EVALUATION OF HYDROGEN EXPLOSION HAZARDS: PHENOMENOLOGY AND POTENTIAL FOR FLAME ACCELERATION AND DDT

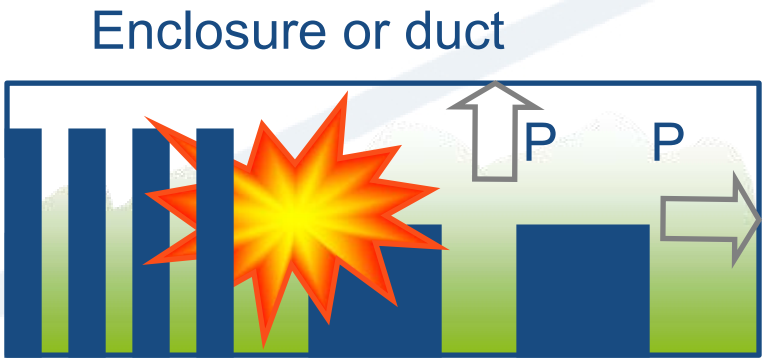
Sergey Dorofeev
FM Global

Prepared for 4th European Summer School on Hydrogen Safety

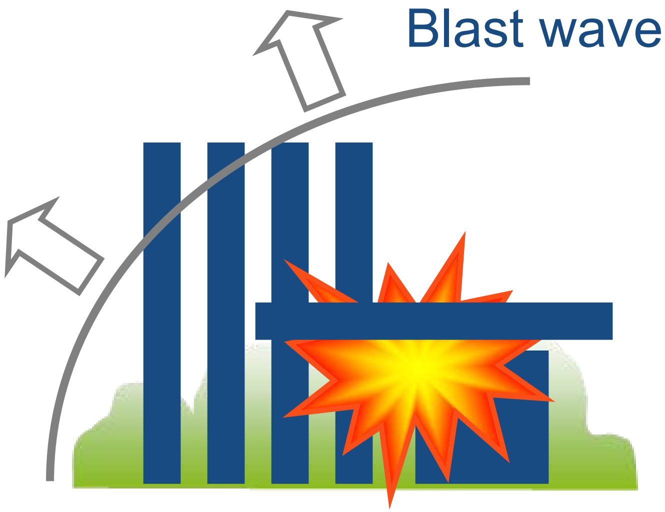
Porticcio, Corsica, France, 7-16 September, 2009

Background

Confined and unconfined explosions



- Confined explosions
    - Internal loads
    - Pressure increase

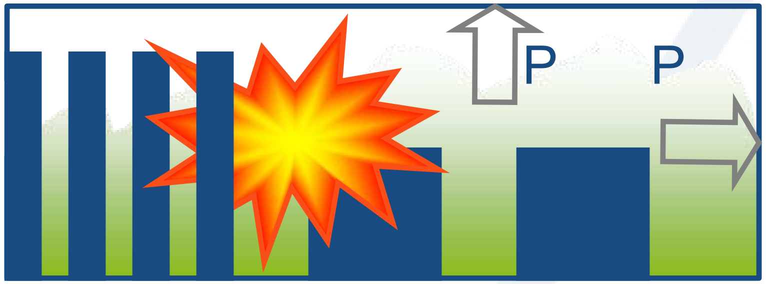


- Unconfined explosions
- Semi-confined
    - External loads
    - Blast waves

Background

Confined explosions

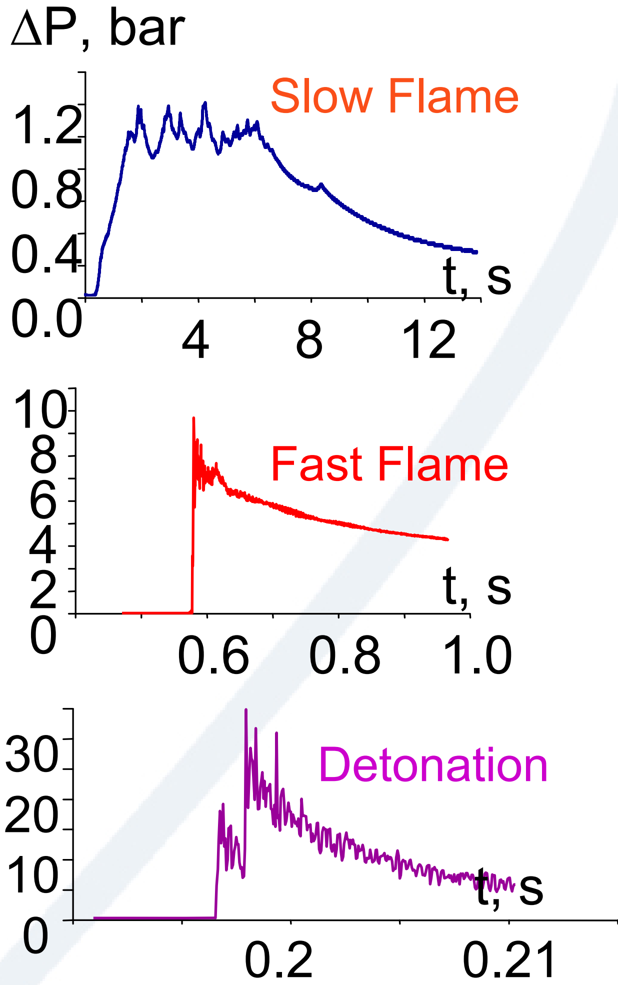
- H_2 releases and transport of H_2- mixtures represent significant safety problem
  - Tubes / ducts
    - Ventilation systems
    - Exhaust pipes
  - Production facilities
  - Tunnels
- Hydrogen: special attention because of high sensitivity to FA



Background

Confined explosions - hazards

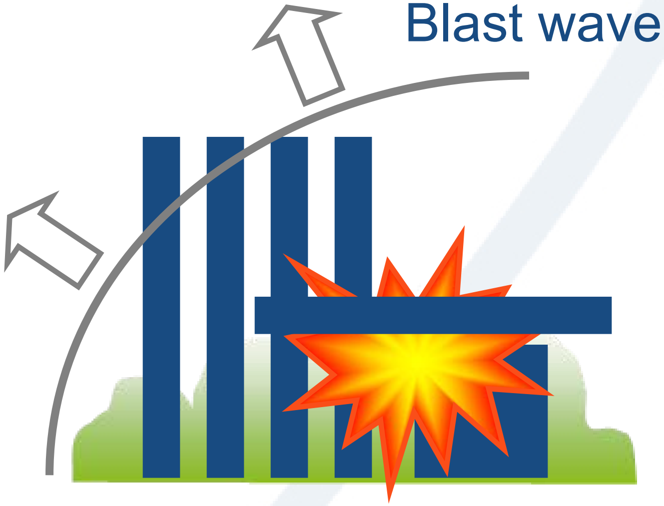
- Slow subsonic flames – mild hazards to confining structures
- Fast flames (supersonic relative to a fixed observer) and detonations – serious hazard
- Possibility of FA to supersonic speeds limits implementation of mitigation techniques
  - explosion suppression
  - explosion venting



Background

Unconfined explosions (VCE)

- Release of hydrogen gas/liquid
- Mixing with air and formation of “Vapor Cloud”
- Ignition and flame propagation
- Generation of air blast wave
- The problem is to evaluate blast parameters (P, I) = f(R) and blast effects



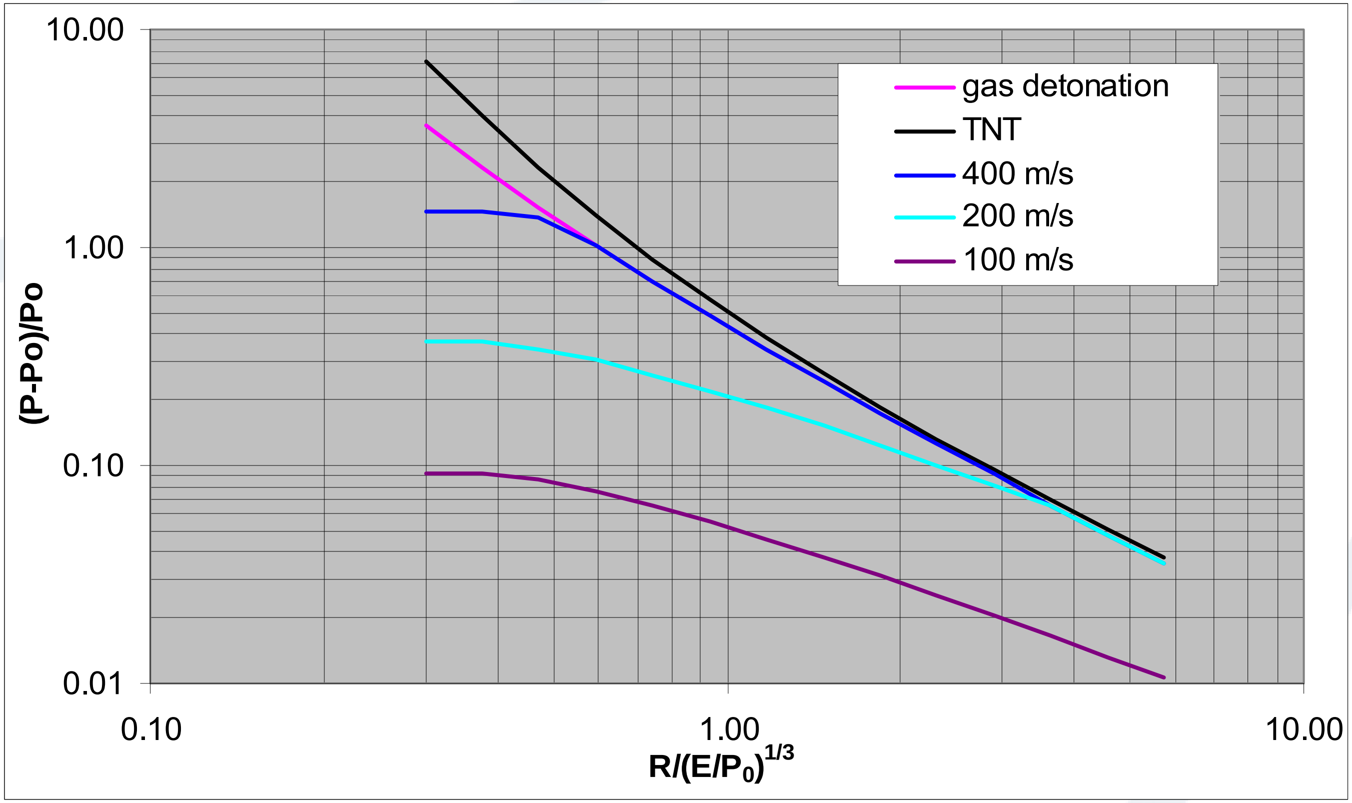
Background

Unconfined explosions (VCE) – hazards

- Amplitudes of pressure waves generated by gaseous explosions depends on flame speed
- There are solutions for P(R), I(R) as a function of flame speed V_f
    - TNO multi-energy method (ME)
    - Baker-Strehlow-Tang (BST)
    - Kurchatov Institute (KI) method
- The problem is to define flame speed and explosion energy

Background

P(R) for Various Flame Speeds



$R^* = R/(E/p_0)^{1/3}$ – Sach's dimensionless distance

Background

Why FA and DDT?

- Explosions almost universally start by ignition of a flame
  - electrical spark
  - hot surface
- Under certain conditions, flame can accelerate and undergo transition to detonation
- Collectively this process is referred to as deflagration-to-detonation transition (DDT)
- It is important to know critical conditions and resulting flame speeds → loads

Background

Understanding of FA and DDT

- Significant advances made in understanding of FA and DDT
  - High resolution Schlieren photography
  - Theoretical and advanced numerical studies
- Basic mechanisms are well understood
- Yet there are limitations in predictive simulations of these complex phenomena
- At present time, quantitative predictions typically rely on experiment based correlations

Background

Objective

- This lecture presents a framework for estimating potential explosion hazards in hydrogen mixtures
- Emphasis is placed on experimental correlations and analytical models
  - Basic physics
  - Simplified models
    - Accuracy within a factor of 2

Background

Outline

- Few comments on basics of deflagrations and detonations
- Description of FA and DDT
- FA and flame propagation regimes
  - FA in smooth tubes
  - FA in ducts with obstacles
  - Effects of initial/boundary conditions on FA
  - FA in unconfined clouds
- Onset of detonations
- Summary of the framework
- Concluding remarks

Deflagrations

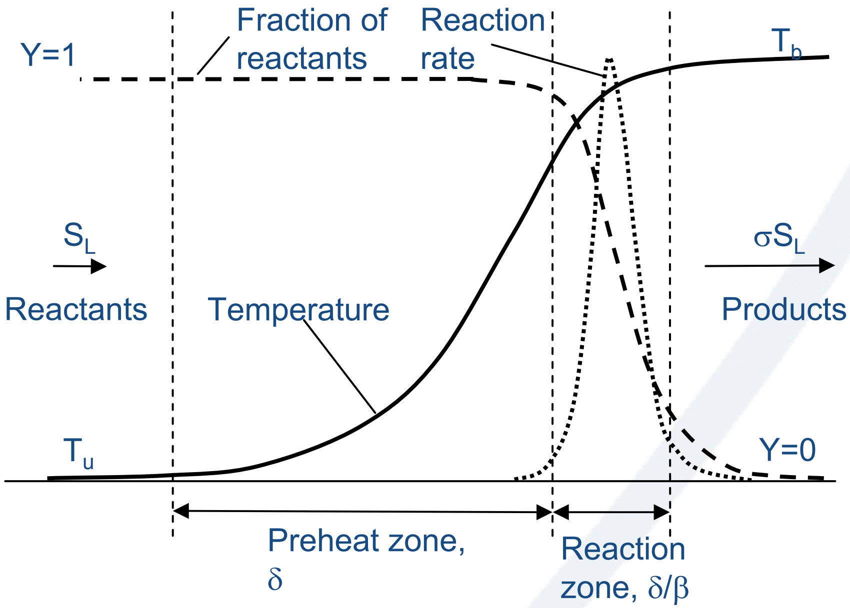
Laminar flames

- Weak ignition results in LAMINAR FLAMES
- Propagation mechanism: diffusion of temperature and species
- Laminar burning velocity

$$S_L \propto \sqrt{\chi/\tau_r} << c_s$$

- Flame thickness

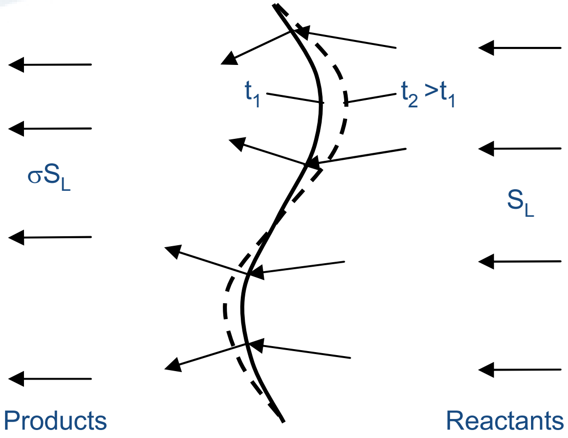
$$\delta = \frac{\rho_b \chi(T_b)}{\rho_u S_L} = \frac{\chi(T_b)}{\sigma S_L}$$

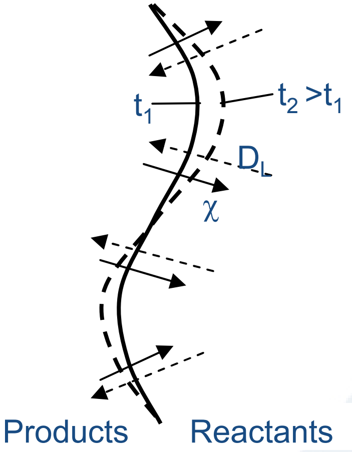


Deflagrations

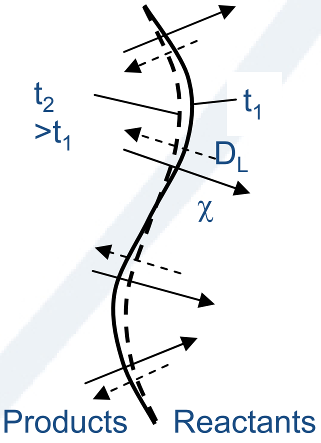
Flame instabilities

- Laminar flames are intrinsically unstable
- Hydrodynamic instability Landau-Darrieus
- Thermal-diffusive instability
  - $Le = \chi/D_L$
  - $Le < 1$ – lean H2 flames





Le<1



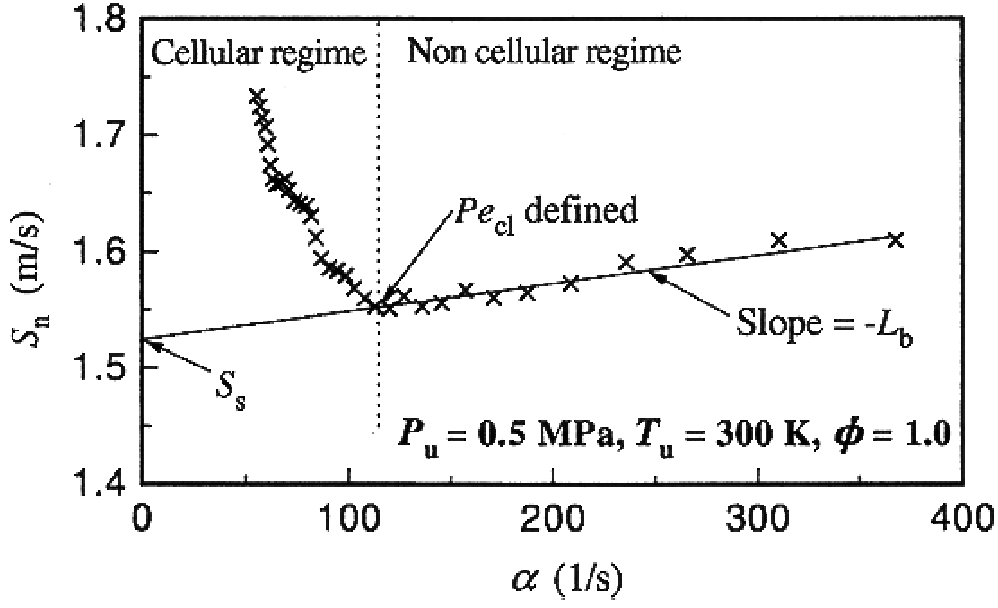
Le>1

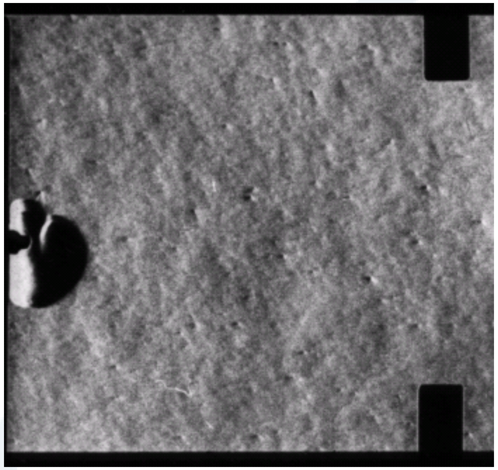
Deflagrations

Instabilities and flame stretch

- Markstein: normal velocity of a curved flame, S_n, may be expressed as in terms of flame stretch, $\alpha = 2S_n/R_f$

$$1-\frac{S_n}{S_L}=\frac{L_b\alpha}{S_L}=Ma\frac{\delta}{S_L}\alpha \qquad Ma = L_b/\delta$$



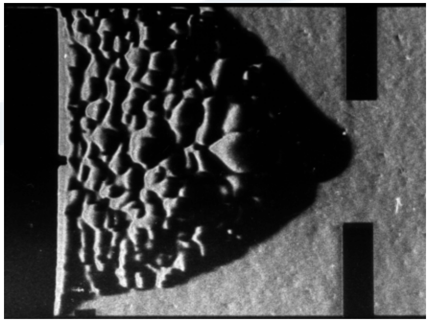


10% H_2/air

Deflagrations

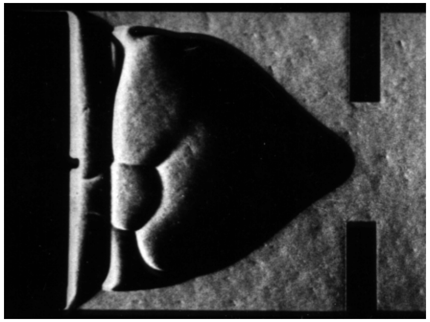
Cellular flames

- Cellular flames in hydrogen mixtures



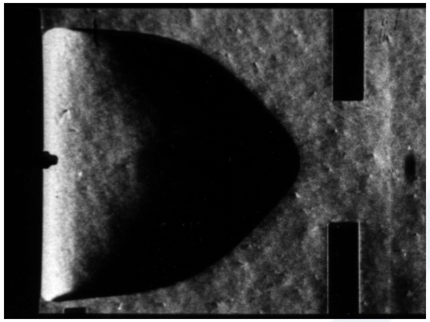
$Le \approx 0.35$

10%H2 in air



$Le \approx 1.0$

10%H2+5%O2+85%Ar



$Le \approx 3.8$

70%H2 in air

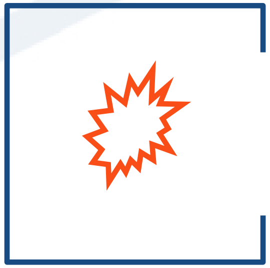
Deflagrations

More flame instabilities

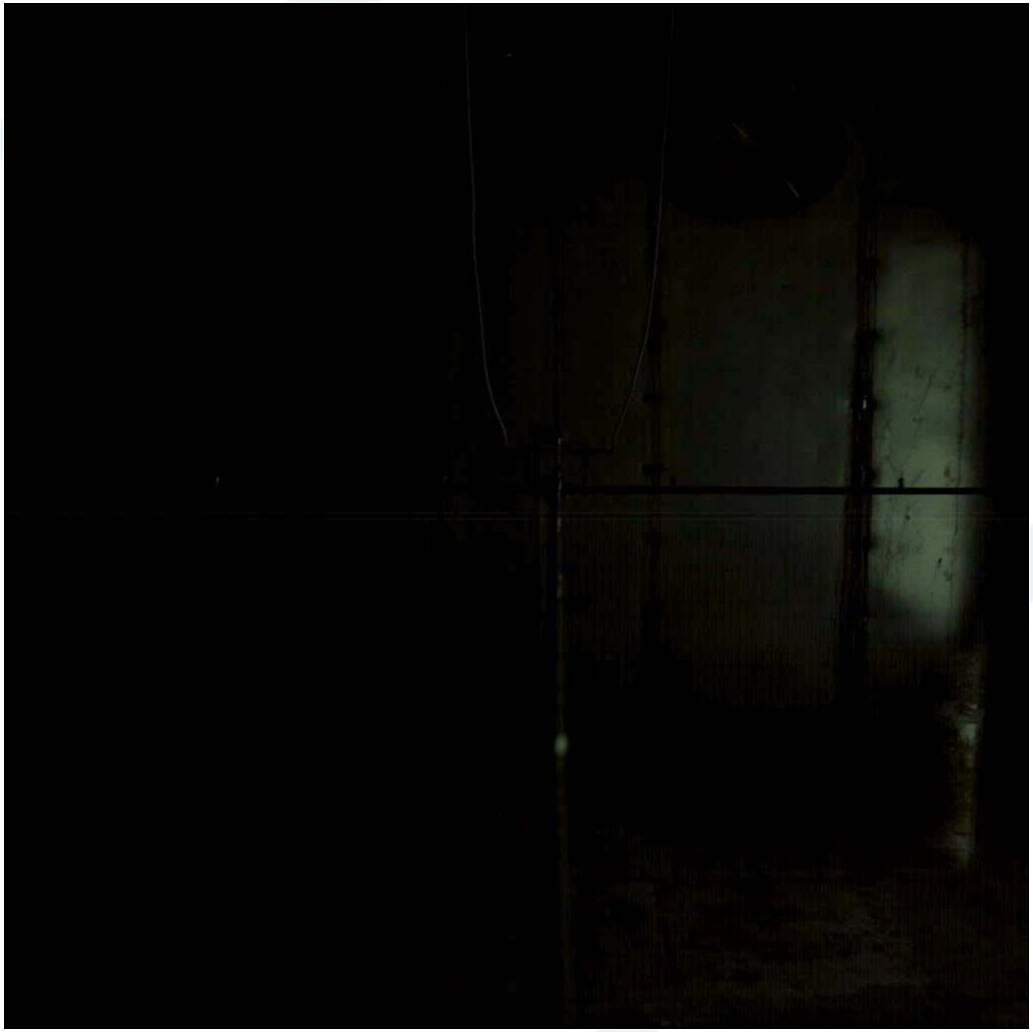
- Acoustic-flame instabilities
- Kelvin-Helmholtz (K-H) – shear instability
- Rayleigh-Taylor (R-T)
- Both K-H and R-T are triggered when flame is accelerated over an obstacle or through a vent
- Powerful mechanisms for ducts with obstacles

