Detonation in Gases

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Combustion Symposium

McGill University August 2008

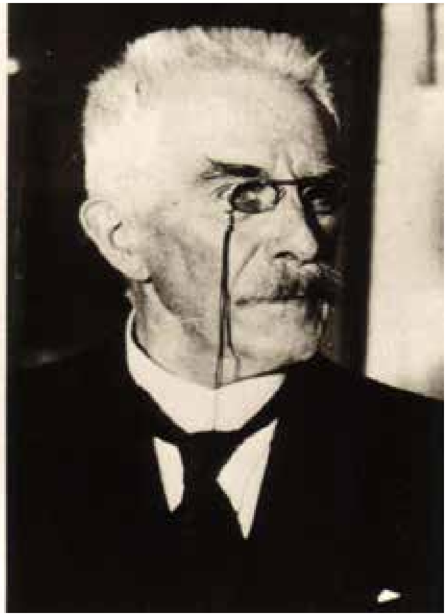
Marcelin Berthelot

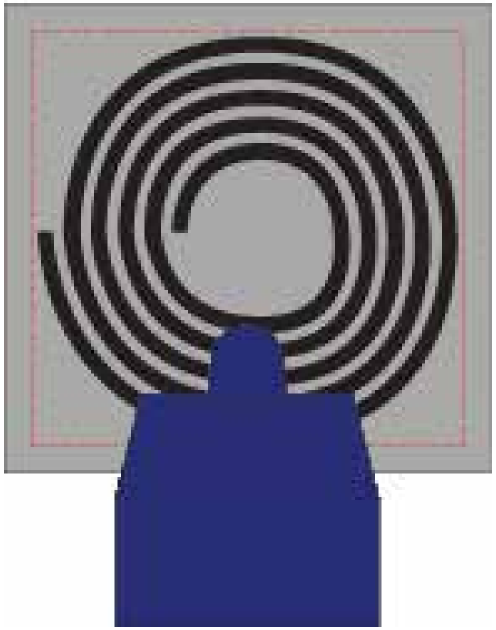
Paul Vielle

1881

Ernest Mallard

Henry Le Chatelier





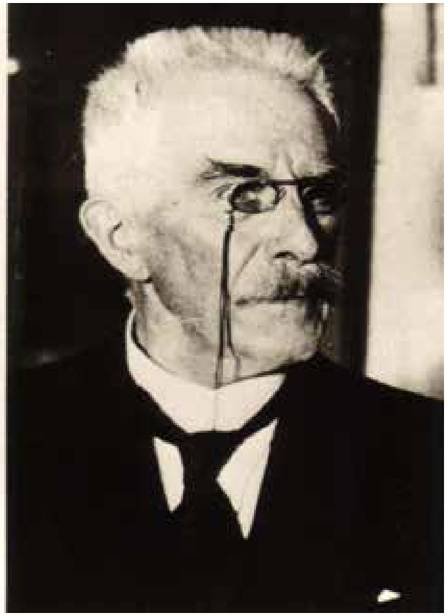
2006

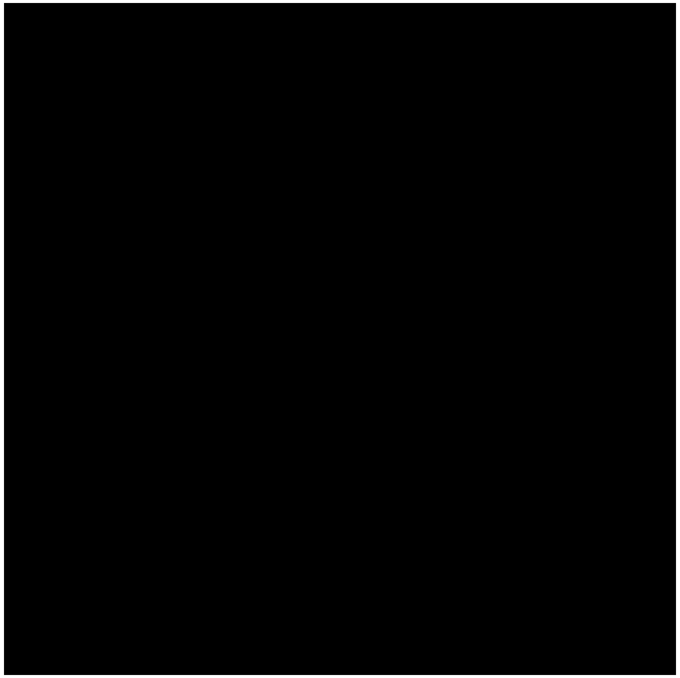
Marcelin Berthelot

Paul Vielle

Ernest Mallard

Henry Le Chatelier





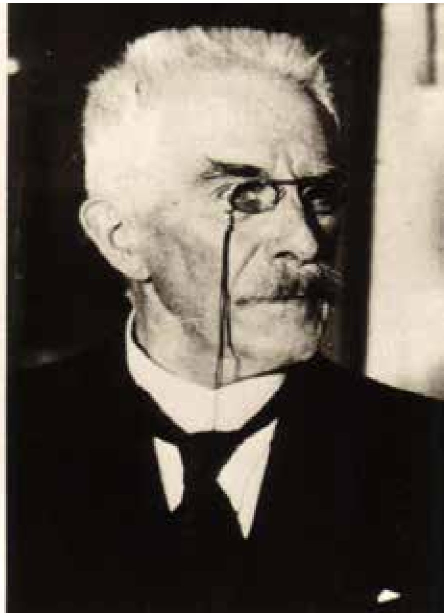
$C_3H_8+5O_2$ 20 kPa

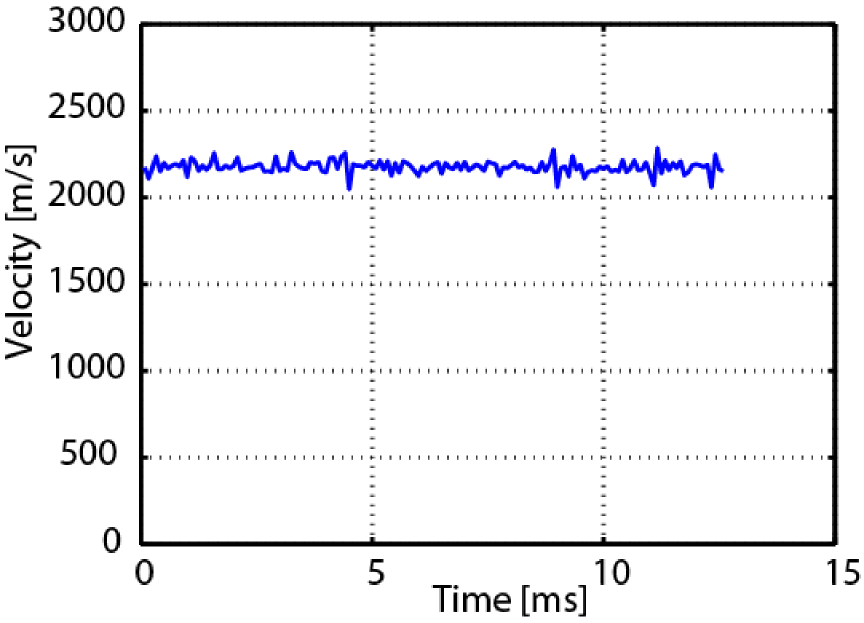
Marcelin Berthelot

Paul Vielle

Ernest Mallard

Henry Le Chatelier

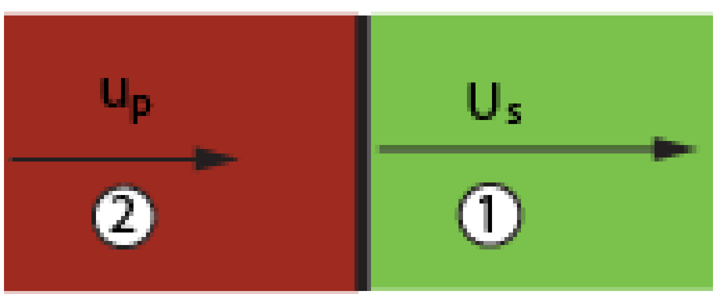




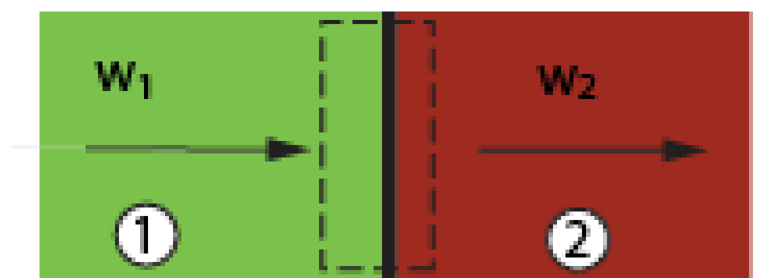
Donald Chapman

Ehrile Jouguet

1889-1905



lab frame



wave frame

Donald Chapman

Ehrile Jouguet

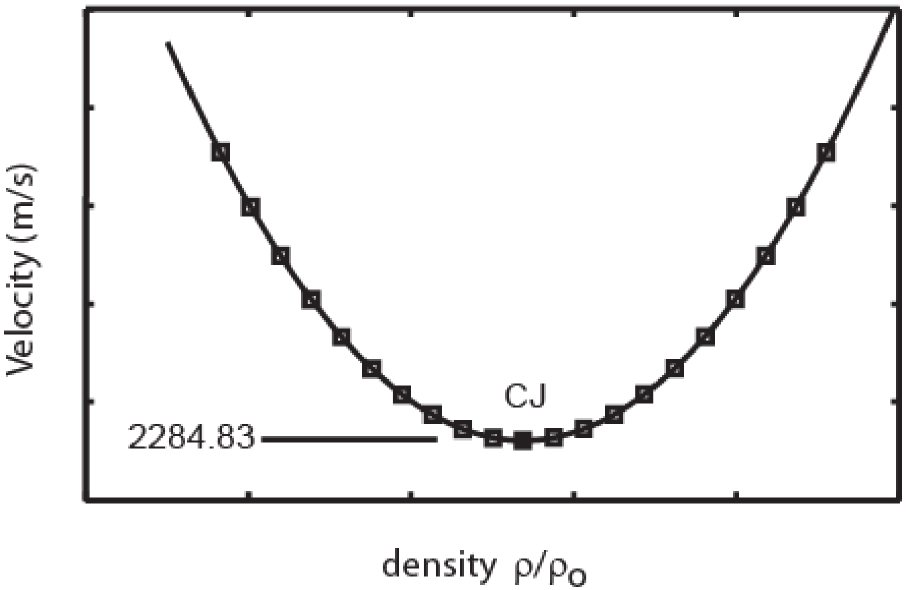
$$\rho_1 w_1 = \rho_2 w_2$$

$$P_1 + \rho_1 w_1^2 = P_2 + \rho_2 w_2^2$$

$$h_1 + \frac{w_1^2}{2} = h_2 + \frac{w_2^2}{2}$$

Donald Chapman

Ehrile Jouguet



or

$$w_{2,CJ} = a_2(T_{CJ}, P_{CJ}, \mathbf{Y}_{CJ})$$

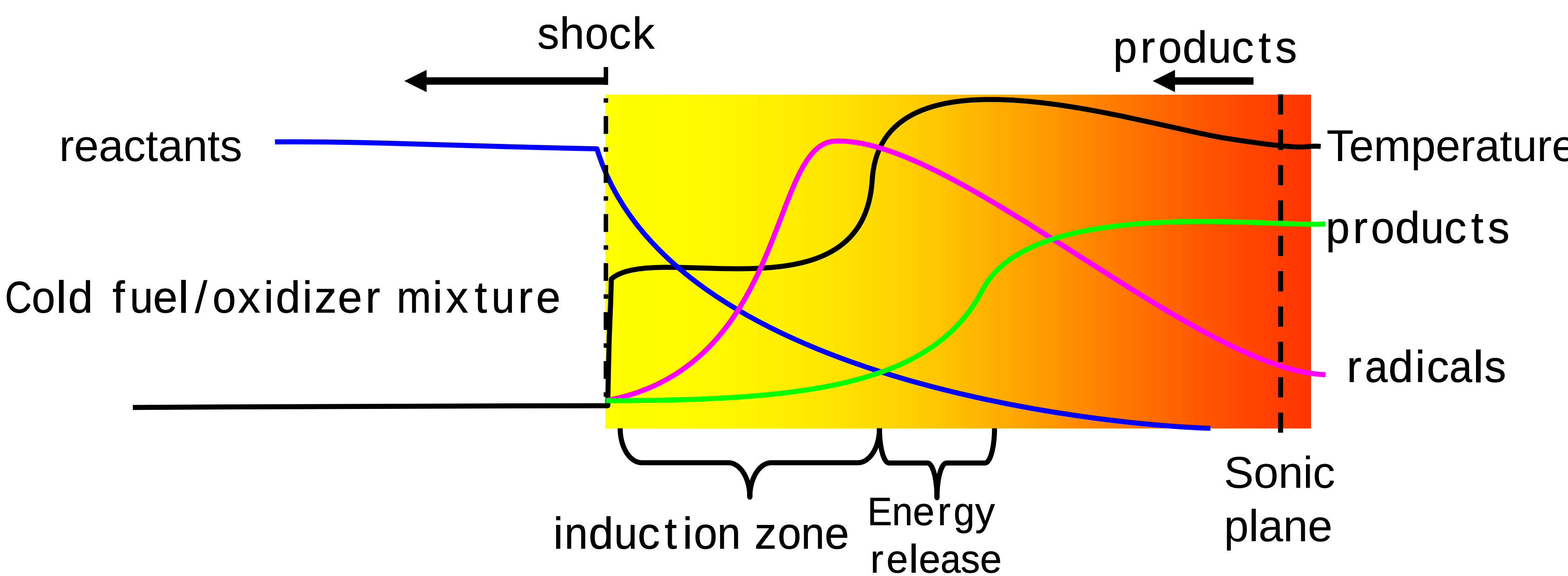
Sonic flow relative to wave

"ZND" 1940-43

Yakov Zel'dovich

John von Neumann

Werner Döring



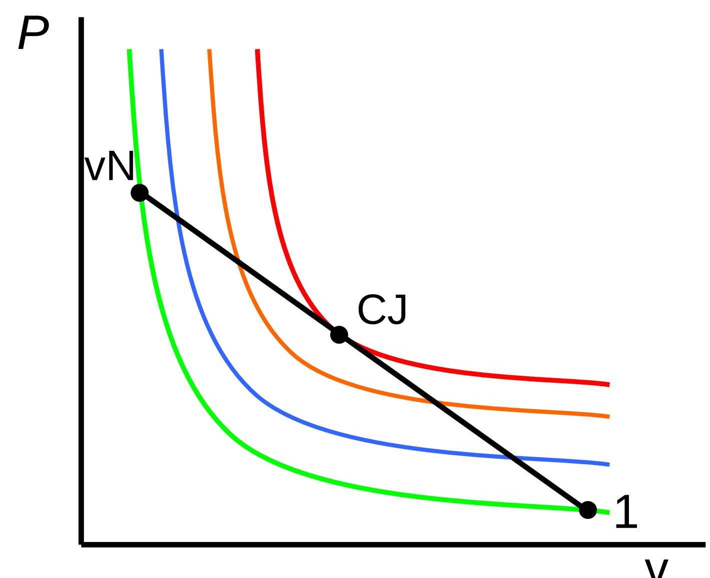
"ZND" 1940-43

$$\rho_1 w_1 = \rho w$$

$$P_1 + \rho_1 w_1^2 = P + \rho w^2$$

$$h_1 + \frac{w_1^2}{2} = h(\mathbf{Y}, P, \rho) + \frac{w^2}{2}$$

$$\frac{DY_i}{Dt} = \Omega_i(\mathbf{Y}, P, \rho)$$



"ZND" 1940-43

thermicity

$$dP = \pm \rho c\, du + \rho c^2 \dot{\sigma}$$

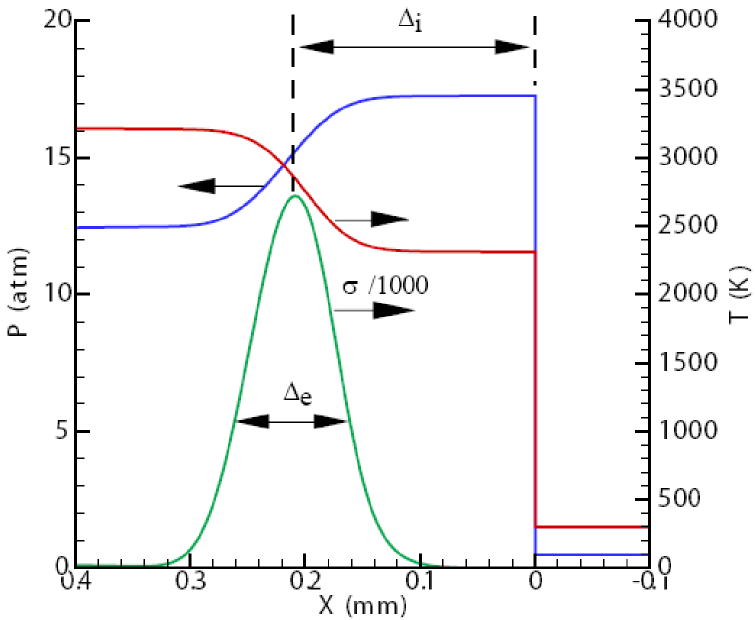
$$u \frac{d\rho}{dx} = \frac{-\rho \dot{\sigma}}{1 - M^2} \qquad u \frac{dY_i}{dx} = \Omega_i$$

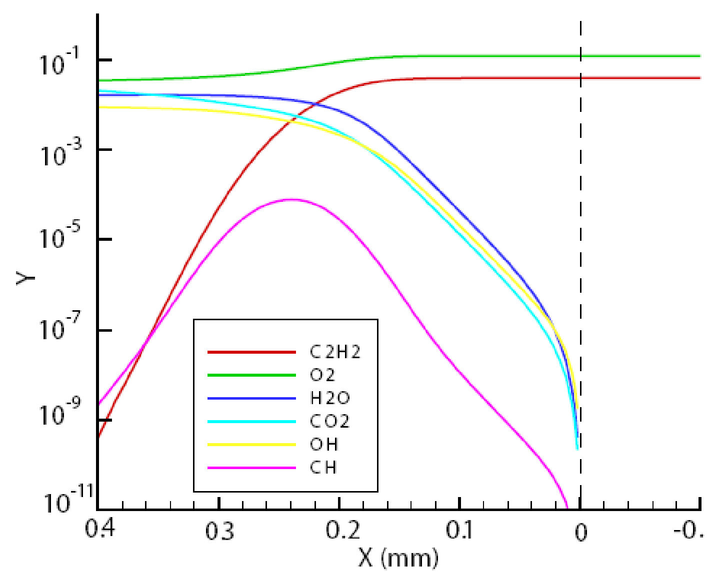
$$u \frac{du}{dx} = \frac{u \dot{\sigma}}{1 - M^2} \qquad \text{where } \dot{\sigma} = \sum_{i=1}^{N} \frac{\Omega_i}{\rho c^2} \left(\frac{\partial P}{\partial Y_i} \right)_{\rho, e, Y_{k \neq i}}$$

$$u \frac{dP}{dx} = \frac{-\rho u^2 \dot{\sigma}}{1 - M^2}$$

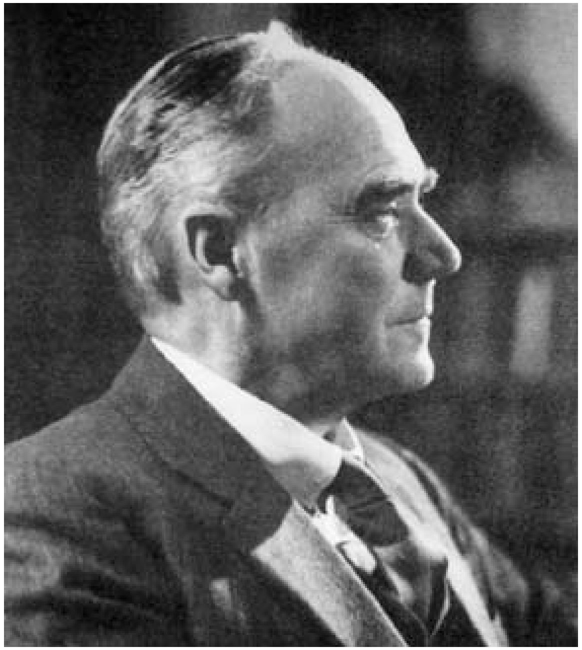
Ω_i : given by kinetic rate law

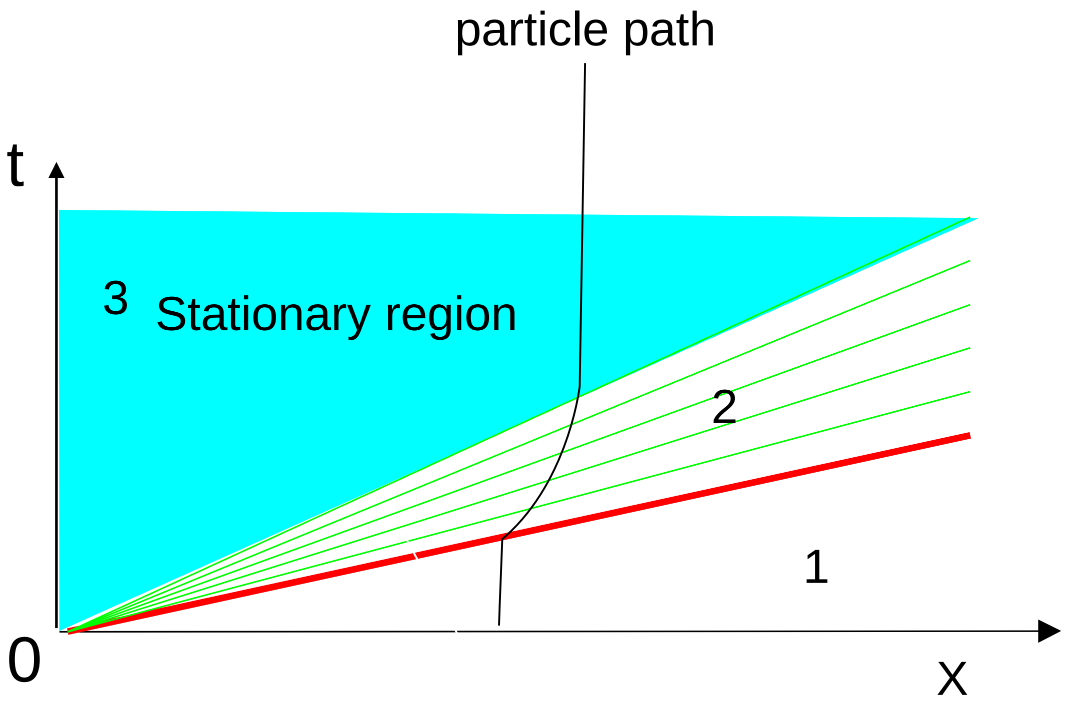
"ZND" 1940-43



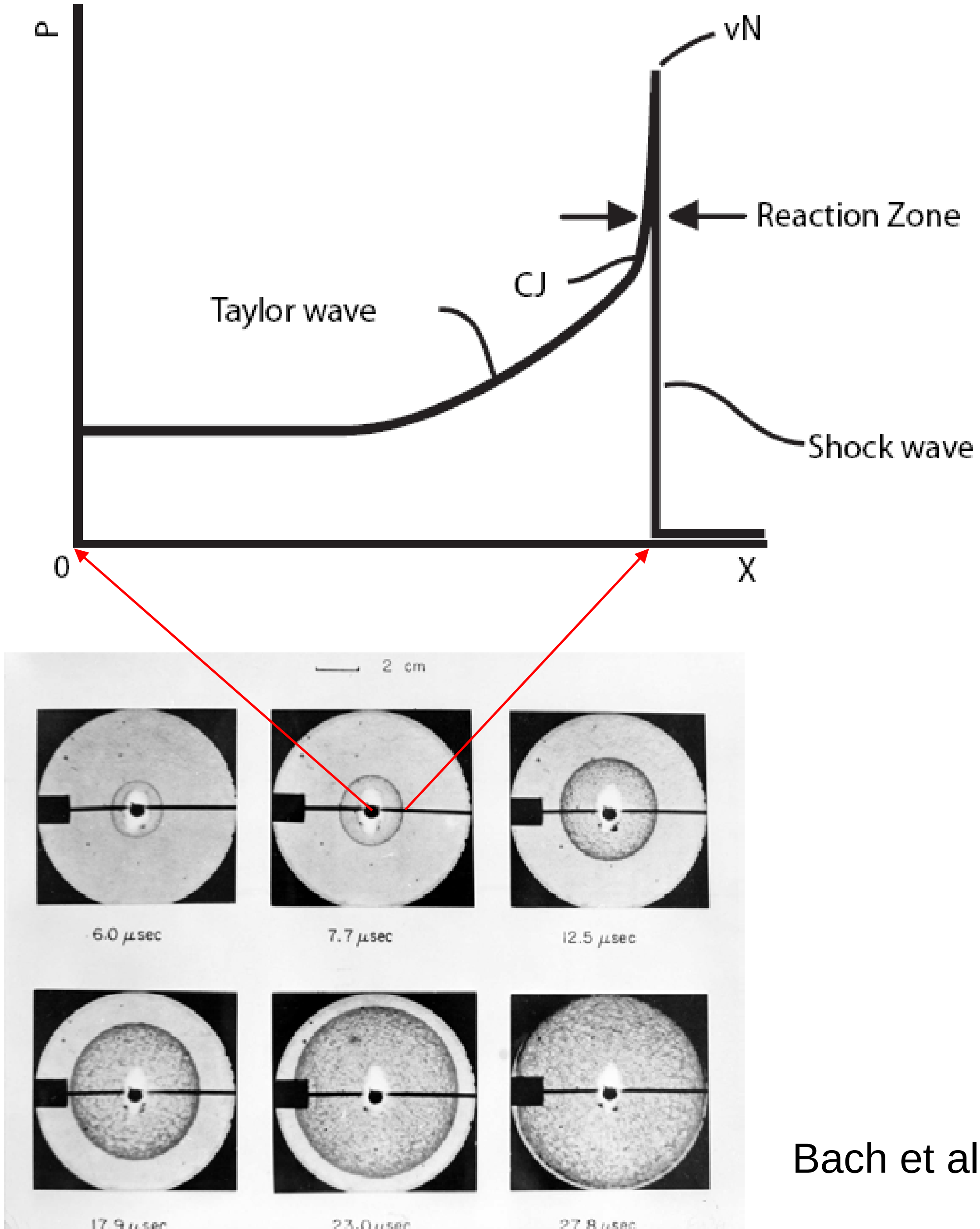


G. I. Taylor

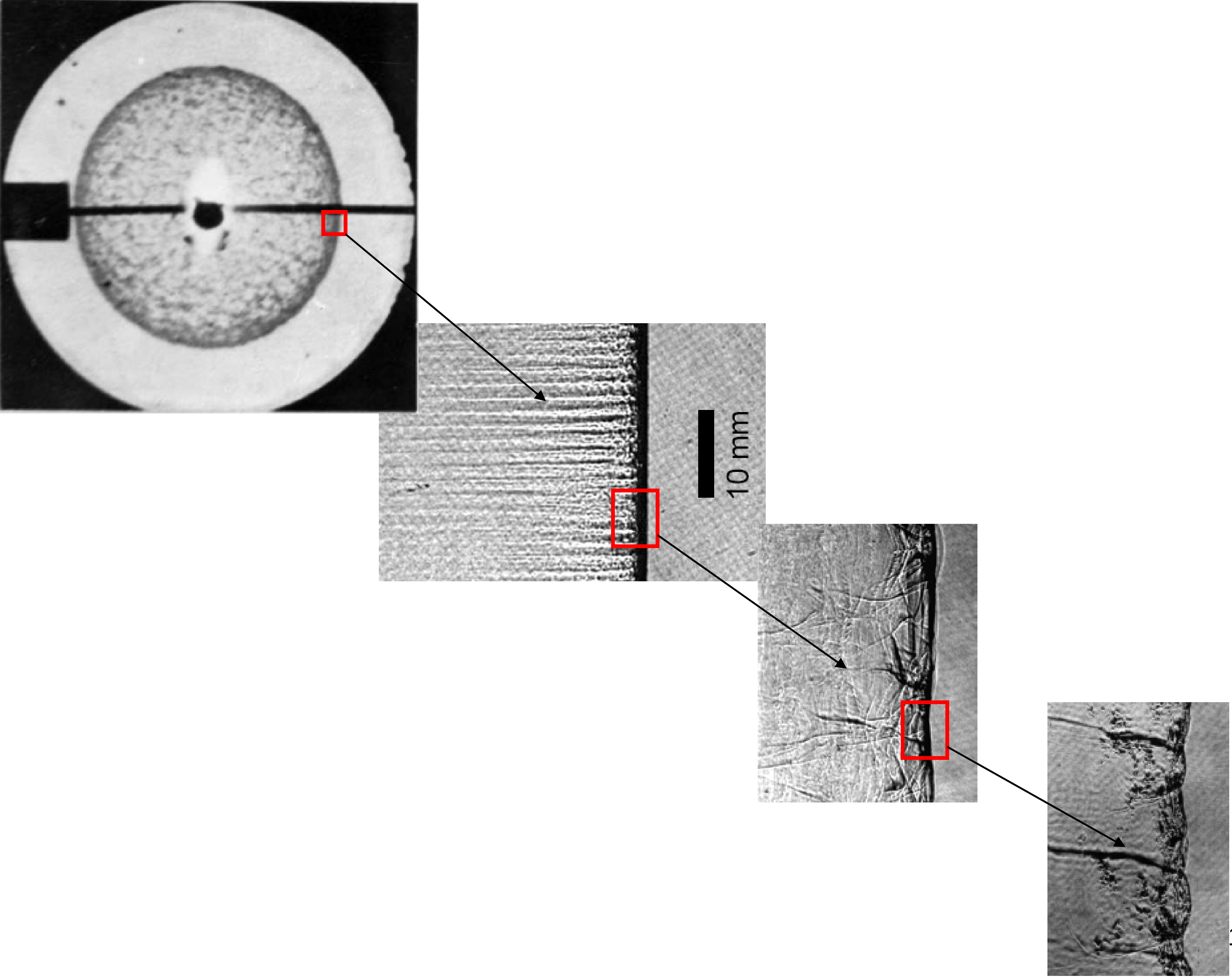




detonation

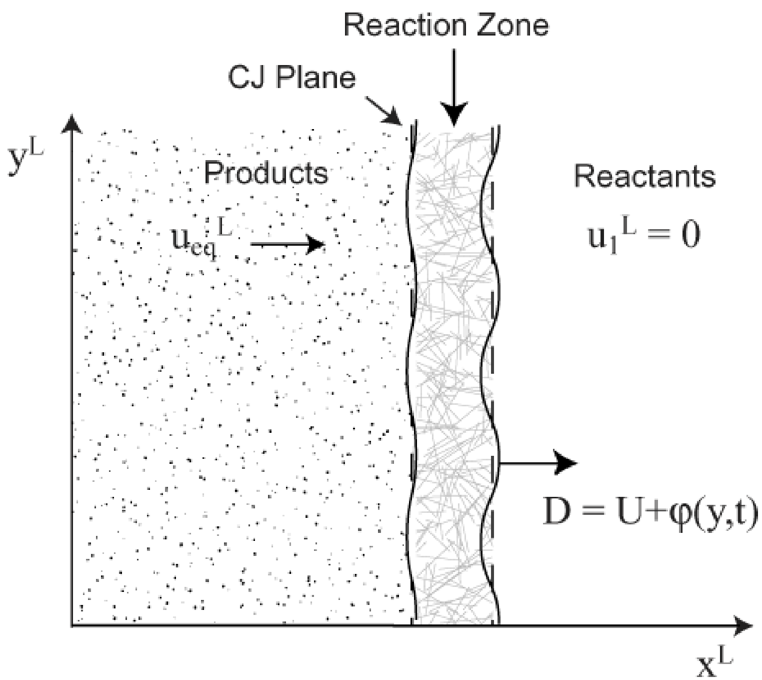


Bach et al 1969


10 mm


НО ТЕОРИЯ ВЕРНАЯ!
BUT THEORi is RIGHT!

