parameters from NASA CEA or Rankine-Hugoniot relation

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Detonation Propagation

- Cracked JP-7/oxygen mixture
  $T = 400\ K$, $p = 1\ MPa$ and $\phi = 1.23$ (O/F=3.04)
- Chapman-Jouguet (C-J) detonation properties from CEC
  - $p/p_1 = 26.884$, $T/T_1 = 10.672$, $\rho/\rho_1 = 1.8384$, and $V_{CJ} = 2580.1\ m/s$
- Unburned and burned gas properties
  - $\gamma_U = 1.2992$ and $R_U = 293.23$ J/kgK
  - $\gamma_B = 1.1484$ and $R_B = 401.79$ J/kgK
  - $q = 1.0422\times10^7$ J/kg
  - Satisfy Rankine-Hugoniot relation

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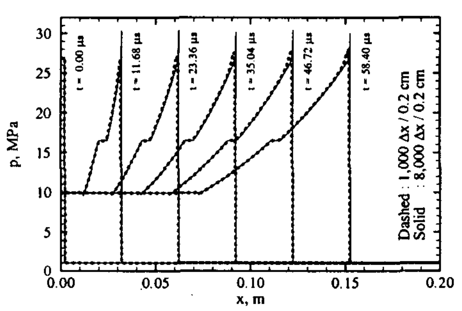
Detonation Propagation (cont'd)



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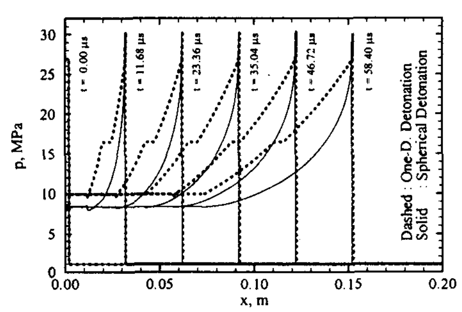
Detonation Propagation (cont'd)



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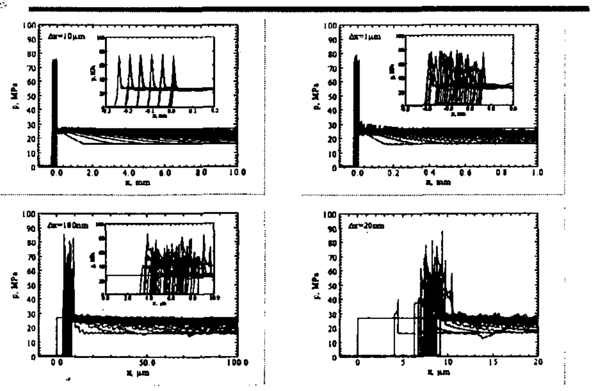
Grid Refinement for Stationary Wave



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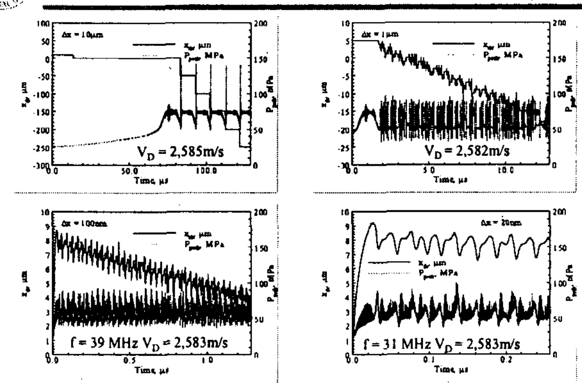
Grid Refinement for Stationary Wave (cont'd)



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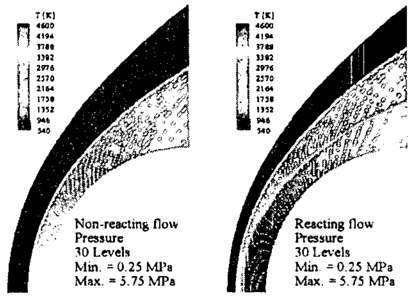
Two-D Formulation

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho e\\ \rho Z\end{bmatrix}+\frac{\partial}{\partial x}\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ (\rho e+p)u\\ \rho Zu\end{bmatrix}+\frac{\partial}{\partial y}\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ (\rho e+p)v\\ \rho Zv\end{bmatrix}+\frac{\alpha}{y}\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2\\ (\rho e+p)v\\ \rho Zv\end{bmatrix}=\begin{bmatrix}0\\ 0\\ 0\\ 0\\ \rho w\end{bmatrix}$$

- TVD upwind discretization – AUSM+/Roe, MUSCL
- Fully-implicit second order time integration
  - Newton sub-iteration, LU-relaxation scheme
  - is computationally efficient by larger time step.
  - is triggering earlier the wave front instability.