Deflagrations

Flame instabilities



64 m^3



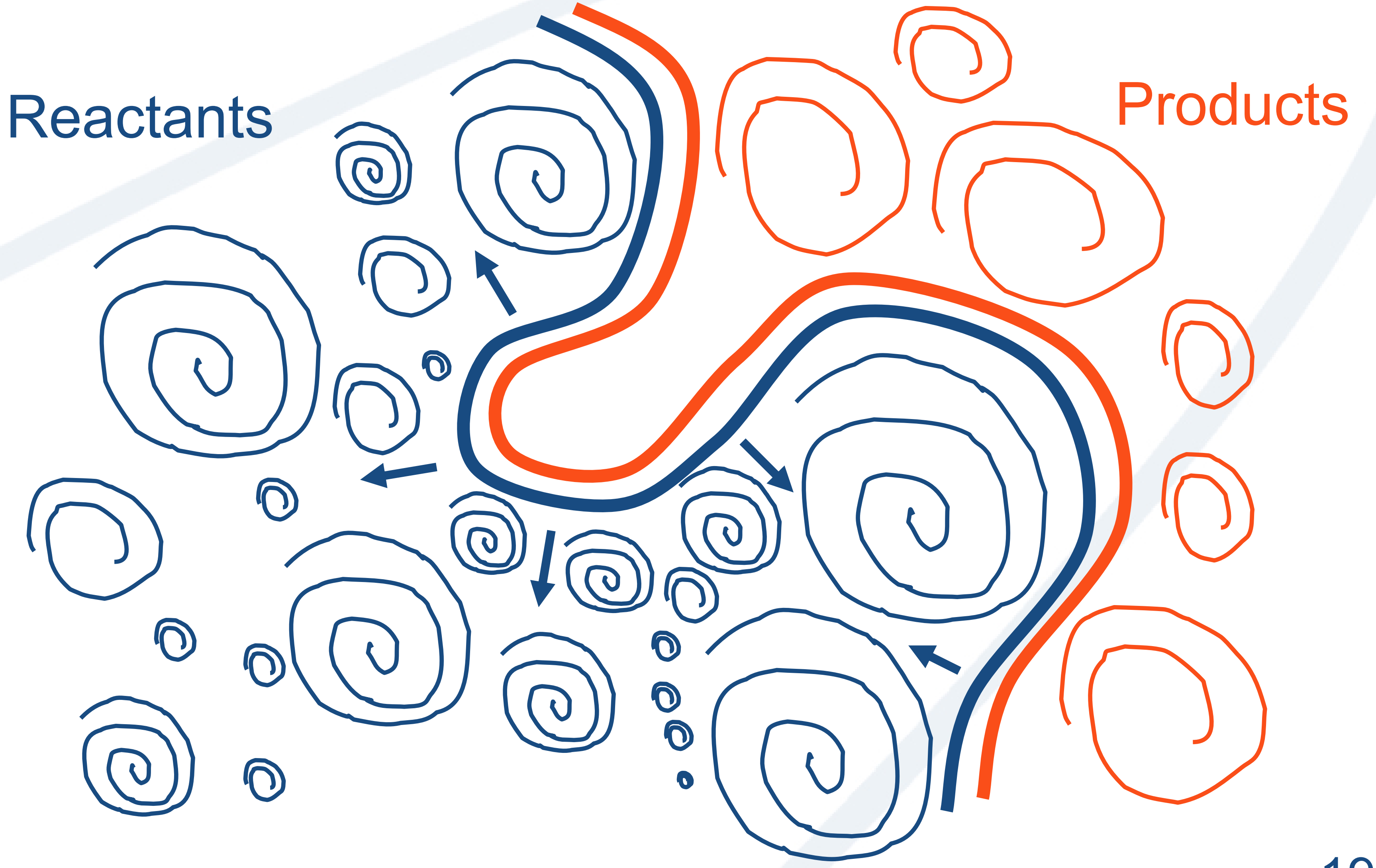
Deflagrations

Turbulent flames

- Laminar flames in initially quiescent mixture become turbulent
  - Development of flame instabilities
  - Growth of turbulence in the flame-generated flow
- Preexisting turbulence

Deflagrations

Flame in turbulent flow



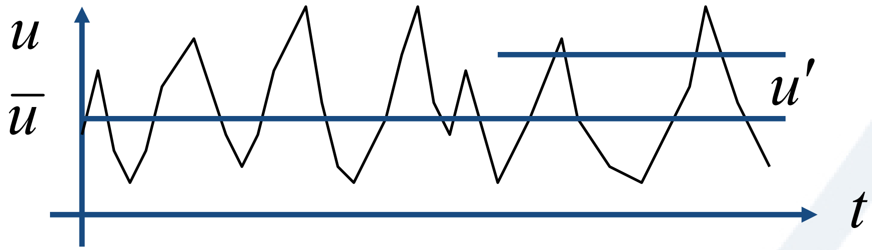
Deflagrations

Scales of turbulence

- Flow instability results in the development of random oscillations superimposed on mean flow

  $u = \overline{u} + u'$

- r.m.s velocity $\overline{u'} \equiv 0$



- Integral length and time scales L_T , τ_T – size and turnover time of the largest eddies
- Kolmogorov length and time scales: l_K , τ_K – size and turnover time of the smallest eddies
  - Viscous dissipation occurs at this scale

Deflagrations

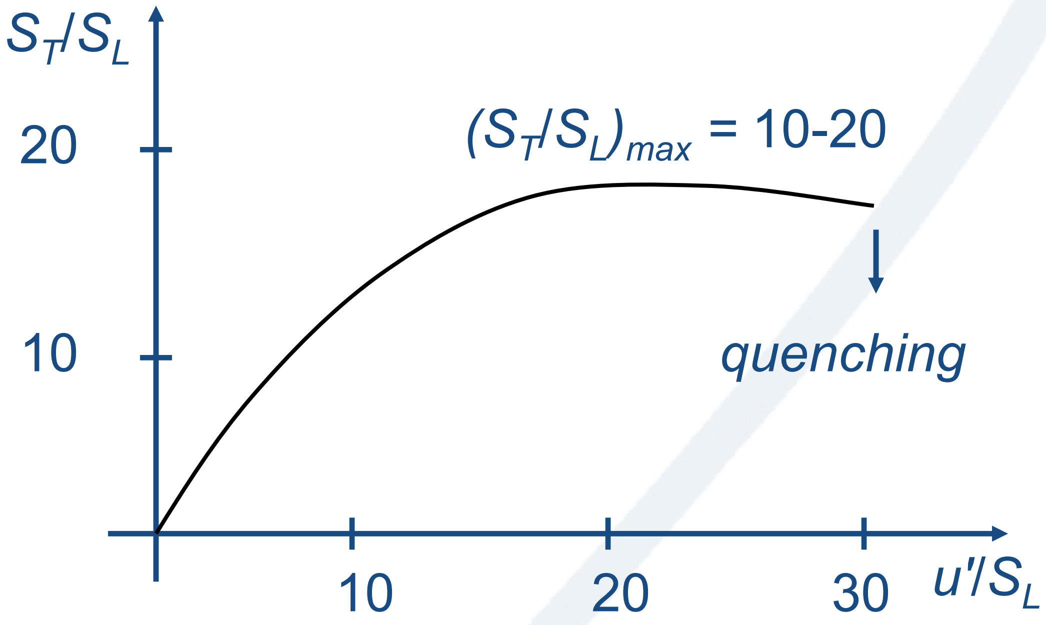
Turbulent burning velocities

- S_T : propagation speed of turbulent reaction zone

$$\frac{S_T}{S_L} = a \cdot \left(\frac{u'}{S_L}\right)^{1/2} \left(\frac{L_T}{\delta}\right)^{1/6} Le^{-n}$$

- *n* is uncertain
  - $n \approx 1$, *Le* = (0.5-1) Kido et al.

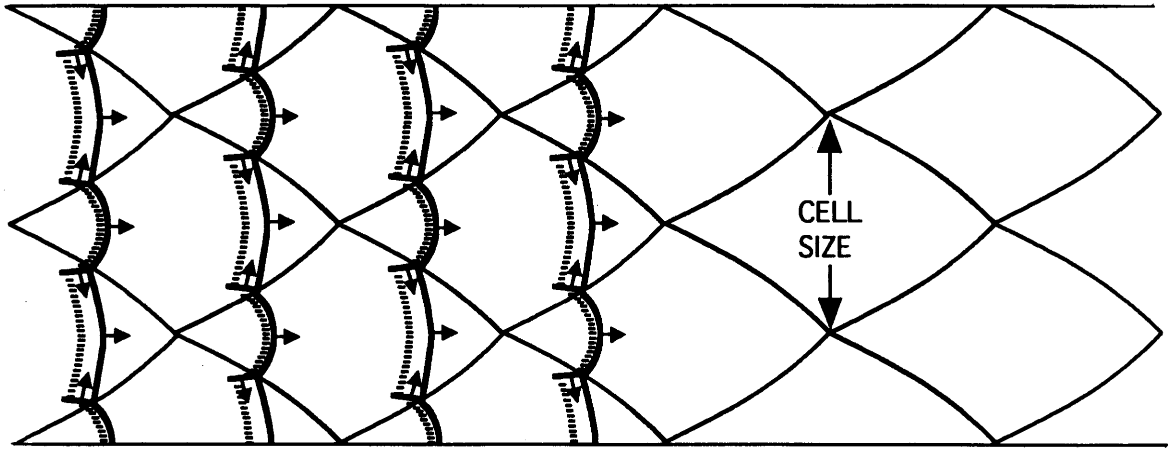
$$\frac{S_T}{S_L} = F\left(\frac{u'}{S_L}, \frac{L_T}{\delta}, Le, \beta, \sigma, n\right)$$

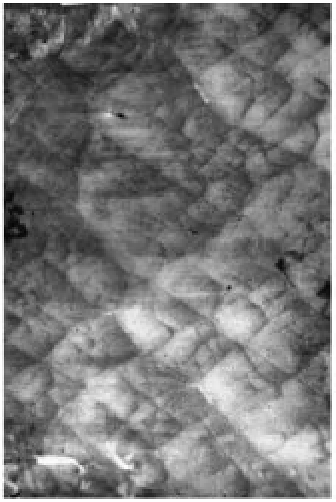


Detonations

Structure of the front

- 1D detonation waves are unstable and transverse perturbations are formed
- Spacing between transverse waves - detonation cell size λ - is important parameter
- The smaller is λ the more reactive is the mixture





Smoked foil after CH_4/air detonation

DDT Phenomenology

Basic studies of DDT

- Early detonation studies (1900+) were in smooth tubes using weak ignition
    - Detonation wave produced at the end of the FA process
    - Flame run-up distance required to form detonation was considered mixture property
- Chapman and Wheeler (1926) were the first to place obstacles in smooth tube to promote FA
- Shchelkin roughened tube by wire coil helix (1940)

DDT Phenomenology

Explosion in the explosion

- Stroboscopic Schlieren photographs by Urtiew and Oppenheim (1966) – a milestone in the study of DDT phenomenon
- Photos showed initiation of detonation from local explosion within shock flame complex “explosion in the explosion”

- Simulations of Elaine Oran and colleagues!

DDT Phenomenology

Detonation onset at flame front

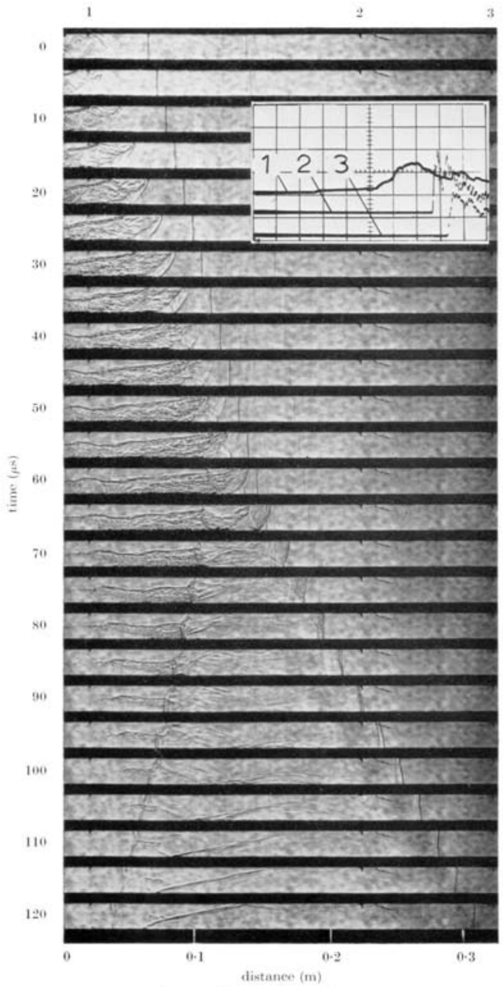


Figure 7. For legend see facing page.

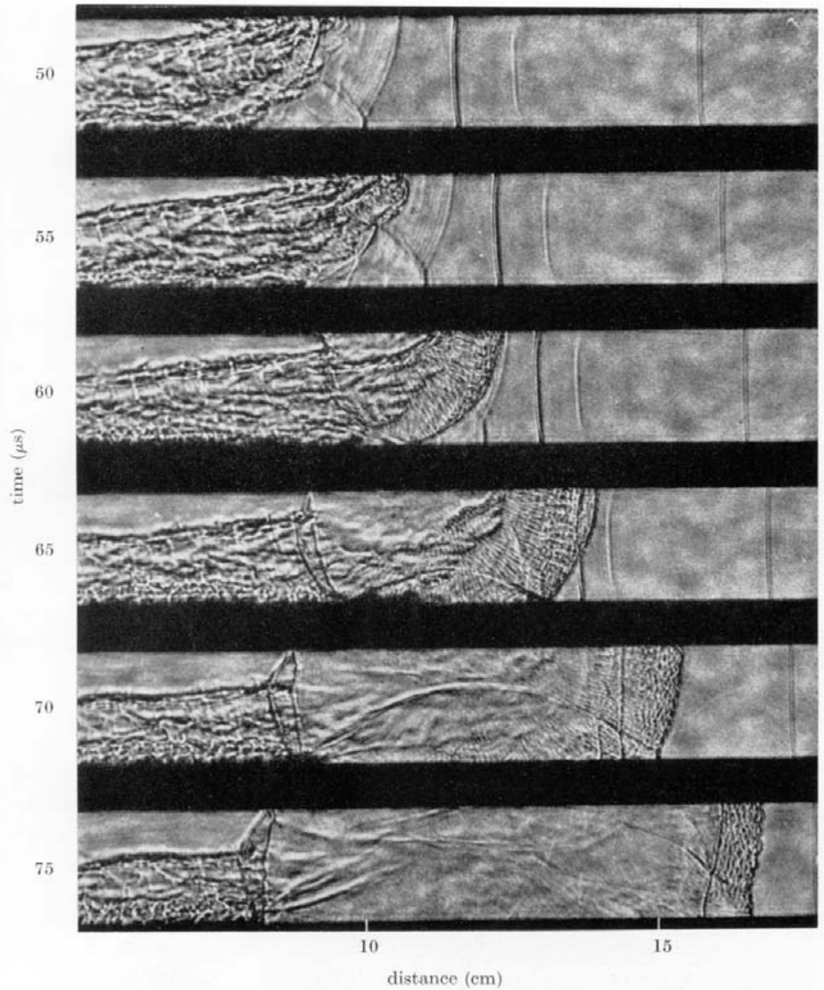


Figure 7 (*a*). Enlargement of frames at 50 to 75 μs of figure 7.

DDT Phenomenology

Studies of DDT

- Processes of DDT have been studied in smooth tubes
  - in channels with repeated obstacles
  - photochemical systems
  - hot turbulent jets
  - shock-flame interactions
  - other experimental situations

DDT Phenomenology

Phases of DDT process

- Following Lee & Moen (1980) and Shepherd & Lee (1991), DDT is divided into two phases:
  1. *Creation of conditions for the onset of detonation* by FA, vorticity production, formation of jets, and mixing of products and reactants;
  2. Actual formation of detonation itself or *the onset of detonation*

DDT Phenomenology

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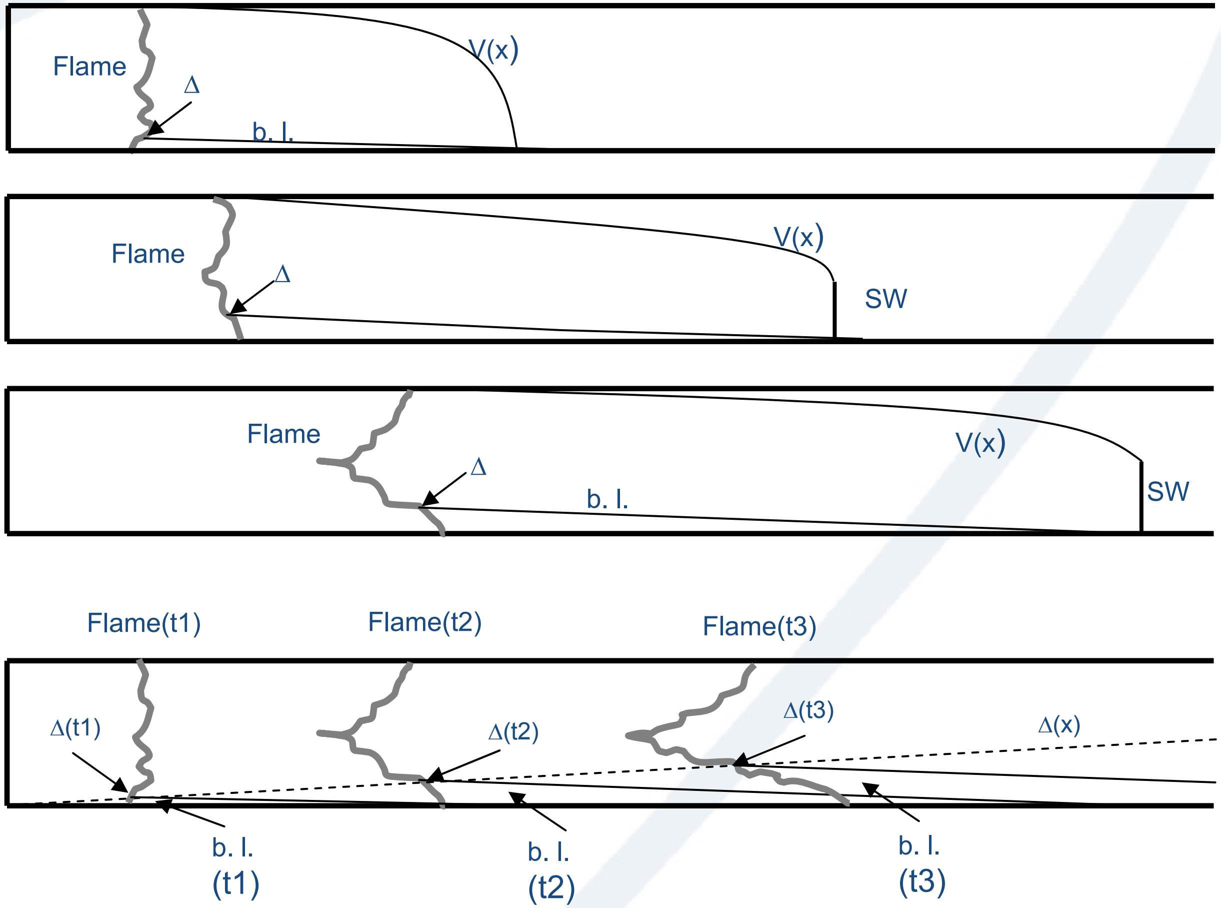
  2. Actual formation of detonation itself or *the onset of detonation*