Erpenbeck 1964, Lee and Stewart 1990, Short, Sharpe, Kasimov, Tumin, …



$$\psi = \psi^1 \exp(\omega t)$$

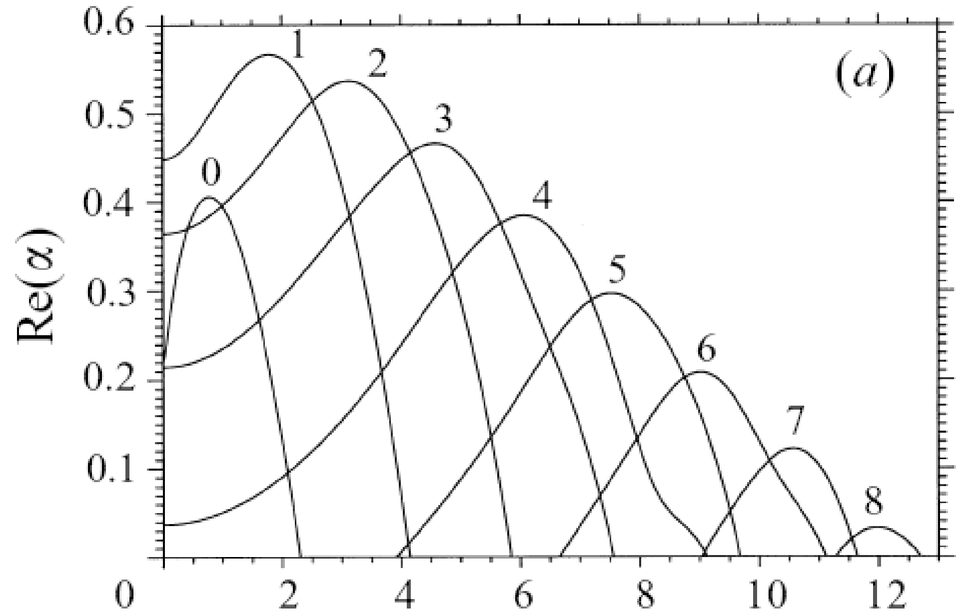
$$v' = v^1(x)\exp(\omega t)$$

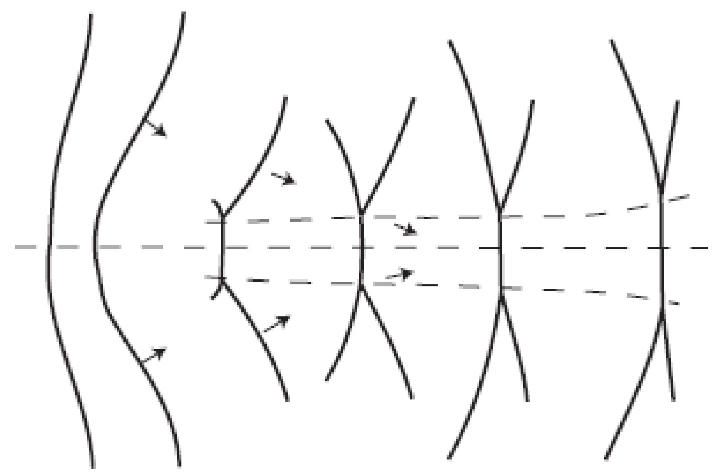
$$\mathrm{u}' = \mathrm{u}^1(x)\exp(\omega t)$$

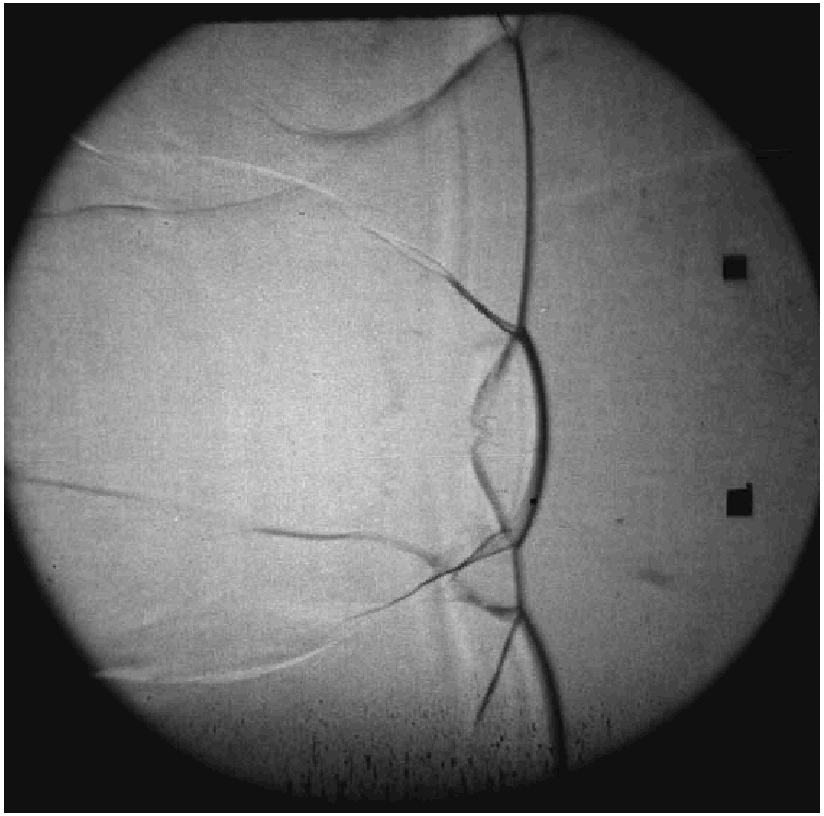
$$P' = P^1(x)\exp(\omega t)$$

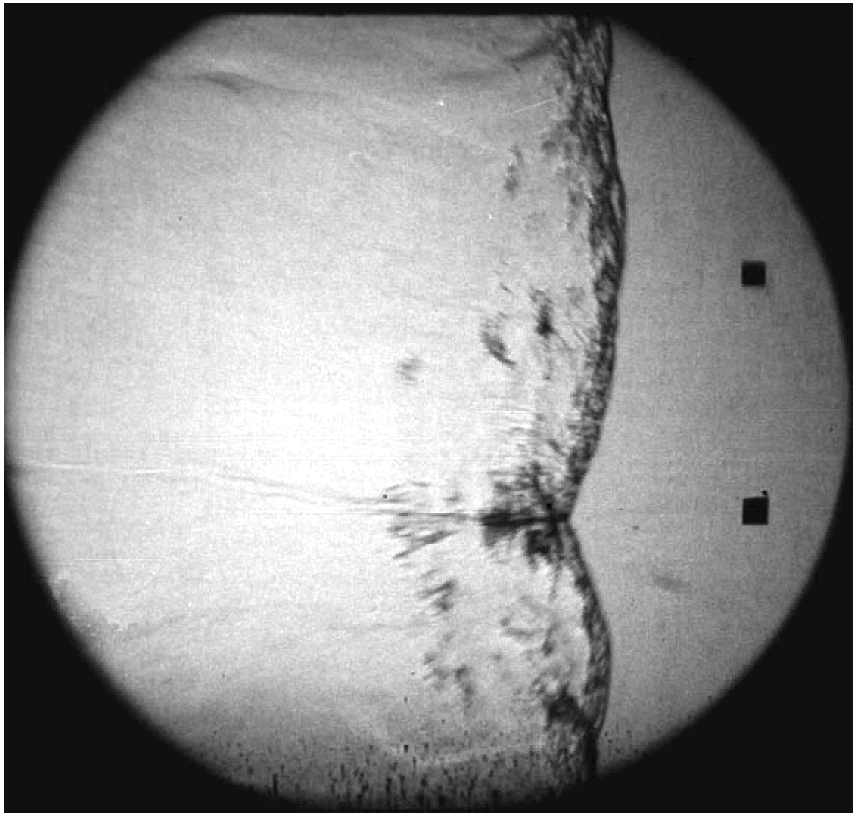
$$y_i' = y_i^1(x)\exp(\omega t)$$

$$\ldots$$



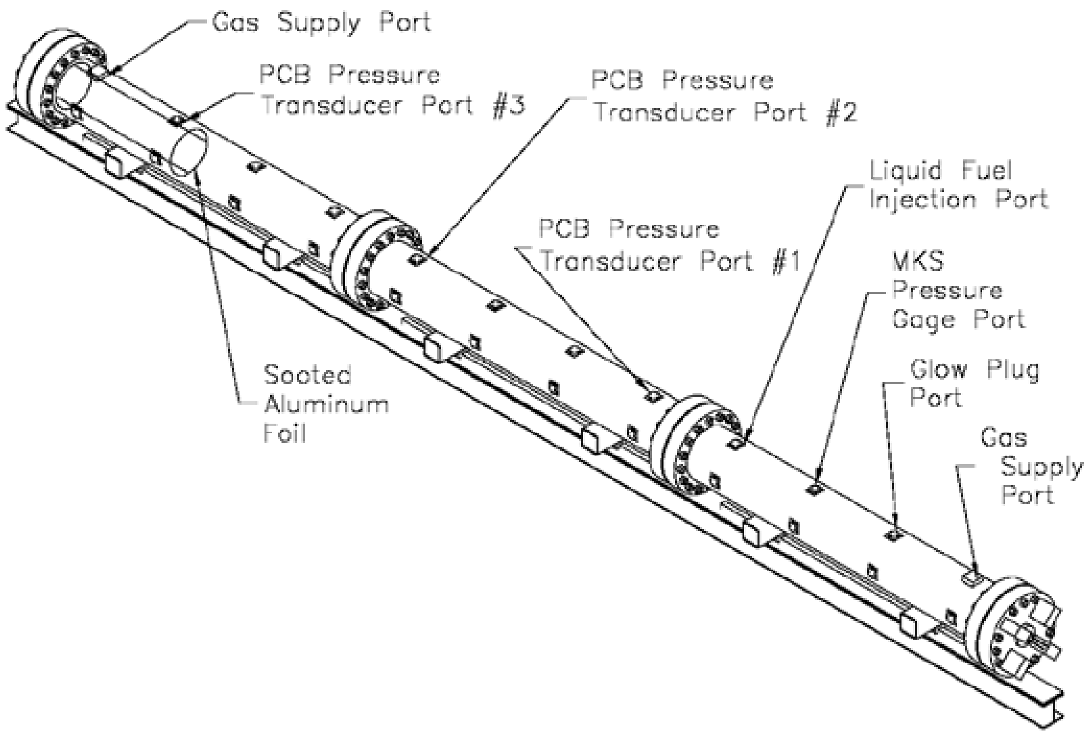




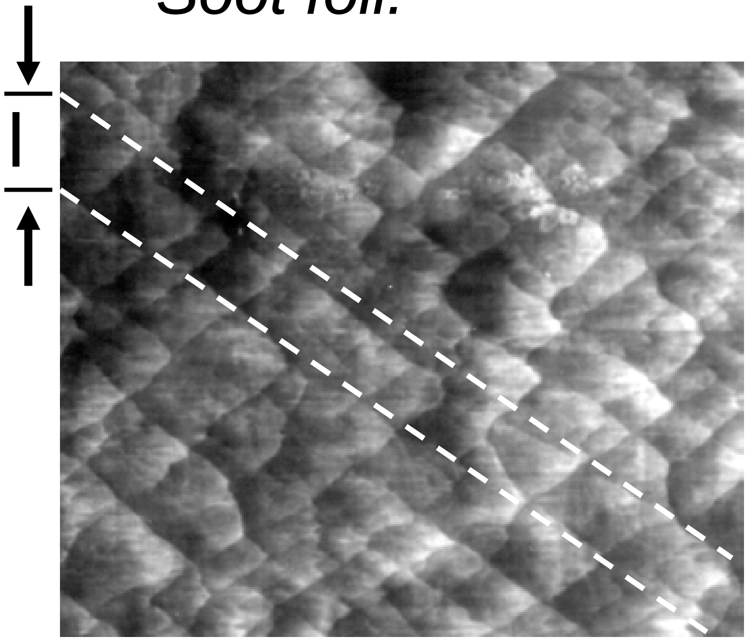


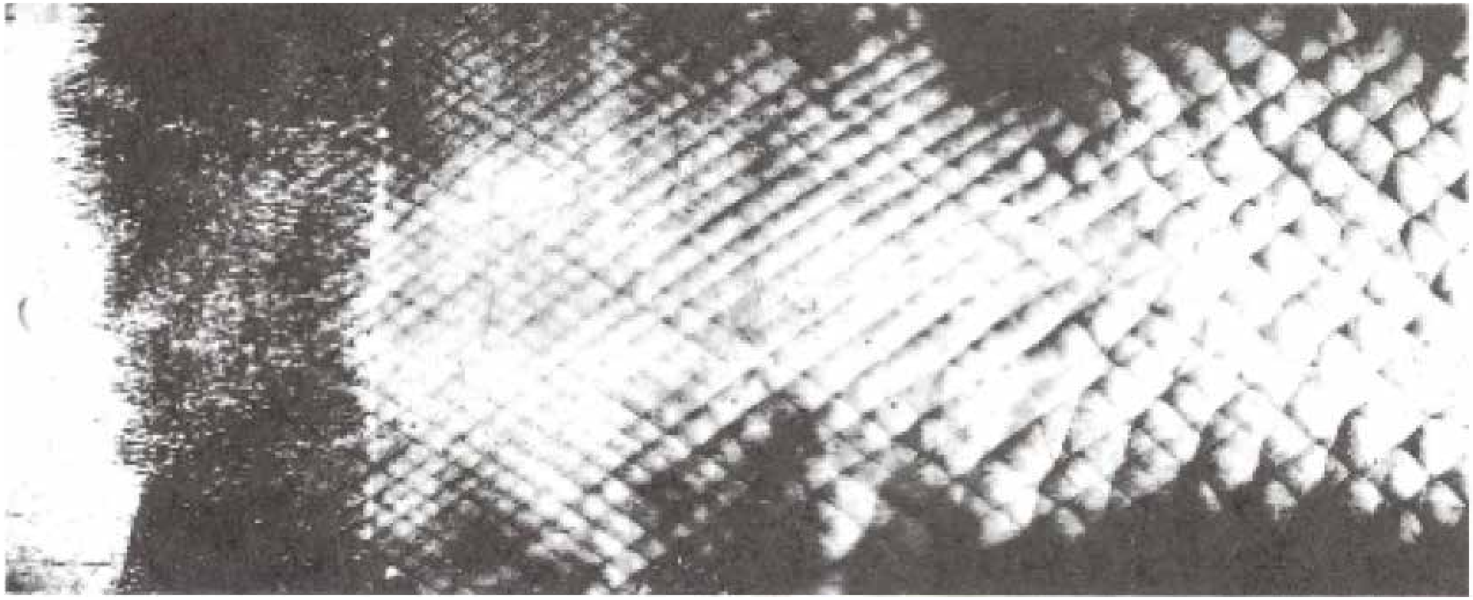
2H2-O2-85%Ar
P_o=20kPa

C3H8-5O2-60%N2
P_o=20kPa

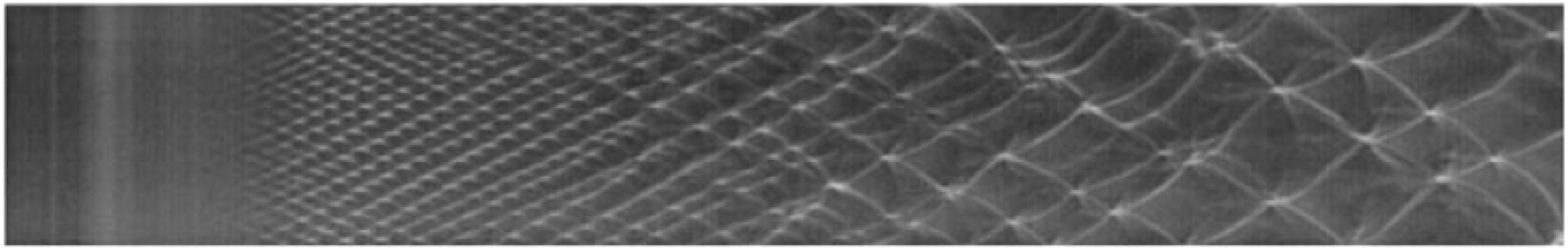

Gas Supply Port
PCB Pressure
Transducer Port #3
PCB Pressure
Transducer Port #2
Liquid Fuel
Injection Port
PCB Pressure
Transducer Port #1
MKS
Pressure
Gage Port
Glow Plug
Port
Gas
Supply
Port
Sooted
Aluminum
Foil

Soot foil:

