Fast deflagrations, deflagration to detonation transition (DDT) and direct detonation initiation in hydrogen-air mixtures

Andrzej Teodorczyk

Waraw University of Technology
Outline

- Flame acceleration in tubes and channels
- DDT in smooth tubes
- DDT in rough tubes (with obstacles)
- DDT in large scale
- Numerical simulation of DDT
- Direct detonation initiation
Regimes of flame propagation in tubes

Tube opened at ignition end

• Acoustic and pressure waves generated by the turbulent flame interact with the flame after reflection from the tube end
• Further instabilities and increase of the flame surface area

Tube closed at ignition end

• 6/7 of reactants vented outside

\[ V_f = \frac{F}{f} \cdot V_n + V_d \]

\( V_d \) – velocity of displacement

• In long tubes: pressure waves ⇒ shock wave ⇒ DDT
Regimes of flame propagation in tubes

- Tube closed at both ends

- First stage $\Rightarrow$ high displacement velocity
- Second stage $\Rightarrow$ low $V_d$
- Oscillations and interactions with acoustic and pressure waves reflected from the closed end
- Long tubes $\Rightarrow$ acceleration $\Rightarrow$ DDT
Flame propagation in tubes

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

- Mild Ignition
- Laminar Flame
- Wrinkled or Cellular Flame
- Turbulent Flame
- Hydrodynamic and Diffusion Instabilities
- Flamelet and Distributed Reaction Zones
- Shock Initiation and SWACER
- DDT
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

$p_0=0.75$ bar

at 210-440 mm from ignition

Ignition by electric spark of 20mJ

(Kuznetsov M., Dorofeev S., 2005)
Mechanisms of flame acceleration

- **Growth of flame surface area:**
  - flame folding
  - velocity gradient in the flow
- **Baroclinic vorticity generation**
  - Density gradient normal to the pressure gradient
- **Hydrodynamic instabilities**
  - Rayleigh – Taylor
  - Richtmyer – Meshkov
- **Microexplosions of vortices**
Mechanisms of turbulence growth

- Initial gas flow turbulence in the mixture
- Gas flow turbulence generated at the shear layer near the wall
- Nonuniform concentration (temperature, pressure) distribution in the flammable mixture
- Interaction of the flame front with an acoustic or pressure wave
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)*
CJ Detonation

Hydrogen-Air CJ Detonation Parameters

- Velocity
- Pressure
- Temperature

Are simple to calculate from equilibrium codes:

NASA
STANJAN
SUPERSTATE
Etc.
Detonation wave structure

2H2+O2+17Ar at 20kPa
(Austin & Shepherd)
Detonation limits

- Propagation limit: $d_{\text{tube}} > d_f$
  
  $$d_f = \frac{\lambda}{\pi}$$

- Critical tube diameter for diffraction: $d_{\text{tube}} > d_c$
  
  Tube: $d_c = 13 \, \lambda$
  
  Square channel: $l_c = 10 \, \lambda$

- Critical energy for direct initiation: $E > E_c$
  
  $$E_c = 430 \rho_0 U_{\text{CJ}}^2 \lambda^3$$
Detonation limits

- propagation limit

\[ d > \lambda/3 \]

\[ h > \lambda \]
Detonation limits

- critical tube diameter for diffraction

\[ d > 13 \lambda \]

\[ h > 10 \lambda \]

\[ h > 3 \lambda \text{ for } w > 3h \]
Detonation cell size

Fuel-air mixtures
Critical tube diameter

Fuel-Air Mixtures ($T_o = 300$ K, $P_o = 1$ atm)
Critical energy for direct initiation

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

Abstract

Welcome to the GALT Explosion Dynamics Laboratory Detonation Database. The goal of this project is to compile, catalog and present experimental data on gaseous detonations. These data currently include cell width, critical tube diameter, initiation energy, and maximum tube diameter. They are formatted in tables and summary graphs, with citations to the original references. A printed version and a World Wide Web version have been prepared. The purpose of this database is to facilitate explosion hazards evaluations and comparisons with numerical simulations of detonation 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.

Edited Last: Jan 29, 2005
Jon Shepherd
Deflagration and detonation pressure

a) Slow deflagration; b) fast deflagration; c) overdriven detonation DDT; d) CJ detonation
Flame acceleration in tube

Open end channel;
Stoichiometric propane-air at 1 bar

(Teodorczyk et al., 1992)
Early accelerating flame

Figure 24. Cinematographic schlieren records of ignition, and initial stages of inflammation in a stoichiometric hydrogen–oxygen mixture.
Borghi Diagram

Flame propagation regimes in terms of:
- turbulence intensity, $u'$,
- laminar burning velocity, $s_l$,
- integral length scale, $L$,
- laminar flame thickness, $d_l$,
- Damköhler number, $Da$,
- Karlowitz number, $Ka$,
- turbulent Reynolds number, $Re_L$.

LIPF images (bottom) of flame structure for the various regimes.