FA in smooth tubes

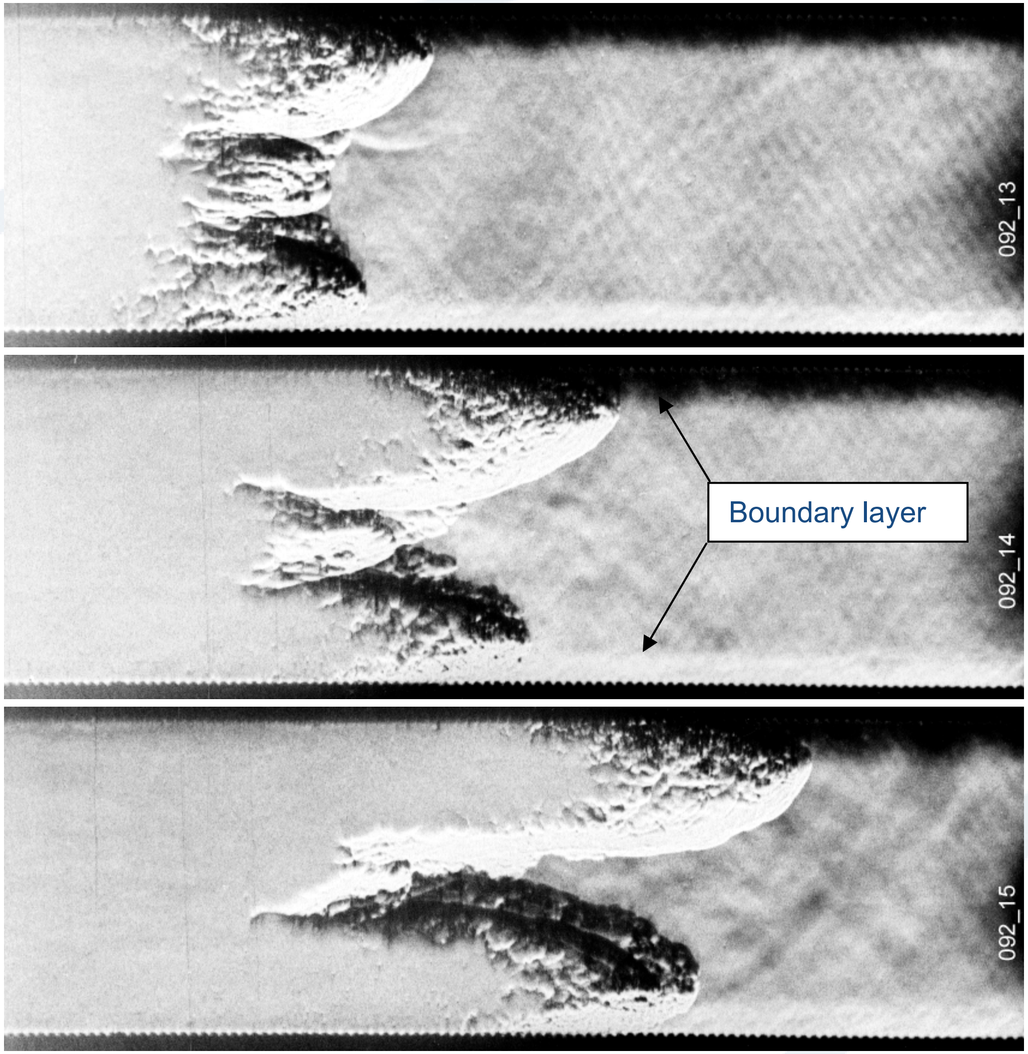
Mechanisms

- Different from tubes with obstacles
- Boundary layer plays an important role
- Thickness Δ of b.l. at flame positions increases during FA



FA in smooth tubes

Flame shapes in smooth tubes

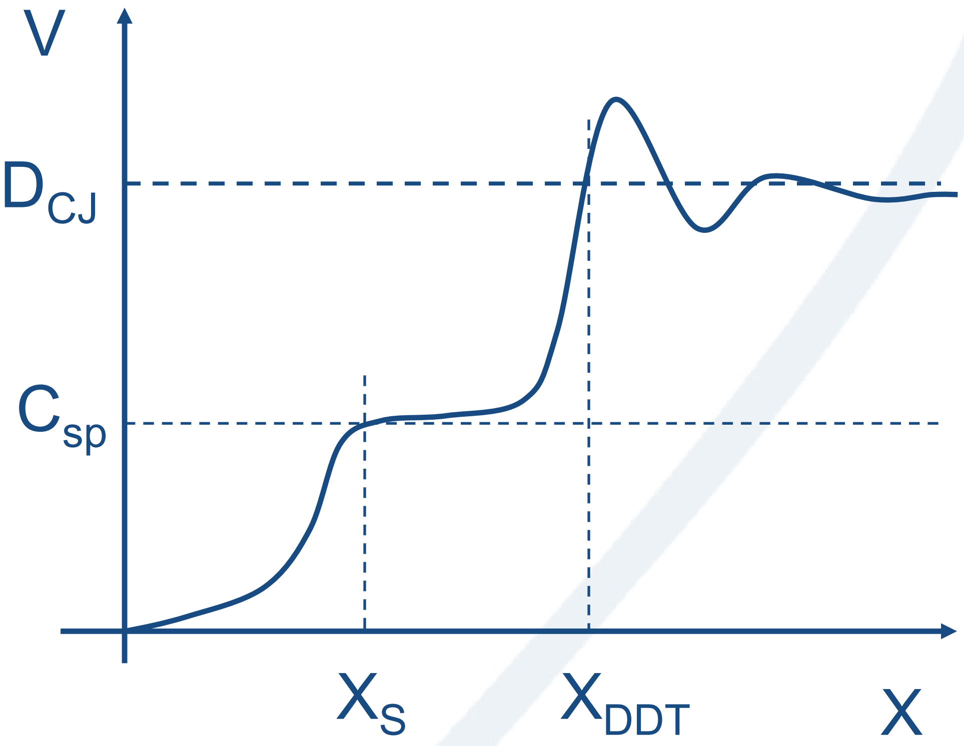


Shadow photos of Kuznetsov, et al.

FA in smooth tubes

Run-up distances in smooth tubes

- Substantial experimental data accumulated on X_{DDT}
- Ambiguous data on the effect of tube diameter and detonation cell size
- Different mechanisms
  - Flame acceleration
  - Onset of detonation



FA in smooth tubes

Run-up distances X_s

- We focus on run-up distances to supersonic flames in relatively smooth tubes
- An approximate analytical model to be described, which is based on the following ideas
  - Relate flame shape / burning velocity evolution and the flame speed
  - Describe boundary layer thickness ahead of an accelerated flame

FA in smooth tubes

X_s in smooth tubes

- Mass balance

$$V\frac{\pi D^2}{4} = \alpha S_T \pi D \Delta(\sigma - 1)\left(\frac{\Delta}{D}\right)^m$$

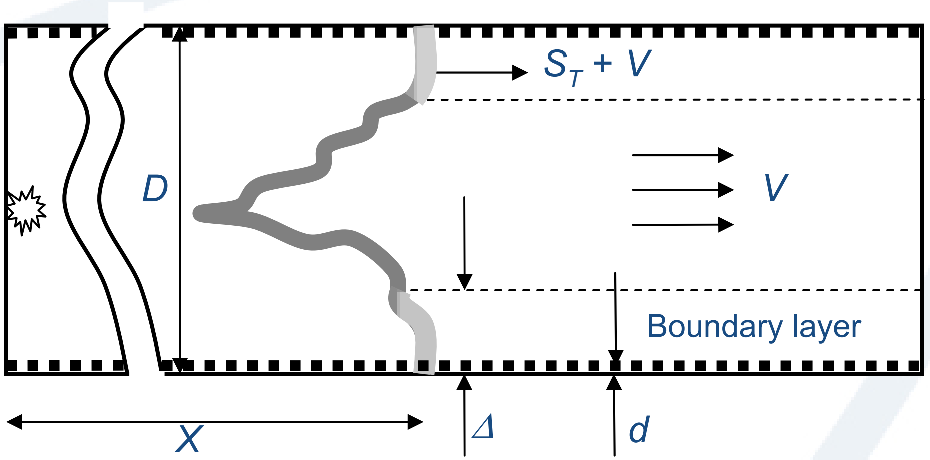
- Burning velocity S_T

$$\frac{S_T}{S_L} = \varphi\left(\frac{u'}{S_L}\right)^{1/2}\left(\frac{L_T}{\delta}\right)^{1/6}$$

- Boundary layer thickness

$$C\frac{X}{\Delta} = \frac{1}{\kappa}\ln\left(\frac{\Delta}{d}\right) + K$$

- X_s: $V+S_T = C_{sp}$



$$\frac{X_S}{D} = \frac{\gamma}{C}\left[\frac{1}{\kappa}\ln\left(\gamma\frac{D}{d}\right) + K\right]$$

$\gamma = \Delta/D$:

$$\gamma = \left[\frac{c_{sp}}{\beta(\sigma - 1)^2 S_L}\left(\frac{\delta}{D}\right)^{1/3}\right]^{\frac{1}{2m+7/3}}$$

Two unknown parameters: *m* and β

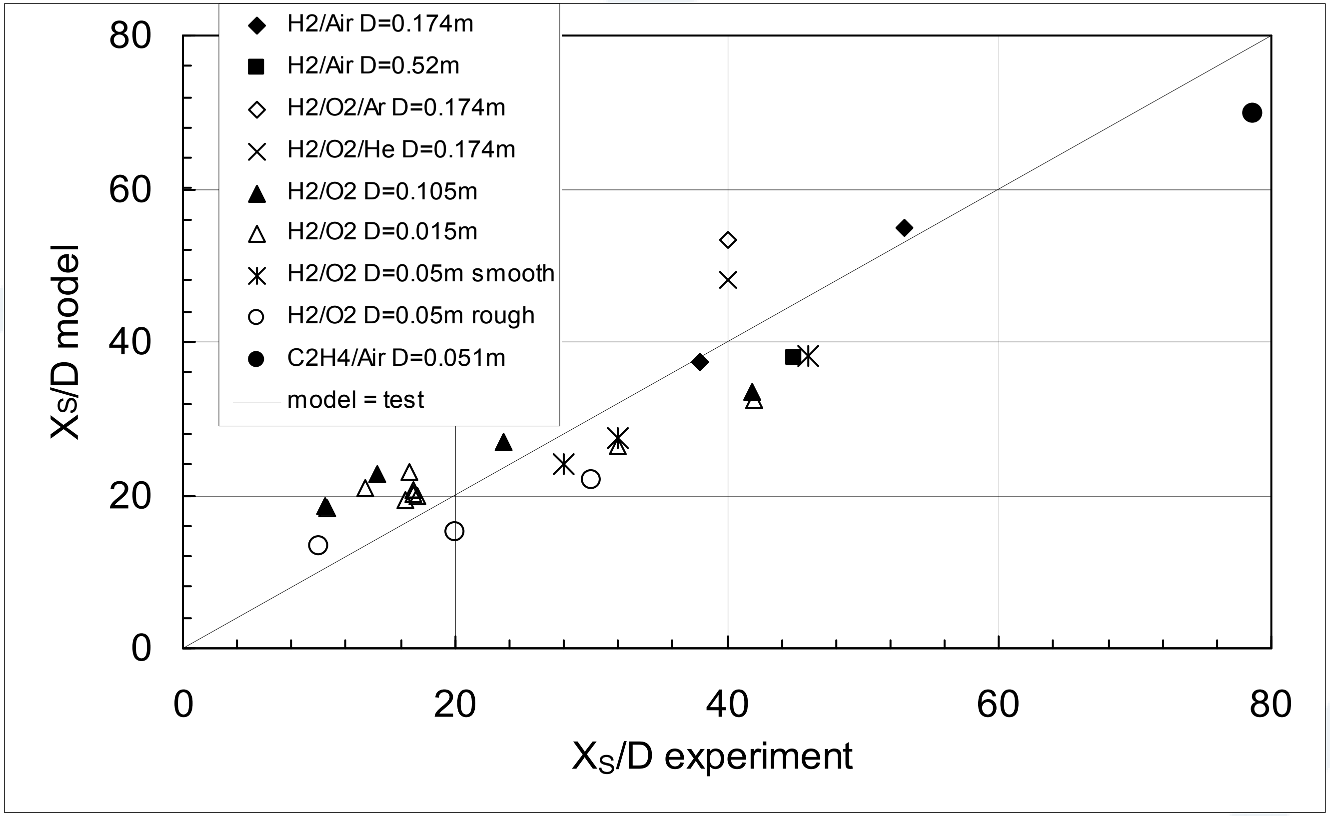
FA in smooth tubes

Experimental data

- Data with V(X)
  - Kuznetsov et al., 1999, 2003, 2005
  - Lindstedt and Michels 1989
- BR: 0.002 – 0.1
- S_L: 0.6 – 11 m/s
- C_{sp}: 790 -1890 m/s
- D: 0.015 – 0.5 m
- X_S/D: 10 - 80

FA in smooth tubes

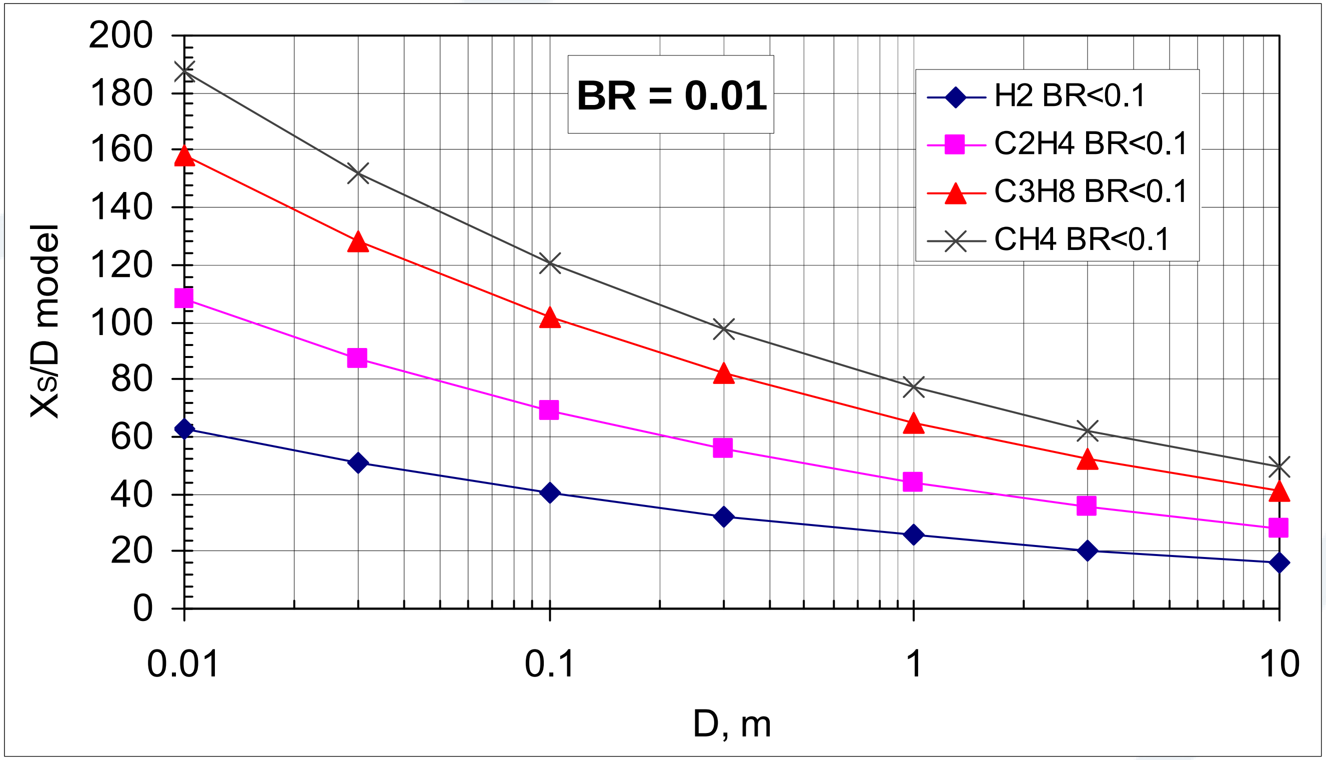
Correlation of model and experimental data



- $\beta = 2.1$
  $m = -0.18$
- Accuracy $\approx \pm 25\%$

FA in smooth tubes

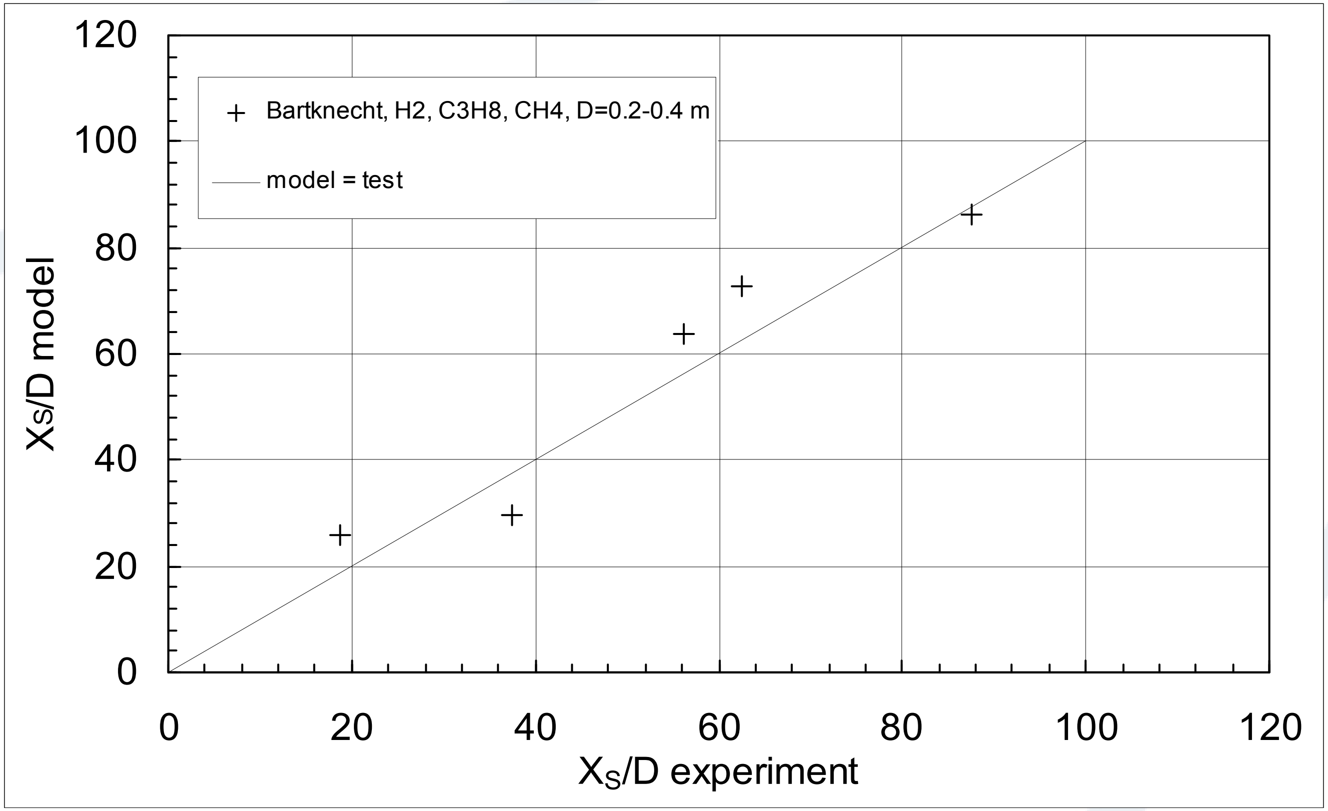
Run-up distances as a function of D



- X_S/D slightly decreases with D for given BR
- Large X_S /D for C_3H_8 and CH_4 – no data on X_S & X_{DDT} in smooth tubes

FA in smooth tubes

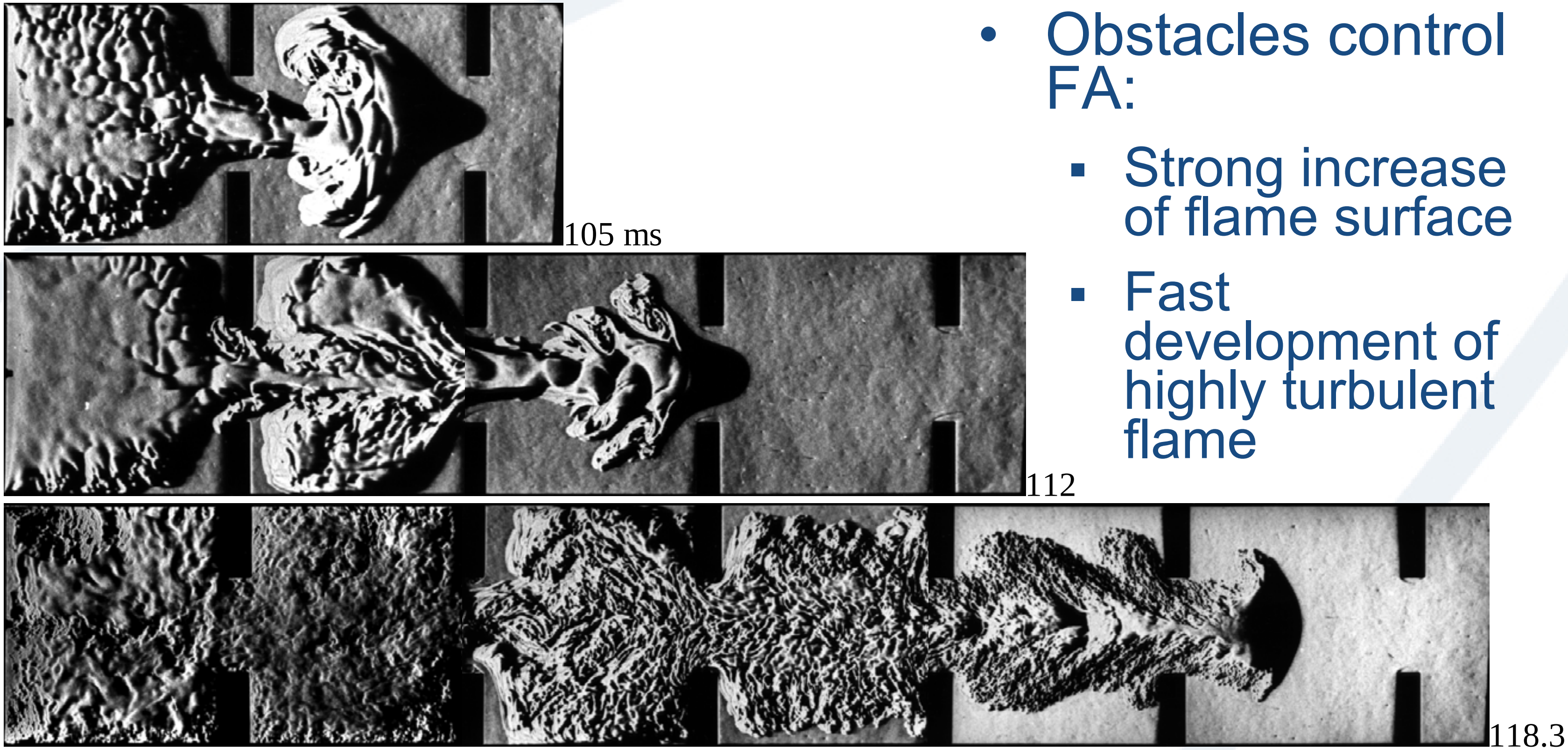
Run-up distances in “turbulent mixtures”



- Only X_S /D-data with initial turbulence for C_3H_8 & CH_4
- Correlate with effective S_L: $S_{Leff} = 2.5S_L$

FA in obstructed channels

Flame evolution in channels with obstacles



- Obstacles control FA:
  - Strong increase of flame surface
  - Fast development of highly turbulent flame

10% H2-air. Shadow photos of Matsukov, et al.