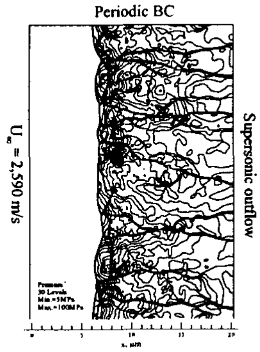
Shock-Induced Combustion

M = 7.0 , p = 0.1 MPa , T = 400 K
80×80 grid , R = 20 μm

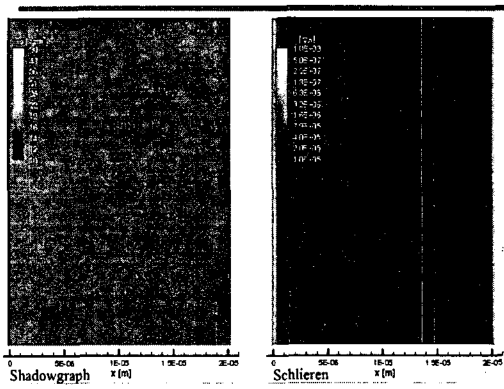


Two-D Detonation Wave

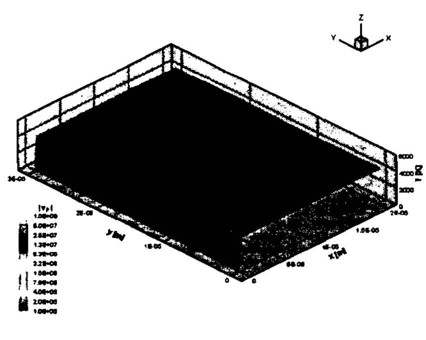
- Cracked JP-7/oxygen mixture
  - $T = 400\ K$, $p = 1\ MPa$
  - $\phi = 1.23$ (O/F=3.04)
- C-J properties as I.C.
  - $p/p_1 = 26.884$
  - $T/T_1 = 10.672$
  - $\rho/\rho_1 = 1.8384$
  - $U_\infty = 2{,}590$ m/s
- Computational domain
  - 20 μm × 30 μm
  - 500×600=300,000 grid points
  - CFL = 1.0



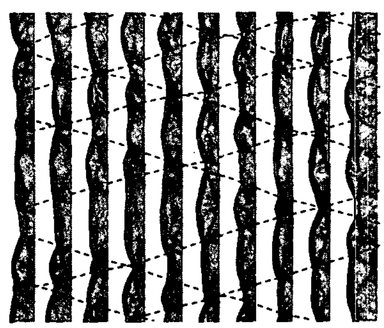
Wave Front Dynamics



Wave Front Dynamics(cont'd)

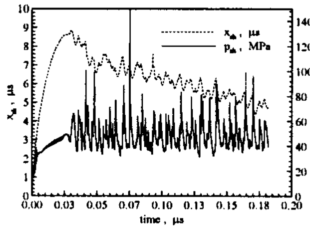


Two-D Cell Structure



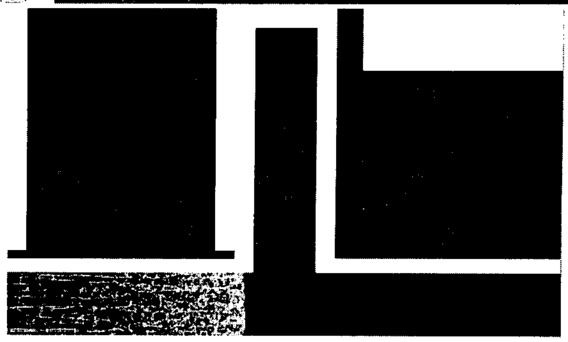
Cell width = 5 ~ 10 μm

Wave Front History



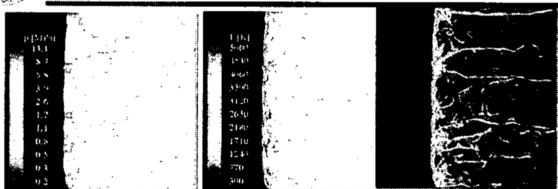
- Pressure oscillation between 35 ~100 MPa.
- Oscillation frequency is approximately 100 MHz.
- Two-dimensional detonation wave speed is 2,920 m/s
  - 1% higher than the C-J detonation speed.
- Irregular cell structure, cell width ranges from 5 to 10 μm .