(Peters, 1986)
Feedback mechanism of flame acceleration

Increase in Burning Velocity

Hydrodynamic instabilities

Increase of temperature and pressure in front of the flame

Generation of pressure waves

Gasdynamic feedback

Decrease of turbulent length scale

Increase of turbulence intensity

Increase of expansion-flow velocity

Fluid-dynamic feedback
Feedback mechanism of flame acceleration

Shadow photographs of later stages of turbulent flame propagation

(Kuznetsov et al., 2005)
Fast deflagration

Schlieren image of a fast deflagration wave (22% H₂ in air), flame velocity 1200 m/s;

OH radical distribution of a fast deflagration wave, flame velocity 850 m/s, 17.5% H₂ in air;

(Eder, 2001)
Flame interaction with shock wave

Butane-air flame; Shock wave of pressure ratio of 1.3

(Markstein, 1968)
Flame interaction with shock wave

Reflected shock (*moving right to left*) emerging following multiple-shock flame interaction. Original incident shock Mach No. 1.7 (incident not shown). Mixture C2H4 + 3O2 + 4N2, initial pressure 13.2 kPa, $\Delta t$ 50 µs

DDT resulting from the interaction of a reflected shock with a flame kernel

*(Bombrey&Thomas, 2002)*
Transition distance to DDT

Depends on:

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

Streak direct photograph

4, 5 - accelerating flame
6 - explosion ahead of the flame
7 - detonation
8, 9 - retonation wave

(Lee, 1978)
DDT in smooth tube

(Myer & Oppenheim, 1965)
DDT in smooth tube

Streak schlieren photograph

(Myer&Oppenheim, 1965)
DDT in smooth tube

Schlieren framing photographs by rotating mirror camera

(Myer&Oppenheim, 1965)
DDT in smooth tube

Schlieren framing photographs by rotating mirror camera

(Urtiev & Oppenheim, 1965)
DDT in smooth tube

Schlieren framing photographs by rotating mirror camera

(Urtiev & Oppenheim, 1965)
DDT in smooth tube

(Urtiev & Oppenheim, 1965)
Flame acceleration over the obstacle

(Wolanski, 1983)

(Hirano, 1987)
Flame acceleration over the obstacle
Flame acceleration in tube

Schlieren CCD camera pictures;
Closed channel
0.5 bar

(Ohyagi et al., 1993)
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).

\[ BR = 1 - \frac{d^2}{D^2} \]  – blockage ratio

\( d \) - orifice diameter
\( D \) - tube diameter

(Lee, 1986)
Regimes of flame propagation in tubes with obstacles

- **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

Stoichiometric hydrogen-oxygen
Pressure 20-150 torr
Ignition by exploding wire

(Teodorczyk, et al., 1988)
Fast deflagration in a channel with obstacles

(TEodorczyk, et al. 1988)
Fast deflagration in a channel with obstacles

(Teodorczyk, et al..1988)
DDT in tube with obstacles

(Teodorczyk, et al..1988)
DDT in rough channel

(Teodorczyk, 1990)
DDT in rough channel

Flame speed 320 m/s

\( p_0 = 0.55 \text{ bar, 1090-1320 mm from ignition} \)

(Kuznetsov M., Dorofeev S., 2005)
Detonation in a channel with obstacles

(Teodorczyk, et al. 1988)
Fast deflagration vs detonation in a very rough channel

(Teodorczyk, 1990)
Flame acceleration and DDT in obstructed channels

(Courtesy of M.Kuznetzov)
RUT experiments on the premixed H2 combustion

Flame acceleration and DDT experiments in complex channel geometry with hydrogen-air mixtures

L = 64 m
S = 2.5x2.25 m²

- 11% H2/air – slow flame:
  p=3-4 bar v = 150-200 m/s
- 12.5% H2/air – sonic flame:
  p=5-7 bar v = 550-600 m/s
- 14% H2/air – detonation:
  p=9-12 bar v = 1400 m/s

(Courtesy of M. Kuznetzov)
DDT in large scale

DDT of a hydrogen/air mixture within a “lane”, simulated by two parallel walls (top view)

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)
DDT in large scale

DDT of a hydrogen/air mixture within a “lane”, simulated by 2 parallel walls (top view)

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)
DDT of a hydrogen/air mixture within a “lane”, simulated by 2 parallel walls (top view)
DDT in large scale

Test set up for igniting a hydrogen/air mixture by means of a flame jet within a “lane“, simulated by two parallel walls

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)
DDT in large scale

Flame jet ignition of hydrogen air cloud within a “lane” with subsequent transition to detonation near the ground.

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)
DDT in large scale

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)
Detonation simulation

DET02D code

Detonation simulation

Simulation: DETO2D

DDT simulation

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

- stoichiometric hydrogen-air mixture at 0.1 MPa
- Channel with obstacles $1m \times 11cm \times 2cm$
Direct initiation of detonation

Stoichiometric hydrogen-chlorine mixture; a) subcritical; b) critical; c) supercritical

(Levin et al. 1978)
Direct initiation of detonation

Critical energy vs equivalence ratio: H2-Air

From detonation database
Direct initiation of detonation

From detonation database

stoichiometric H2-O2 mixture;
at49a: T = 293 K;
at49b: T = 123 K;
Direct initiation of detonation

(Schauer et al. 2005)