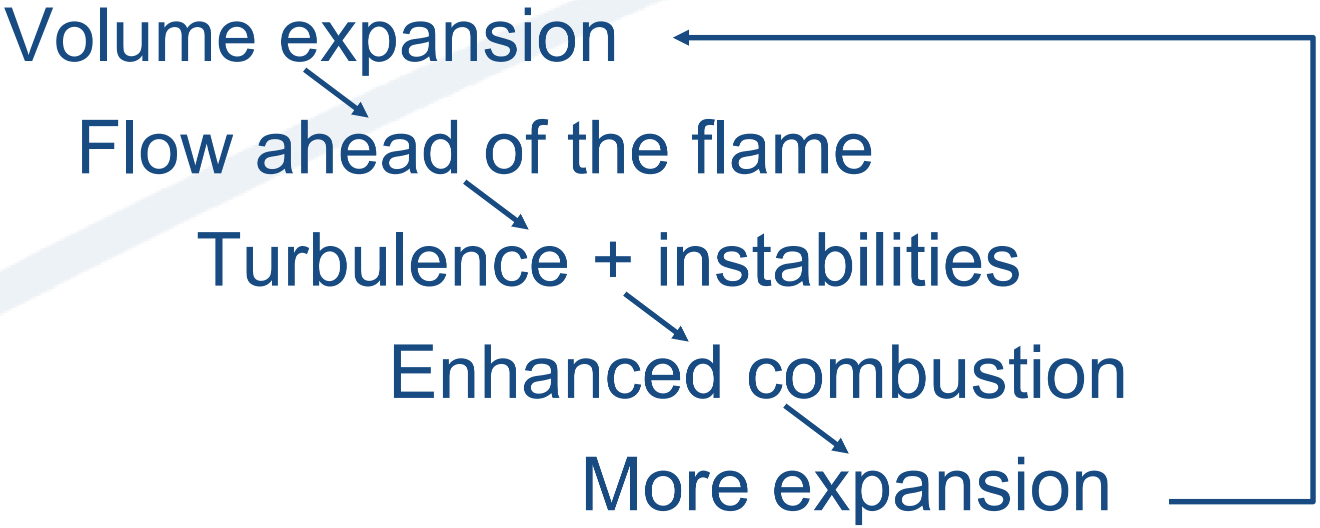
FA in obstructed channels

Two effects responsible for FA

- Flame surface increase
  - Flame speed relative to fixed observer: $V_f = S_L \sigma$(Flame area)/(Flow cross-section) > $10S_L$
- Turbulence generated in the flow ahead of the flame affect the burning velocity S_T
  - Increase of burning velocity S_T/S_L up to about 10 to 20
- Total increase of flame speed relative to fixed observer: $V_f > 100\mathrm{S}_\mathrm{L}$

FA in obstructed channels

FA – Feedback mechanism



Volume expansion

Flow ahead of the flame

Turbulence + instabilities

Enhanced combustion

More expansion

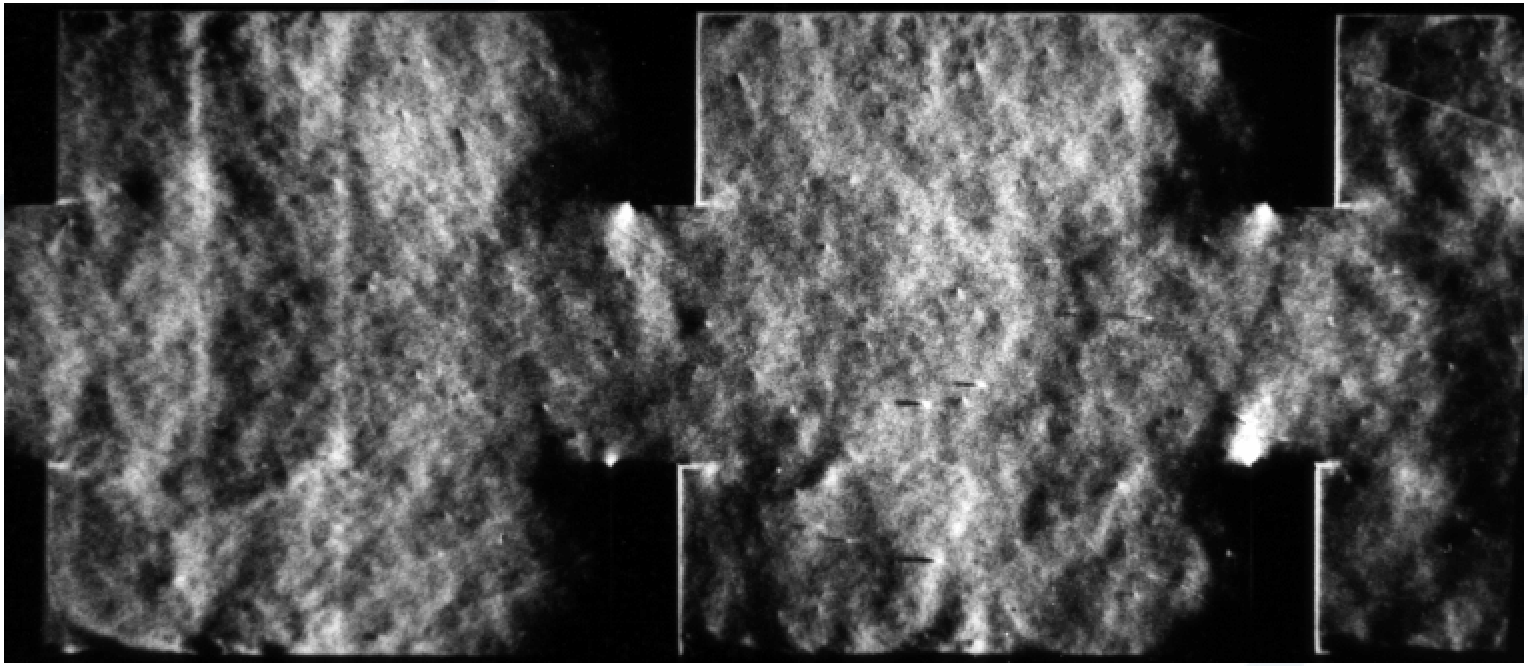
FA in obstructed channels

Weak and strong FA

- *Weak* FA results in slow unstable turbulent flame regimes
- *Strong* FA leads to fast flames propagating with supersonic speed relative to a fixed observer

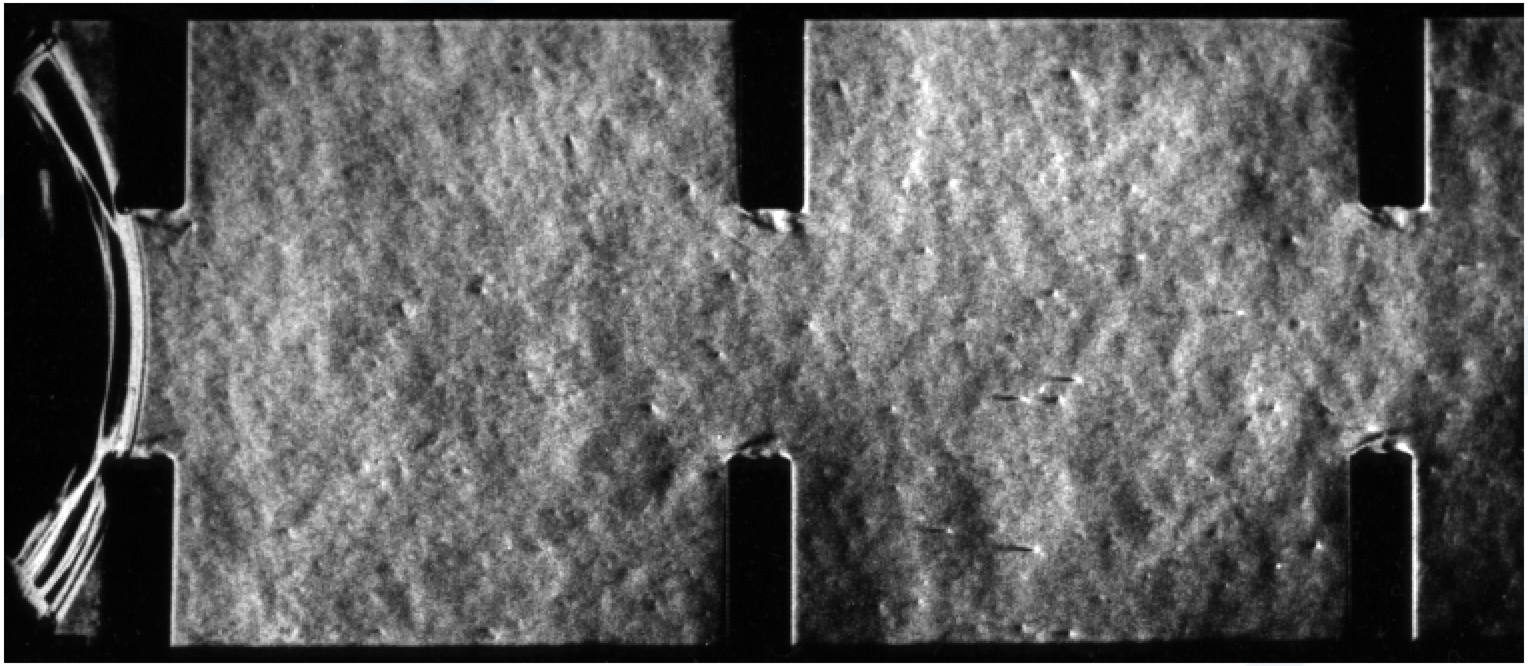
FA in obstructed channels

Flame structure – *weak* FA



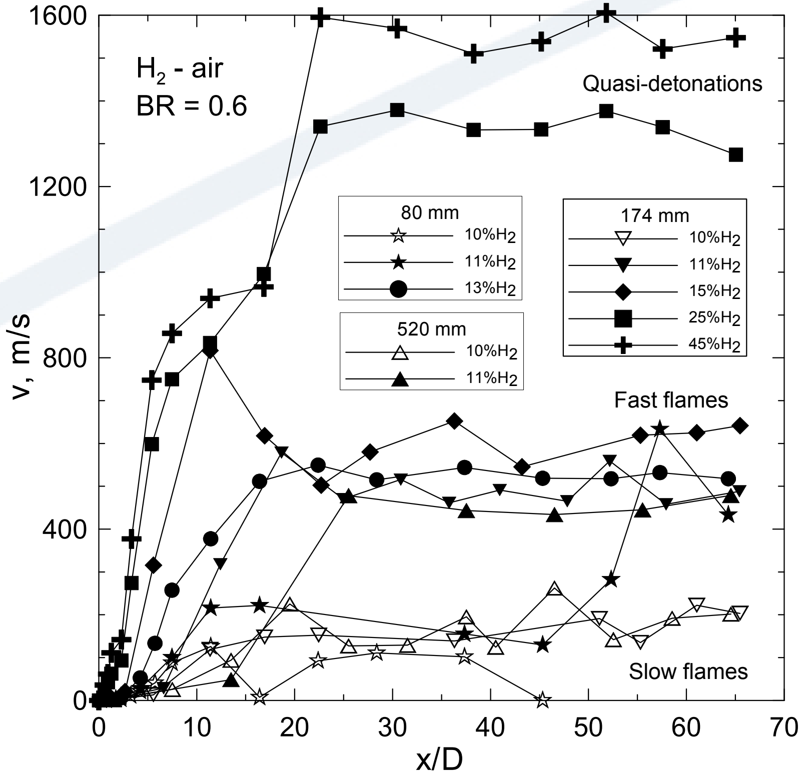
FA in obstructed channels

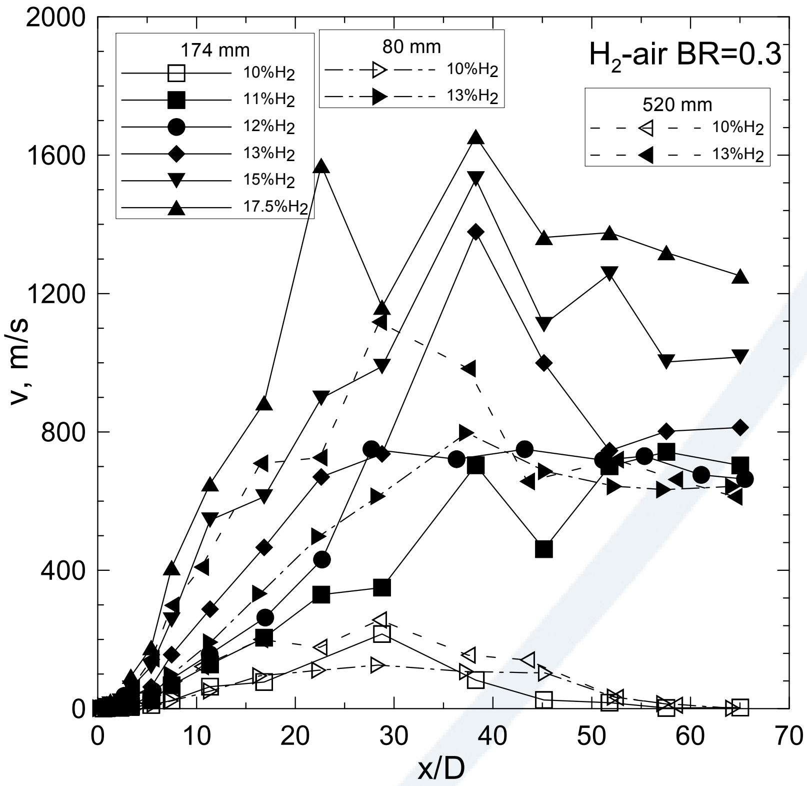
Flame structure – *strong* FA



FA in obstructed channels

Flame speeds as a function of distance





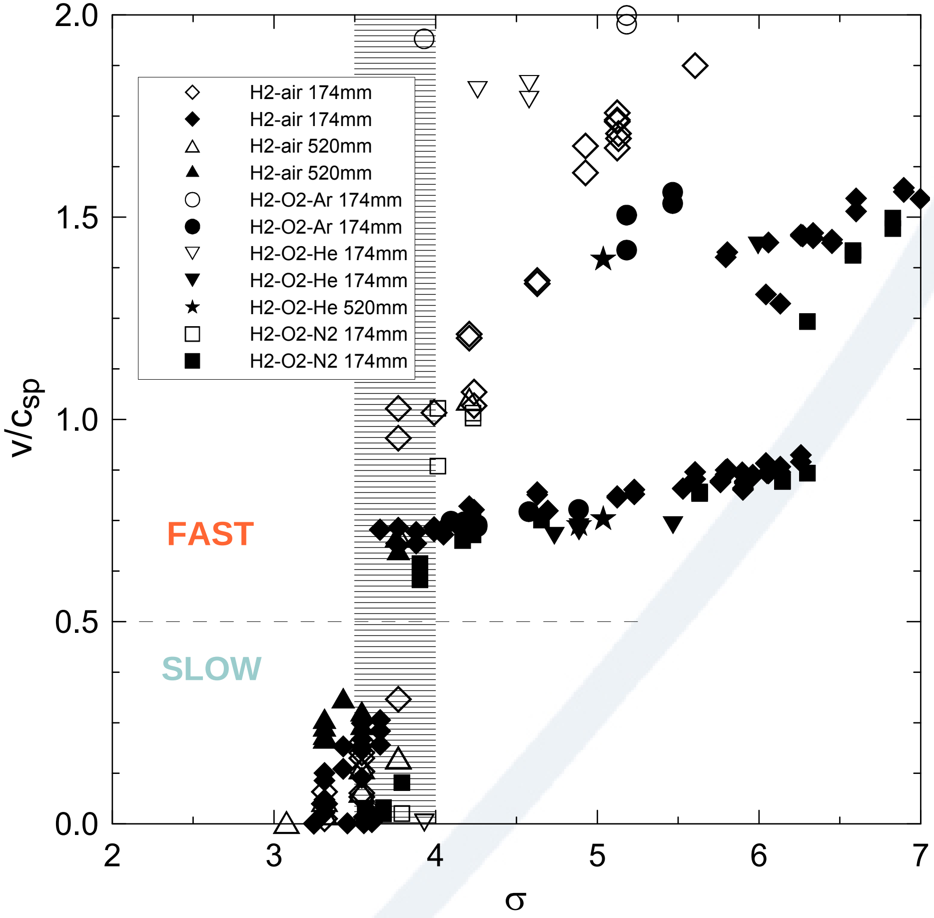
H$_2$-air

FA in obstructed channels

Criteria for strong/weak FA

Effect of expansion ratio

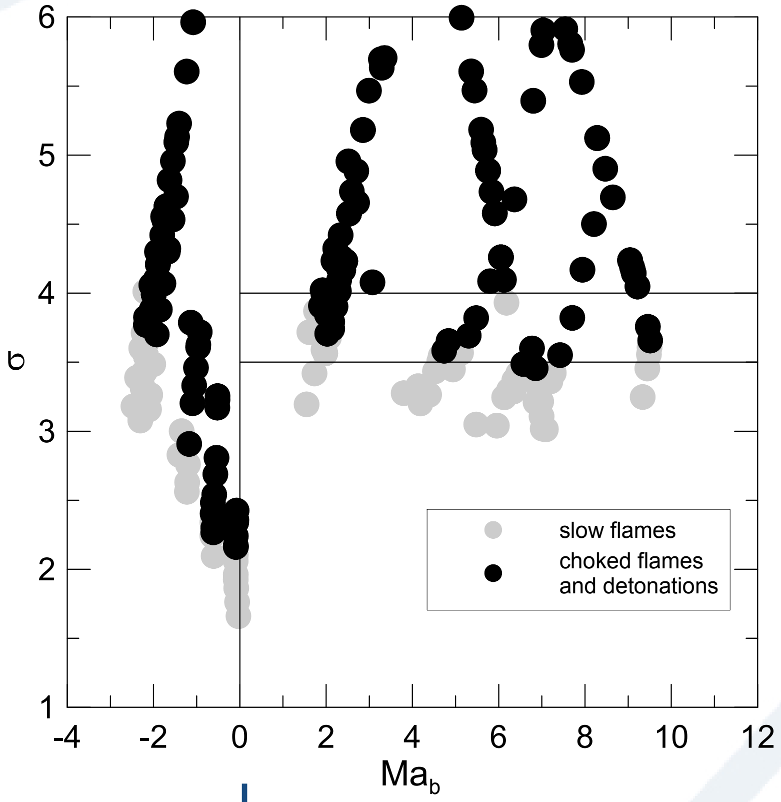
H_2-air at normal T, p



FA in obstructed channels

Criteria for strong/weak FA

Effect of Markstein number



Increase of burning velocity with stretch

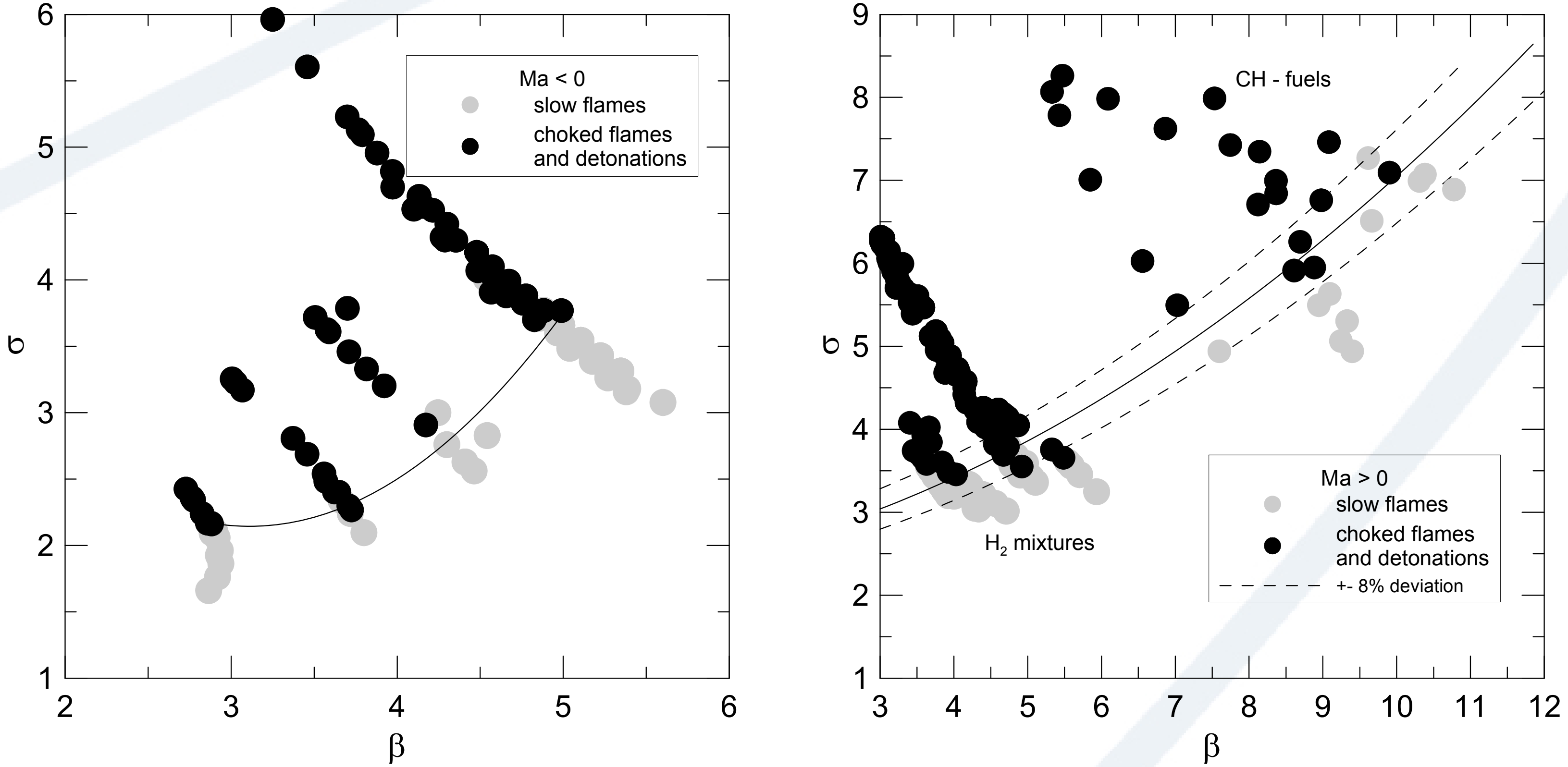
Decrease of burning velocity with stretch