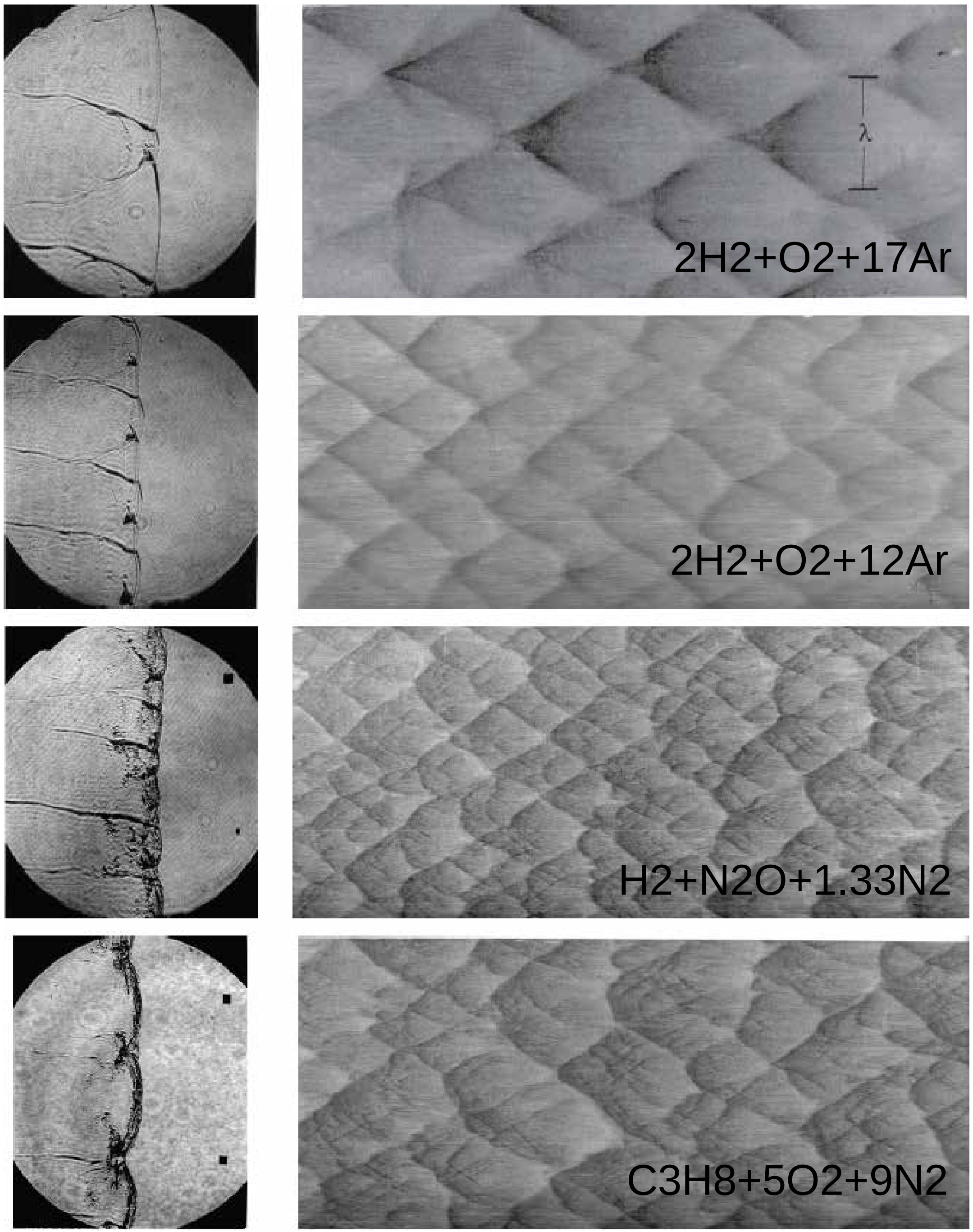


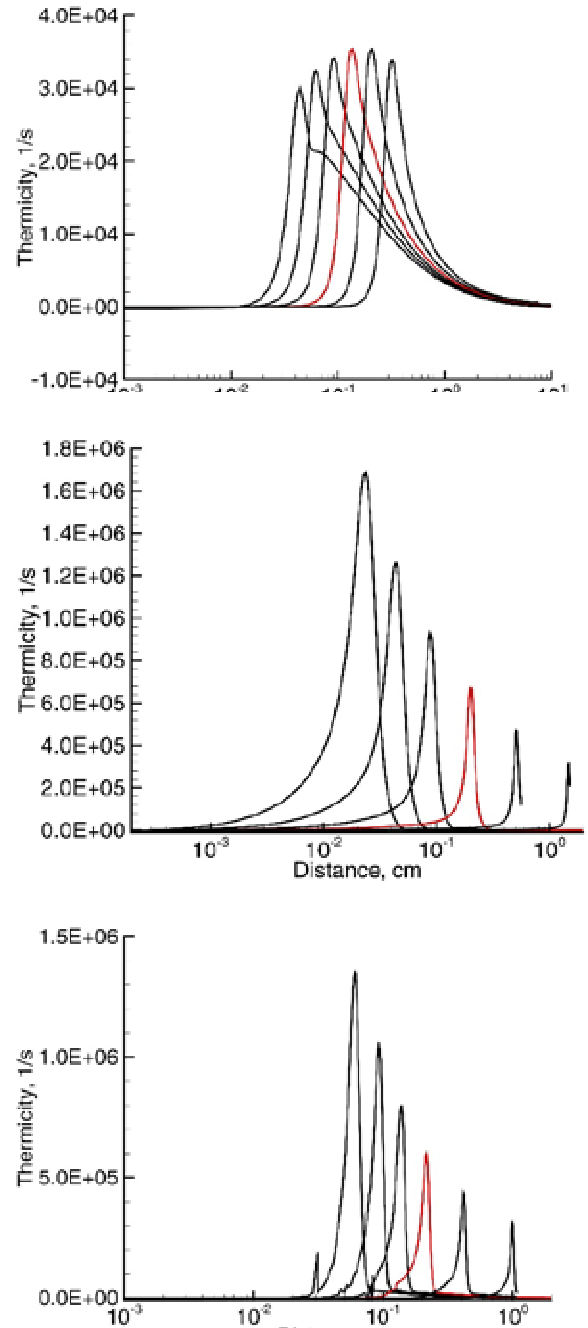


Strehlow 1967 $2H_2+O_2+7Ar$

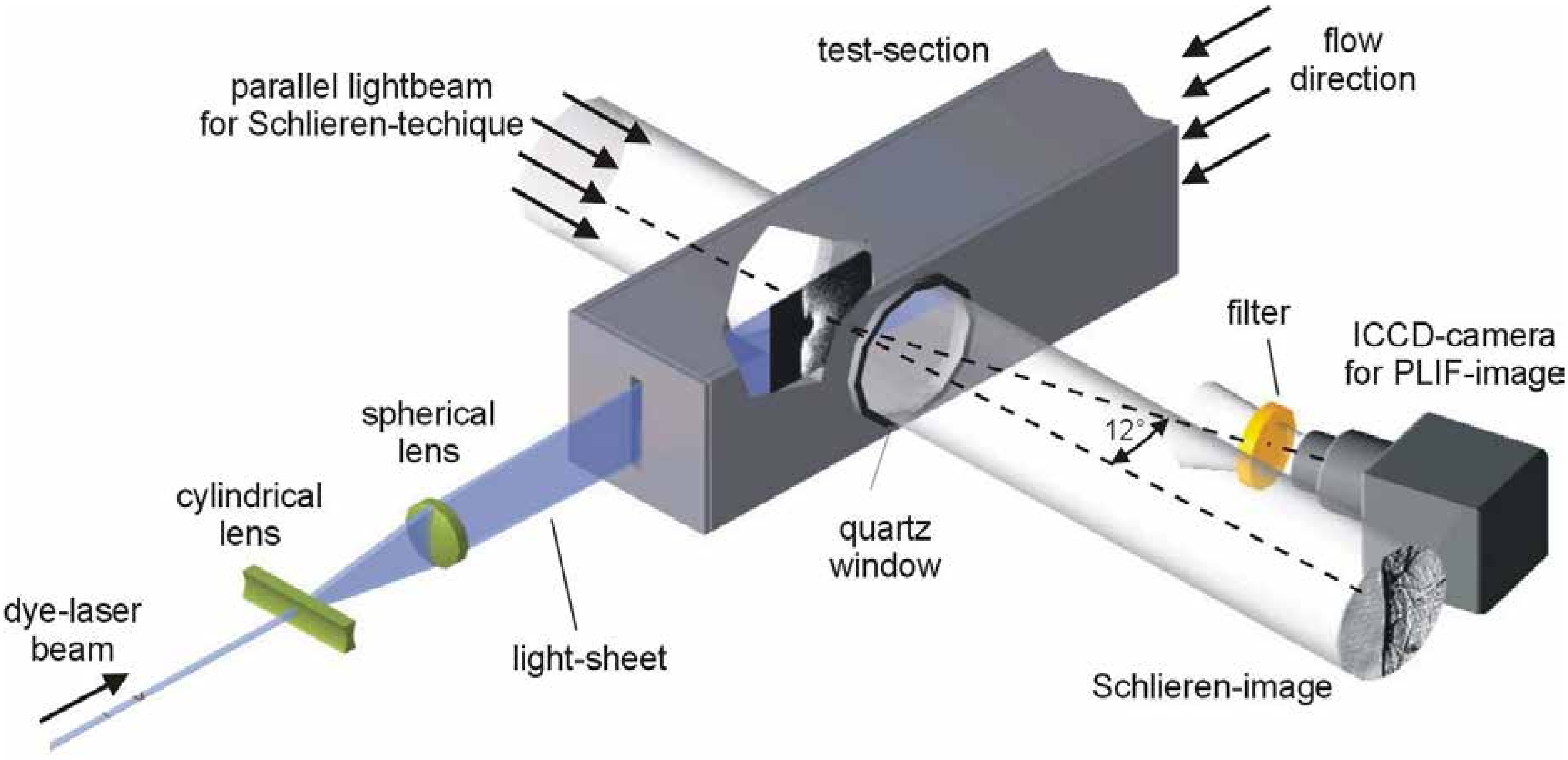


Gamezo et al 1999 $E/RT = 7.4$ $DY/Dt = -A(1-y) \exp(-E/RT)$


λ
2H2+O2+17Ar
2H2+O2+12Ar
H2+N2O+1.33N2
C3H8+5O2+9N2

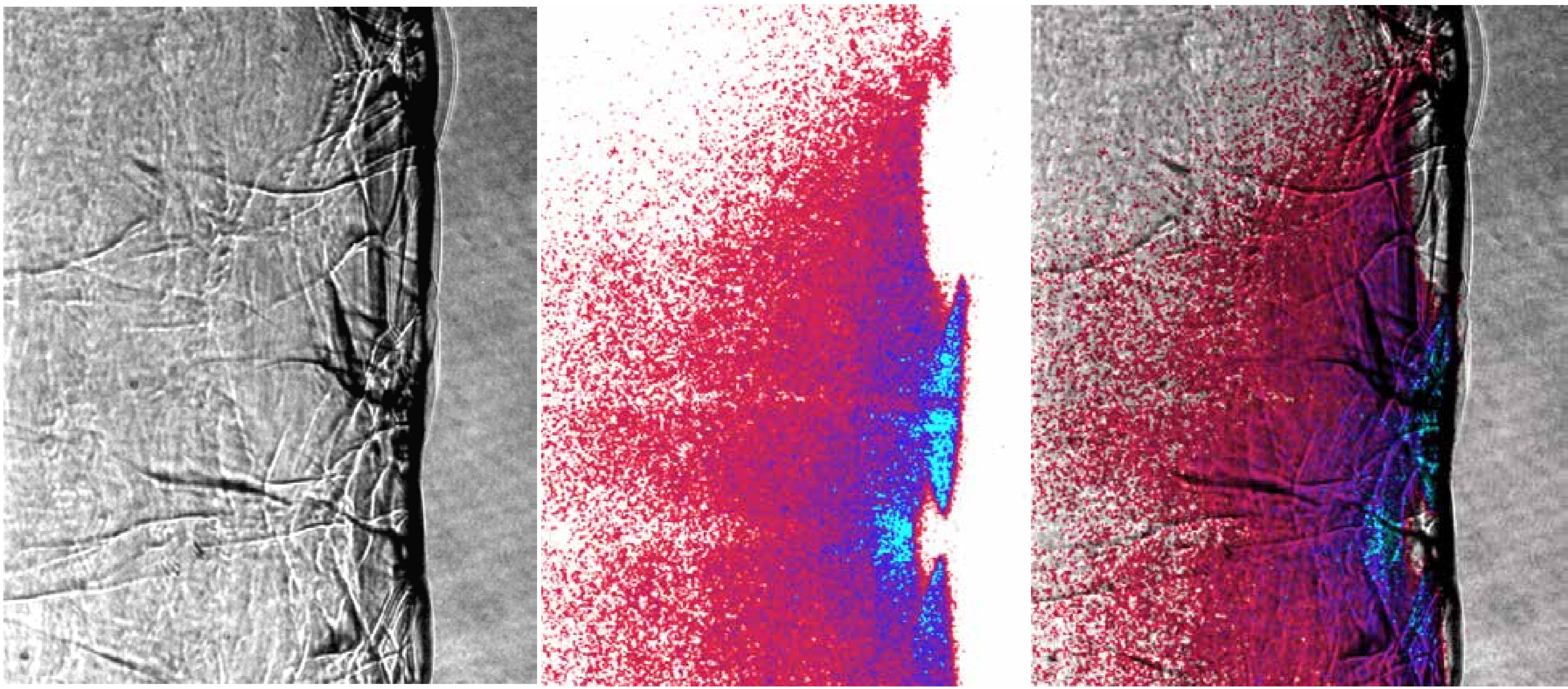

Thermicity, 1/s
4.0E+04
3.0E+04
2.0E+04
1.0E+04
0.0E+00
-1.0E+04
1.8E+06
1.6E+06
1.4E+06
1.2E+06
1.0E+06
8.0E+05
6.0E+05
4.0E+05
2.0E+05
0.0E+00
Distance, cm
1.5E+06
1.0E+06
5.0E+05
0.0E+00

Austin 2003



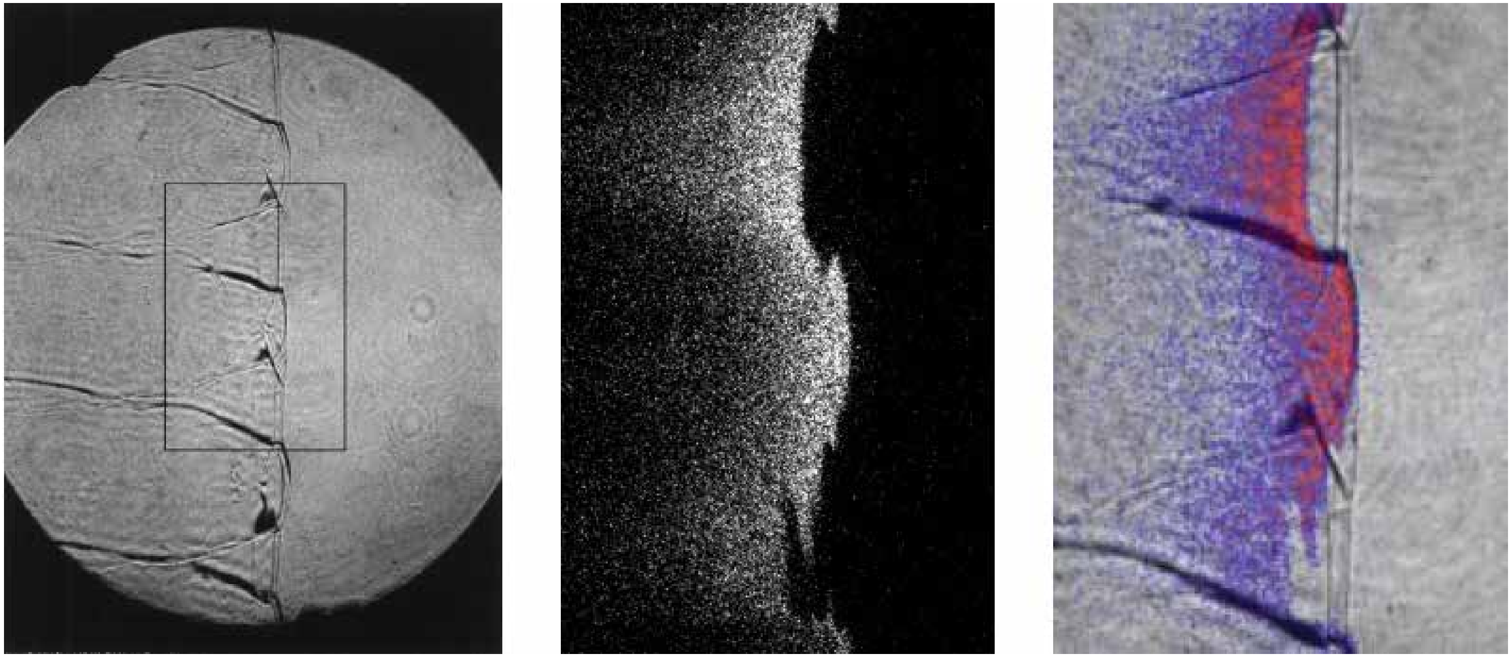
Pintgen et al 2003

$2H_2+O_2+17Ar$, 20kPa   cellsize: 48 mm
ZND-calculated Induction-zone-length at CJ-state: 1.6 mm

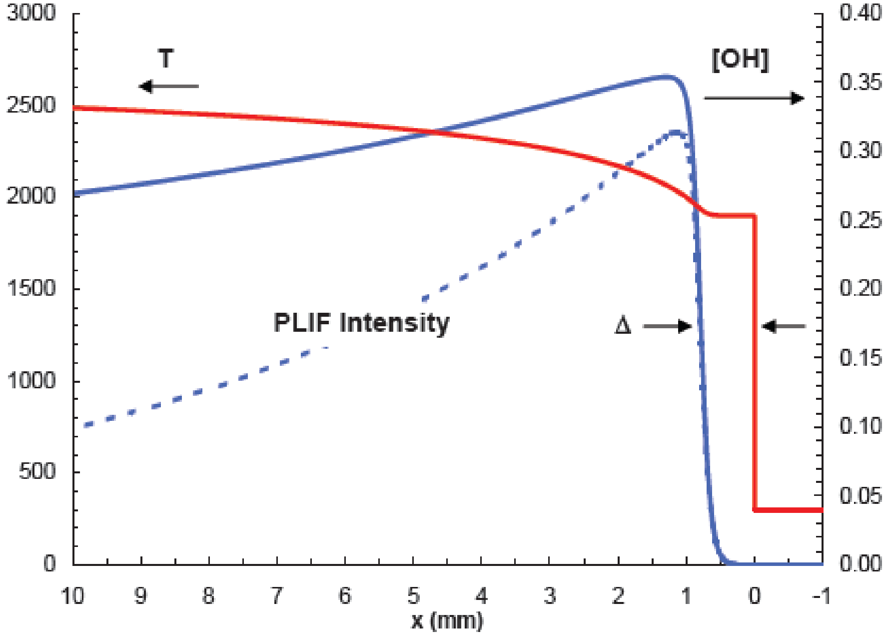
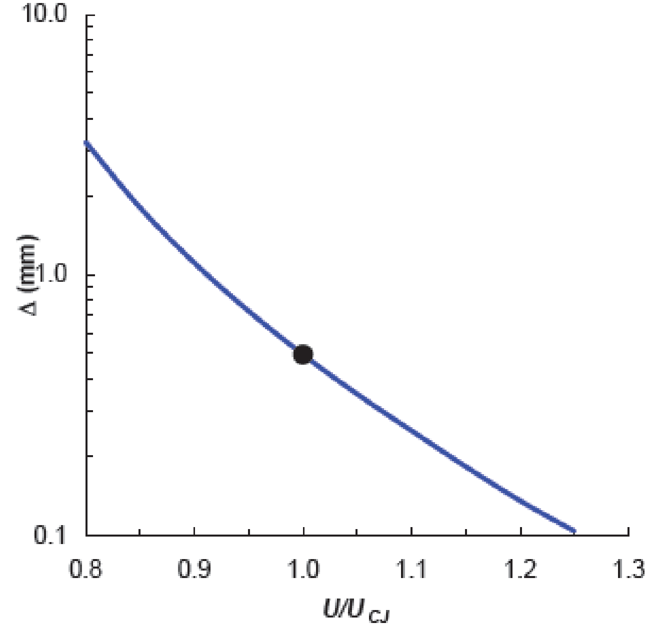


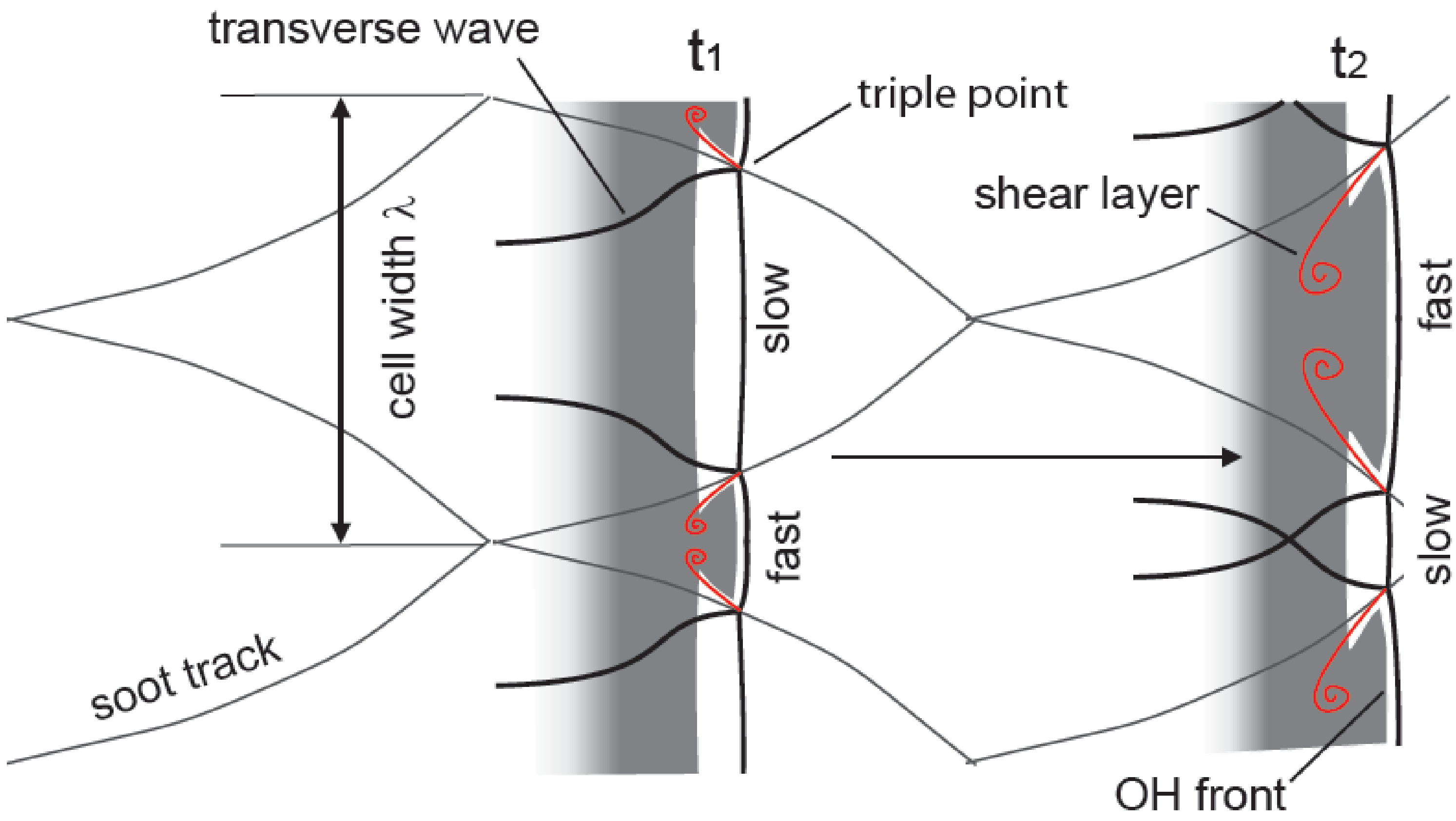
Ñr   [OH]

Pintgen 2000



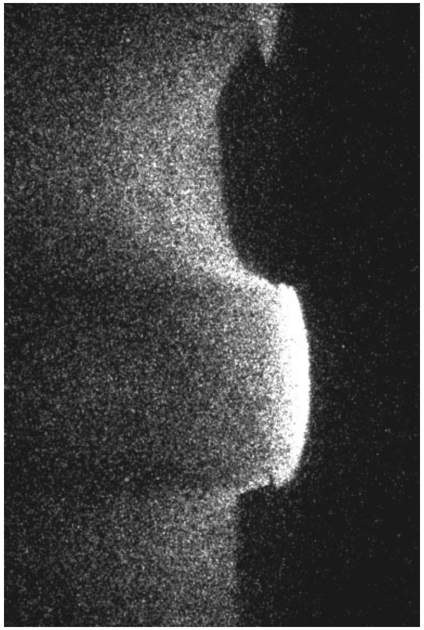
Austin 2003


3000
2500
2000
1500
1000
500
0
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
T
[OH]
PLIF Intensity
Δ
10
9
8
7
6
5
4
3
2
1
0
-1
x (mm)

10.0
1.0
0.1
Δ (mm)
0.8
0.9
1.0
1.1
1.2
1.3
U/U CJ



transverse wave
t1
triple point
t2
shear layer
cell width λ
slow
fast
fast
slow
soot track
OH front

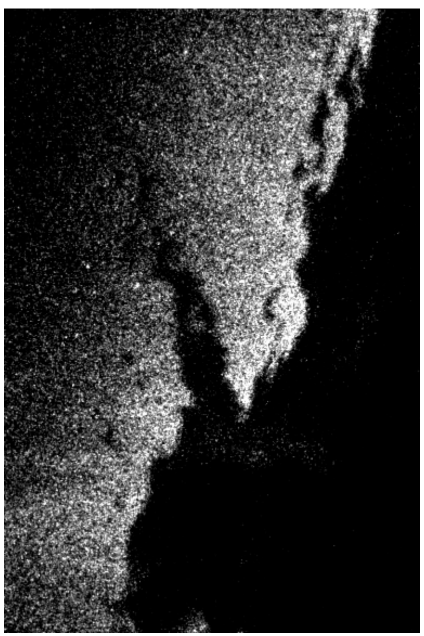
$2H_2+O_2+17Ar$



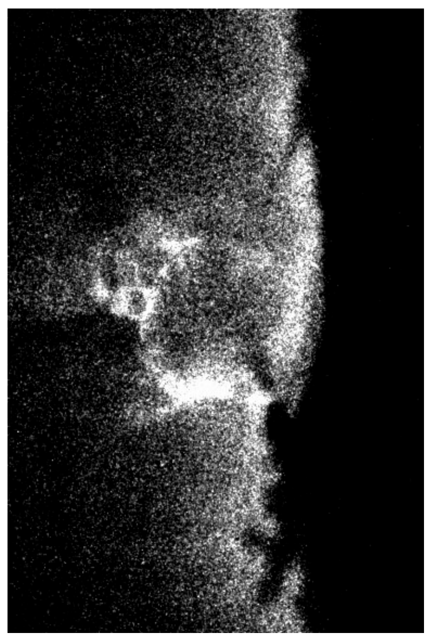
$2H_2+O_2+8N_2$

$H_2+N_2O+3N_2$

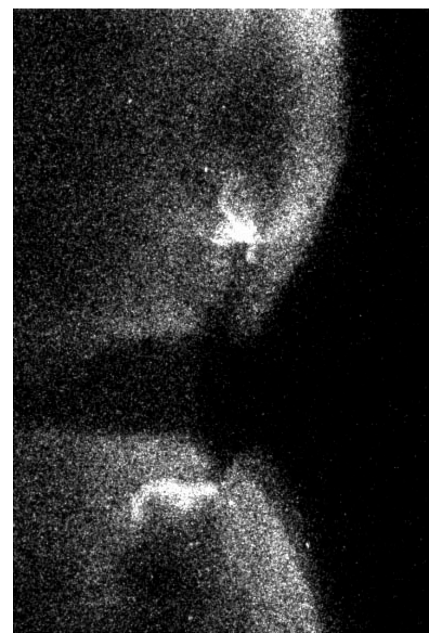
C_2H_4-$3O_2$-$10.5N_2$

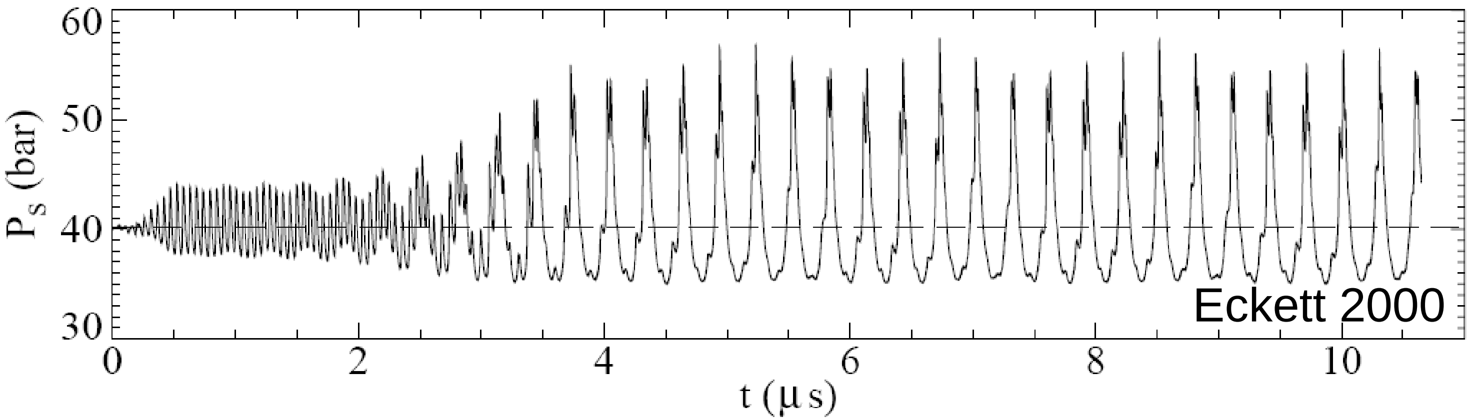


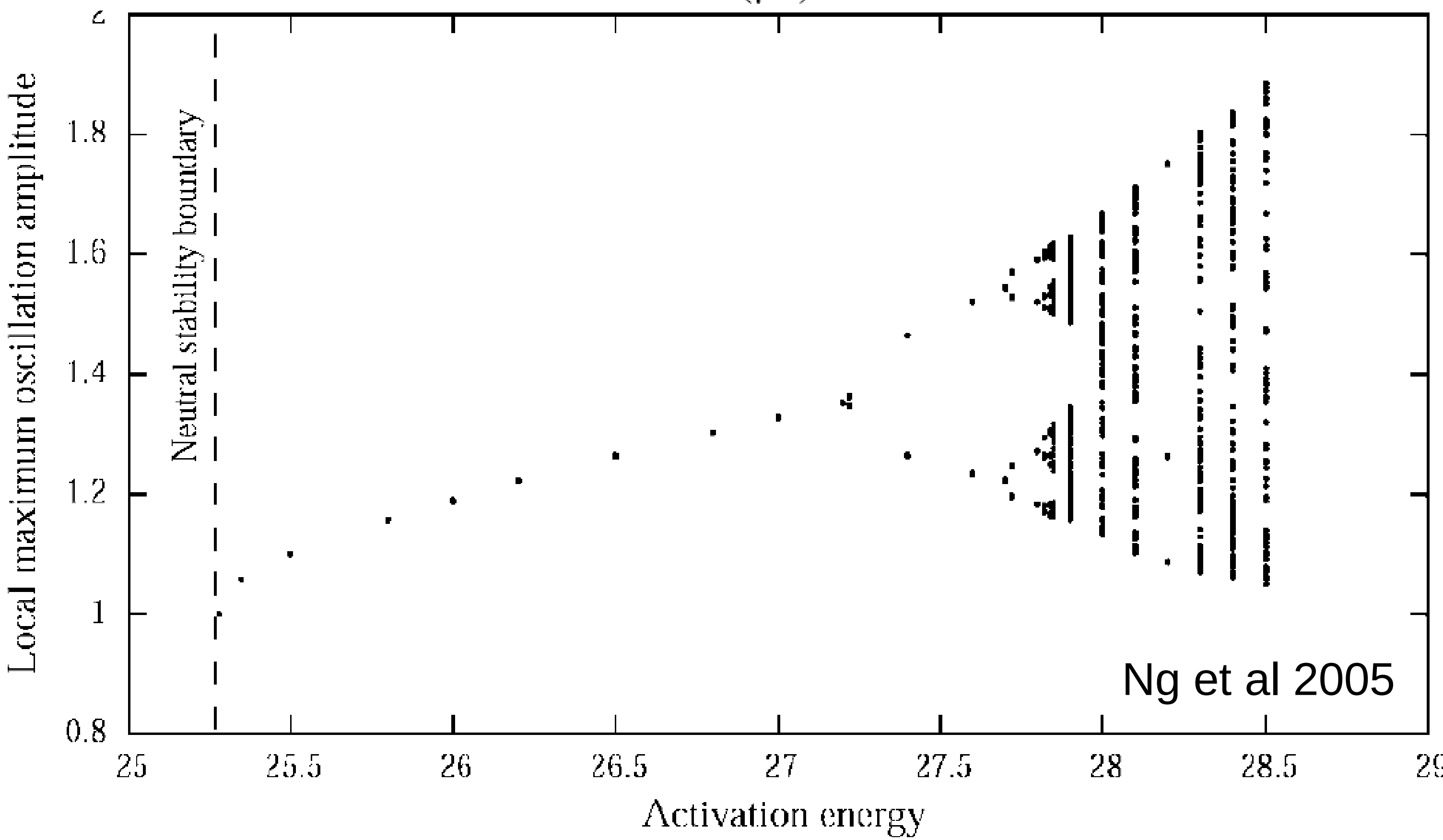
C_3H_8-$5O_2$-$9N_2$

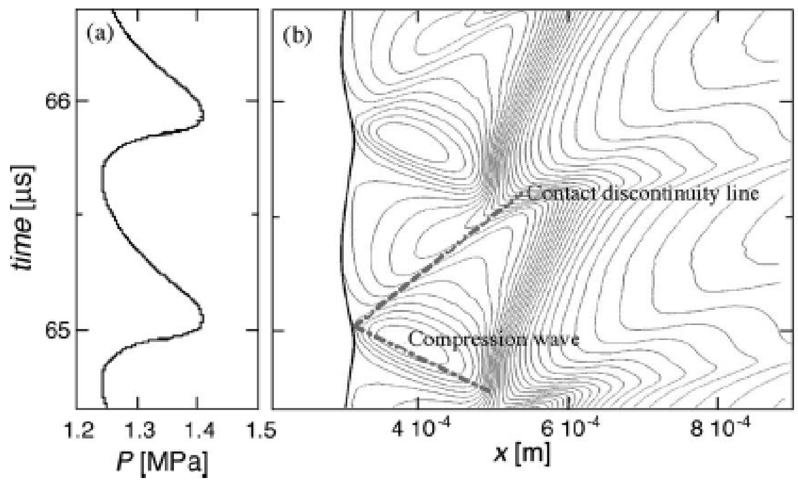


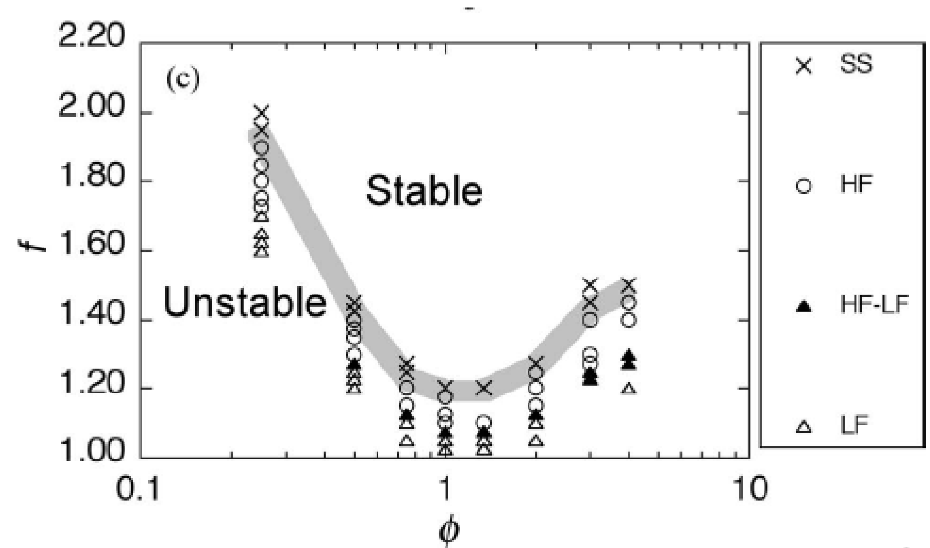
C_3H_8-$5O_2$-$9N_2$



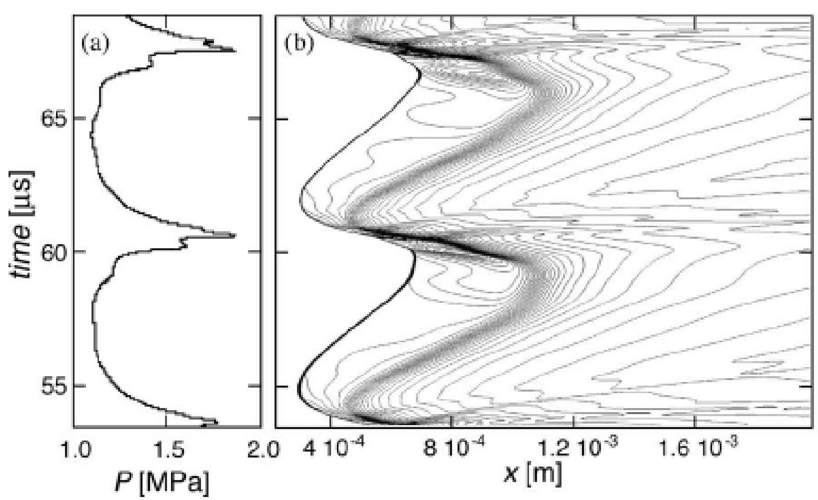

60
50
40
30
P_S (bar)
0
2
4
6
8
10
t (μ s)
Eckett 2000

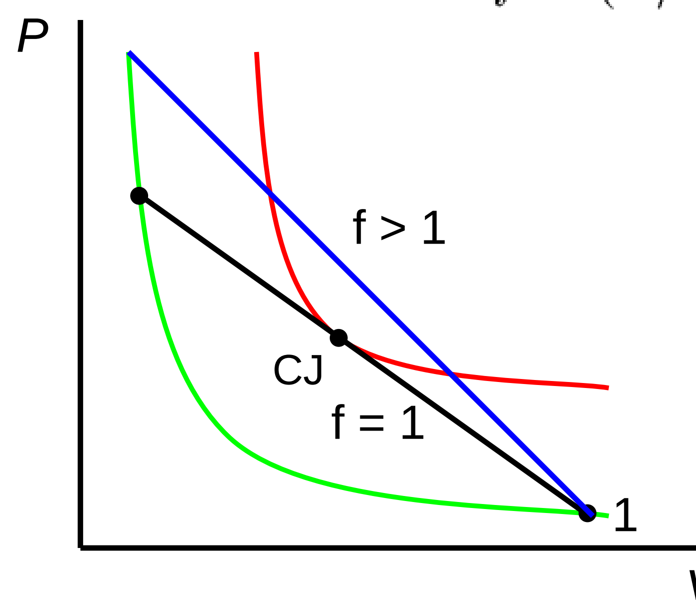

Local maximum oscillation amplitude
0.8
1
1.2
1.4
1.6
1.8
Neutral stability boundary
25
25.5
26
26.5
27
27.5
28
28.5
29
Activation energy
Ng et al 2005





