



# LIMITS

# OF STEADY PROPAGATION OF HYDROGEN DEFLAGRATIONS AND DETONATIONS

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- Lower limit  $\Rightarrow$  LAMINAR FLAME (m/s)
- Upper limit  $\Rightarrow$  CJ DETONATION (km/s)
- Between limits ⇒ spectrum of TURBULENT FLAMES depending on:
  - Initial conditions: pressure, temperature, composition
  - Geometry: size, obstacles, etc.
- Smooth tubes  $\Rightarrow$  continuous flame acceleration and abrupt DDT
- Rough (obstructed) tubes  $\Rightarrow$  several distinct regimes of steady flame propagation



## **Experimental Composition Limits**



Mixture	Deflagration lean limit [% fuel by vol.]	Detonation lean limit [% fuel by vol.]	Detonation rich limit [% fuel by vol.]	Deflagration rich limit [% fuel by vol.]
$H_{2} - O_{2}$	4.6	15	90	93.9
H <sub>2</sub> – air	4	18.3	59	74
$CO - O_2$	15.5	38	90	93.9
(CO+H <sub>2</sub> )–O <sub>2</sub>	12.5	17.2	91	92
(CO+H <sub>2</sub> )–air	6.05	19	59	71.8
$NH_3 - O_2$	13.5	25.4	75	79
$C_{3}H_{8} - O_{2}$	2.4	3.2	37	55
$C_2H_2 - O_2$	2.8	3.5	92	93
$C_4H_{10}O - air$	1.85	2.8	4.5	36.5

#### Source: Kuo, Principles of Combustion, 2005



#### **Progress of DDT event in a smooth tube**





- a) the initial configuration showing a smooth flame and the laminar flow ahead;
- b) first wrinkling of flame and instability of the upstream flow;
- c) breakdown into turbulent flow and a corrugated flame;
- d) production of pressure waves ahead of the turbulent flame;
- e) local explosion of a vertical structure within the flame;
- f) transition to detonation.

(Shepherd&Lee, 1992)



# Effect of boundary layer on the flame acceleration and DDT



Premixed flames in smooth closed tube - stoichiometric hydrogen-oxygen



Shadow photograph of early stage of flame propagation p<sub>0</sub>=0.75 bar at 210-440 mm from ignition Ignition by electric spark of 20mJ

(Kuznetsov M., Dorofeev S., 2005)



#### **Regimes of flame propagation leading to DDT**





Zel'dovich number:

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

Expansion ratio:

$$\sigma = \frac{\rho_u}{\rho_h}$$

Source: S.Dorofeev et al., Journal of Loss Prevention in the Process Industries 14 (2001) 583–589



#### **Regimes of flame propagation leading to DDT**





Explosion limits for H2/air/H2O mixtures at T=500 K and p=1 atm. Range of uncertainty of fast flame boundary is shown by dotted lines

Source: S.Dorofeev et al., Journal of Loss Prevention in the Process Industries 14 (2001) 583–589