FA in obstructed channels

Criteria for strong/weak FA

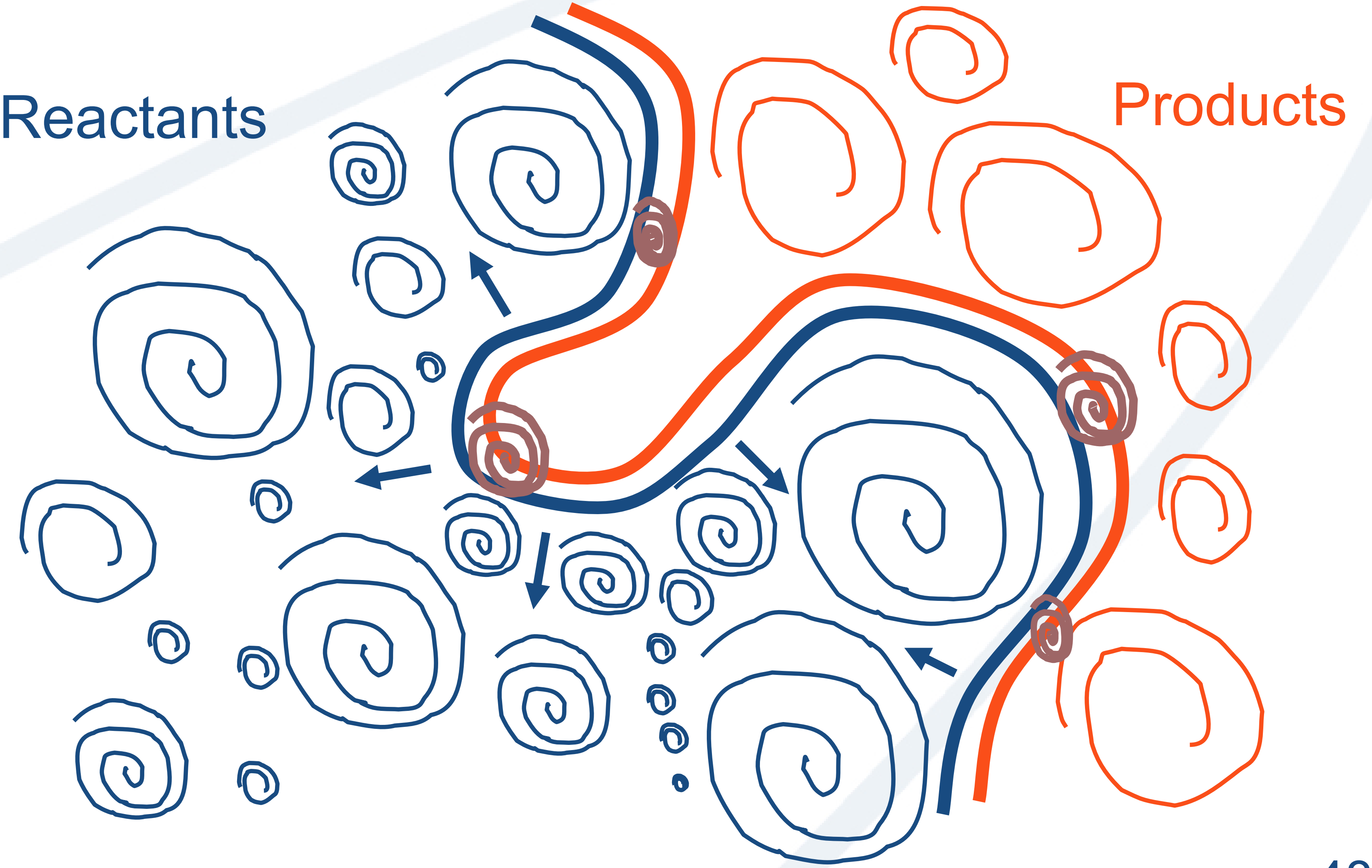
Effect of Zeldovich number, *β*

$$\beta = \frac{E_a (T_b - T_u)}{R T_b^2}$$



FA in obstructed channels

Flame – high turbulence (u'/S_L)



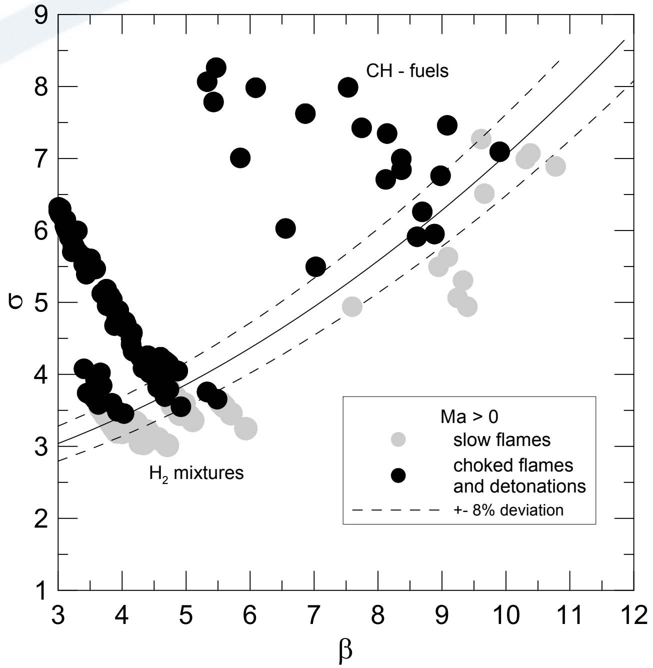
FA in obstructed channels

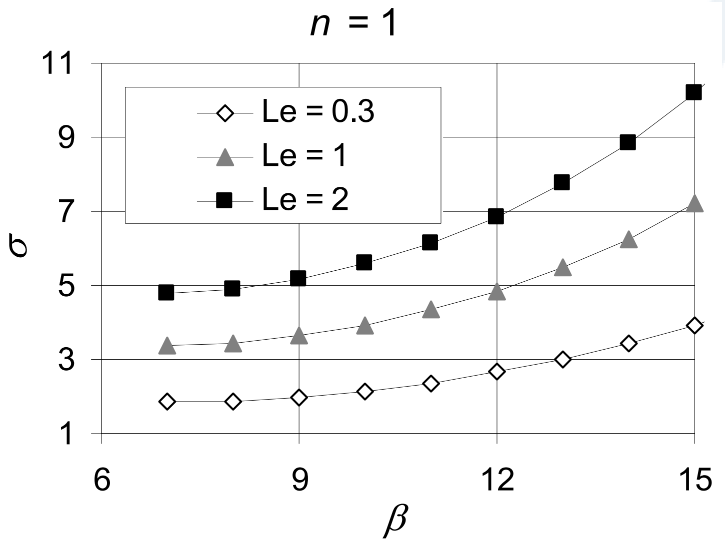
Criteria for strong/weak FA

Quenching of the largest (=ALL) mixed eddies :

$$\frac{\sigma^2 \beta^2 (\beta/2-1)^n e^{1-\beta/2}}{6 Le^n \Gamma_{n+1} \kappa} = 1$$

Only mixture properties





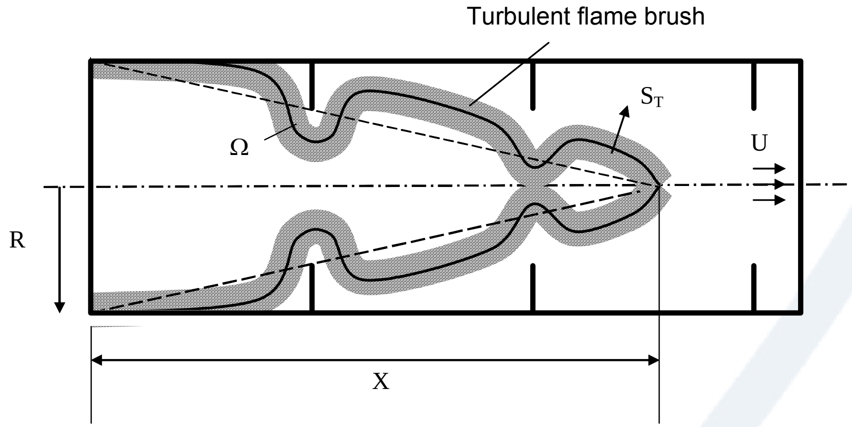
Experiment

Theory

FA in obstructed channels

Run-up distances X_s

- Flame shape is given by obstacle field
- Burning velocity S_T is constant and equal to its max value
  $S_T \approx 10S_L$
- X_S is the distance where flame speed approaches C_{sp}



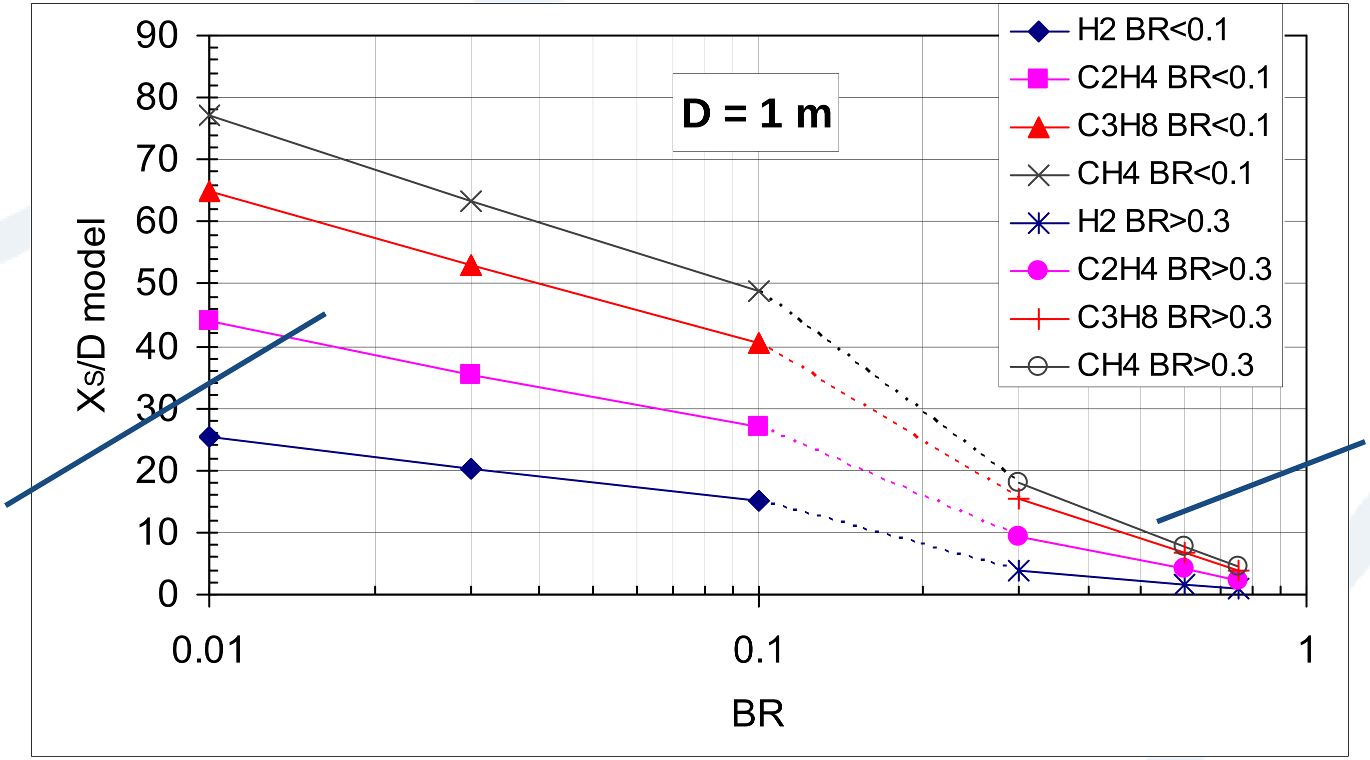
$$\frac{X_S}{R}\frac{10S_L(\sigma-1)}{c_{sp}} \approx a\frac{1-BR}{1+b\cdot BR}$$

- $X_S \propto D$ for given mixture, BR, and initial T, p

Data:
SL: 0.1–1.5 m/s
C_{sp}: 640–1900 m/s

Variations of Xs

Run-up distances as a function of BR



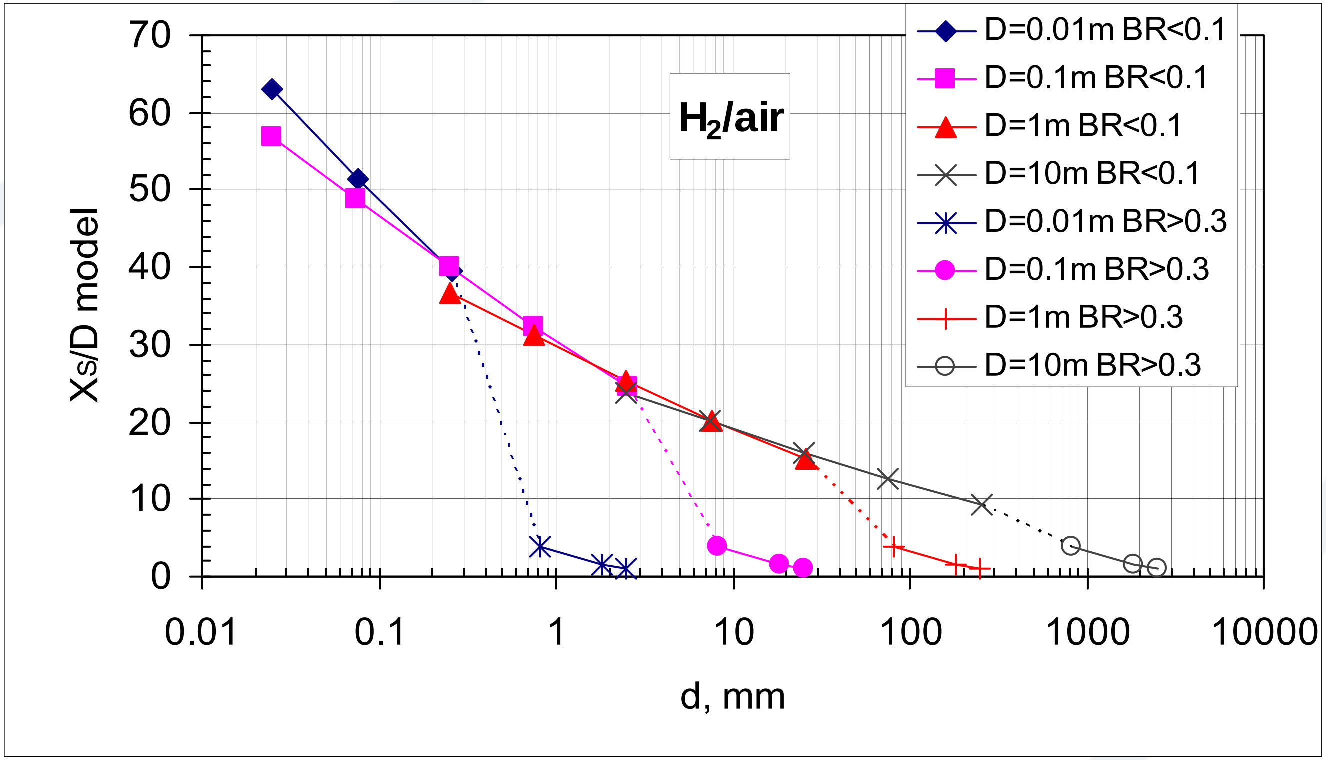
Smooth tube

Obstructed tube BR>0.3

- X_S/D decreases with BR for given D
- FA is strongly promoted by obstructions

Variations of Xs

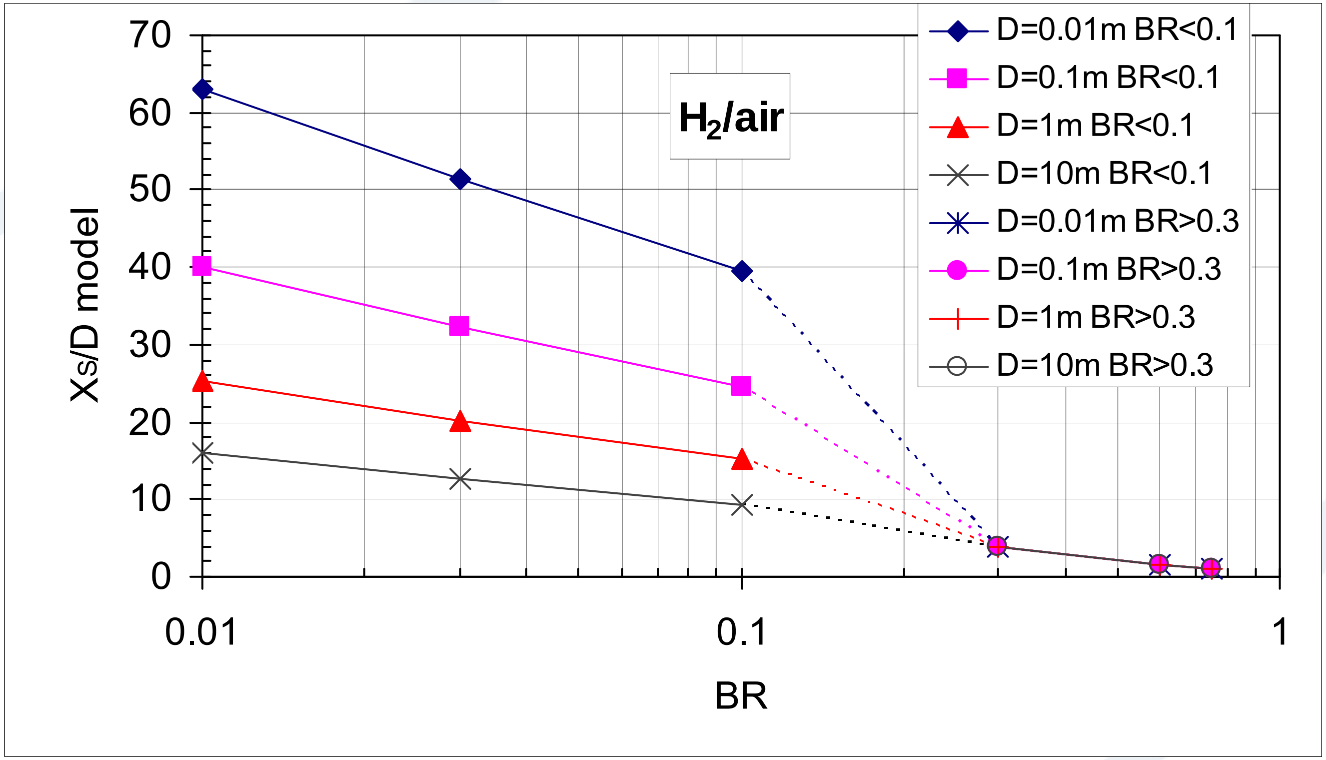
Run-up distances versus tube roughness, d



- X_S/D slightly decreases with D
- At sufficiently large d (so that BR>0.1) X_S/D drops

Variations of Xs

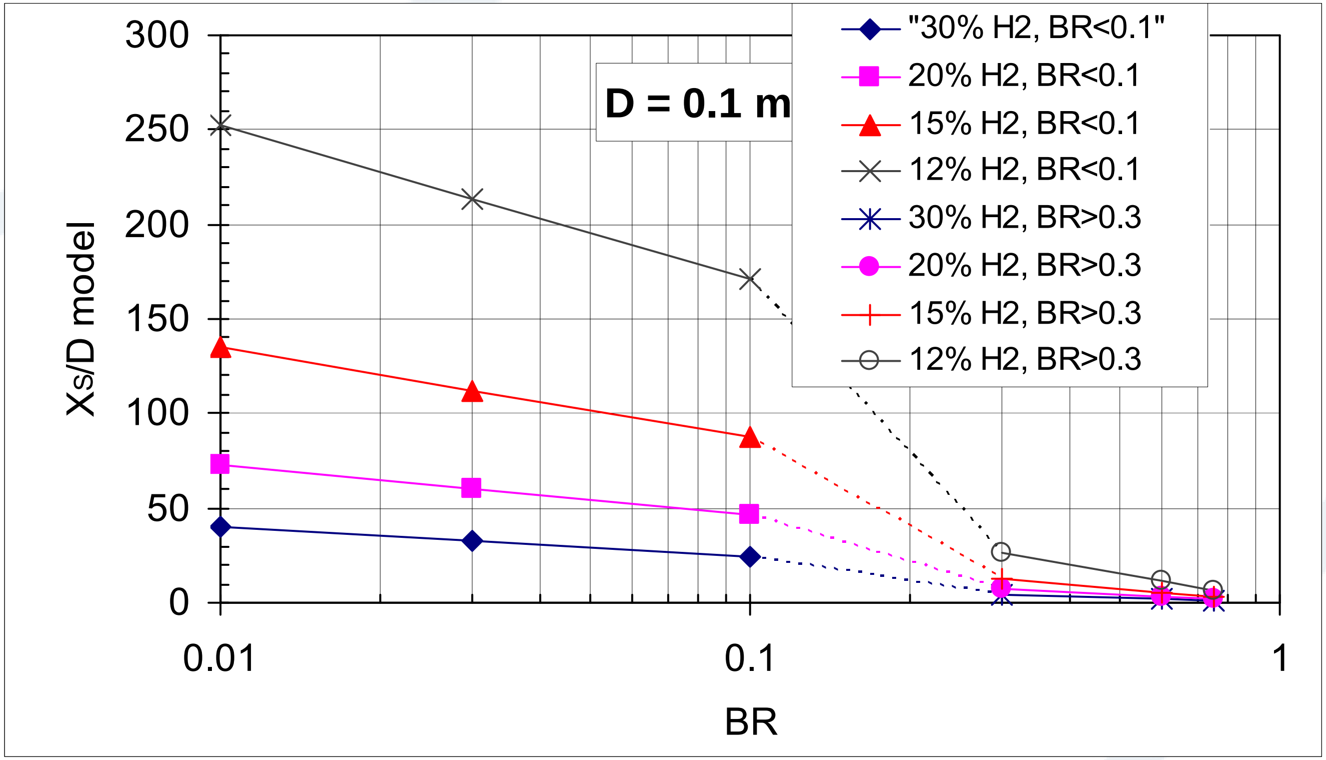
Run-up distances for various D



- Smooth tubes: X_S/D slightly decreases with D
- Obstructed tubes (BR>0.3): X_S/D independent of D