$$f = (U/U_{CJ})^2$$



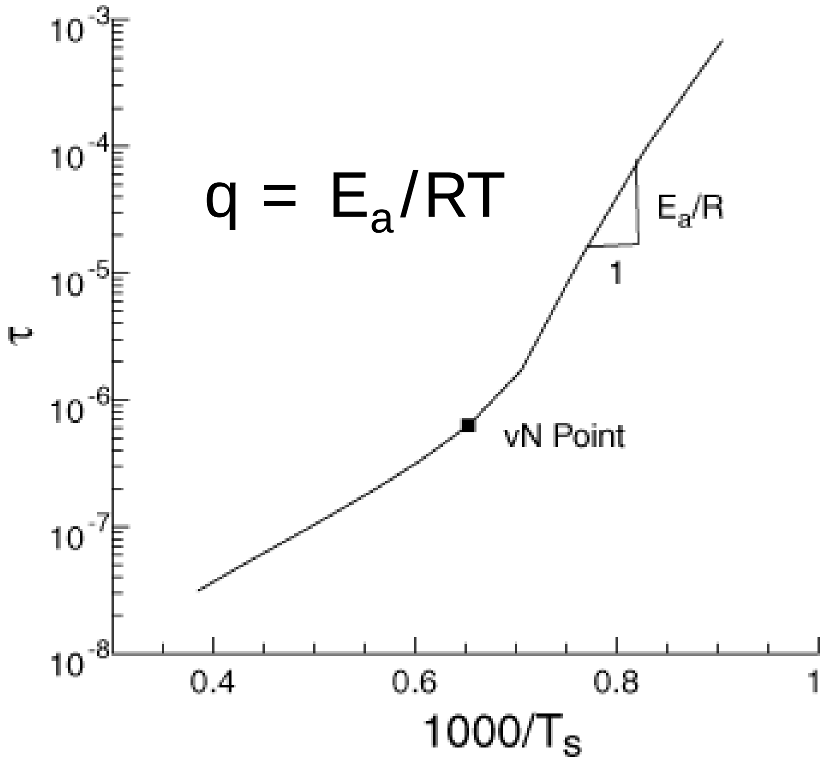


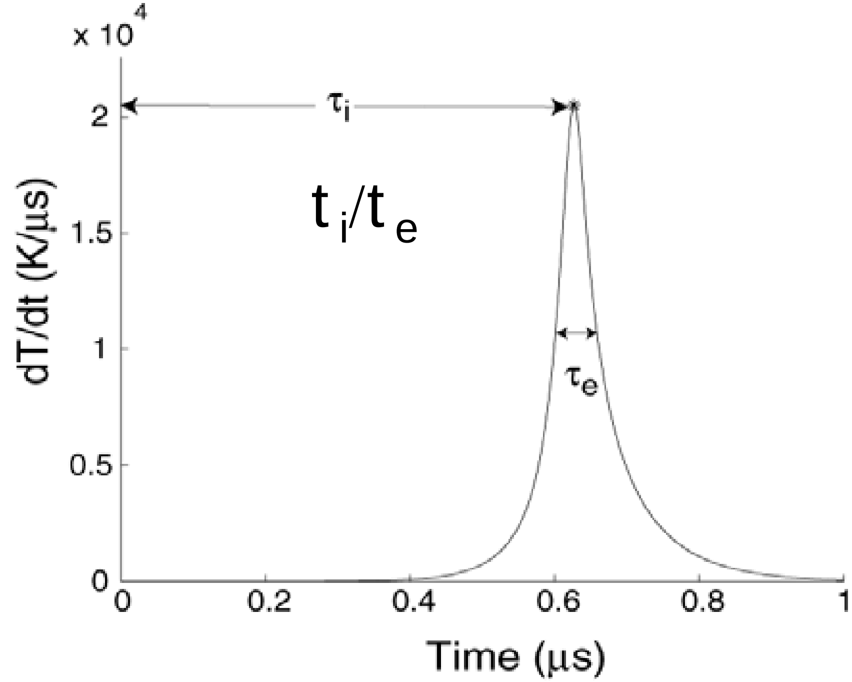
Daimon & Matsuo 2008

q – Reduced Effective Activation Energy

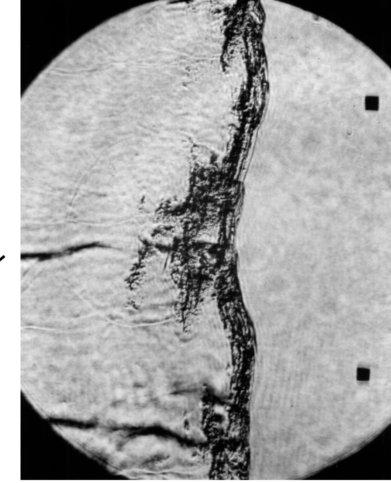
t_i – Induction Time

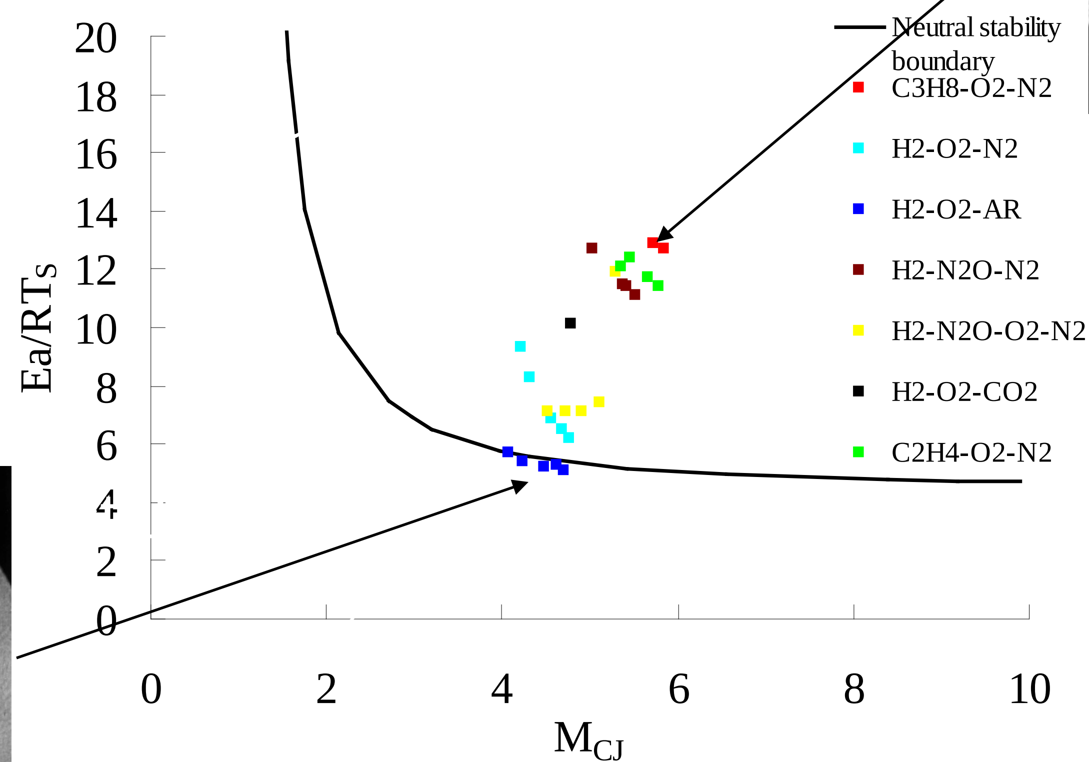
t_e – Energy Release Pulse Width





$$\frac{E_a}{RT} = \frac{T}{\Delta_i} \frac{\partial \Delta_i}{\partial T}$$

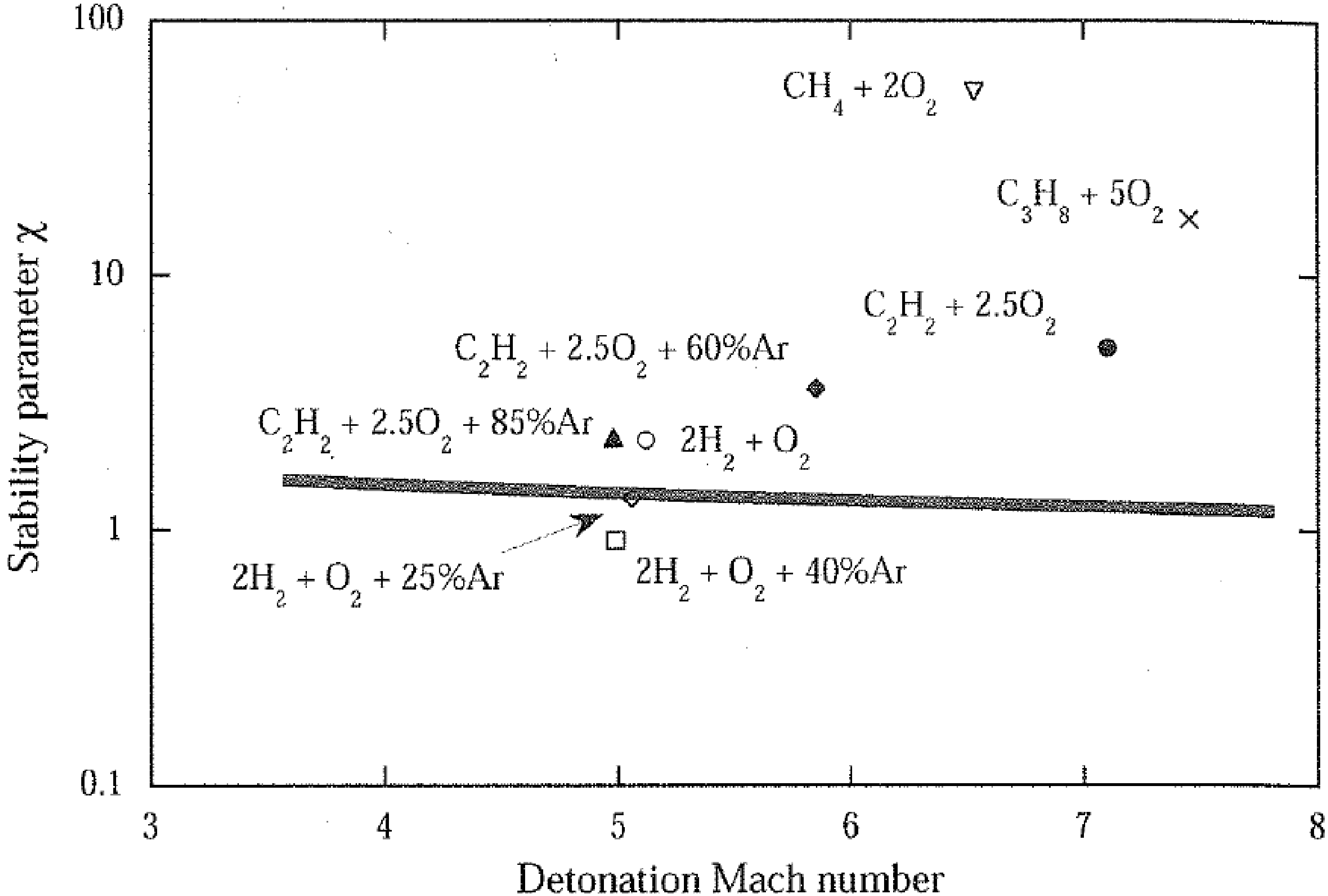




highly unstable
(high E_a/RT_S)

weakly unstable
(low E_a/RT_S)

$$\chi = \frac{E_a}{RT}\frac{\Delta_i}{\Delta_e}$$

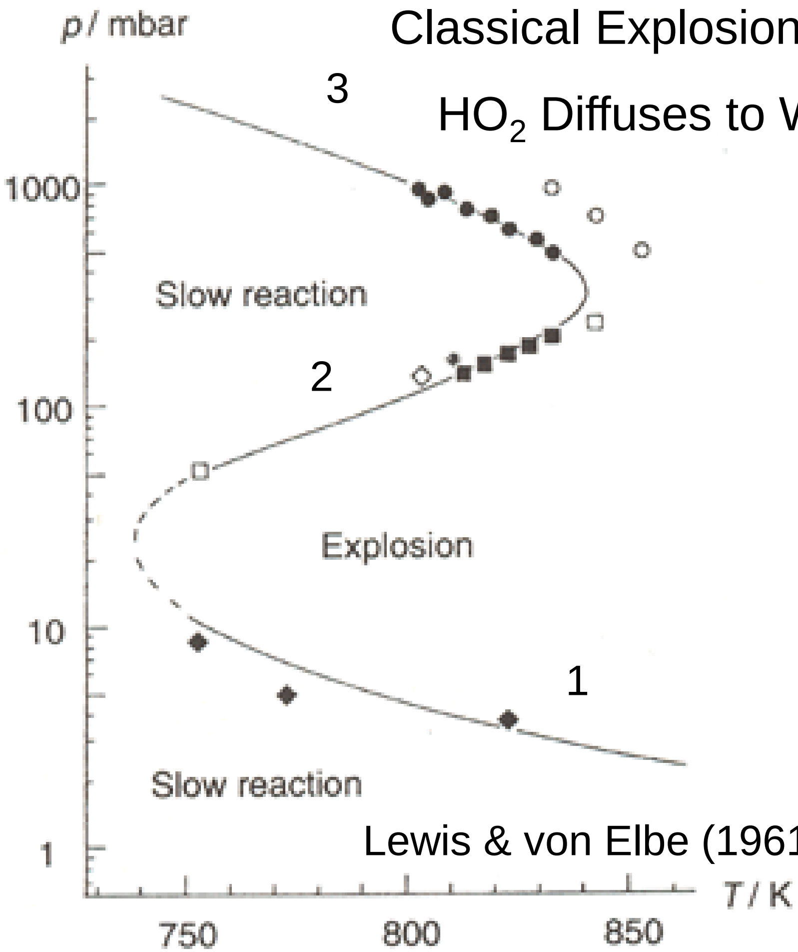


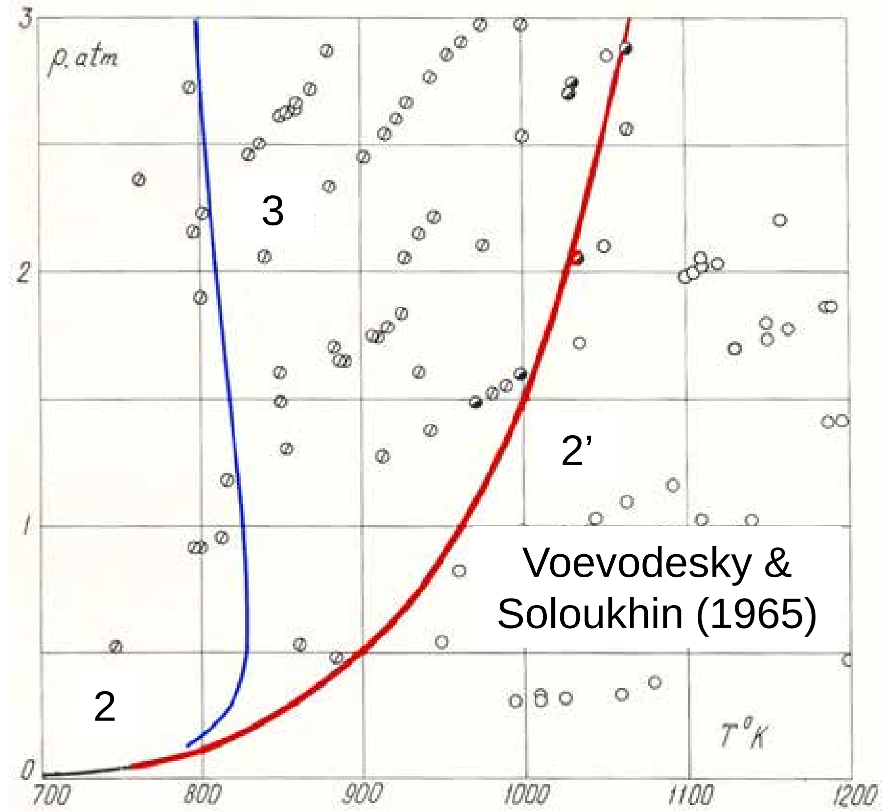
Ng et al 2005

H_2-O_2 Chemistry: Explosion Limits

Classical Explosion Limits

HO_2 Diffuses to Walls

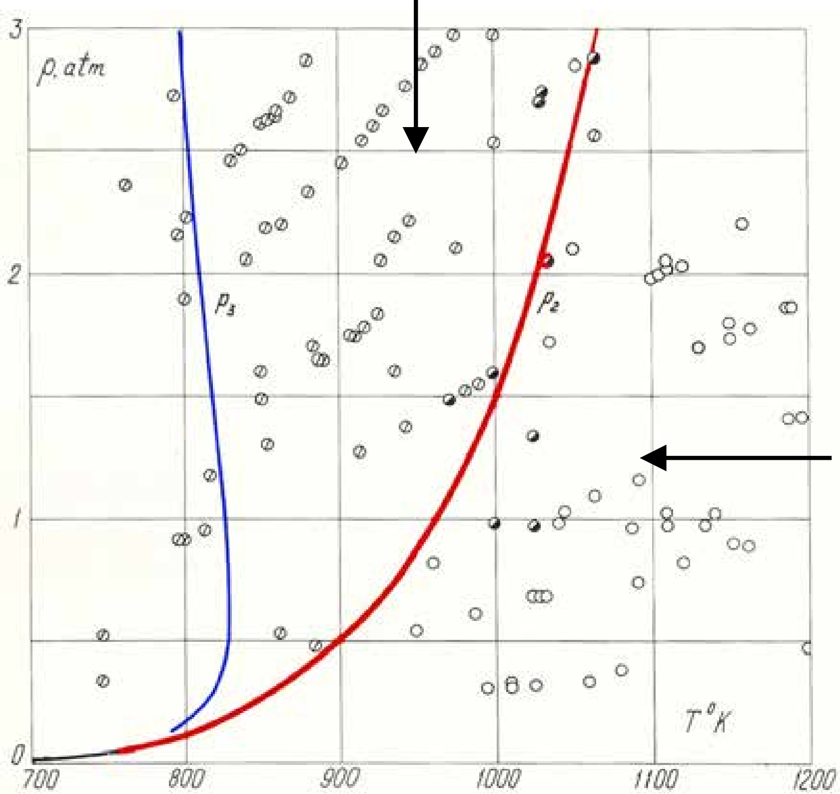




Extended Second Limit

H_2O_2 Enables Explosion

H_2-O_2 Chemistry: Two Pathways



- Peroxide Straight-Chain Pathway

$H + O_2 + M\ !\ HO_2 + M$

$HO_2 + HO_2\ !\ H_2O_2 + O_2$

$H_2O_2 + M\ !\ 2\ OH + M$ R1

(Rate Limiting Step)

- Chain-Branching Pathway

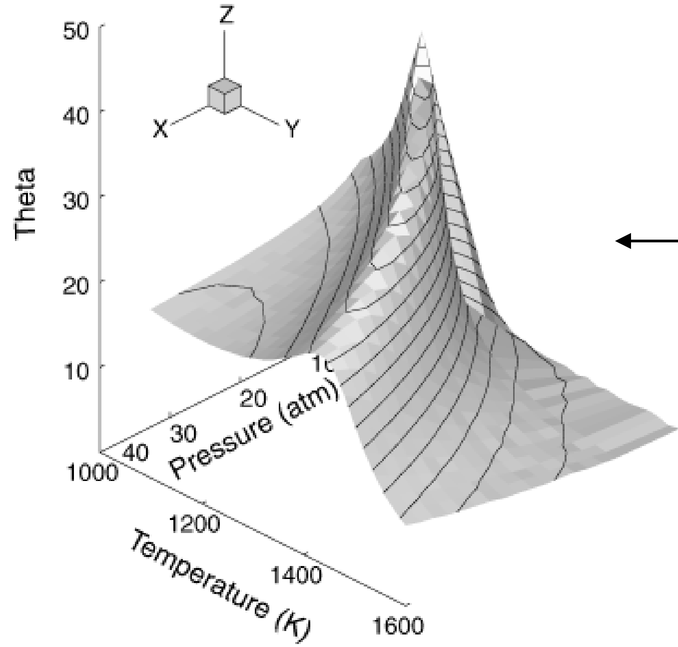
$H + O_2\ !\ OH + O$ R2

(Rate Limiting Step)

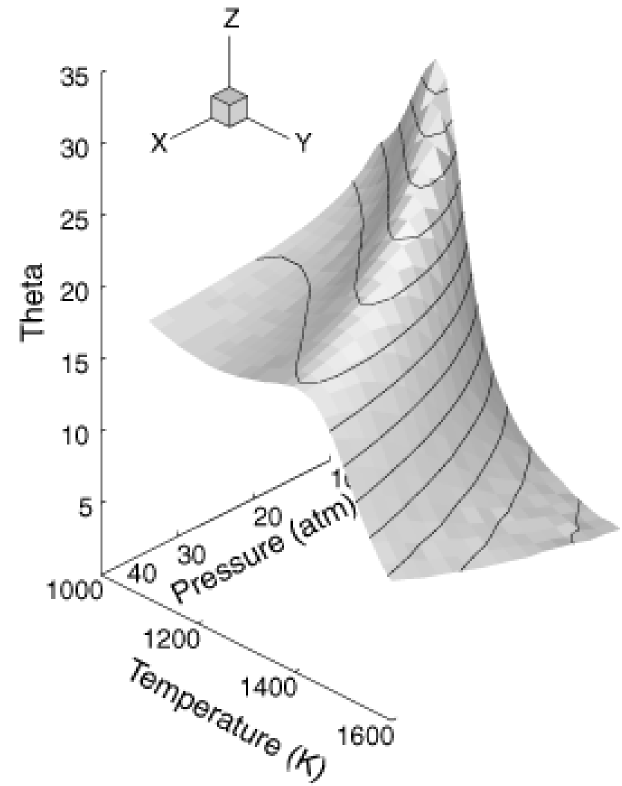
$O + H_2\ !\ OH + H$

$OH + H_2\ !\ H_2O + H$

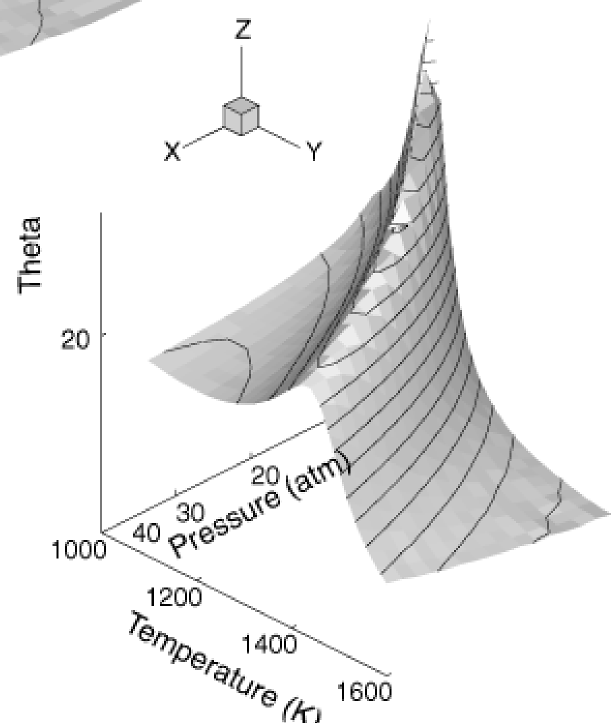
$$\theta = \frac{T}{\Delta_i}\frac{\partial \Delta_i}{\partial T} \approx \frac{E_a}{RT}$$