### **CJ Detonation**



F	uel	% vol.	U <sub>cJ</sub> [m/s]	P <sub>cJ</sub> [bar]	т <sub>сл</sub> [K]	P <sub>vN</sub> [bar]	Т <sub>vN</sub> [K]
			Fuel –air	mixtures			
hydrogen	H <sub>2</sub>	29.6	1971	15.6	2949	27.7	1532
acetylene	C <sub>2</sub> H <sub>2</sub>	7.75	1867	19.1	3113	34.8	1674
ethylene	C <sub>2</sub> H <sub>4</sub>	6.54	1825	18.4	2926	33.5	1592
ethane	C <sub>2</sub> H <sub>6</sub>	5.66	1825	18.0	2816	33.0	1542
propane	C <sub>3</sub> H <sub>8</sub>	4.03	1801	18.3	2823	33.6	1543
butane	C <sub>4</sub> H <sub>10</sub>	3.13	1800	18.4	2828	34.4	1554
methane	CH <sub>4</sub>	9.48	1804	17.2	2781	31.2	1530
octane	C <sub>8</sub> H <sub>18</sub>	1.62	1796	18.6	2832	30.3	1541
		•	Fuel – oxyg	en mixtures			
hydrogen	H <sub>2</sub>	66.7	2842	18.9	3683	33.1	1770
acetylene	C <sub>2</sub> H <sub>2</sub>	28.6	2425	33.9	4213	64.5	2239
ethylene	C <sub>2</sub> H <sub>4</sub>	25.0	2376	33.5	3938	64.1	2037
ethane	C <sub>2</sub> H <sub>6</sub>	22.2	2373	34	3803	65.6	1933
propane	C <sub>3</sub> H <sub>8</sub>	16.7	2360	36.3	3830	70.4	1931
butane	C <sub>4</sub> H <sub>10</sub>	13.3	2358	39.1	3854	76.3	1987
methane	CH <sub>4</sub>	33.3	2394	29.4	3728	55.6	1907
octane	C <sub>8</sub> H <sub>18</sub>	7.4	2343	39.9	3868	78.3	1932







#### **CJ** Detonation







#### **ZND Detonation**







## **ZND Detonation**



Calculated values of the physical parameters of ZND model for various hydrogen and propane detonations (Glassman I., Combustion, 1996)

		1	1'	2	
13 - P	H2 – air ( $\Phi$ = 1.2)				
11 -	М	4.86	0.41	1.00	
9 - T	U [m/s]	2033	377	1129	
7 Induction period	P [bar]	1	28	16	
5 Chemical reaction	Т [К]	298	1546	2976	
3- -	ρ/ρ <sub>1</sub>	1.00	5.39	1.80	
	H2 – O2 ( $\Phi$ = 1.1)				
*1.0 cm	Μ	5.29	0.40	1.00	
	U [m/s]	2920	524	1589	
	P [bar]	1	33	19	
	Т [К]	298	1773	3680	
	ρ/ρ <sub>1</sub>	1.00	5.57	1.84	
	23 13 14 9 7 5 5 5 5 5 5 5 5 11 1 1 1 1 1 1 1 1 1 1 1 1	$ \begin{array}{c} 23 \\ 13 \\ 14 \\ 9 \\ 7 \\ 5 \\ 10 \\ 7 \\ 7 \\ 5 \\ 10 \\ 11 \\ 11 \\ 11 \\ 11 \\ 11 \\ 11 \\ 11$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	



#### **Detonation wave structure**









#### **Detonation cell size**



1000 500 ( w w )  $\circ$ 200 " ۲ " 100 DETONATION CELL WIDTH 50 20 10 5 OMETHANE CH4 RUTANE CAHIO П C<sub>3</sub>H<sub>B</sub> 2 C2 H4 O HYDROGEN H. Δ ACETYLENE C. 3 2 0 1 EQUIVALENCE RATIO

Fuel-air mixtures



### **Detonation cell size**



#### hydrogen-air mixtures





### **Detonation cell size**



#### hydrogen-oxygen mixtures





## **Detonation limits**



• propagation limit:  $d_{tube} > d_{f}$ 

$$d_f = \lambda/\pi$$

• critical tube diameter for diffraction:  $d_{tube} > d_{c}$ 

Tube:  $d_c = 13 \lambda$ 

Square channel:  $I_c = 10 \lambda$ 



• Critical energy for direct initiation:  $E > E_c$ 

$$E_c = 430 \rho_0 U_{CJ}^2 \lambda^3$$





• single spin (head)





## **Single spin detonation**





Experimental soot traces for CH4 + 2O2 mixture at P0 = 50mbar.