Variations of Xs

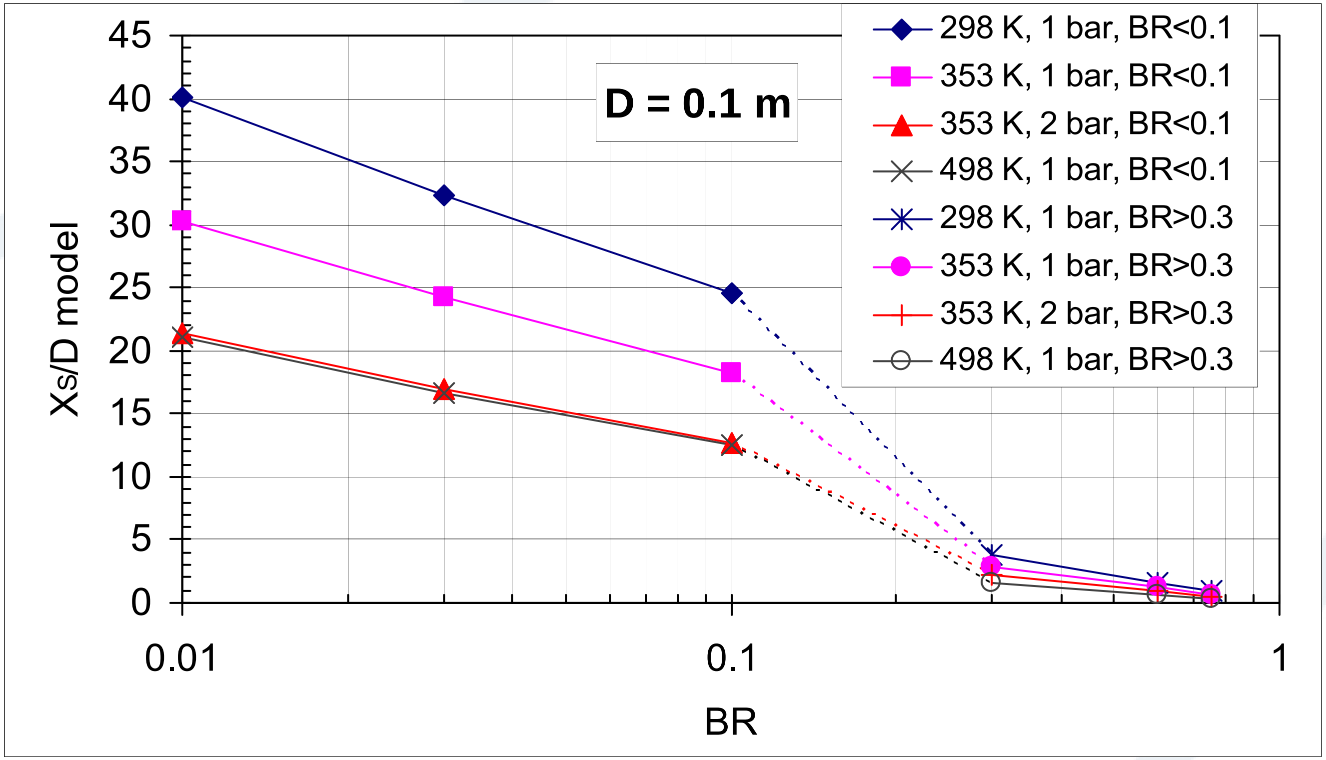
Effect of mixture composition



- Decrease of the H2 from 30 to 12% leads to the increase of the run-up distances by a factor of 5

Variations of Xs

Effect of T and P on run-up distances



- Initial T and p affect S_L, C_{sp}, and σ
- Changes are specific to particular mixture

FA in unconfined clouds

Flame speeds

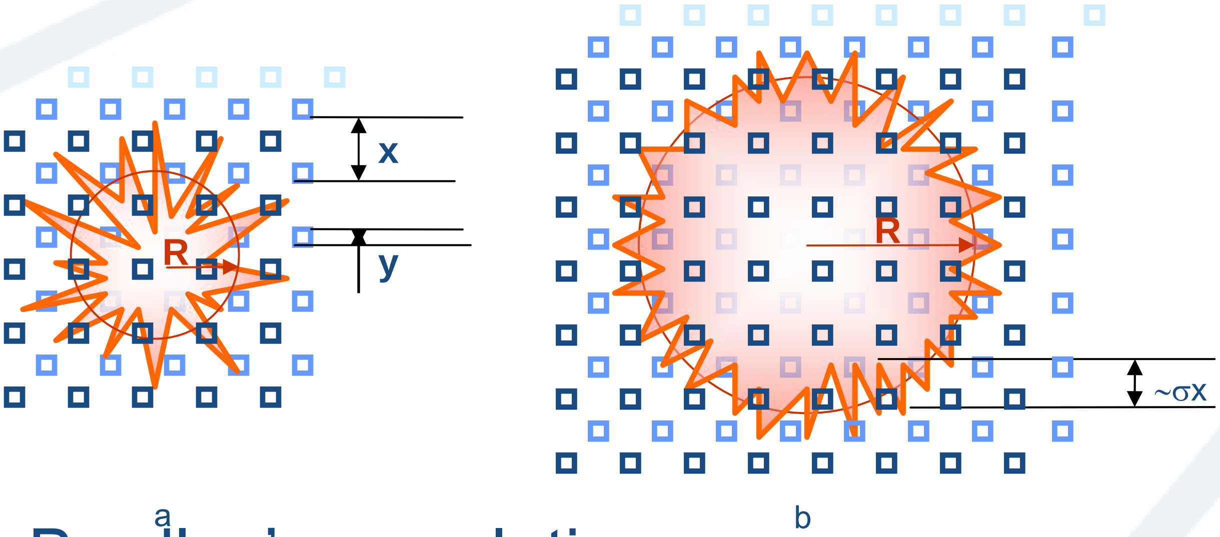
- Pressure effect of a gas explosion essentially depends on the maximum flame speed
- Congested and free clouds are of interest
- Flame speed increases due to:
  - Increase of the flame area in an obstacle field
  - Increase of the turbulent burning velocity during flame propagation

$$V_f = \sigma S_T \frac{A_f}{A_R}$$

FA in unconfined clouds

Model for flame speeds

- Flame area – flame folding due to obstacles



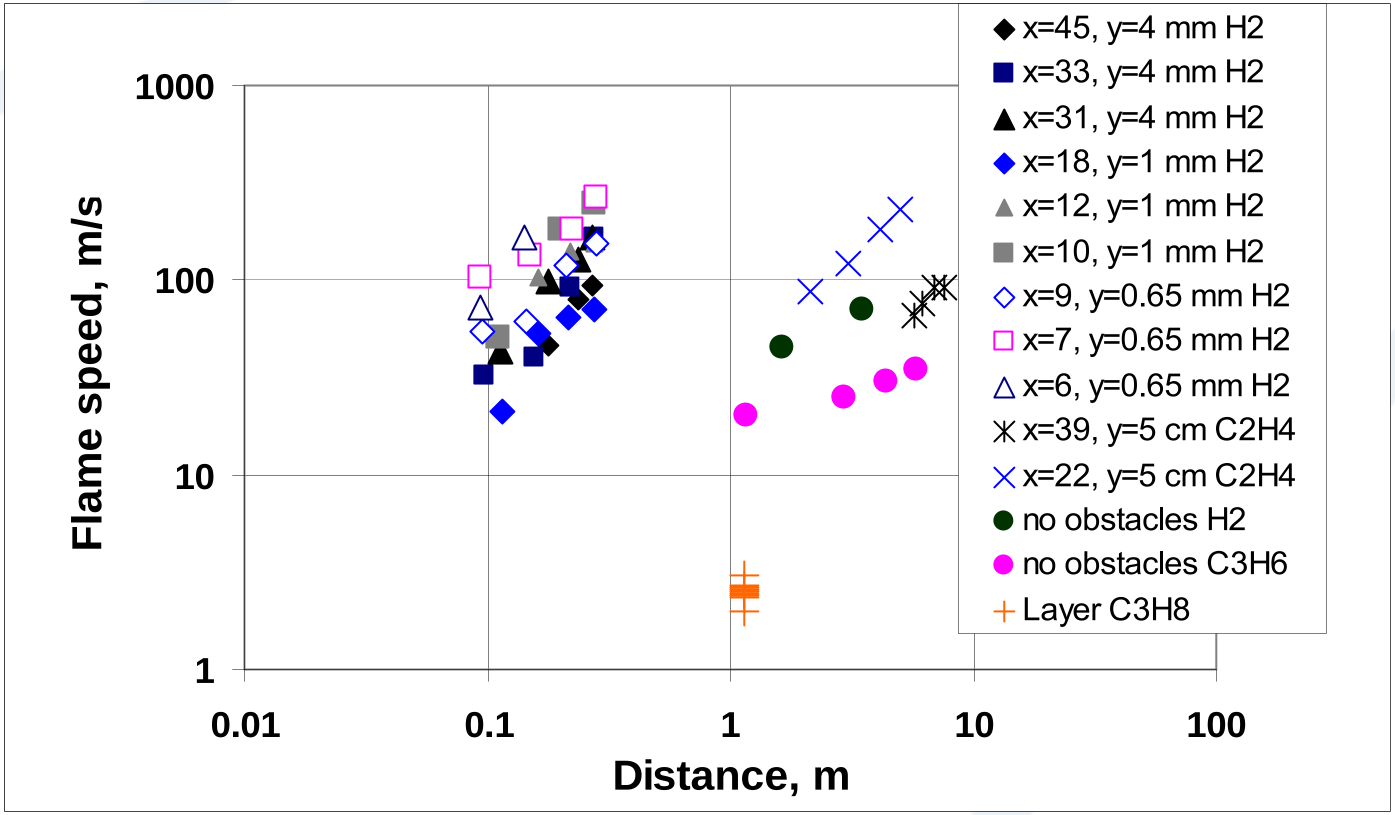
- S_T – Bradley's correlation

$$V_f = a^2 b\sigma(\sigma - 1)S_L\left(1 + \frac{4}{3}\frac{\sigma y}{x}\frac{R^\alpha}{(\sigma x)^\alpha}\right)^2\left(\frac{R}{\delta}\right)^{1/3}$$

FA in unconfined clouds

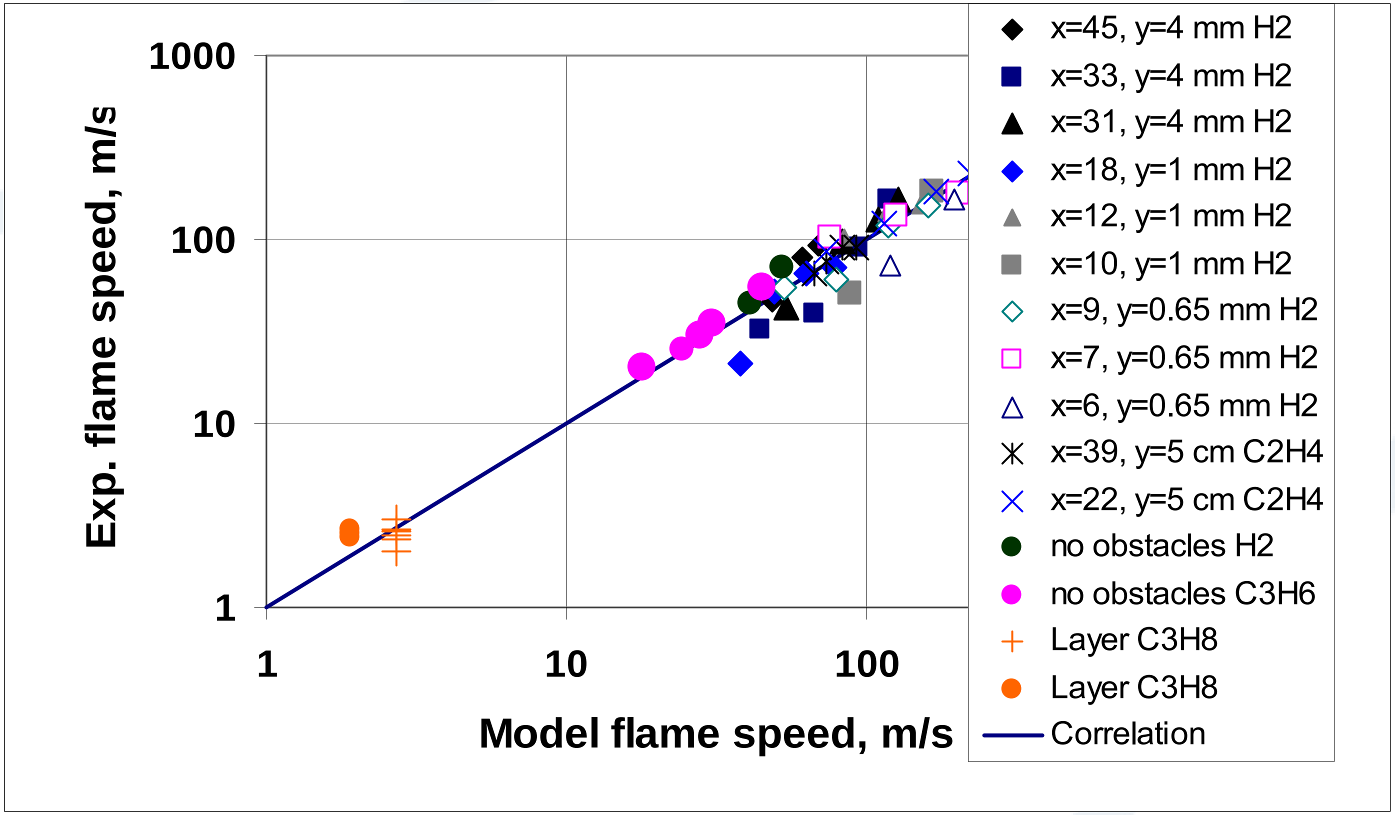
Flame Speeds: Data

- Range of data used for evaluation of unknown parameters



FA in unconfined clouds

Flame Speeds: Model Calibration



FA in unconfined clouds

Link to blast parameters

- KI method (published in 1996)
- Dimensionless *P** and *I** are functions of flame speed, V_f, and *R**

$$P^* = \min(P_1^*, P_2^*) \qquad I^* = \min(I_1^*, I_2^*)$$

$$P_1^* = 0.34/(R^*)^{4/3} + 0.062/(R^*)^2 + 0.0033/(R^*)^3$$

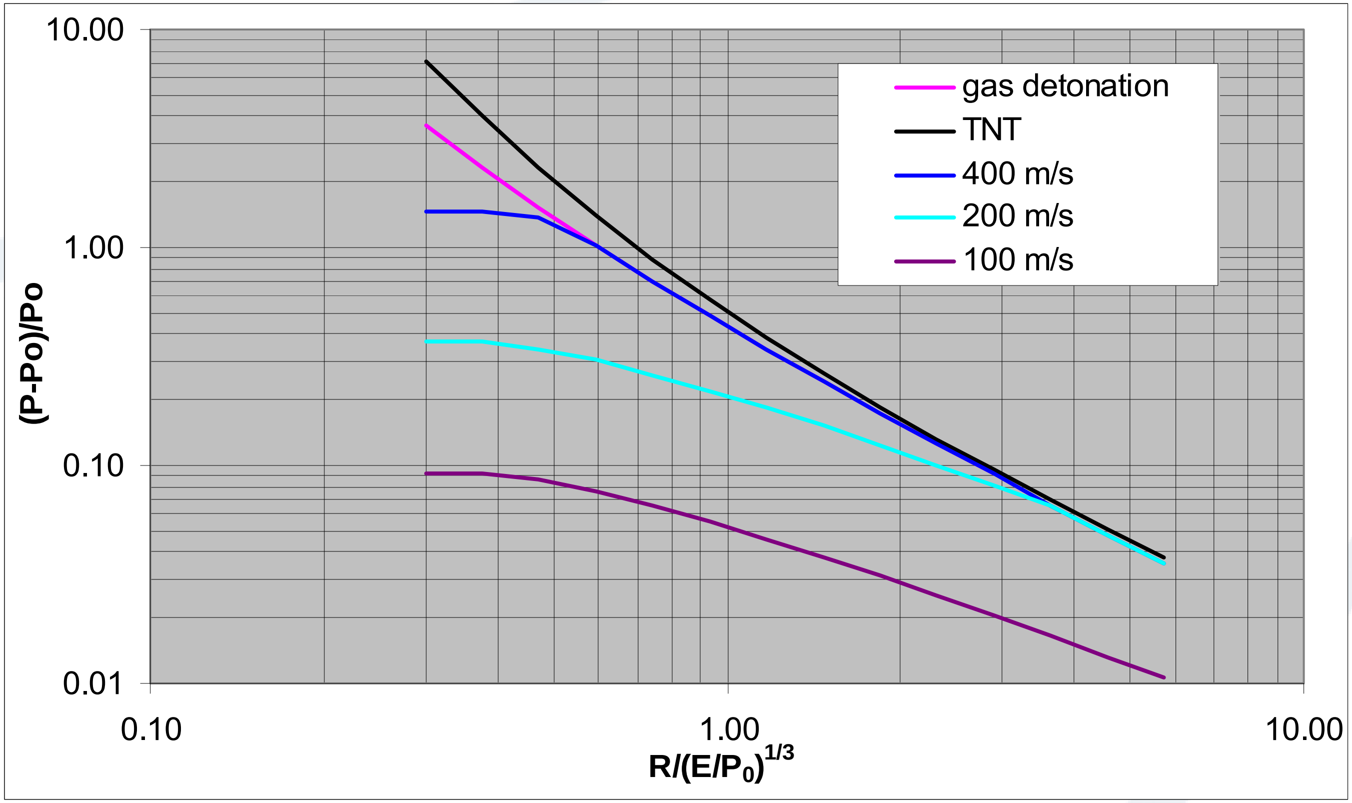
$$I_1^* = 0.0353/(R^*)^{0.968}$$

$$P_2^* = \frac{V_f^2}{c_0^2}\frac{\sigma-1}{\sigma}(0.83/R^* - 0.14/(R^*)^2)$$

$$I_2^* = \frac{V_f}{c_0}\frac{\sigma-1}{\sigma}\left(1-0.4\frac{V_f}{c_0}\frac{\sigma-1}{\sigma}\right)(0.06/R^* + 0.04/(R^*)^2 - 0.0025/(R^*)^3)$$

FA in unconfined clouds

P(R) for Various Flame Speeds

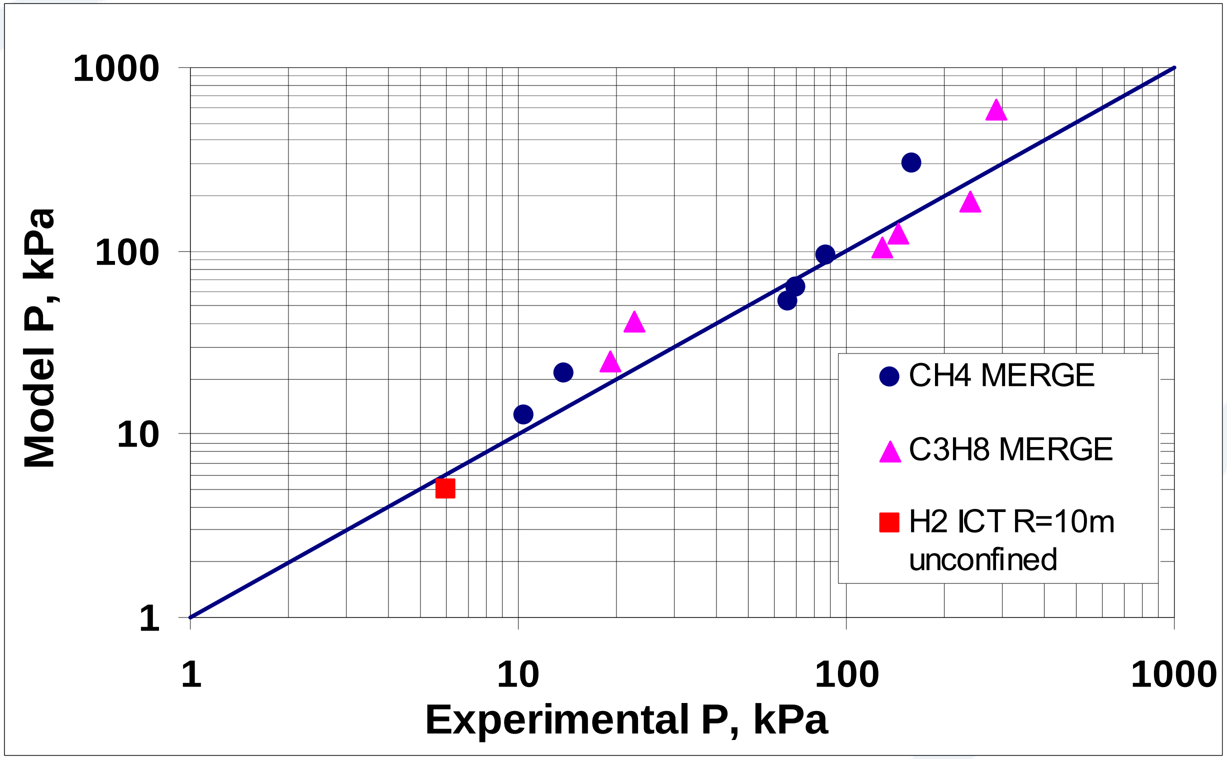


R* = R/(E/p$_0$)$^{1/3}$ – Sach's dimensionless distance

FA in unconfined clouds

Validation - example

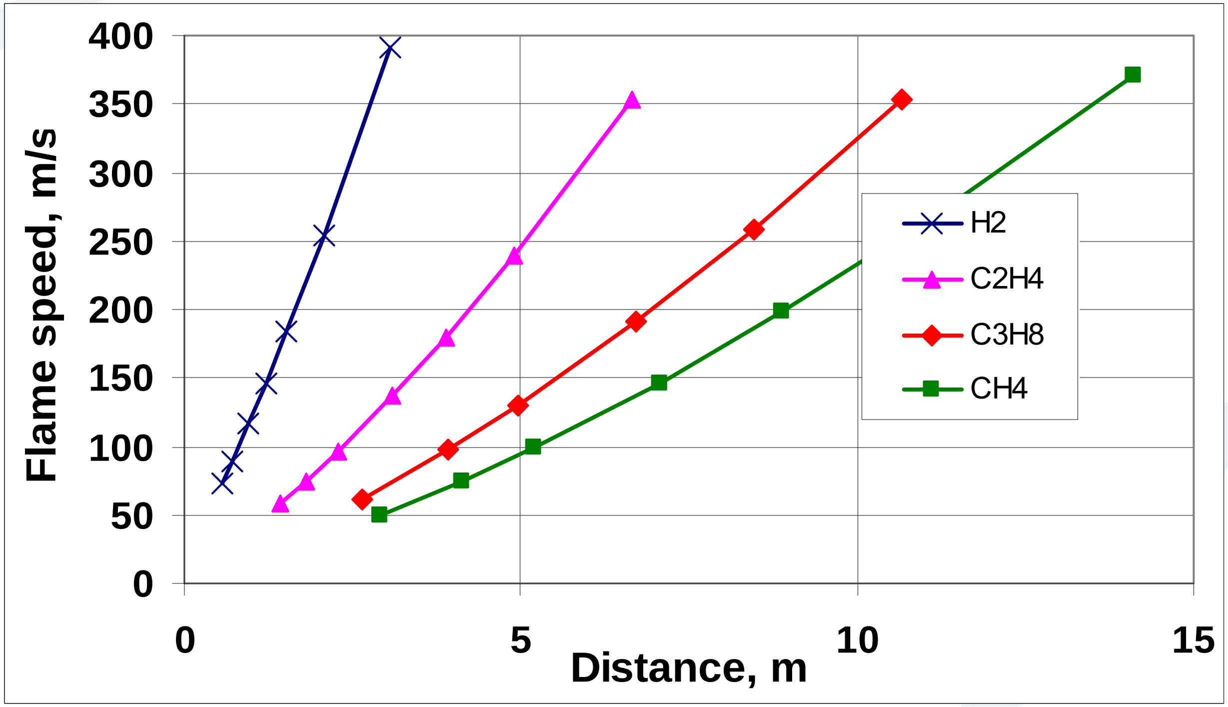
- MERGE data – heavy congestion and IST data – unconfined H_2/air (R=10m)