Stoichiometric H_2-Air



Lean H_2-Air φ = 0.8



Rich H_2-Air φ = 3.0

Lean H_2-Air φ = 0.35

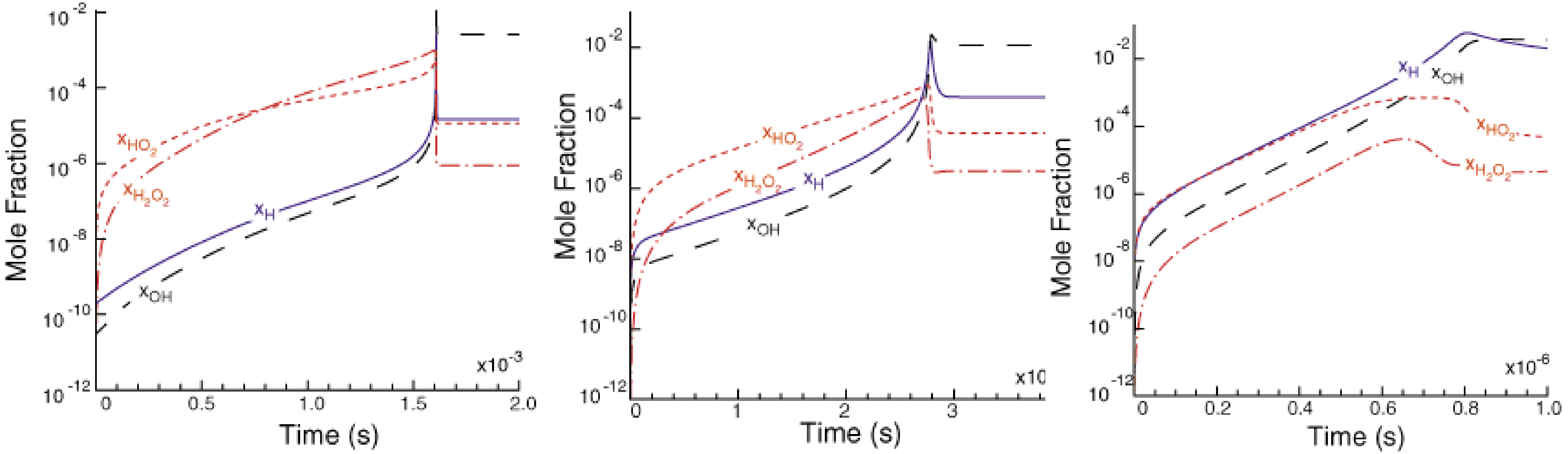
Peroxide Pathway Dominant

Lean H_2-Air φ = 0.5

Competition

Stoichiometric H_2-Air

Branching Pathway Dominant

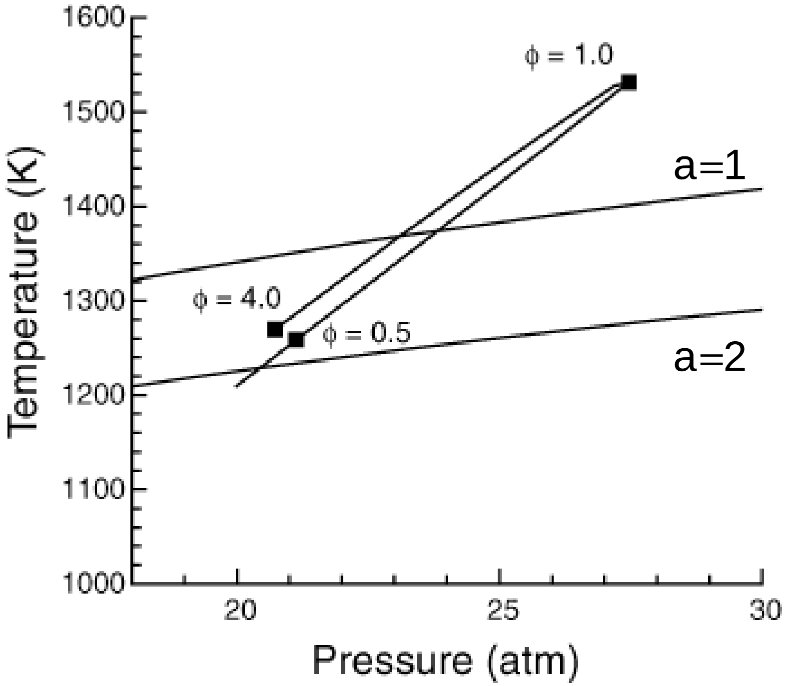


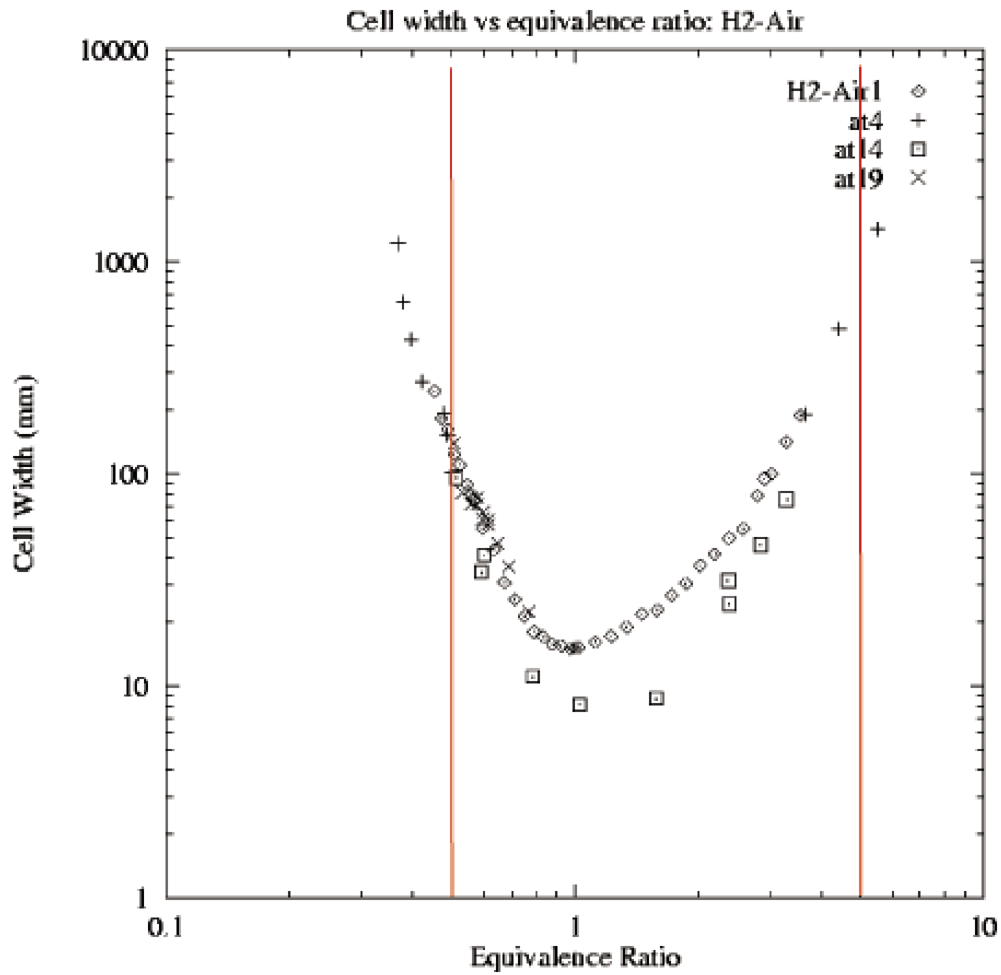
Initial Conditions

T = 300 K, P = 0.7 atm

Browne, Liang, Shepherd 2005

Detonation limits?





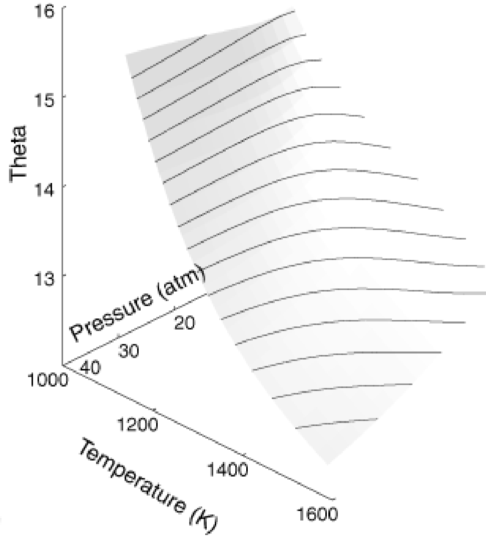
$H + O_2$! $OH + O$ R1

$H + O_2 + M$! $HO_2 + M$ R2

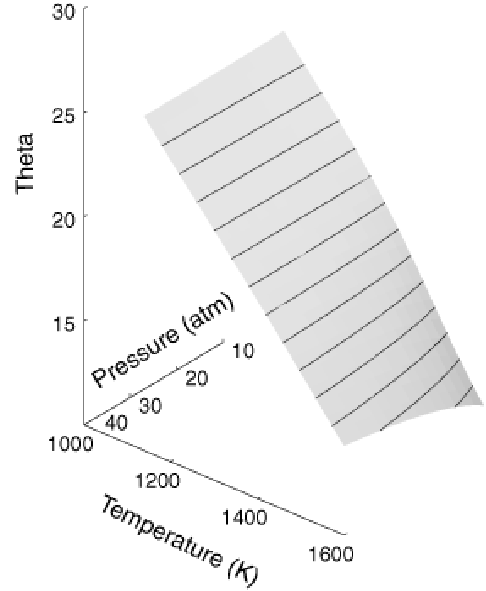
$r_2/r_1 = a$

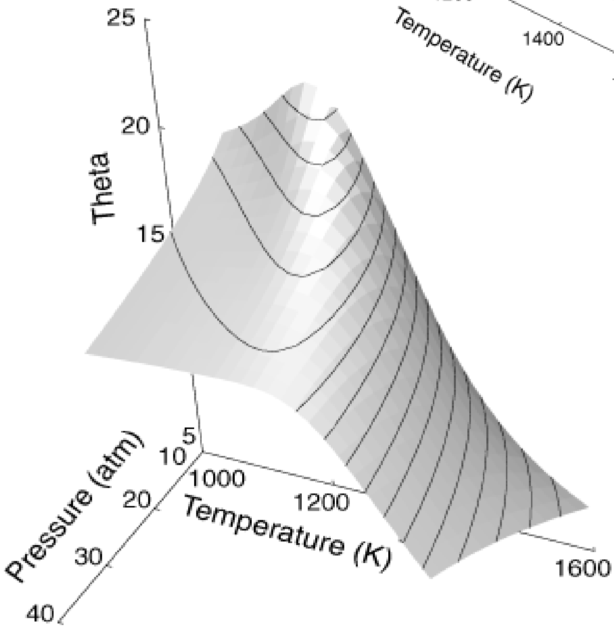
Cross-over Temperature Cannot Predict Limits

Stoichiometric
CH_4-Air

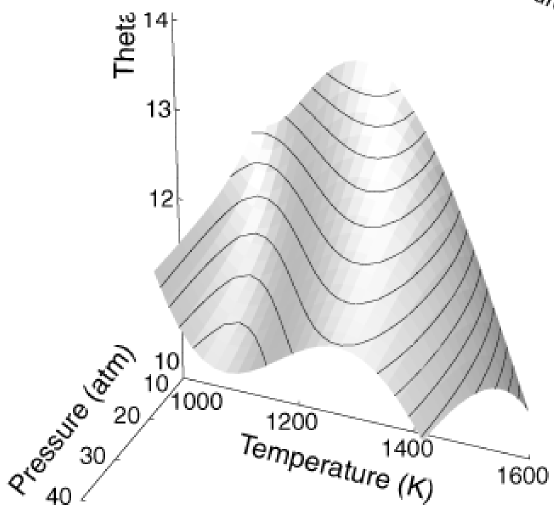


Stoichiometric
C_2H_6-Air

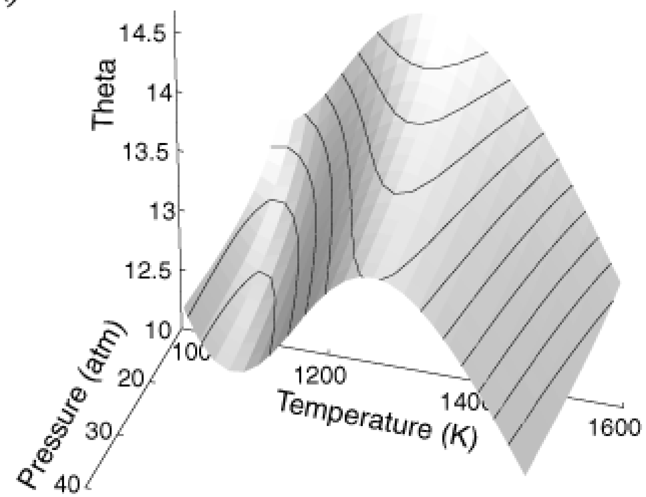




Stoichiometric
C_2H_4-Air

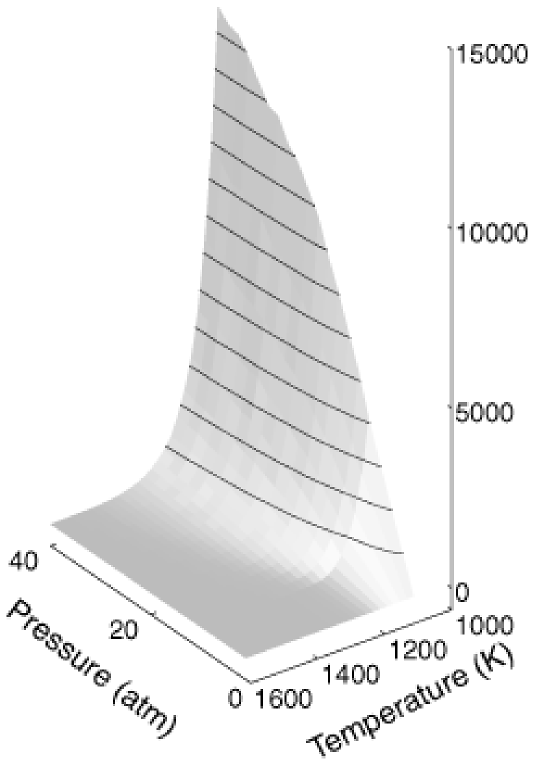


Stoichiometric
C_2H_2-Air

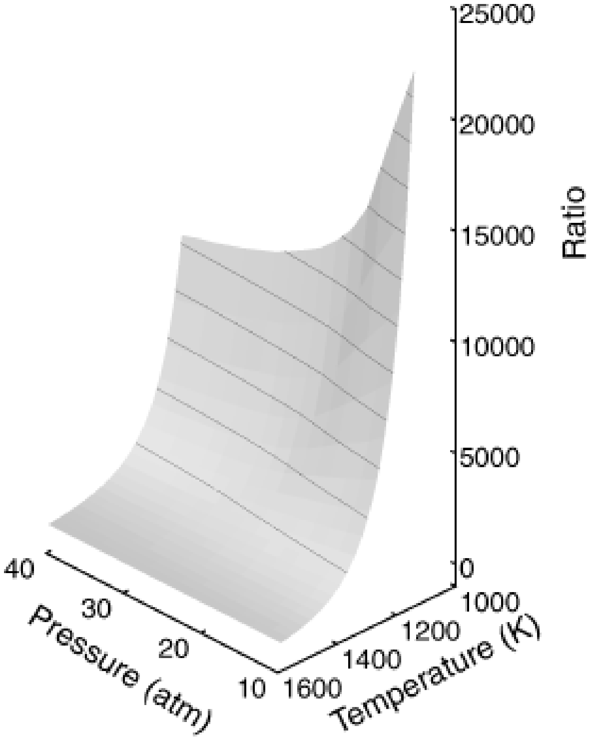


Stoichiometric
C_3H_8-Air

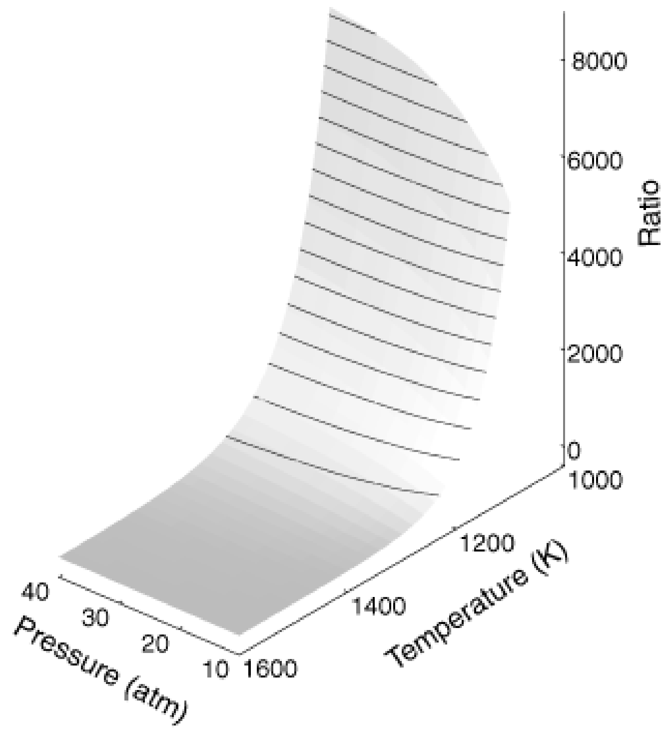
Ratio of Time Scales (τ_i/τ_e)



Stoichiometric H_2-Air



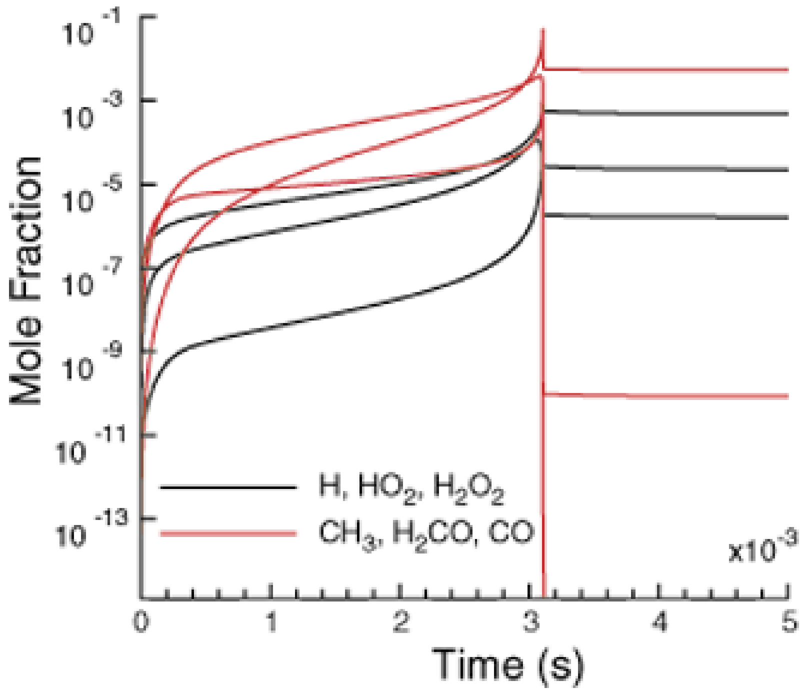
Stoichiometric CH_4-Air



Stoichiometric C_2H_2-Air

Hydrocarbon Oxidation

- Many Pathways



Additional Pathways Can Bypass Competition Effect

NO CROSS-OVER TEMPERATURE

CO Oxidation

- CO + O_2 ! CO_2 + O
- CO + OH ! CO_2 + H
- CO + HO_2 ! CO_2 + OH

CH_4 Oxidation

- CH_4 + *X* ! CH_3 + *X*H
- CH_3O + M ! H_2CO + H + M
- H_2CO + *X* ! HCO + *X*H
- HCO + M ! H + CO + M

Modeling Competing Radicals

Chemistry

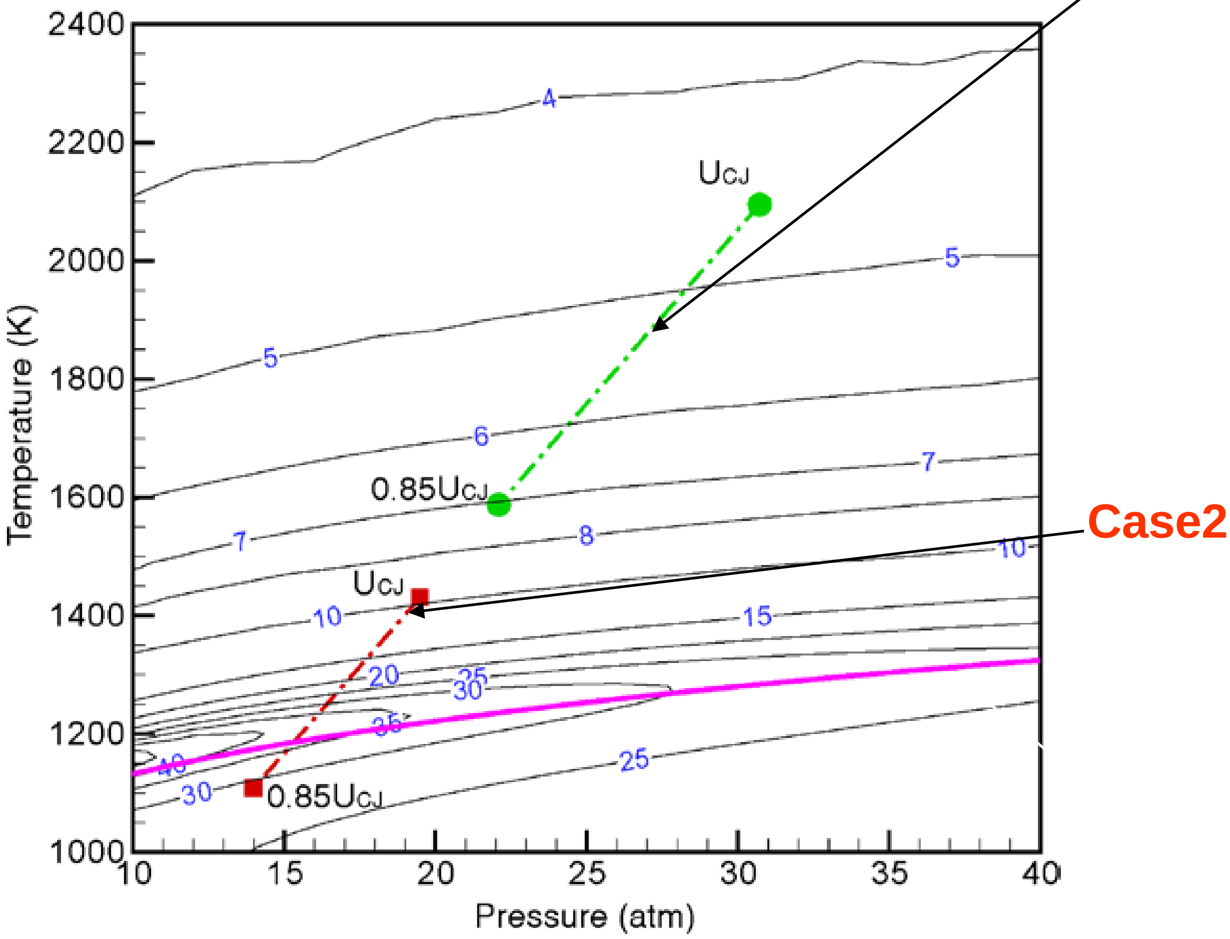
	Dold & Kapila *CF* 91, Short & Quirk 97 *JFM*	**Shepherd *PAA* 86**
	(1) $R \xrightarrow{K_1} B$	$H_2 + O_2 \rightarrow HO_2 + H$
pathway	(2) $R + B \xrightarrow{K_2} 2B$	$\begin{cases} H + O_2 \leftrightarrow OH + O \\ O + H_2 \leftrightarrow OH + H \\ OH + H_2 \leftrightarrow H_2O + H \end{cases}$
	(3) $R + B + M \xrightarrow{K_3} C + M$	$H + O_2 + M \leftrightarrow HO_2 + M$
	(4) $C \xrightarrow{K_4} 2B$	$\begin{cases} HO_2 + HO_2 \rightarrow H_2O_2 + O_2 \\ H_2O_2 + M \leftrightarrow 2OH + M \end{cases}$
	(5) $B + B + M \xrightarrow{K_5} \mathrm{Pr} + 2M$	$H + OH + M \leftrightarrow H_2O + M$

Psuedo species: R (**H_2, O_2**), B (**OH, H, O**), C (**HO_2, H_2O_2**), Pr(**H_2O**)

Browne, Liang, Shepherd 2005

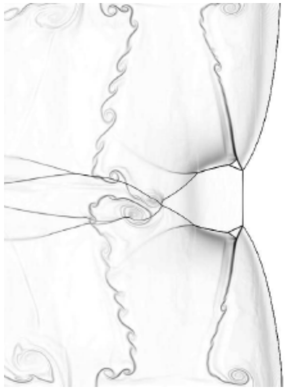
Effective Activation Energy q

Case1



Extended second limit

Ucj=1785 m/s	**q=4.3**
U=0.85Ucj	**q=7.2**



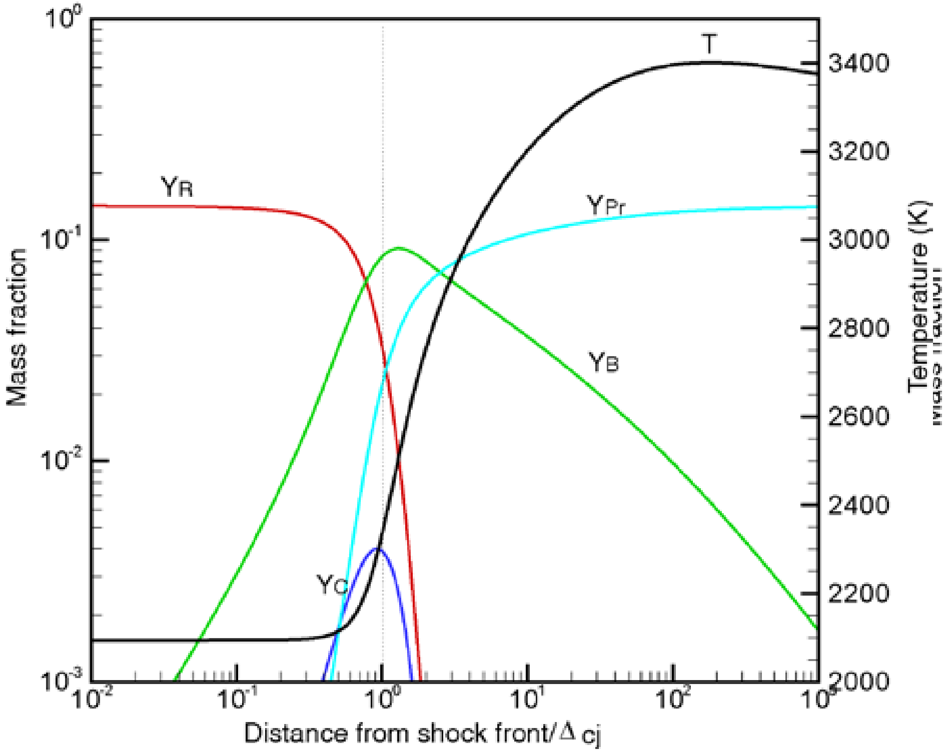
Ucj=1390 m/s	**q=10**
U=0.85Ucj	**q=29**

ZND Structures

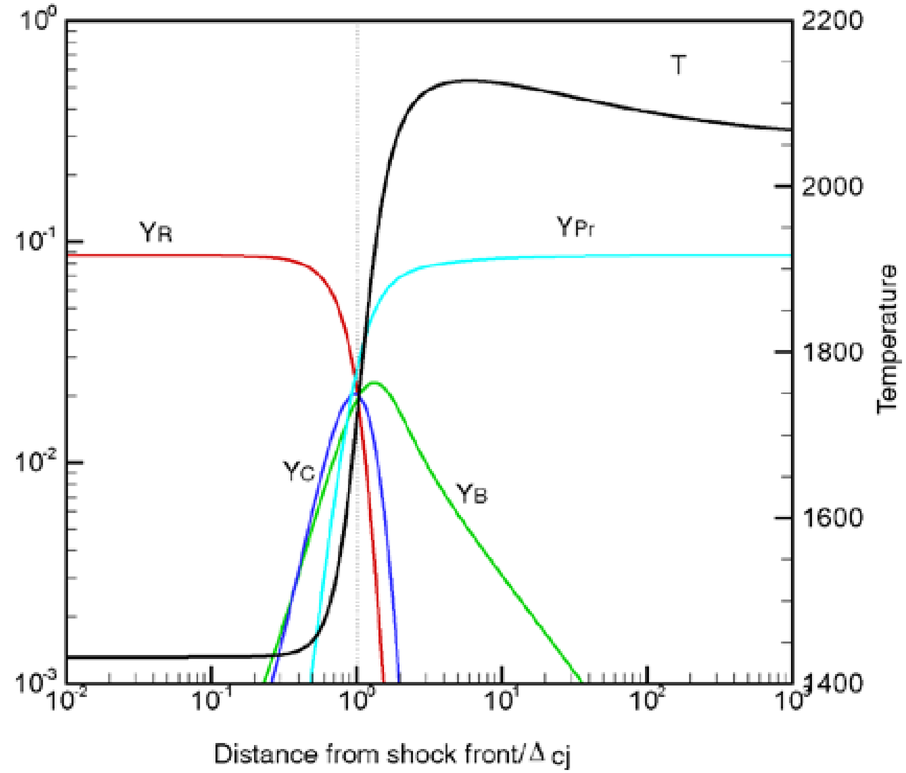
Case 2

Ucj →	**D=0.029 mm**	**D_i/D_e=0.9**
85%Ucj →	**D=0.16 mm**	**D_i/D_e=1.5**

Ucj →	**D=0.64 mm**	**D_i/D_e=1.3**
85%Ucj →	**D=275 mm**	**D_i/D_e=33**



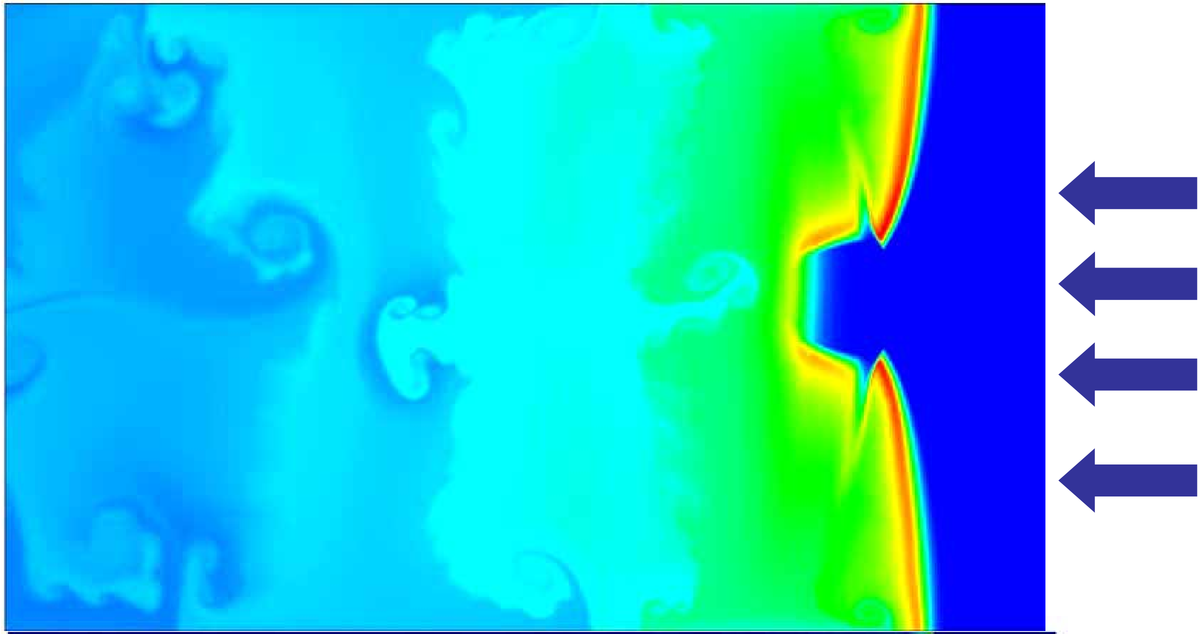
Y_B is much larger than Y_C



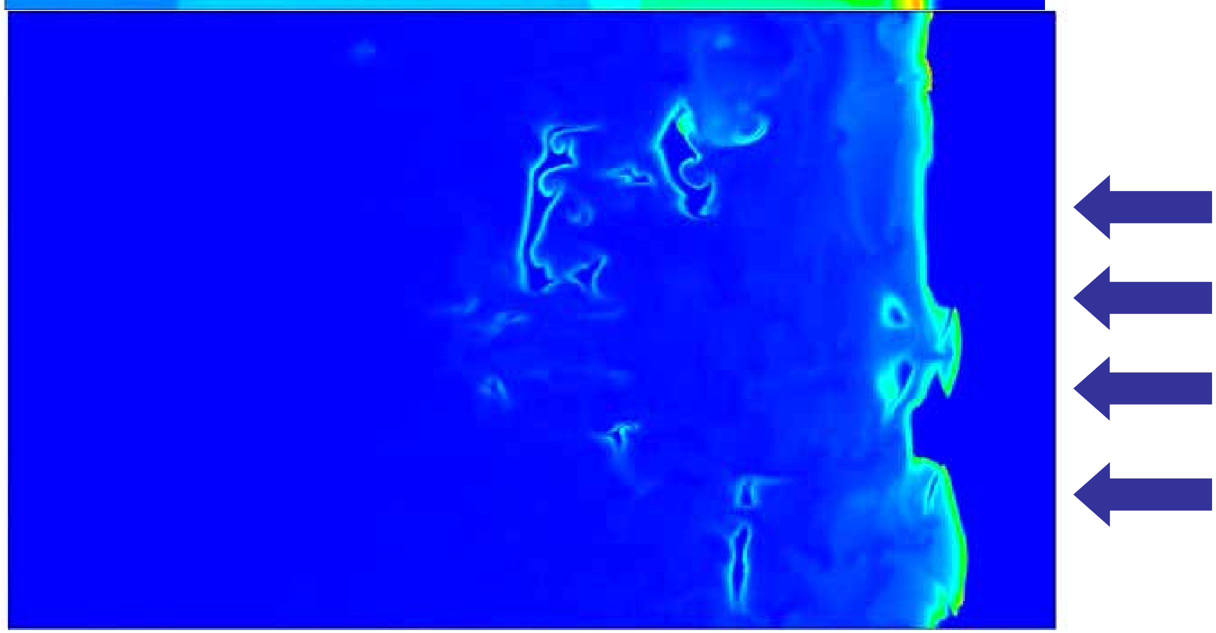
Y_B is comparable with Y_C

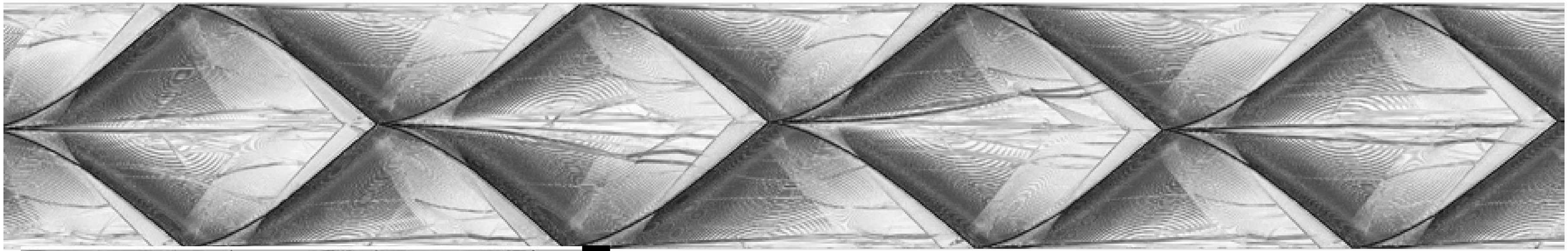
Species "B" (OH, H, or O)