Detonation Propagation in T-branch

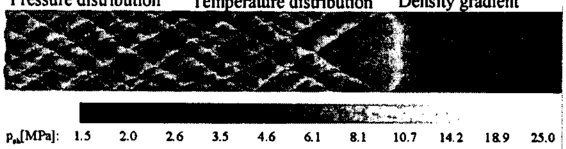


$3600 \times 400 + 400 \times 1600 \geq 2{,}000{,}000$

Standing Wave Simulation

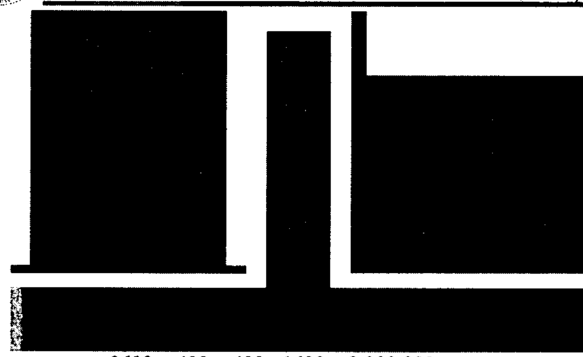


Pressure distribution Temperature distribution Density gradient



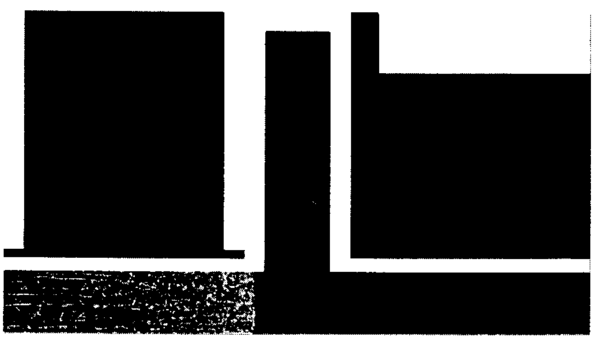
Numerical smoked-foil record

Detonation Propagation in T-branch, (cont'd)

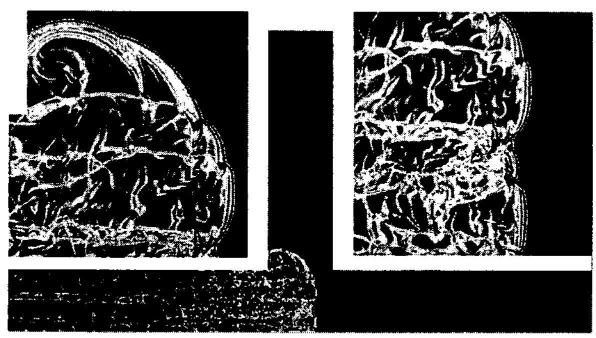


$3600 \times 400 + 400 \times 1600 \geq 2{,}000{,}000$

Snap Shot 1

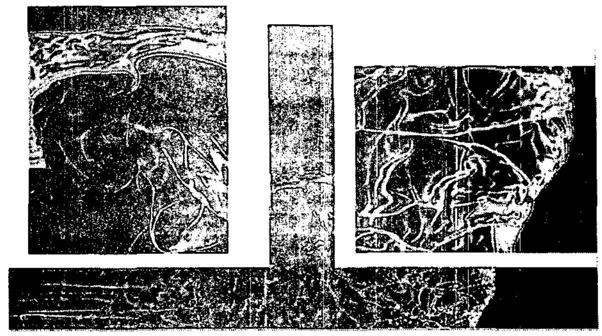


Snap Shot 2



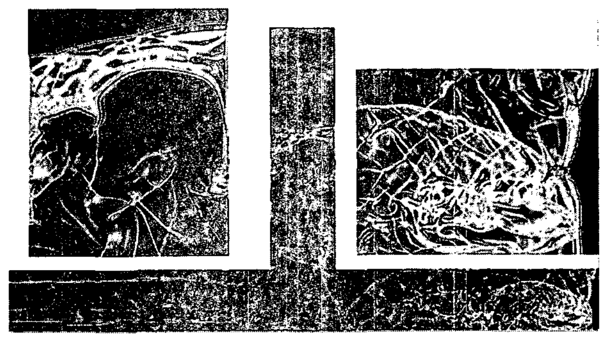
Snap Shot 3

Snap Shot 4

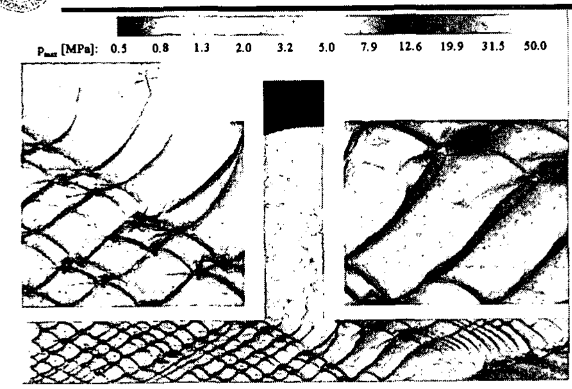


Snap Shot 5

Snap Shot 6



Numerical Smoked Foil Record



Conclusions

- Development of IPM (induction parameter modeling) PROCEDURE.
  - Based on detailed kinetics mechanisms
  - Applied for Hydrocarbon fuel/Oxidizer mixture
  - Efficiency
  - Accuracy
- One-D code construction with IPM implementation
  - One-dimensional detonation wave propagation
  - Grid refinement study for wave front dynamics
- Time efficient two-D code construction with IPM
  - Two-dimensional detonation wave simulations
  - Investigation of Detonation wave Propagation in T-branched tubes
- Further applications are expected.
  - Other fuel/Oxidizer mixture
  - Other combustion phenomena (premixed combustion including detonation)