FA in unconfined clouds

Flame speeds -examples

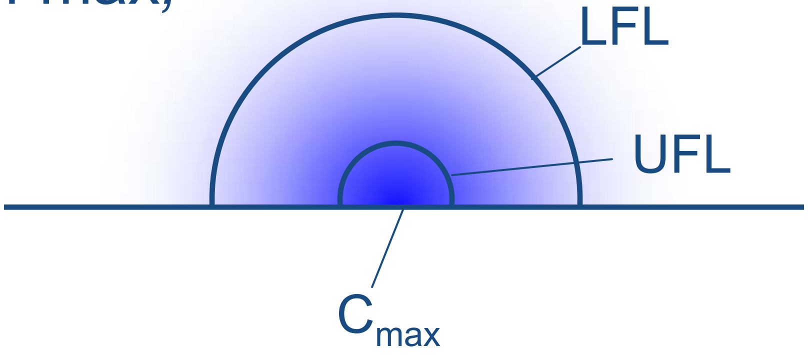
- Stoichiometric mixtures and medium congestion
  y/*x* = 0.33 and *x* = 1 m



FA in unconfined clouds

Nonuniform cloud – ‘worst case’

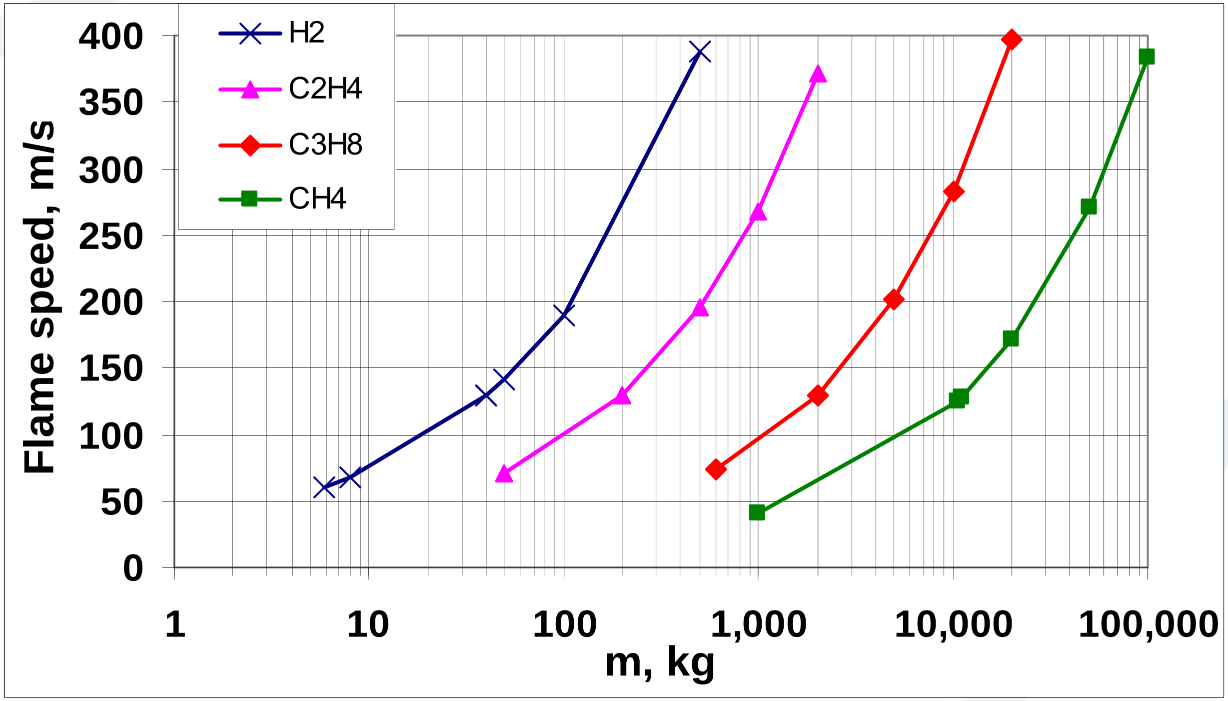
- Variable concentration
- Maximum concentration in the center, C_{max}
- ‘Worst case’: maximum flame speed parameter $<\gamma>=<\sigma(\sigma\text{-}1)S_L>$, averaged between UFL and LFL
- Properties of ‘worst case’:
  - Flame speed is a fraction of max,
  - Energy is a fraction of total chemical energy



FA in unconfined clouds

Flame speeds - examples

- ‘Worst case’ clouds and medium congestion
  y/*x* = 0.33 and *x* = 1 m



FA in unconfined clouds

High pressure releases of H_2

- Total amount of H_2 near the source is limited by buoyancy
- Maximum mass of H_2 near release can be estimated as
  - Engineering correlation for release rate

    $$m' = K C_d A_r \sqrt{2 \rho_v P_v}$$

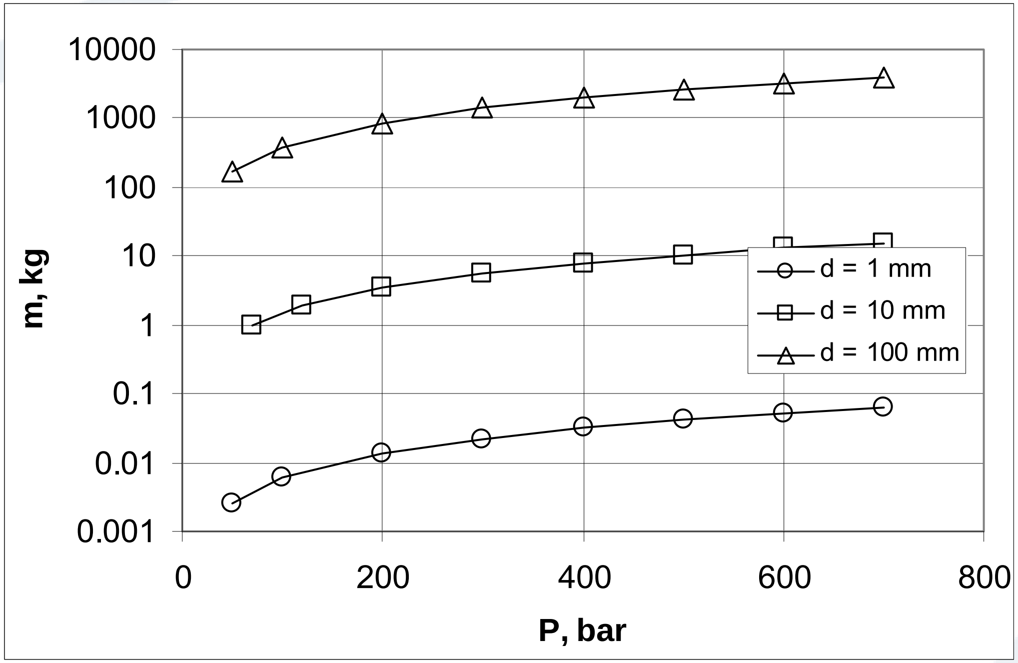
  - Release time *t** is time for buoyant displacement of cloud with C_{LFL}=0.04 to be equal to size of cloud with $C = C_{LFL}$.

    $$t^* = \xi \left(\frac{m'}{C_{LFL} \rho_{H2}} \right)^{1/5} \left(\frac{\rho_{air} - \rho_{cloud}}{\rho_{cloud}} \frac{g}{2} \right)^{-3/5}$$

FA in unconfined clouds

High pressure releases of H_2

- Estimate of maximum mass of H_2 near the source



Release orifice *d* >10mm and high P are necessary for H_2 clouds with m >10 kg and flame speeds > 80 – 100 m/s

DDT Phenomenology

Phases of DDT process

- Following Lee & Moen (1980) and Shepherd & Lee (1991), DDT is divided into two phases:
  1. *Creation of conditions for the onset of detonation* by FA, vorticity production, formation of jets, and mixing of products and reactants;
  2. Actual formation of detonation itself or *the onset of detonation*

Onset of detonations

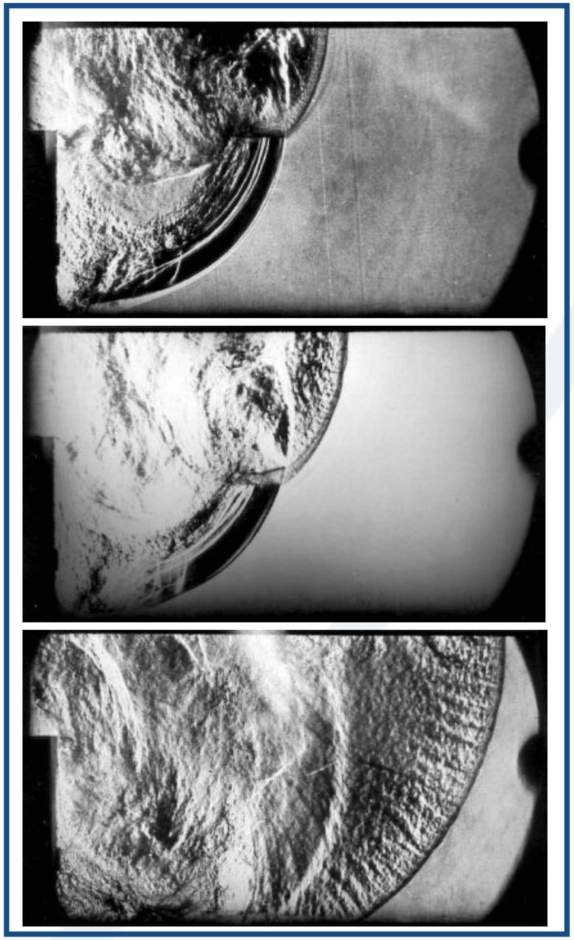
Types of detonation onset phenomena

- The key is to create conditions of localized explosion somewhere in the mixture
- Two types of detonation onset phenomena:
  1. Detonation initiation from shock reflection or focusing
  2. Onset of detonation caused by instabilities and mixing processes
     - instabilities near the flame front
     - explosion of a quenched pocket of mixture
     - P and T fluctuations in the flow and boundary layer
     - …

Onset of detonations

Shock induced detonation initiation

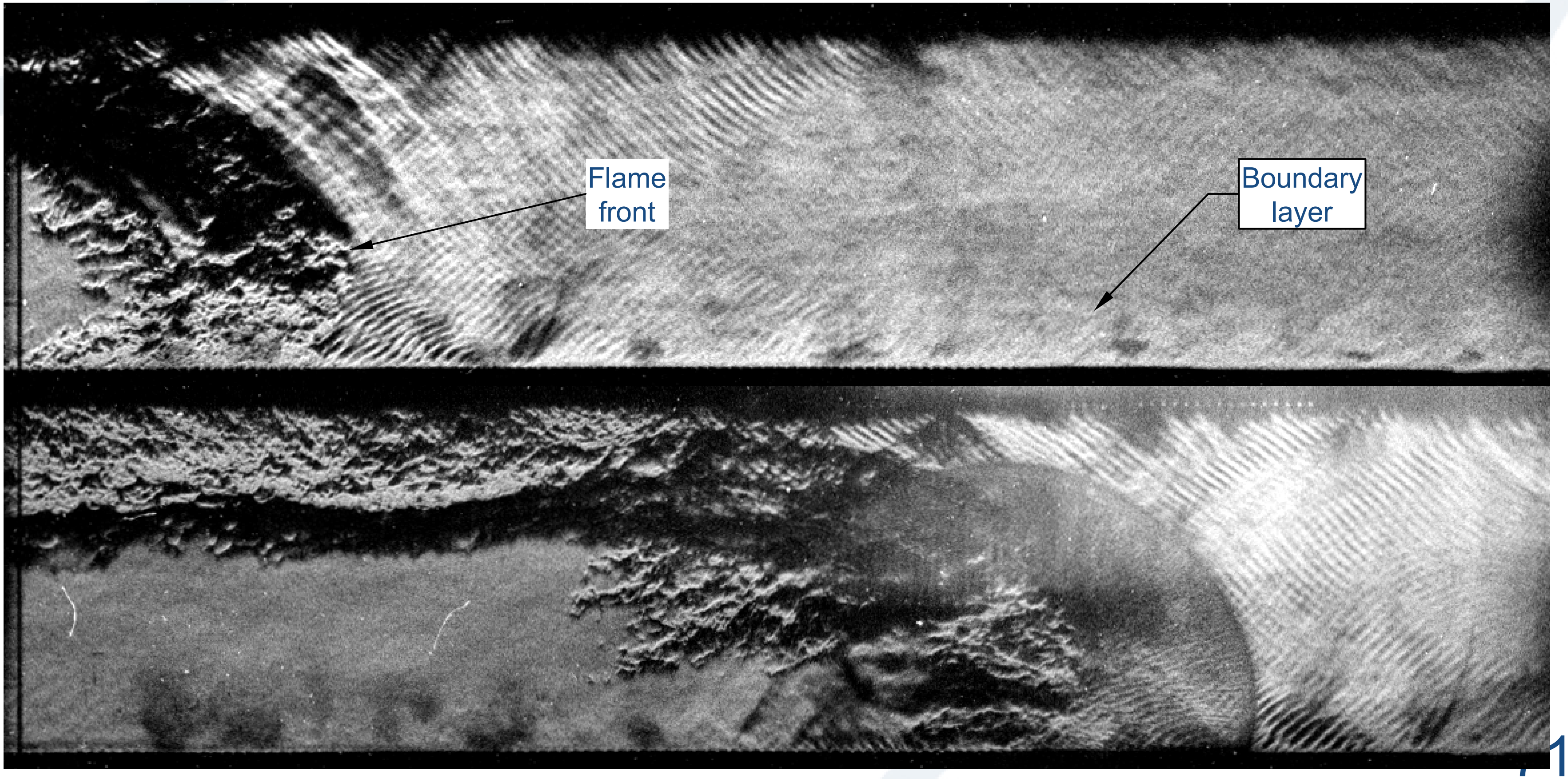
- Onset of detonation resulting from Mach reflection of lead shock of fast deflagration



Onset of detonations

Onset of detonation caused by instabilities

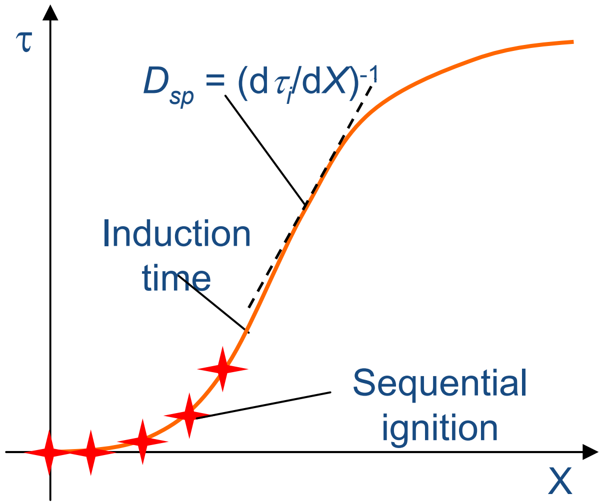
- Onset of detonation triggered by interactions of pressure waves, flame, and boundary layer



Onset of detonations

Underlying mechanism

- Seemingly unrelated phenomena may be controlled by a single underlying mechanism
  - Shock Wave Amplification by Coherent Energy Release (SWACER)

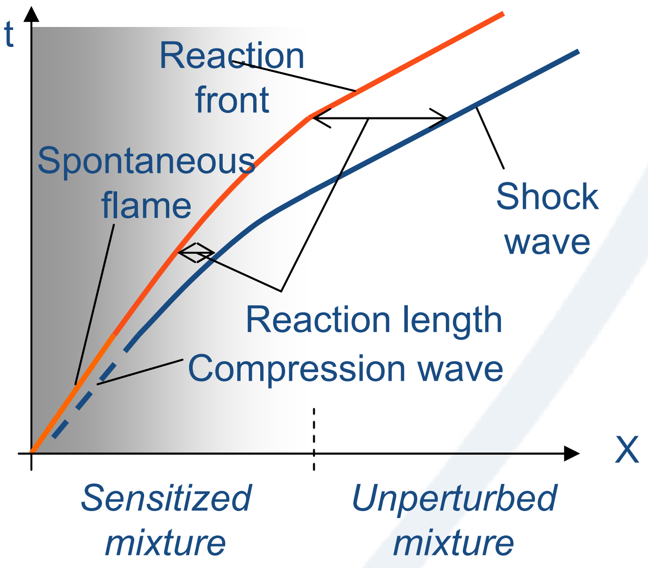


Zeldovich et al. theory 1970
Lee et al. experiments and SWACER concept 1978

Onset of Detonations

Requirements

1. Conditions for localized autoignition should be created
2. Gradient of induction time should provide coupling of chemistry and gasdynamics to create explosion wave
3. This wave should survive propagating thorough gradient of induction time and adjust itself to the chemical length scale of ambient mixture



- 1 and 2 require sufficiently high flame speed ($\sim c_{sp}$)
- 3 requires sufficiently large size of sensitized region ($\sim 10\lambda$)

Onset of D in smooth tubes

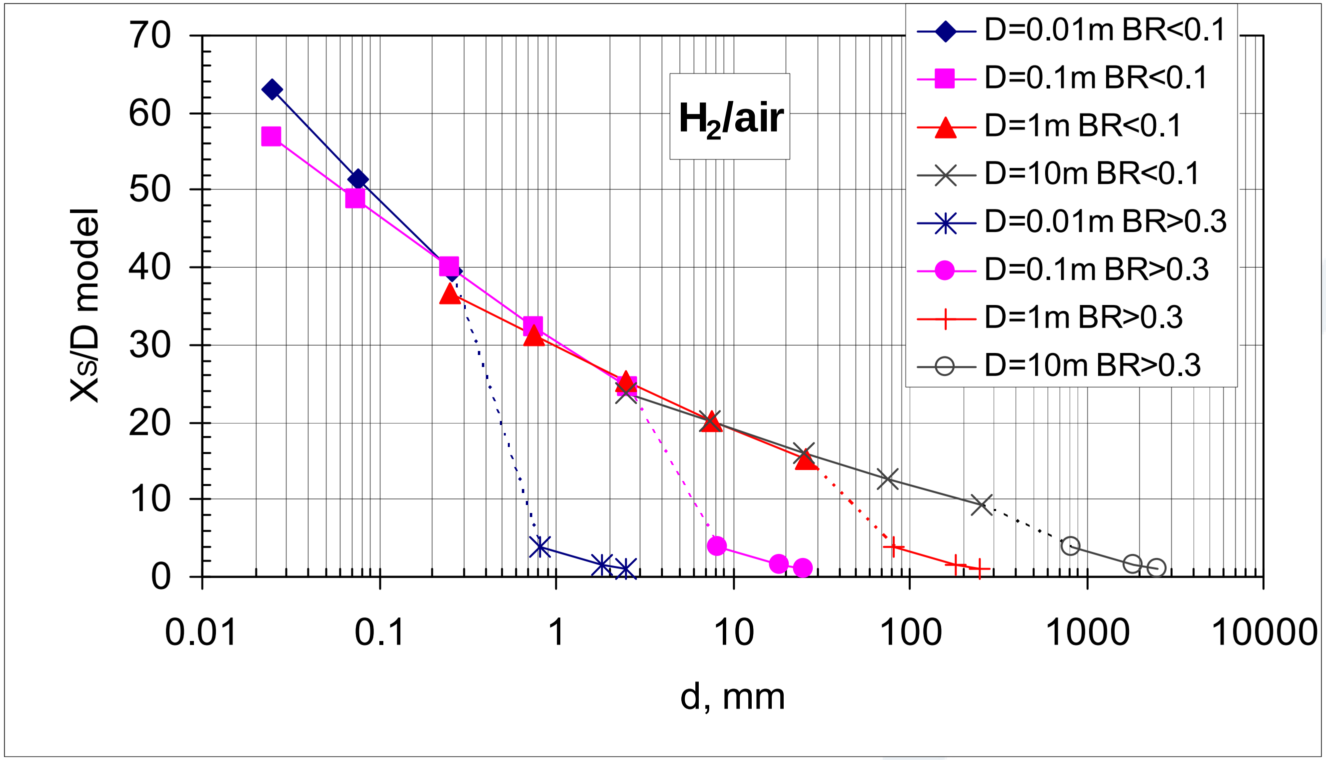
Necessary conditions

- Flame should reach a speed of about c_{sp}
    - See FA correlations
- Min. scale requirement related to the tube size
    - Tube diameter should be greater than the detonation cell width $D > \lambda$ (Peraldi et al.)
    - Kogarko & Zeldovich, and Lindstedt et al., argued that $D > \lambda/\pi$ should be used
    - Most conservative $D > \lambda/\pi$ preferable for applications