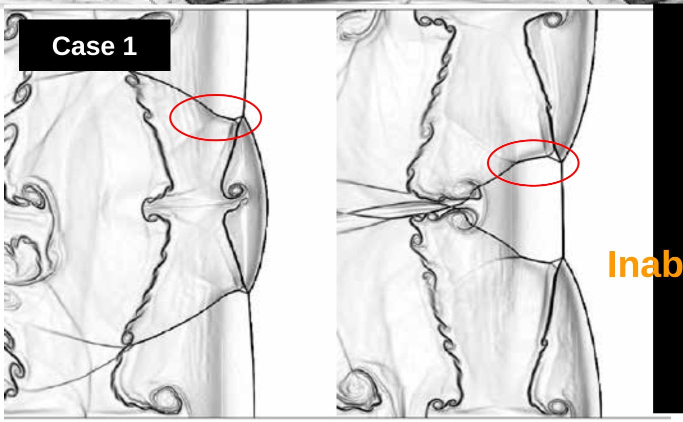
Y_B (OH)



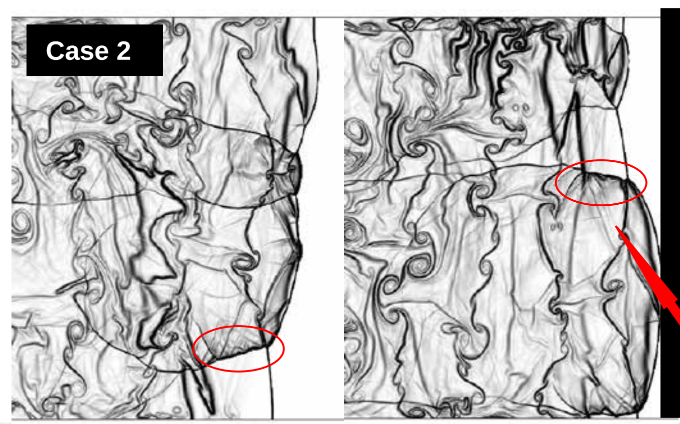
Y_B (OH)



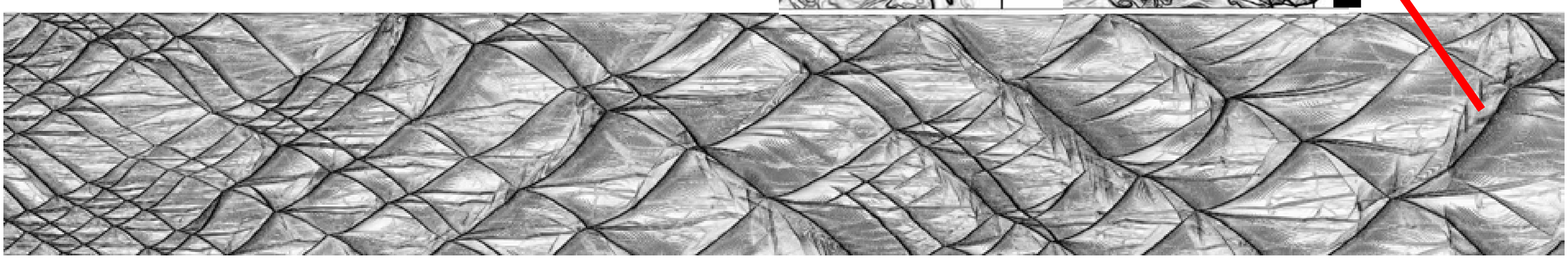




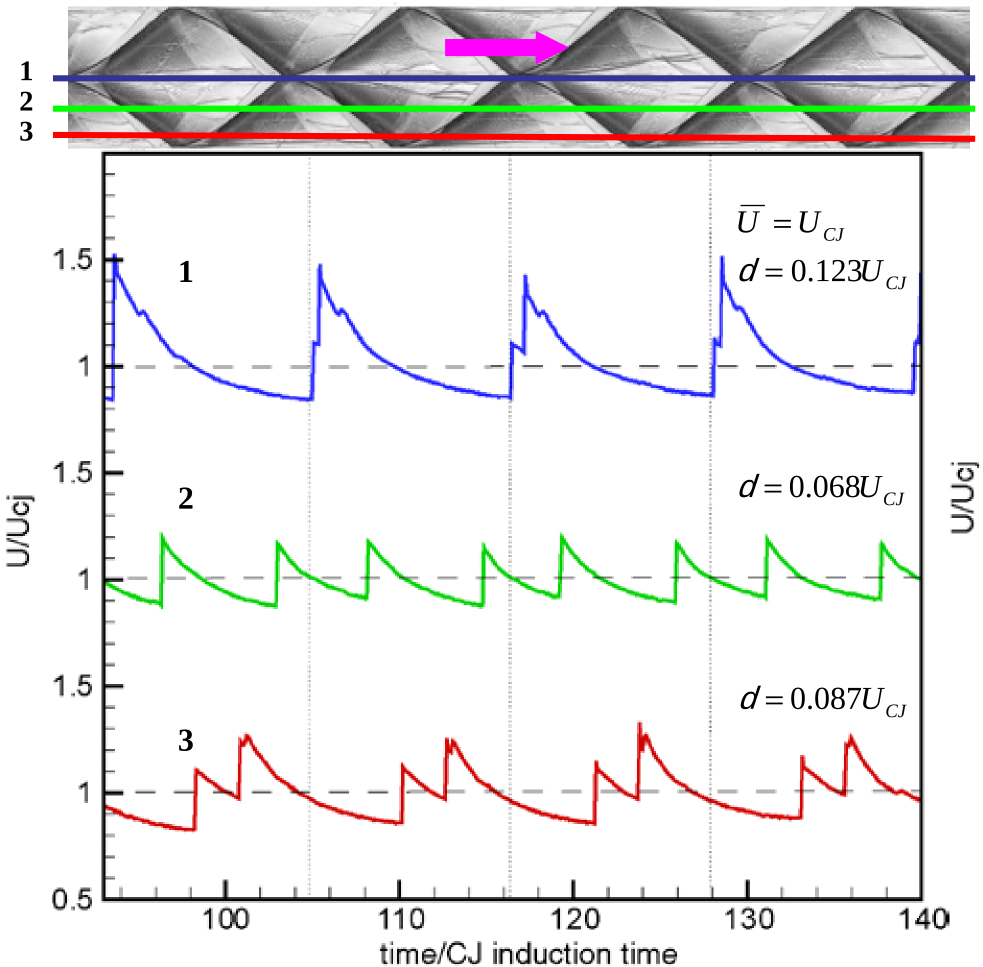
Inaba & Matsuo
2001

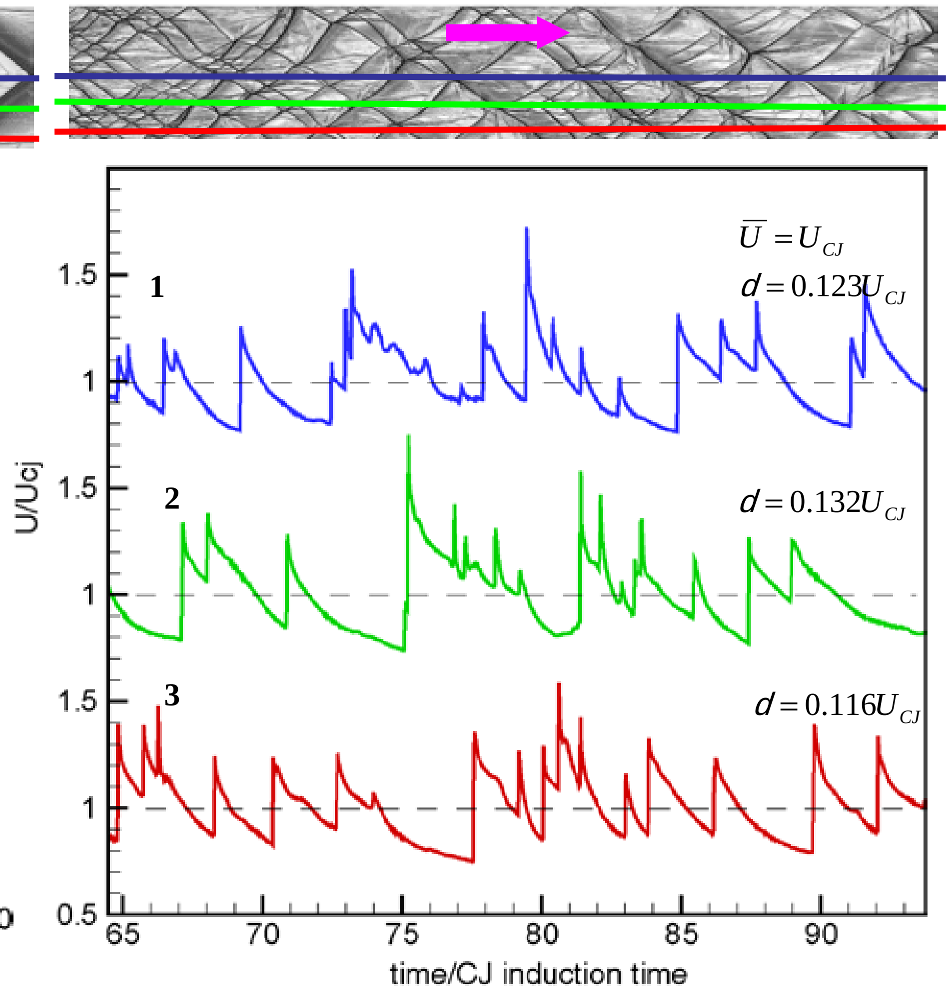


Gamezo et.al
2000

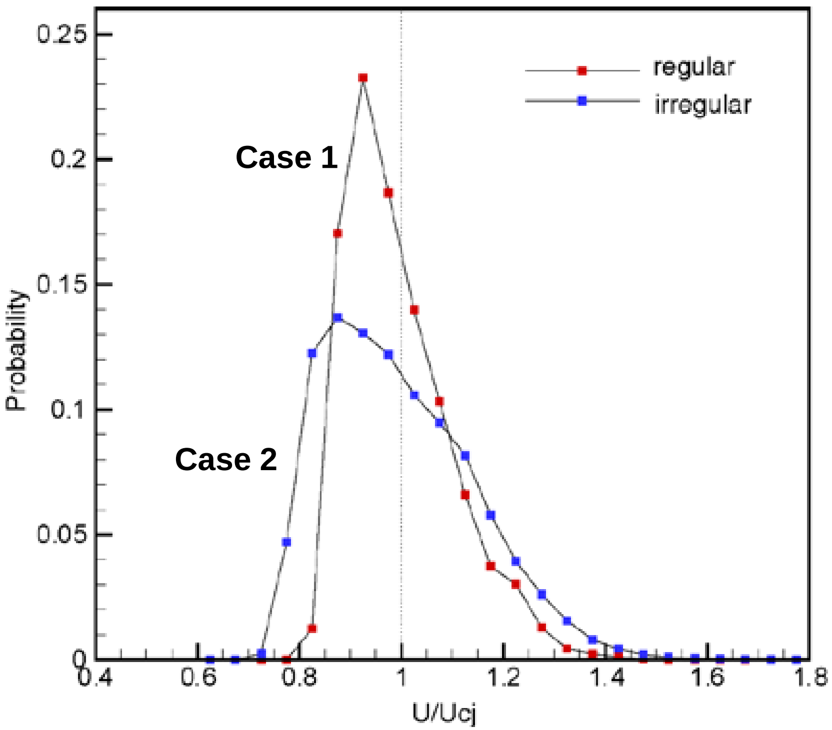


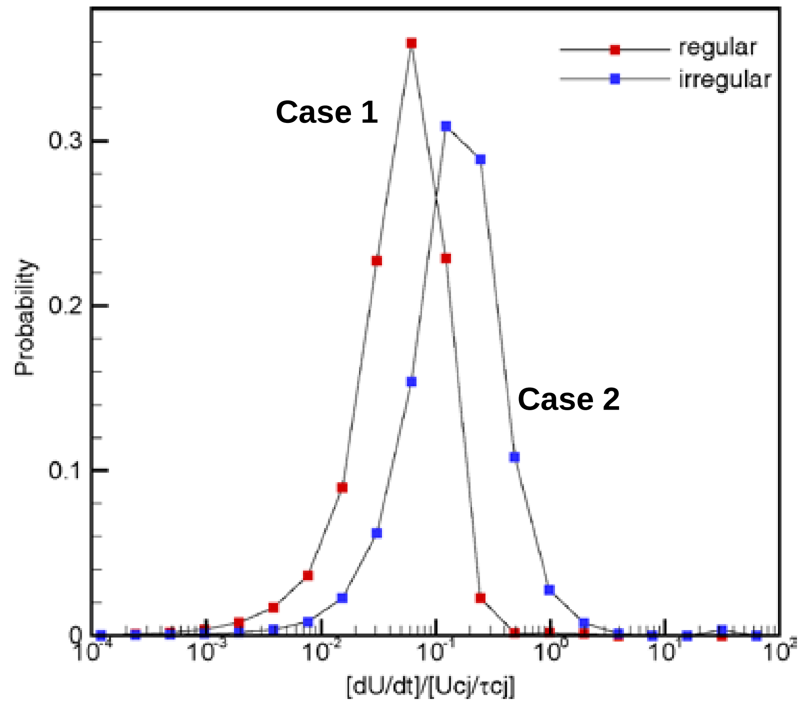
Fluctuations in Shock Velocity





PDF – Velocity, Acceleration

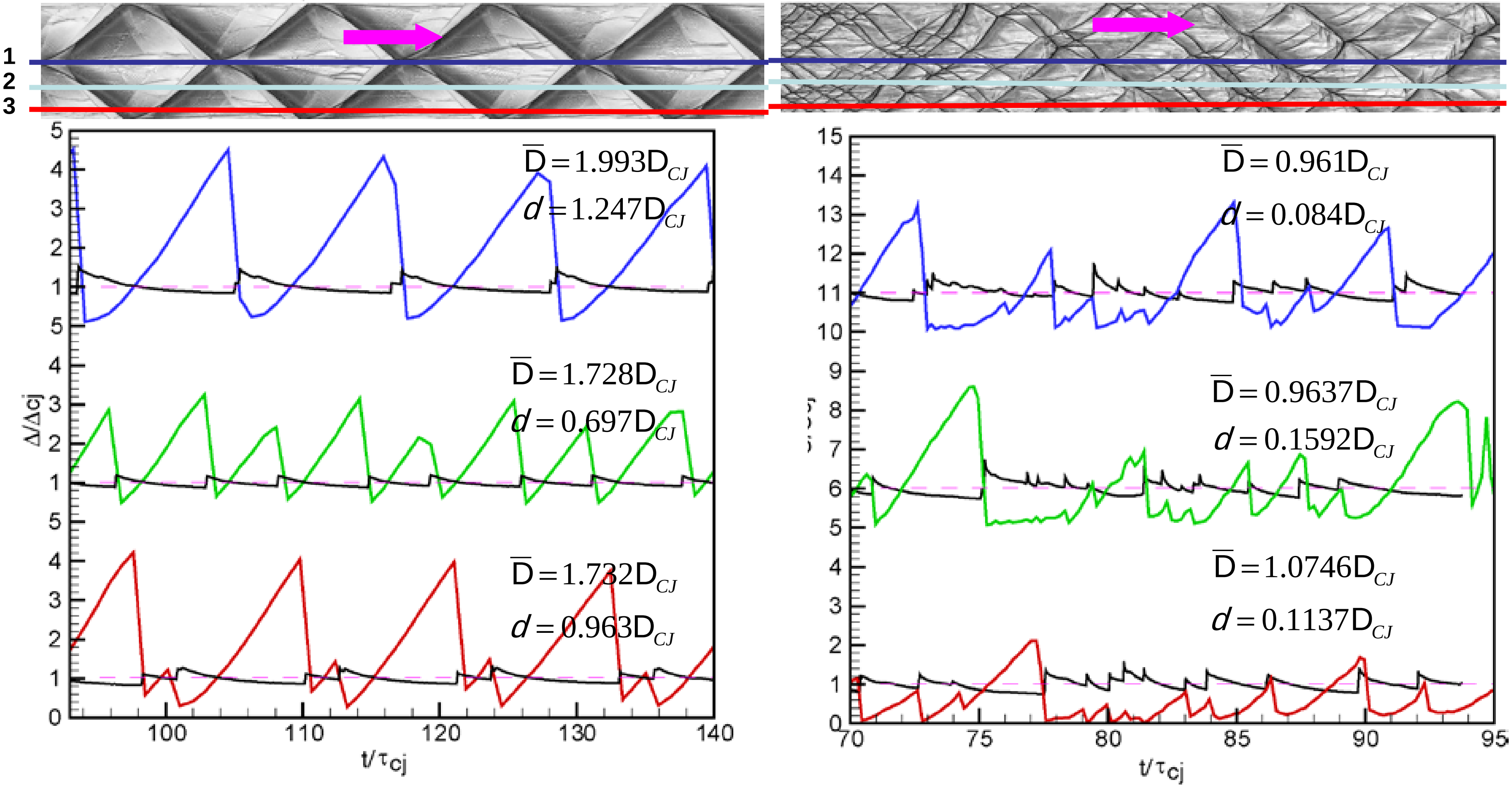




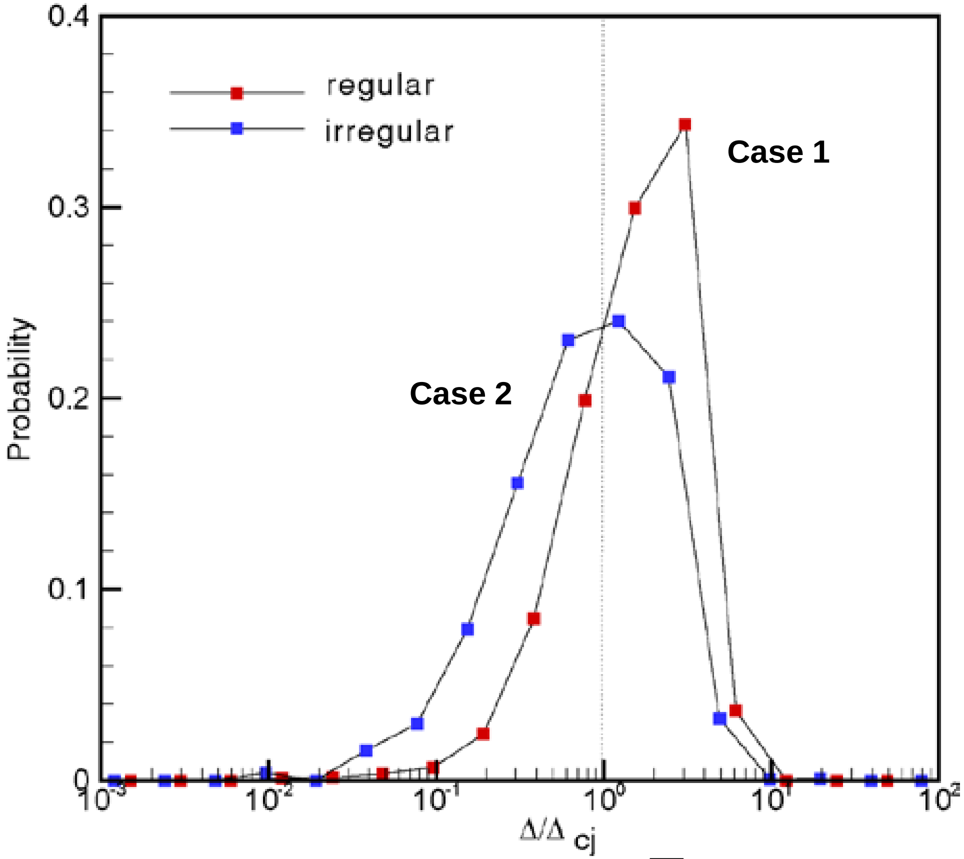
- Mean velocity $\overline{U} = U_{CJ}$ for both cases
- Most likely velocity $U < U_{CJ}$ for both,
  lower for irregular mixture
- Regular mixture: 0.8 U_{CJ}~1.35 U_{CJ}
- Irregular mixture: 0.7 U_{CJ}~1.5 U_{CJ}

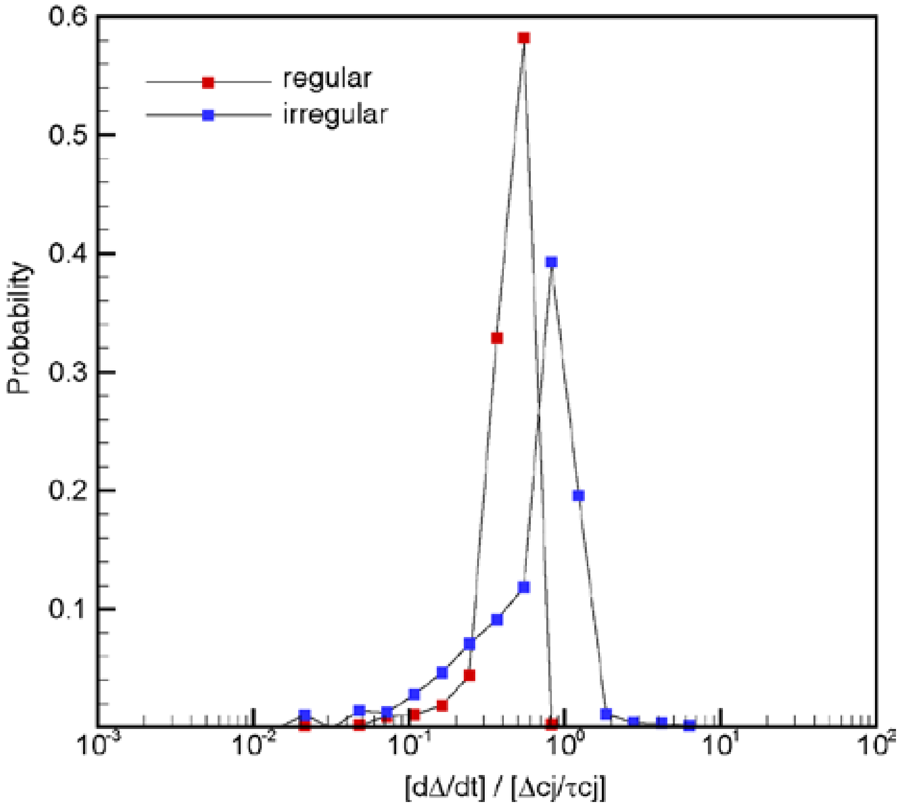
- **Regular mixture:**
  - **most likely** $-\frac{dU}{dt} \approx 0.08\frac{U_{CJ}}{t}$
- **Irregular mixture**
  - **most likely** $-\frac{dU}{dt} \approx 0.2\frac{U_{CJ}}{t}$
  - **faster decay rate!**