CH4/O2 spinning detonation simulation

Source: F.Virot et al., 21st ICDERS, Poitiers, 2007



Comparison of pressure contours on the wall

Source: N.Tsuboi et al., 21st ICDERS, Poitiers, 2007

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## **Detonation limits**





• propagation limit







## Minimum tube diameter





at28e: T = 298 K, P = 100 kPa, Φ = 1, 86% He







# **Detonation critical tube diameter**



 critical tube diameter for diffraction to unconfined space





## Critical tube diameter



Fuel-Air Mixtures ( $T_o = 300$  K,  $P_o = 1$  atn





## Critical tube diameter





Second European Summer School on Hydrogen Safety, Belfast, 30 July-8 August 2007



## **Critical mixture layer**







# Critical energy for direct initiation



Fuel-Air Mixtures ( $T_o = 300$  K,  $P_o = 1$  atm





#### **Detonation database**



🗱 Detonation Database - Mozilla	
Plik Edycja Widok Przej <u>d</u> ź Zakładki <u>N</u> arzędzia <u>O</u> kno Pomo <u>c</u>	
Image: Constraint of the second se	💌 🧟 Szukaj 🗳 👻 🚺
👔 🚮 Strona domowa 🛛 😻 Zakładki 🥒 mozilla.org 🥠 mozilla.Zine 🥠 mozdev.org	
Detonation Detological	E
Database	
Accessing the Data   Summary Graphs   Data Sets   References   Database Search	
Abstract	
Welcome to the GALCIT Explosion Dynamics Laboratory Detonation Database. The goal of this project is to compile, catalog and present experimental data on gaseous de include cell width, critical tube diameter, initiation energy, and minimum tube diameter. They are formatted in tables and summary graphs, with citations to the original referen Wide Web version have been prepared. The purpose of this database is to facilitate explosion hazards evaluations and comparisons with numerical simulations of detonation	etonations. These data currently .ces. A printed version and a World . behavior.
Introduction to the Detonation Database project.	
Contributors. Authors of the database.	
Disclaimer. We're not perfect.	
Citations. Using the data in publications.	
How to Access the Data. Some useful information and tips.	
How the Database Works. For those who are interested.	
The Database. Links to the different branches.	
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#### **Deflagration and detonation pressure**







## **Transition distance to DDT**



## Depends on:

- Combustible mixture (chemistry and thermodynamics)
- Tube diameter for hydrogen-air in smooth tube:
  - $\cdot$  8 m in 50 mm tube
  - 30 m in 400 mm tube
- Ignition source
- Obstacles, wall roughness
- Initial conditions
- · ???



## **DDT in tube with obstacles**



- Flame velocity versus fuel concentration for H2-air mixtures
- 10 m long tubes of 5 cm, 15 cm and 30 cm in internal diameter with obstacles (orifice plates).
- BR = 1 d2/D2 blockage ratio
- d orifice diameter
- D tube diameter



(Lee, 1986)





- **quenching regime** flame fails to propagate,
- **subsonic regime** flame is traveling at a speed that is slower than the sound speed of the combustion products,
- **choked regime (CJ Deflagration)** flame speed is comparable with the sound speed of the combustion products,
- quasi-detonation regime velocity between the sonic and Chapman-Jouguet (CJ) velocity,
- CJ detonation regime velocity is equal to the CJ detonation velocity



#### **DDT in tube with obstacles**







#### **Regimes of flame propagation leading to DDT**





Propagation speeds of flames and detonations along the tube versus ratio of distance, x, to tube diameter, D (hydrogen—air mixtures).

Source: S.Dorofeev et al., Journal of Loss Prevention in the Process Industries 14 (2001) 583–589



## Flame acceleration and DDT in obstructed channels





(Courtesy of M.Kuznetzov)







Geometrical size

$$L = \frac{L_1}{1 - \alpha}$$

where

$L_{1} =$	L + H
	2

$$\alpha = \frac{1-h}{H}$$

L – distance between obstaclesH – channel heighth – obstacle height

(Courtesy of S.Dorofeev)



# Run-up distance for DDT in obstructed channels



In tubes at 0.1 MPa, H<sub>2</sub>-air





## **DDT simulations**



V.Gamezo et al., 31st Symposium International on Combustion, Heidelberg 2006

- stoichiometric hydrogen-air mixture at 0.1 MPa
- Reactive Navier-Stokes equations with one-step Arrhenius kinetics
- 2D channel with obstacles