Onset of D in smooth tubes

Example

- Stoichiometric H_2-air, roughness=0.1mm, λ=10mm
  - DDT possible with D=10 cm at X > Xs ≈ 4.5 m
  - Onset of D impossible with D < 3mm ($D > \lambda/\pi$)



Onset of D in channels with obstacles

Necessary conditions: d/λ

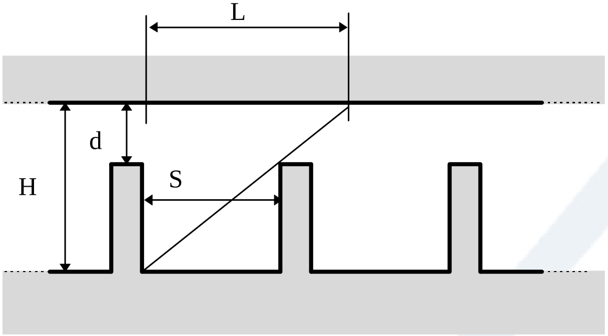
- Flame should reach a speed of about c_{sp}
- Scale requirement related to tube size
  - Size of unobstructed passage $d/\lambda > 1$
  - d/λ increases with decrease of obstacle spacing and with increase of BR
  - Variations of critical d/λ can be quite large, from 0.8 to 5.1 for BR from 0.3 to 0.6

Onset of D in channels with obstacles

Necessary conditions: *L/λ*

- Scale requirement related to possible macroscopic size of the sensitized mixture or characteristic mixture size *L*
  - For a channel or room with obstacles the characteristic size *L* is given by

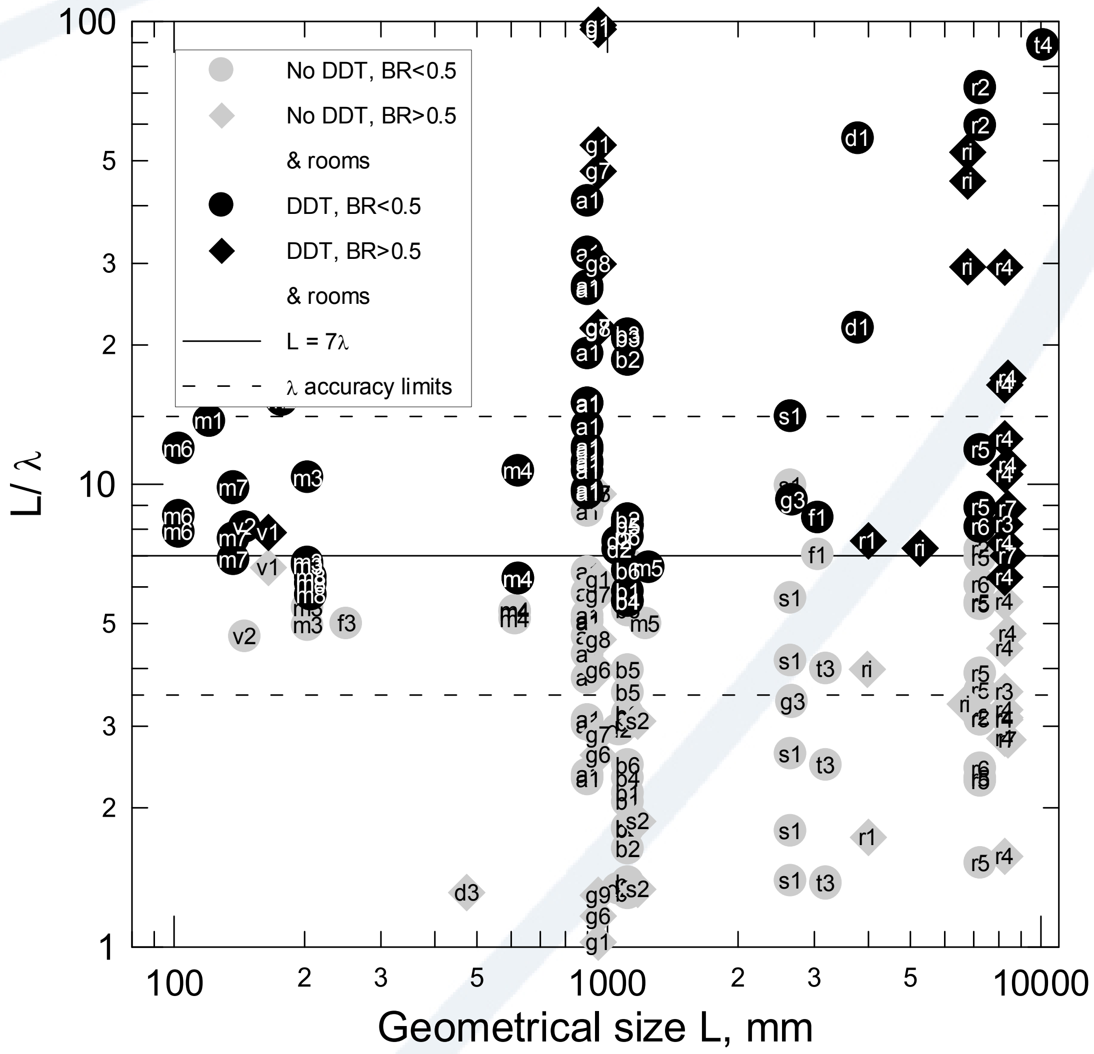
$$L = \frac{(H+S)/2}{1-d/H}$$



Onset of D in channels with obstacles

L/λ-criterion

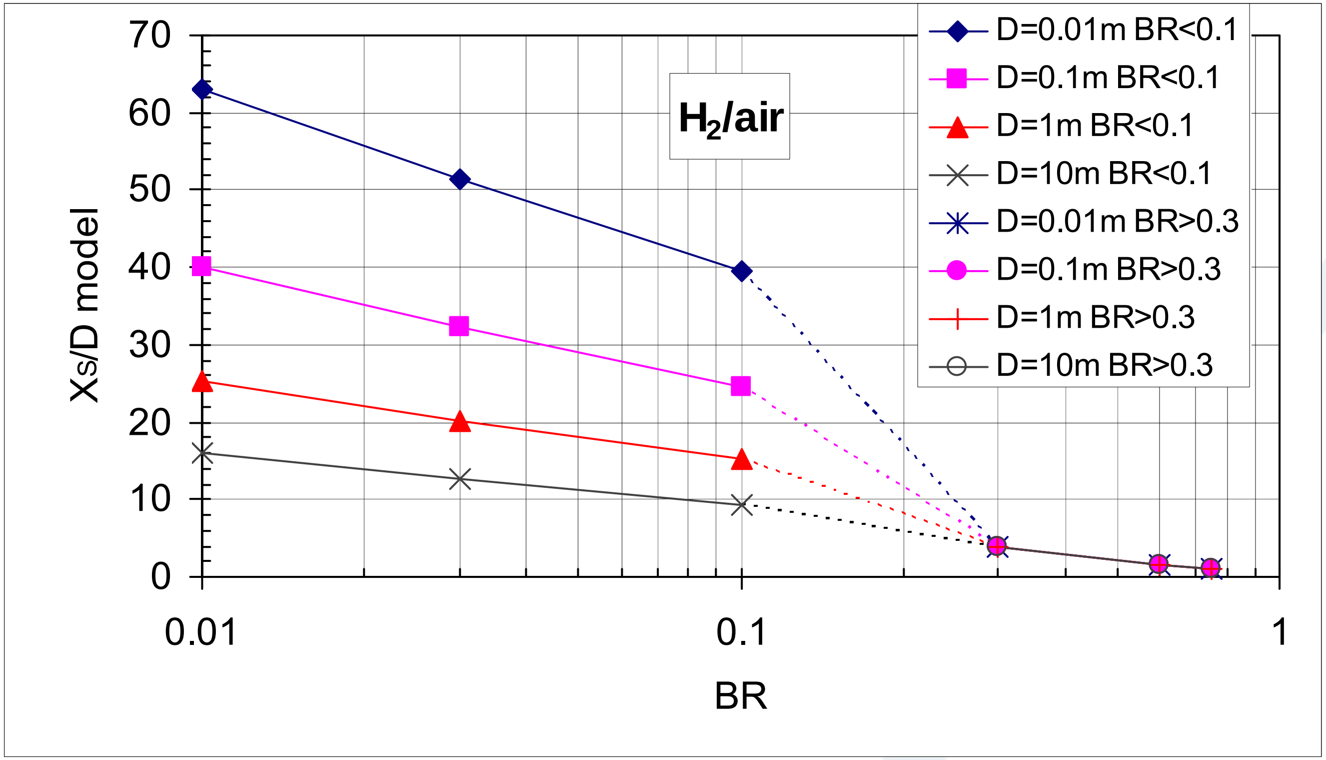
- *L/λ*>7 correlation for predicting DO is applicable over wide range of scales



Onset of D in channels with obstacles

Example

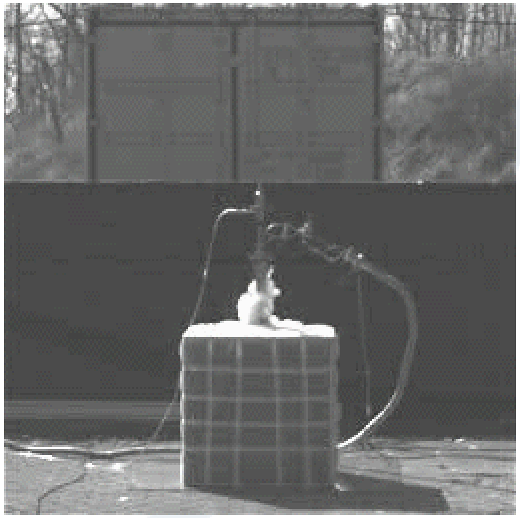
- Stoichiometric H_2-air, λ=10 mm
  - DDT possible with D=10 cm, BR=0.3 at X > Xs ≈ 0.4m
  - Onset of D impossible with D = 1cm, BR = 0.6 (L<7λ)



Onset of D in unconfined mixtures

Congested areas

- There are several observations of onset of detonations
  - DO was observed as soon as flame speed reached a value of about 700±200 m/s
  - With stoichiometric H2-air DDT observed in cloud containing 4 g of H2



Onset of D in unconfined mixtures

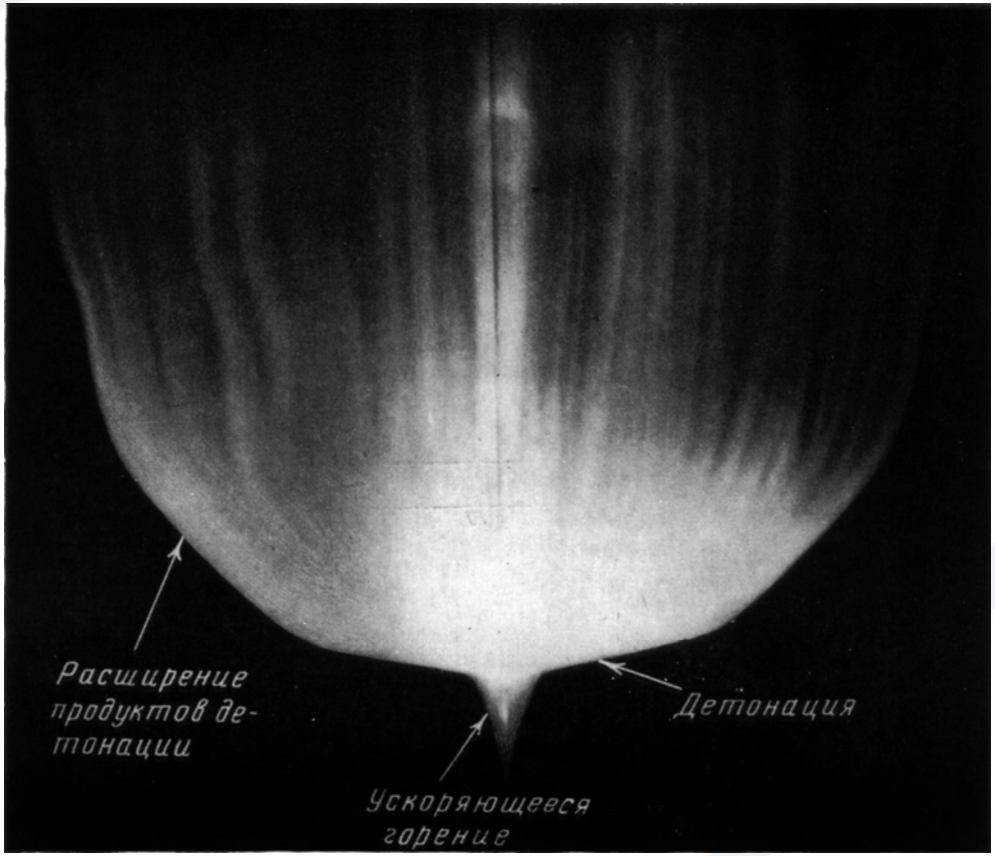
No obstructions

- No convincing observations of DO under truly unconfined conditions
    - Turbulent jet initiation
    - Sensitive mixtures in envelopes
        - Shchelkin 22% C_2H_2 +78%O_2 in 420mm rubber sphere – DO at 50 mm
        - Gostintsev et al. no transition, same mixture, rubber sphere 600mm

Onset of D in unconfined mixtures

Nearly unconfined DDT

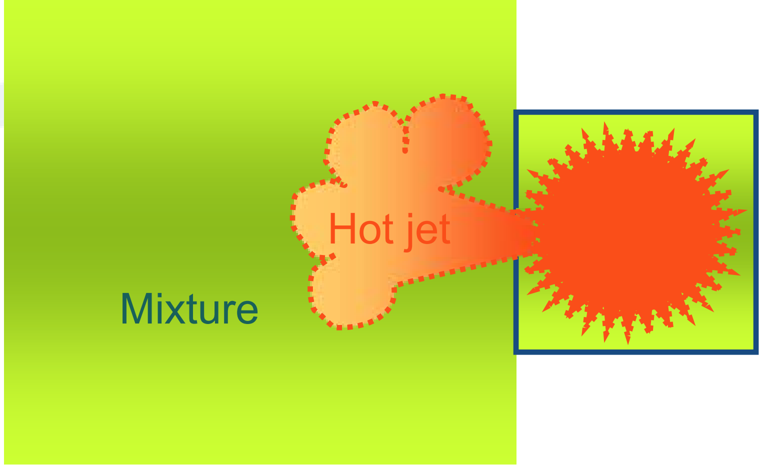
- Shchelkin 22% C_2H_2 +78%O_2 in 420mm rubber sphere – DO at 50 mm



Onset of D in unconfined mixtures

Turbulent jet initiation

- Critical conditions: $D_{jet} \geq (14\text{-}24)\lambda$



215 m^3

Detonation of H2-air initiated by hot turbulent jet of combustion products

Summary

Evaluation of potential for FA and DDT

1. In order for FA to be *strong*, a sufficiently large expansion ratio $\sigma = \rho_u/\rho_b > \sigma^*$ is necessary
   - σ^* depends on the mixture composition and initial T and P
2. Even if $\sigma > \sigma^*$, tube diameter should be $> 10^2$ laminar flame thickness (δ)
3. If *strong* FA is possible ($\sigma > \sigma^*$, $D > 10^2\delta$), a sufficiently large run-up distance X_s is necessary for actual development of supersonic combustion regimes

$$\boxed{V_{flame} = f(R) \leq C_{sp}}$$

Summary

4. If supersonic regime is developed, detonation may only occur if the size of a duct or mixture volume is sufficiently large compared to λ
   - $D \geq \lambda/\pi$, where D is the internal diameter of a smooth tube
   - $d \geq \lambda$, where d is the transverse dimension of the unobstructed passage in a channel with obstacles
   - $L \geq 7\lambda$, where L is a more general characteristic size defined for rooms or channels
   - $D_{jet} \geq (14\text{-}24)\lambda$, where D_{jet} refers to the exit diameter of the jet

Detonation is possible

Concluding Remarks 1

- There are many spatial and temporal physical scales involved in FA and detonation
- These scales are given by chemistry, turbulence, and confinement
- The interplay of these scales control major features and thresholds,
  - Onset of instabilities & flame structure,
  - Onset & structure of detonations
- Wide range of the scales makes it difficult to resolve all the phenomena from first principles
- However, it is the comparison of scales that give us a way to approach practical problems

Concluding Remarks 2

- Critical conditions for strong FA and the onset of detonation are formulated as *necessary criteria*
- Uncertainties are related to
  - Critical values of mixture expansion ratio,
  - Detonation cell size data
  - Laminar burning velocity and flame thickness
  - Effect of the Lewis number
  - Issues in respect to changes of thermodynamic state of unburned mixture during FA, which can change the critical conditions for DDT
- All should be taken into account in practical applications

Questions?

Deflagrations

Laminar flames – one step reaction

- Laminar burning velocity

$$S_L = \frac{1}{\sigma}\sqrt{2\Gamma_{n+1}Le^n \frac{\chi(T_b)}{\beta^{n+1}\tau_r}}$$

- Zeldovich number

$$\beta = \frac{E_a(T_b - T_u)}{RT_b^2}$$

- Flame thickness

$$\delta = \frac{\rho_b\chi(T_b)}{\rho_u S_L} = \frac{\chi(T_b)}{\sigma S_L} \qquad \delta = \frac{\nu}{S_L}$$

Deflagrations

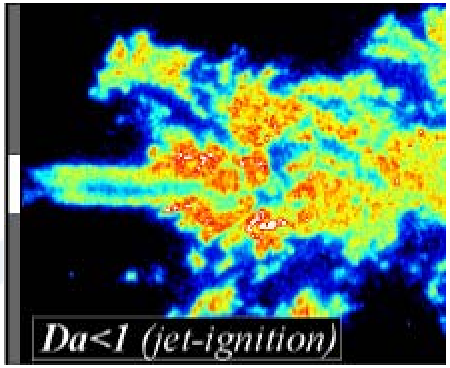
Markstein number

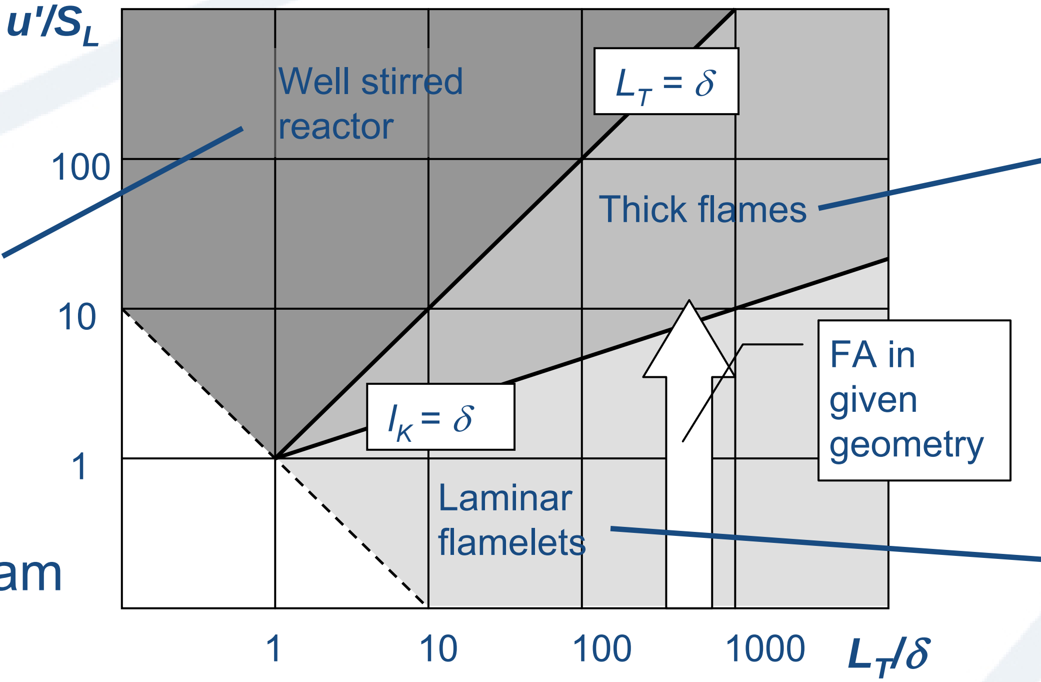
- Stretch may be created by both flame curvature (α_c) and strain rate (α_s) $S_L - S_n = Ma_c \delta \alpha_c + Ma_s \delta \alpha_s$
- Flames with negative *Ma*, such as lean H_2-air mixtures, are known to be extremely unstable
- For β >> 1, parameter $\beta(Le - 1)$ defines the value and the sign of *Ma*

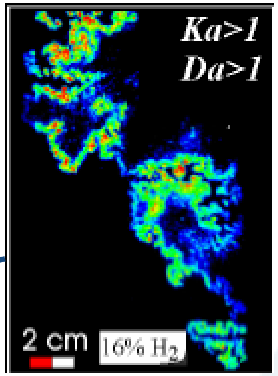
$$Ma_b = \frac{\sigma}{\sigma - 1}\left(\ln \sigma + \frac{\beta(Le-1)}{2(\sigma-1)} \cdot \int_0^{\sigma-1} (\sigma - 1)\frac{1+x}{x} dx\right)$$

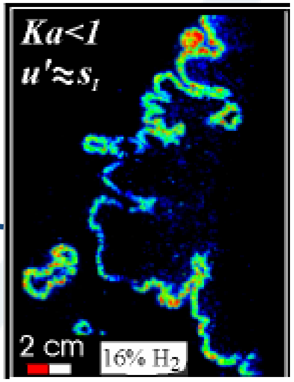
Deflagrations

Turbulent combustion regimes









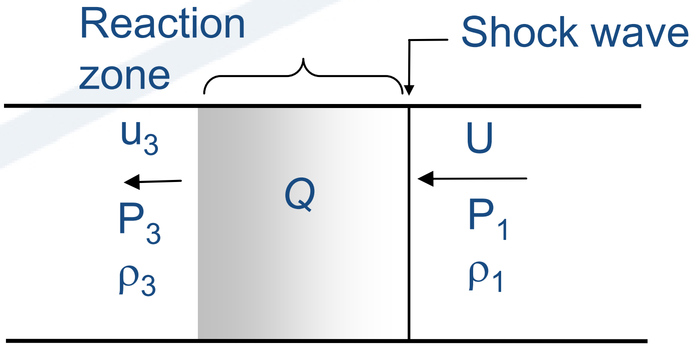
Borghi diagram

PLIF images of flame structure for various regimes – U-Munich

Detonations

Chapman Jouguet Detonation

- 1D model



$$D_{CJ} \cong \sqrt{2Q(\gamma_3+1)} >> a_1$$