Fluctuations in Reaction Length



PDF – Reaction thickness

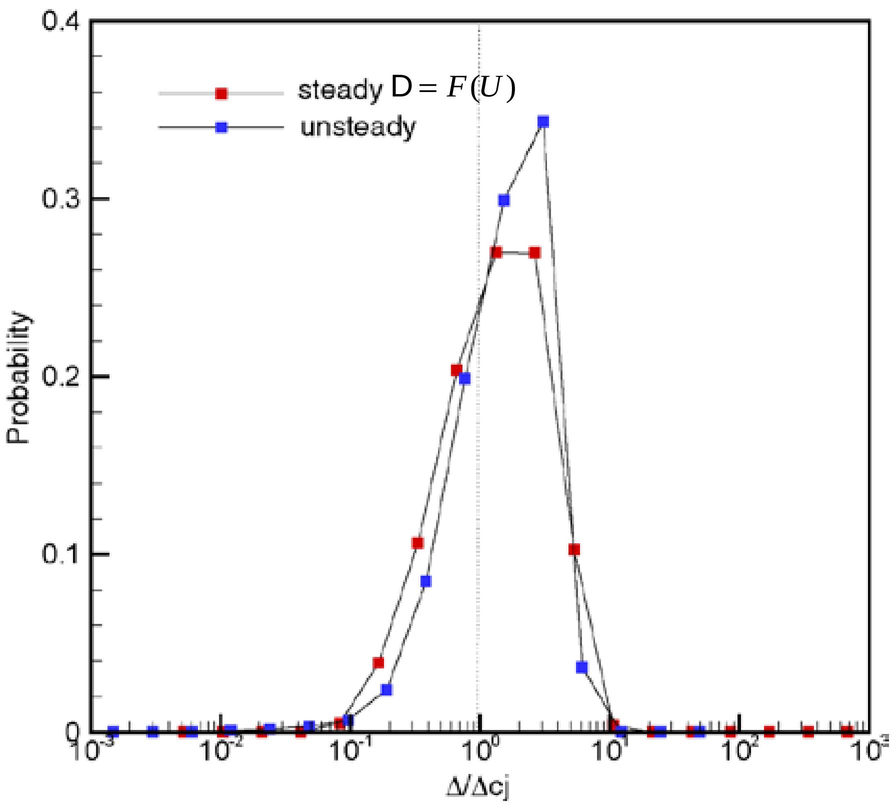


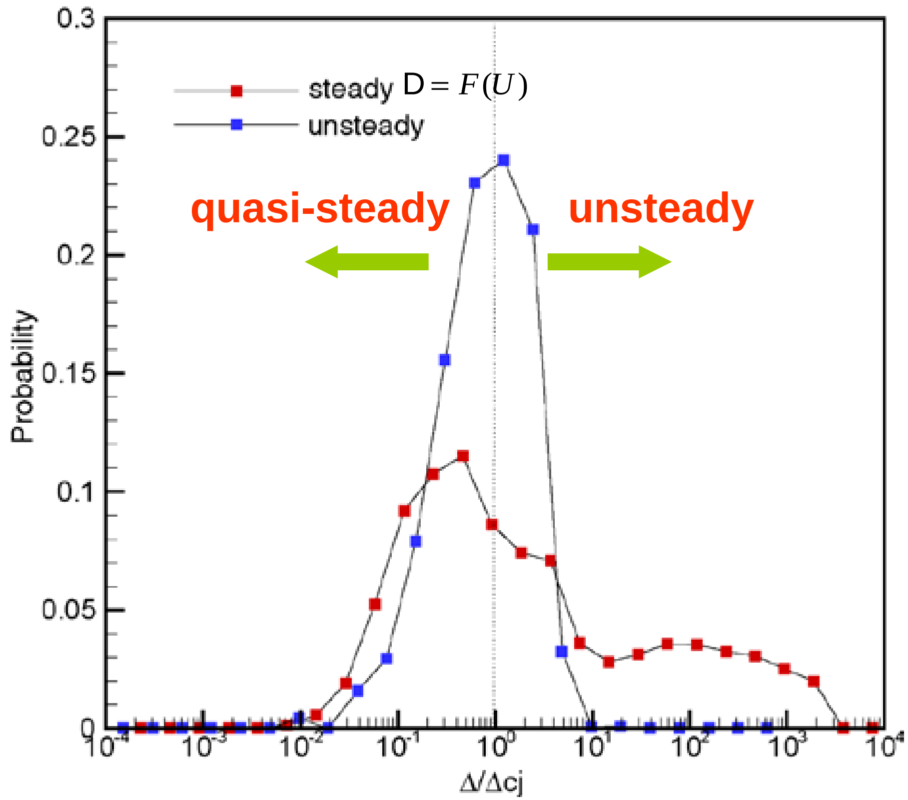


- Regular mixture ➡ $\bar{D} > D_{CJ}$
- Most likely $D > D_{CJ}$
- Irregular mixture ➡ $\bar{D} \sim D \sim D_{CJ}$

- Regular mixture ➡ slower acceleration
- Irregular mixture ➡ faster acceleration

Influence of Unsteadiness





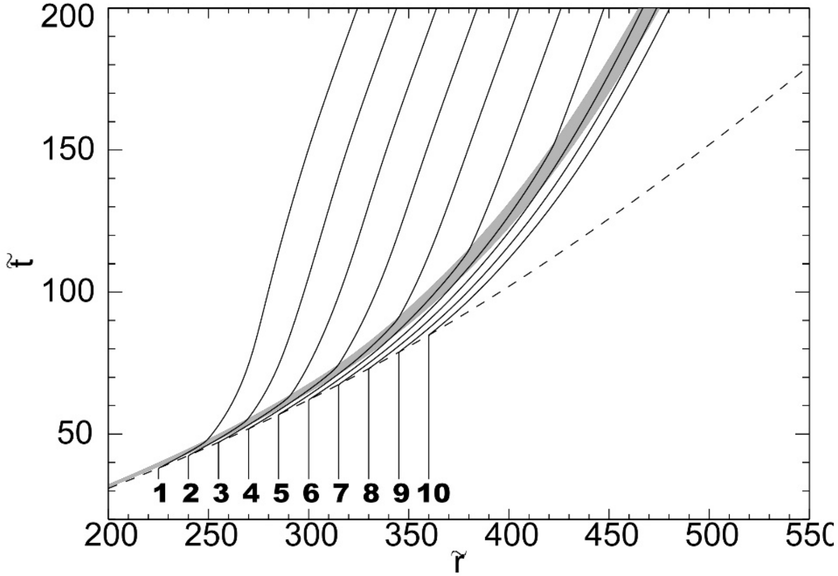
regular mixture ➡

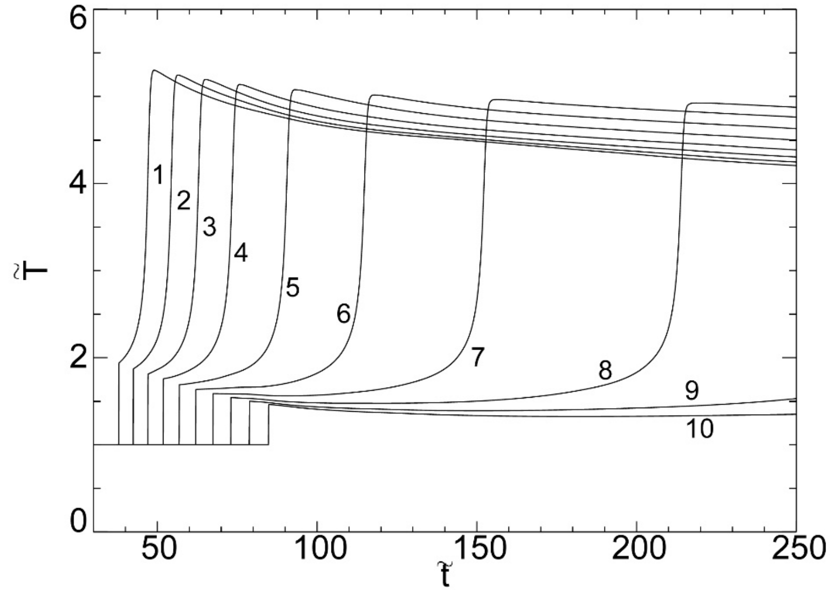
- steady (F(U)) and unsteady (**D**) reaction thickness is highly correlated;
- quasi-steady reaction zone.

irregular mixture ➡

- steady (F(U)) and unsteady (**D**) reaction thickness is less correlated;
- unsteady reaction zone

$$\left(1-M^2\right)C_P\frac{DT}{Dt}=\left(1-\gamma M^2\right)Qk\left(1-Z\right)\exp\left(-\frac{E_a}{RT}\right)+\frac{j}{R-x}u^2\left(U-u\right)+u\frac{dU}{dt}-u\frac{\partial u}{\partial t}+\frac{1}{\rho}\frac{\partial P}{\partial t}$$





$$\frac{\mathrm{D}\hat{T}_1}{\mathrm{D}\zeta}=\mathrm{e}^{\hat{T}_1}-\alpha \qquad \alpha=-\frac{\theta\tau}{(1-M_s^2)C_P T_s}\left(w_s\frac{\mathrm{d}U}{\mathrm{d}t}-w_s\frac{\mathrm{d}w_s}{\mathrm{d}t}+\frac{1}{\rho_s}\frac{\mathrm{d}P_s}{\mathrm{d}t}\right)$$

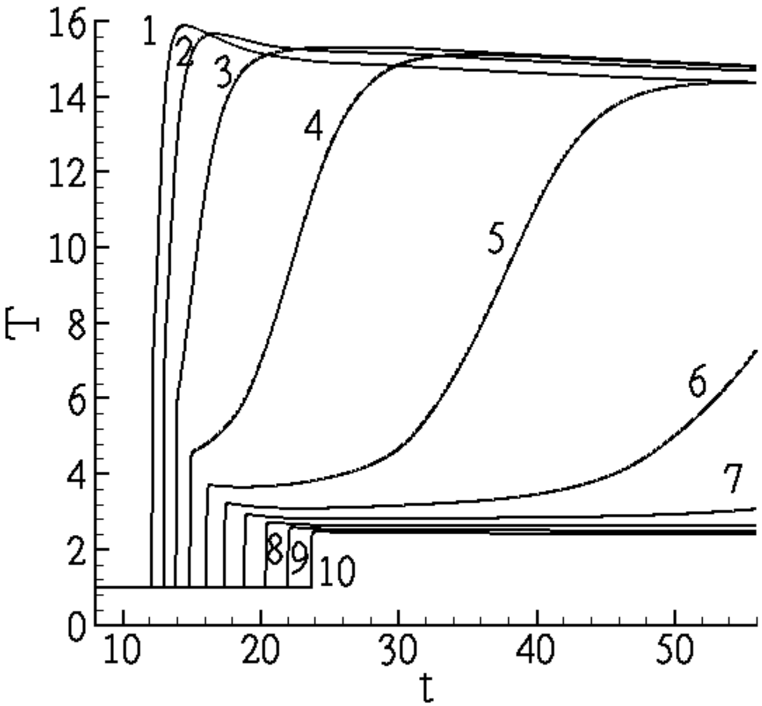
Critical shock decay rate

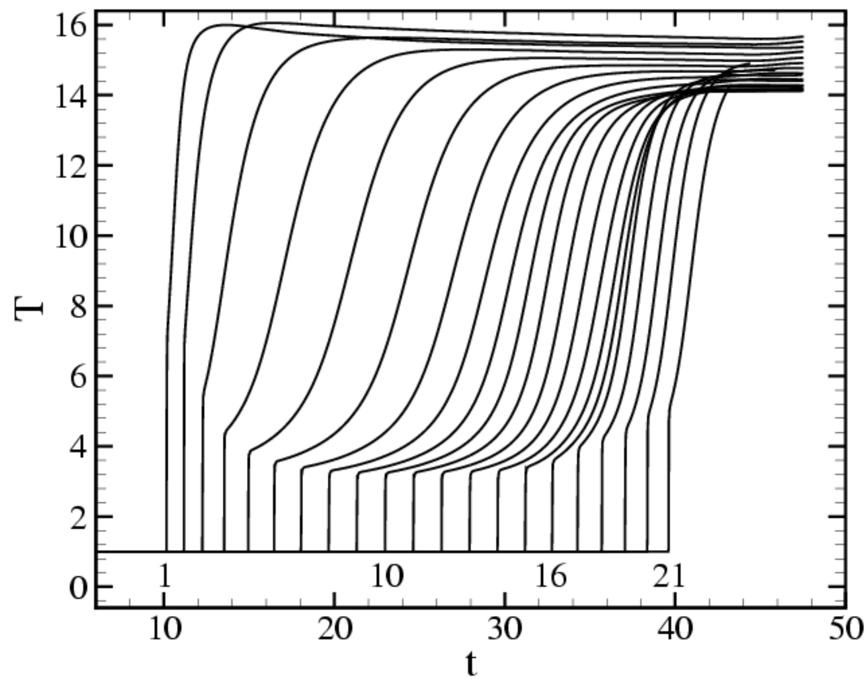
$$\frac{1}{t_d}=\frac{1}{U}\frac{dU}{dt} \qquad t_{d,c}=6\frac{\gamma-1}{\gamma+1}\frac{E_a}{RT_S}t$$

Eckett, Quick, Shepherd JFM 2000

Quenching $t_d < t_{d,c}$.

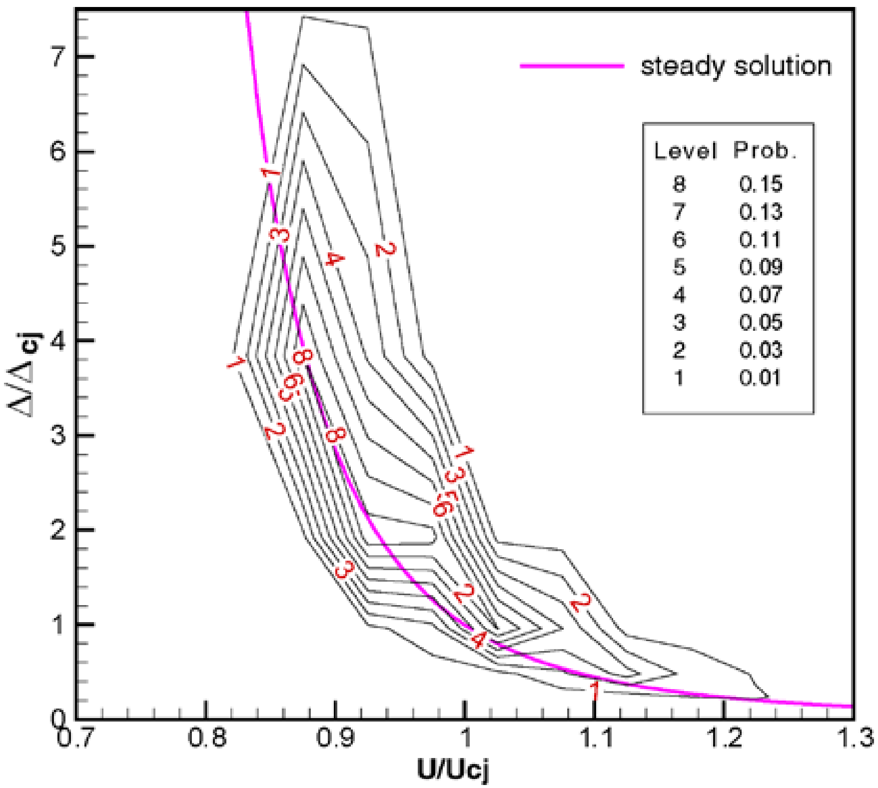
Coupling, $t_d > t_{d,c}$.

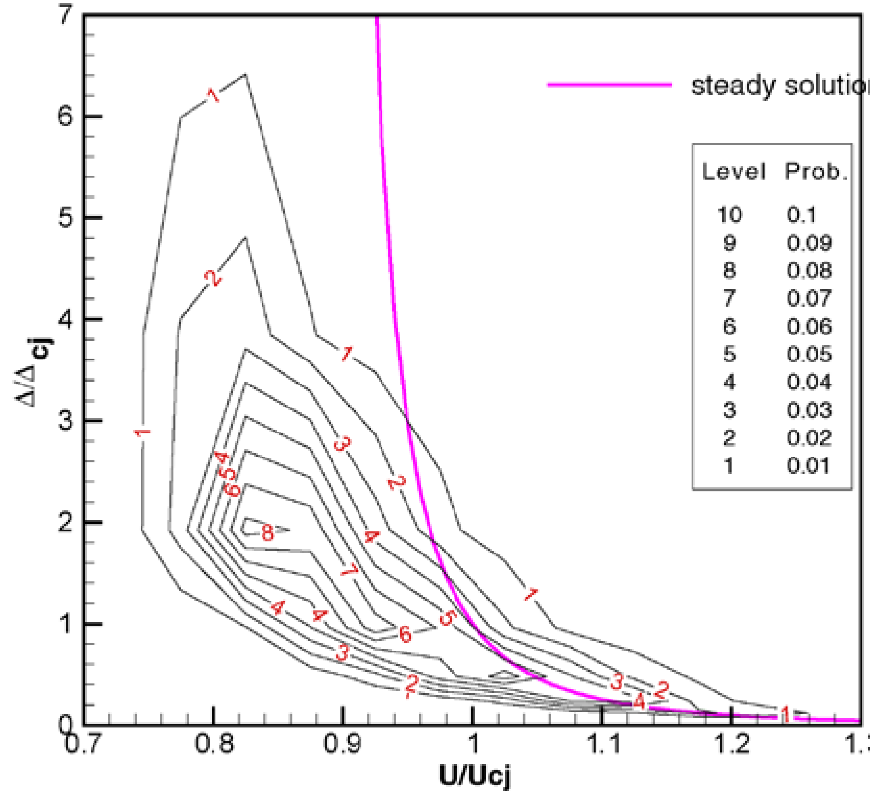




Eckett et al 1999

Joint PDF (D, *U*)





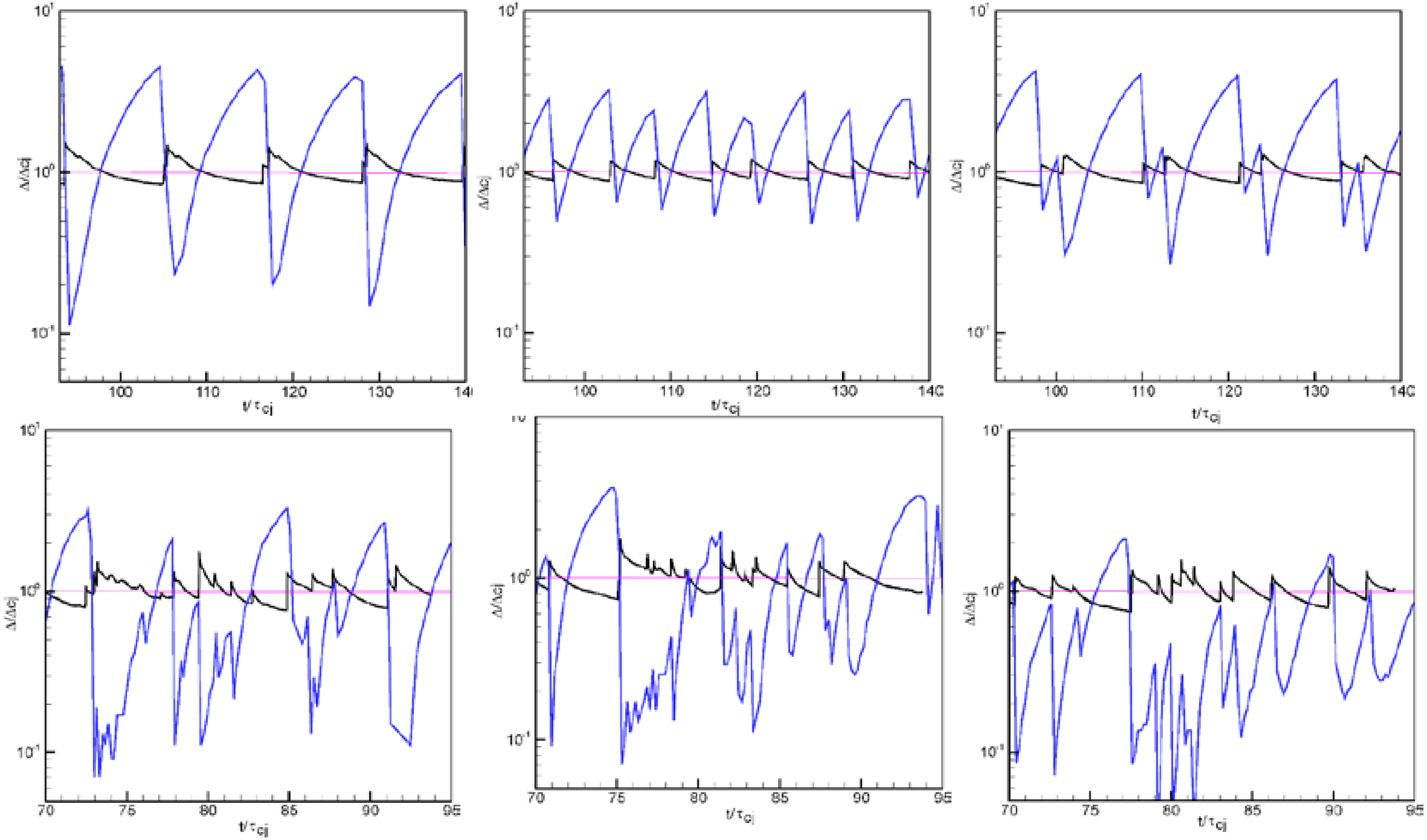
regular mixture ➡ steady relation of U and D is close to the most likely unsteady solution.

irregular mixture ➡ large difference between steady and unsteady relation.

Fluctuations in spatial scales

Case 1 regular structure

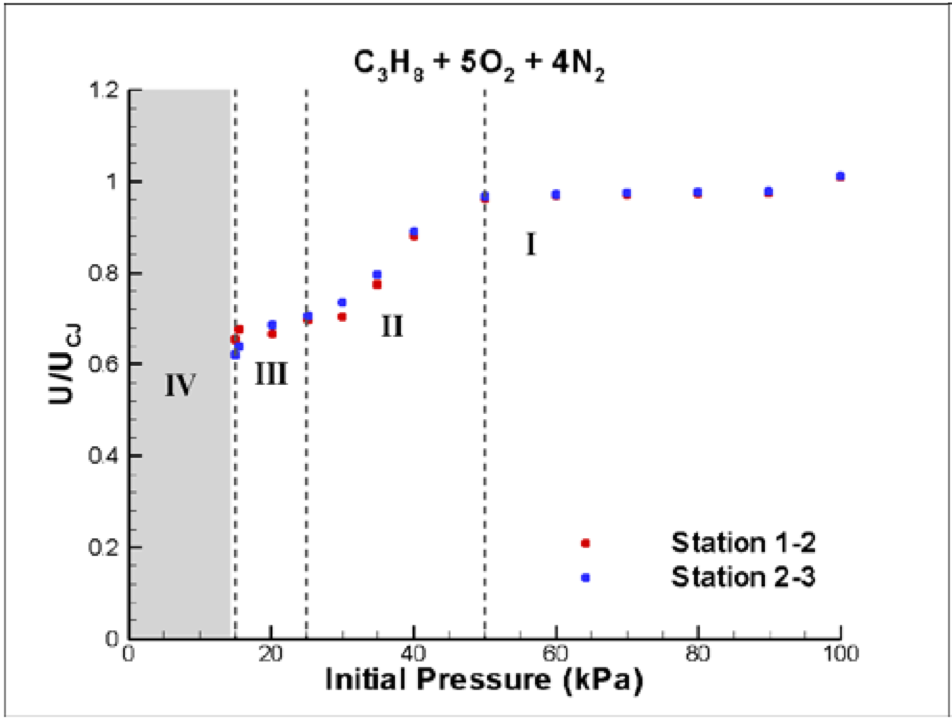
Case 2 irregular structure

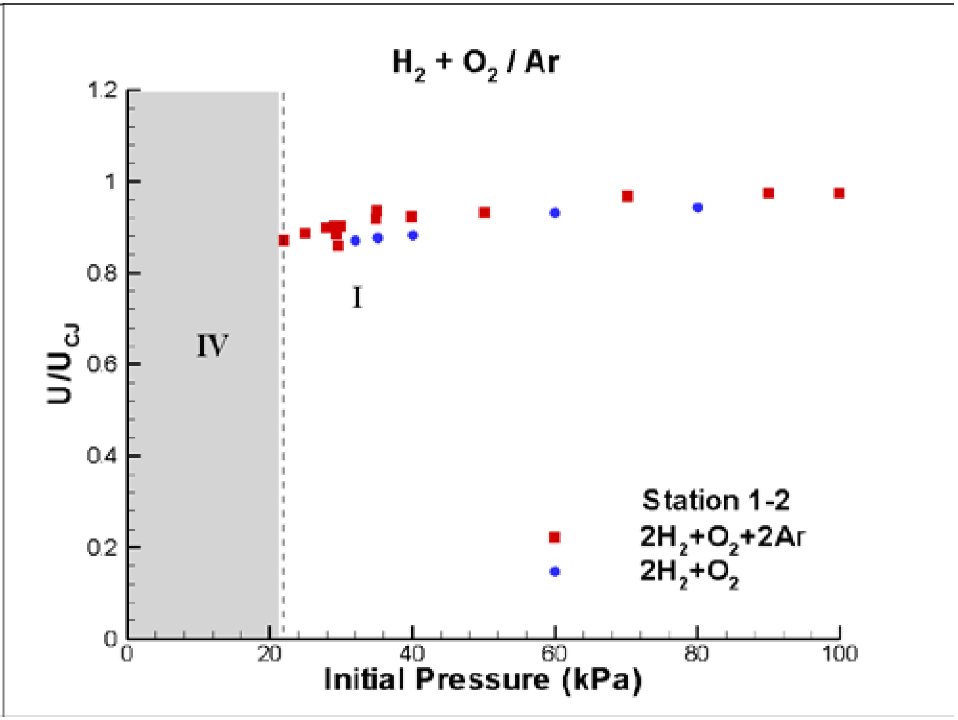


- **Irregular structure ➡ larger ratio between max D and min D**

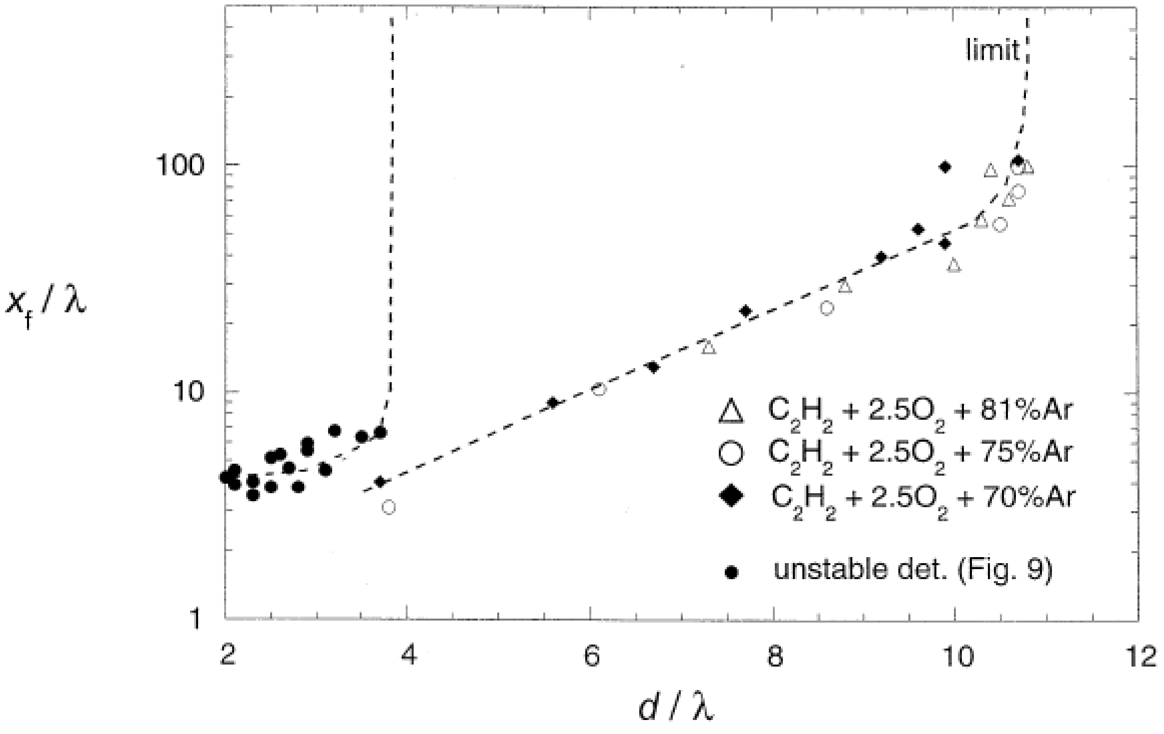
  challenge for experimental measurements and computations

Propagation limit in small tubes



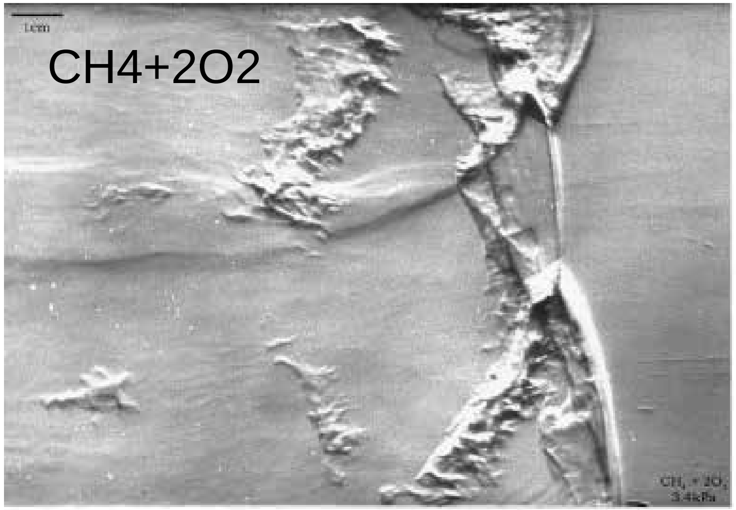


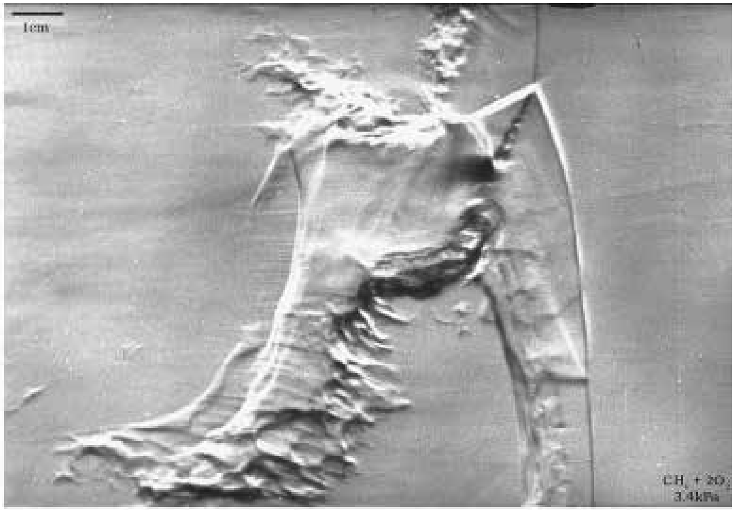
Quenching in porous tubes

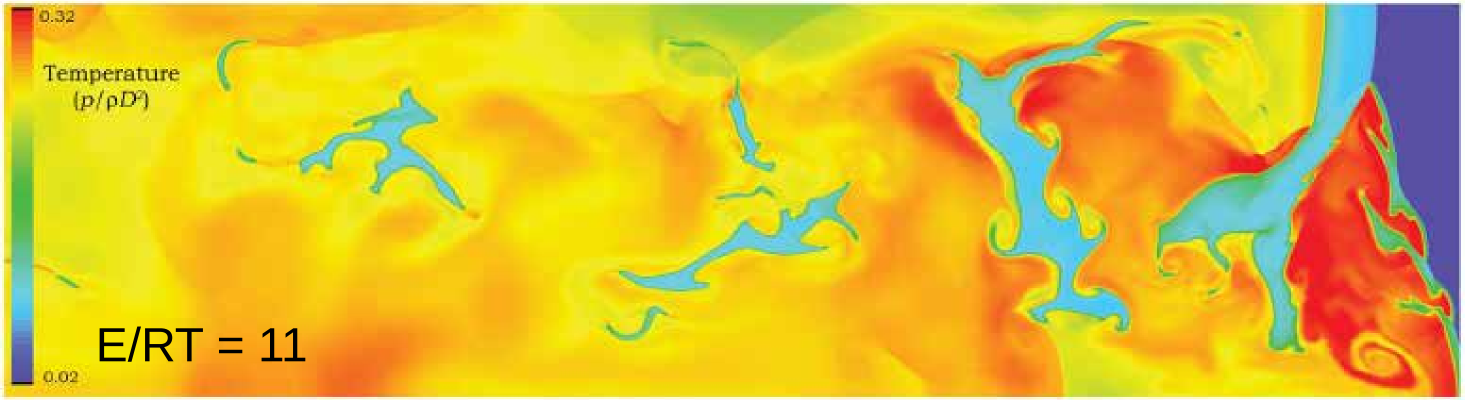


Radulescu and Lee Comb Flame 2002

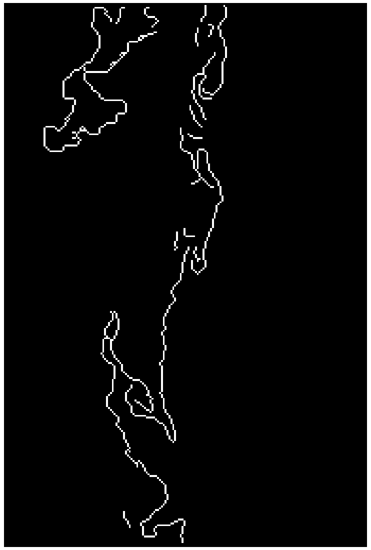
Formation of unburned “pockets”



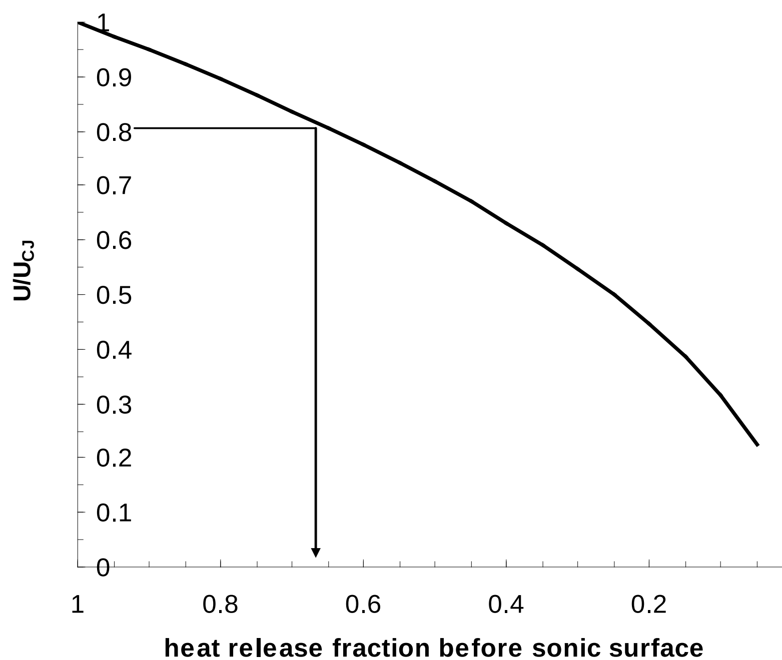




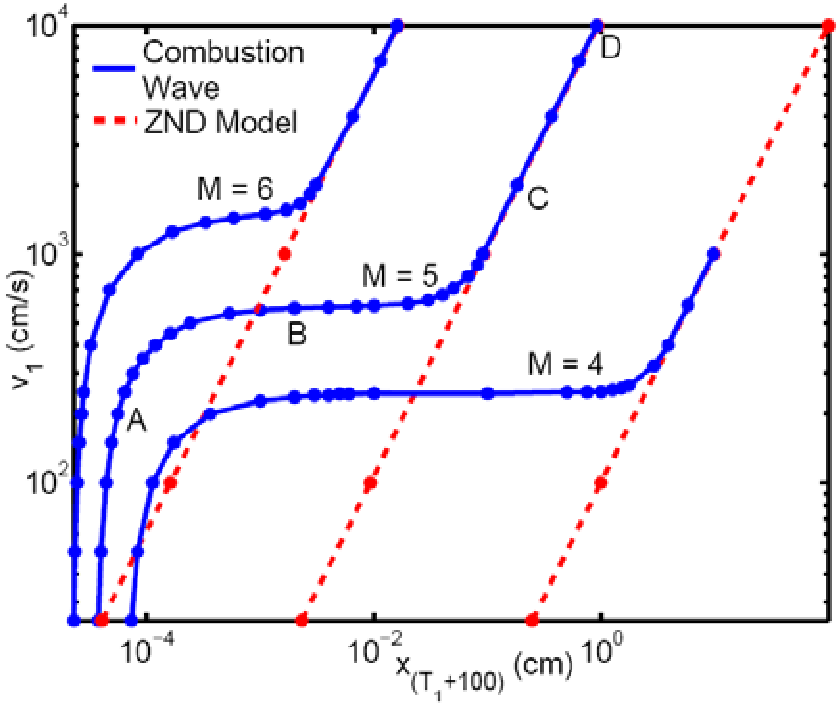
Radelescu et al 2005, Radelescu, Law, Sharpe 2005

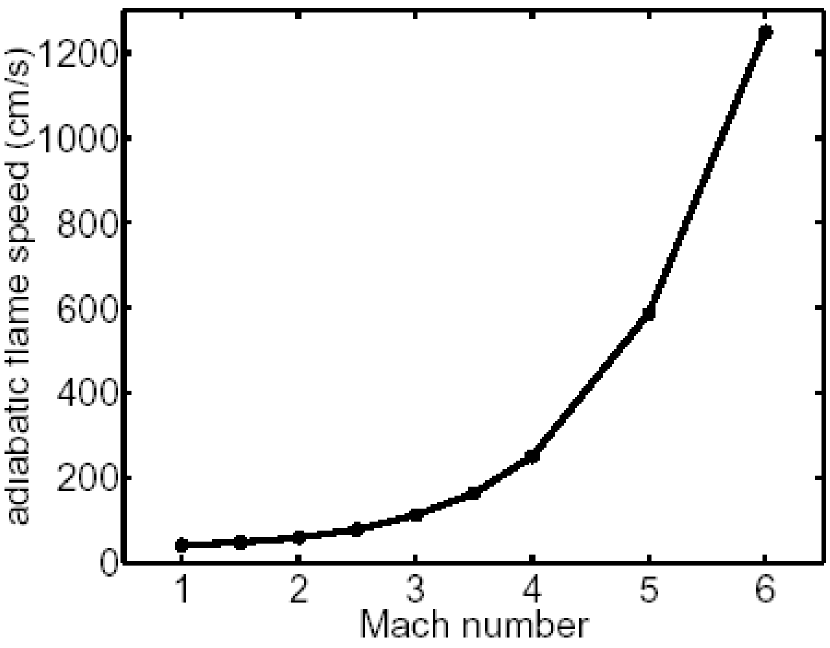


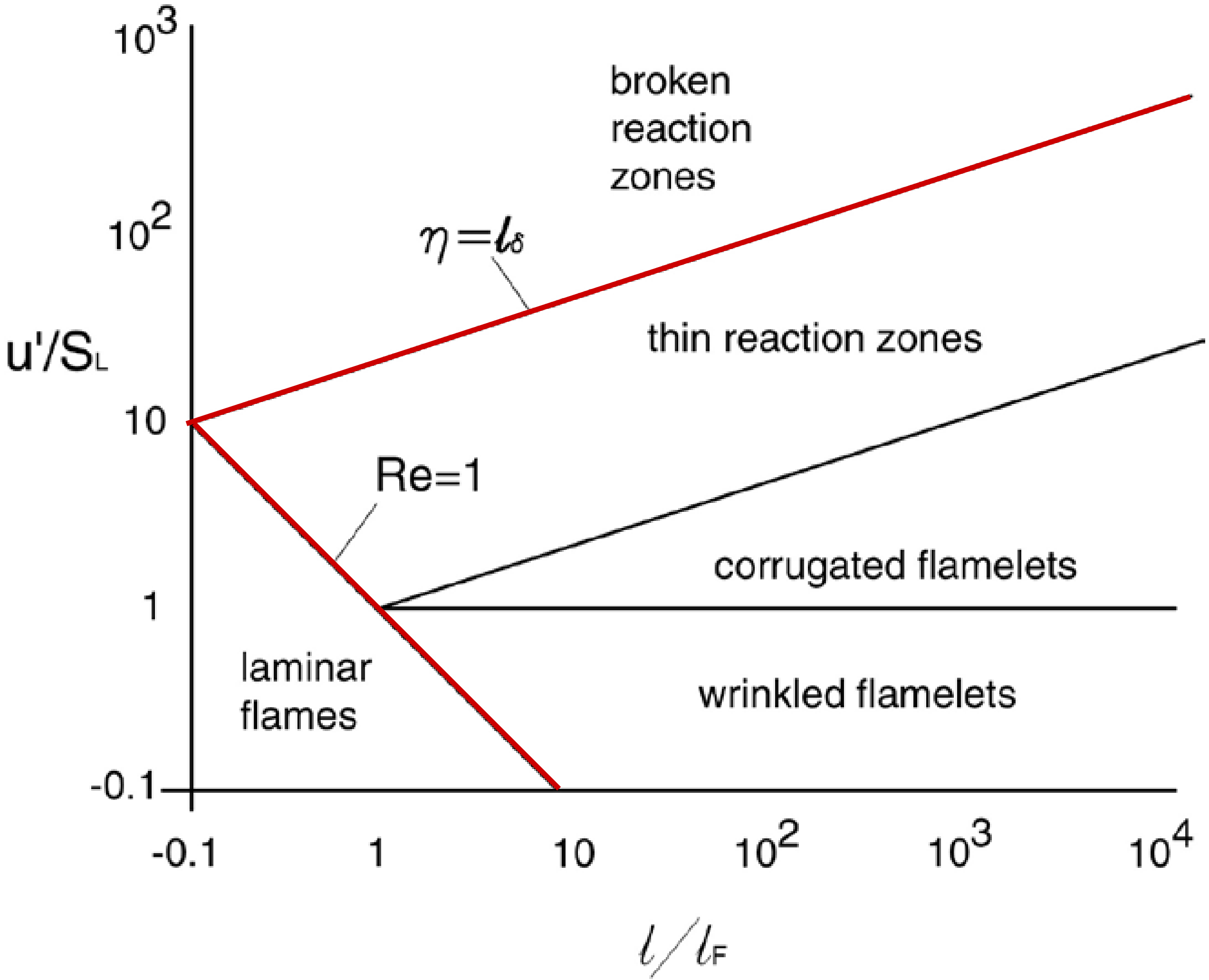
Diffusive burning?



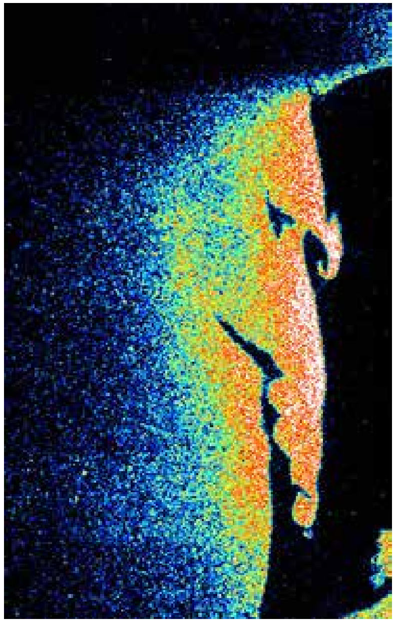
CH4-air

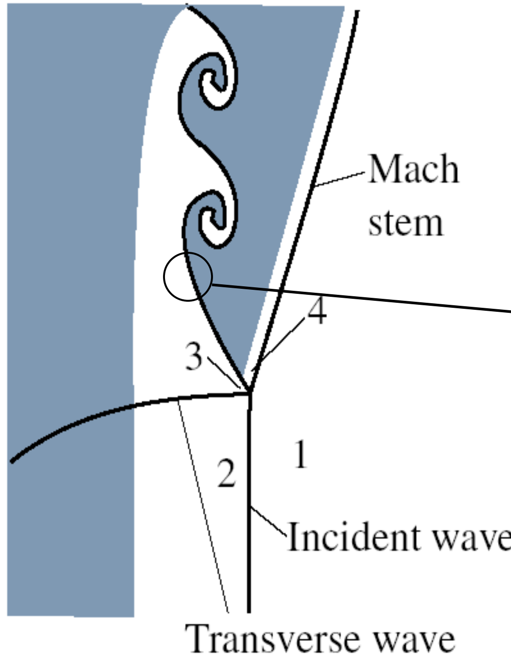

Combustion Wave
ZND Model
M = 6
M = 5
M = 4
A
B
C
D
10^4
10^3
10^2
v_1 (cm/s)
10^{-4}
10^{-2}
10^0
$x_{(T_1+100)}$ (cm)


adiabatic flame speed (cm/s)
0
200
400
600
800
1000
1200
1
2
3
4
5
6
Mach number

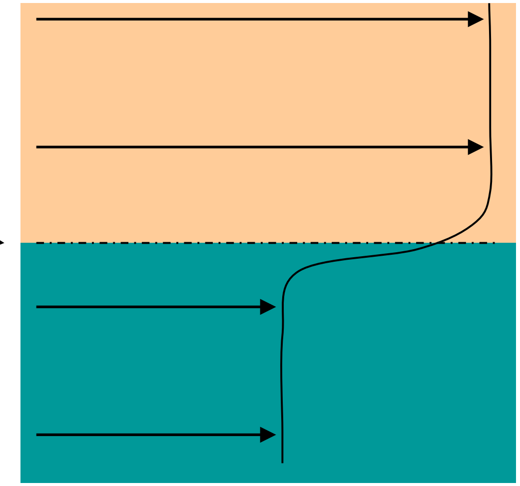


from N. Peters (2000) Turbulent Combustion



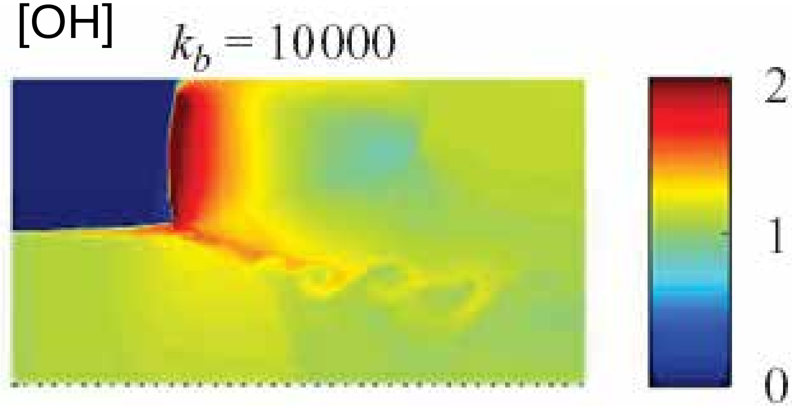


Warm reactants

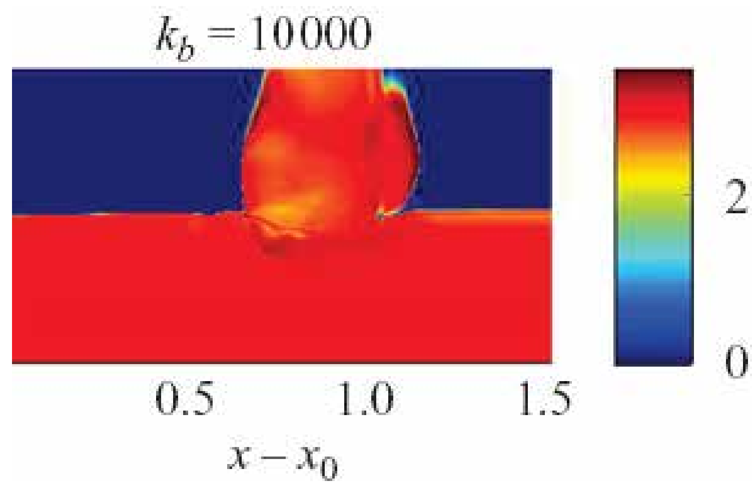


Hot products

[OH]



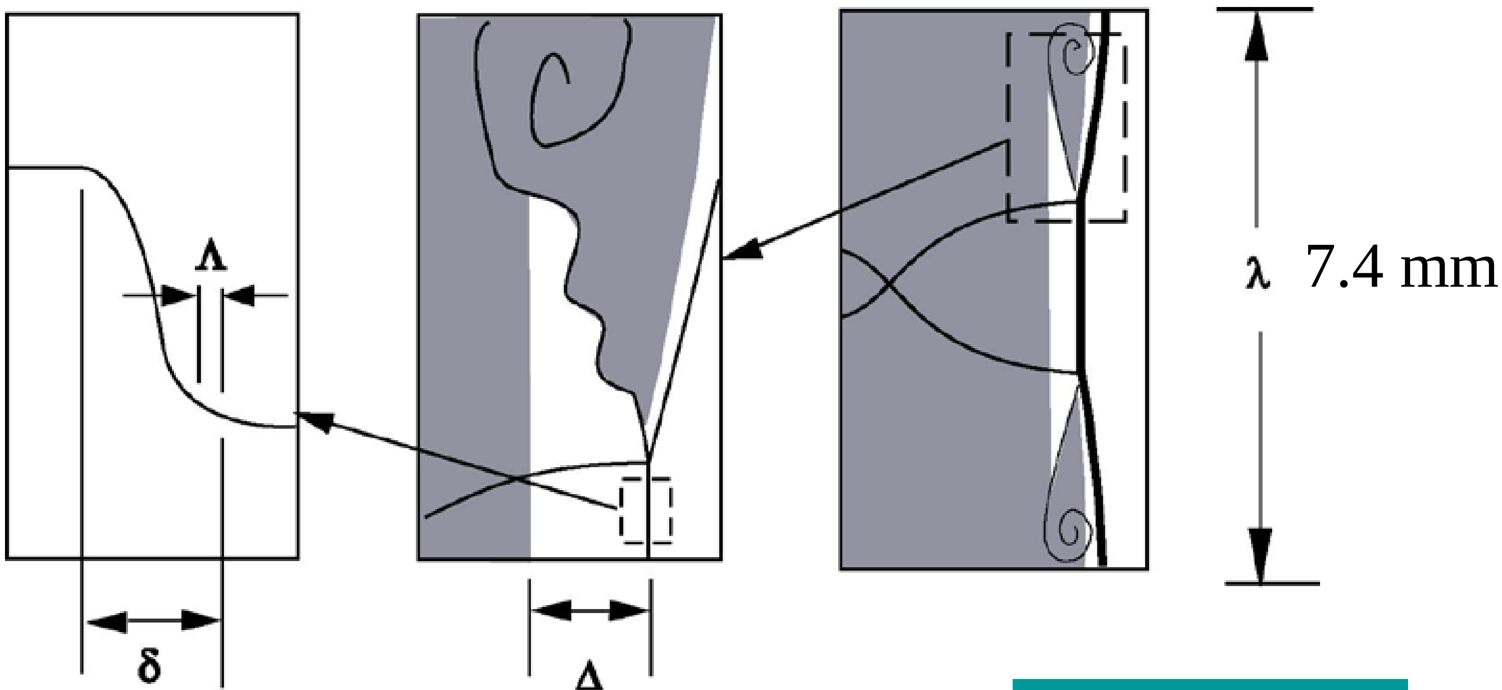
$2H_2$–O_2–$5.6N_2$



C_3H_8–$5O_2$–$9N_2$

Massa, Austin, Jackson 2007

Large range of spatial & temporal scales

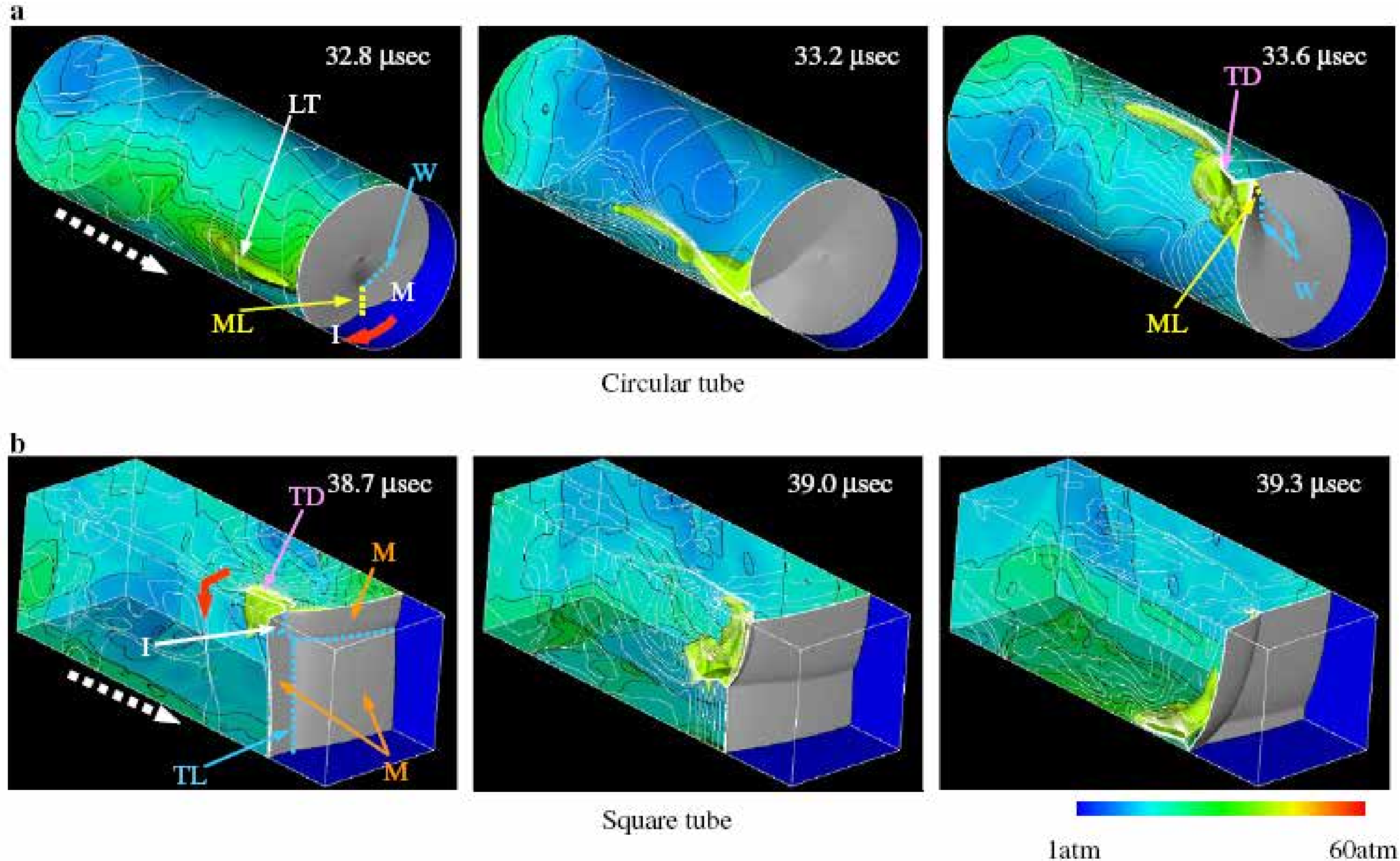


500 nm

77 mm

l /L = 74,000

Stoichiometric hydrogen-oxygen mixture at an initial pressure of 20 kPa



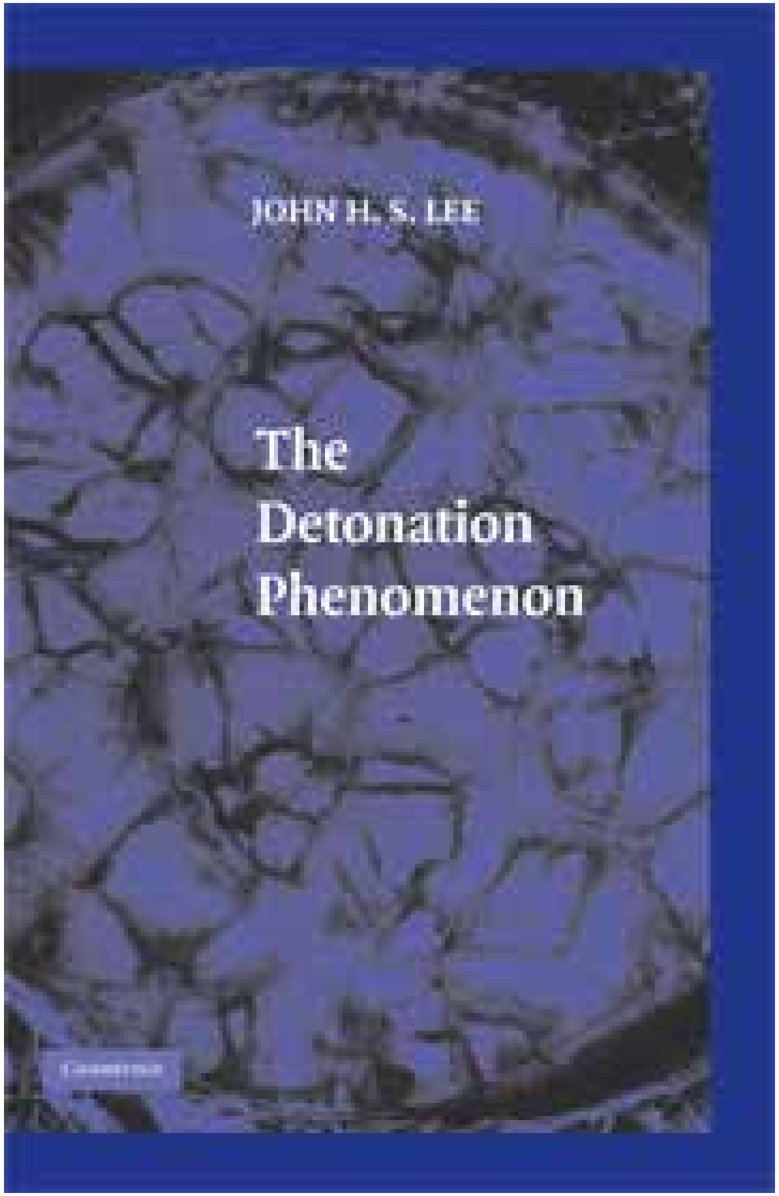
N. Tsuboi & A. K. Hayashi 2007

Needs

- Scientific studies of turbulence
  - Experiments with quantitative data on statistics of flow field
  - Statistical analysis of high-fidelity numerical simulations
- Engineering models of turbulent fronts
  - Subgrid scale models for quantitative prediction and analysis

Thank You!

- Past students and postdoctoral scholars, particularly
  - Joanna Austin
  - Florian Pintgen
  - Rita Liang
- Financial and Institutional support
  - California Institute of Technology
  - US DOE
  - US NRC
  - ONR
  - GE Global Research
  - Sandia, Los Alamos, and Lawrence Livermore National Laboratories


JOHN H. S. LEE
The Detonation Phenomenon