TEL AVIV UNIVERSITY אוניברסיטת תל אביב

Numerical Simulations in Deflagration-to-Detonation Transition Research

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jointly with G. Sivashinsky

Introduction

A self-sustained wave of an exothermic chemical reaction spreading through a homogeneous combustible gas mixture is known to occur either as a subsonic deflagration (premixed gas flame) or supersonic detonation.

	Deflagration	Detonation
Speed	subsonic	supersonic
Ignition	mild (spark)	strong (explosion)
Mechanism	diffusivity	shock wave
Pressure	almost adiabatic	high pressure

It is know however, that in the presence of obstacles or confinement the initially formed deflagration undergoes gradual acceleration abruptly converting into detonation.
Despite more than a century of research, identification of the crucial flame-flow interaction involved is still far from complete, and DDT remains one of the major areas of activity in combustion research.

Outline of the problem

Deflagration-to-detonation transition (DDT) occurring in smooth-walled channels, narrow enough to ensure the laminar character of the developing flow, is the simplest system for theoretical/numerical exploration of the DDT.
Yet, even under these benign conditions the emerging dynamical picture is quite complex for a straightforward identification of the mechanisms involved.
The present review is intended as a wide brush discourse on the fifteen years of theoretical and numerical efforts in this area undertaken at Tel Aviv University.

Topics

A) 1D Fanno Model. CTM **2**, 429. (1998)

1) Multiplicity of combustion regimes. C&F **122**, 130 (2000)

B) 2D Deflagration-to-detonation Transition. C&F **134**, 389 (2003)

1) Bimolecular reaction: Isotherm vs adiabatic walls. FTC **84**, 423 (2010)

2) Channels vs. Tubes. FTC **84**, 423 (2010)

3) Narrow channel limit. Proc. Comb. Inst. **35**, 913 (2015)

4) Flame folding vs. Hydraulic resistance. CTM **20**, 798 (2016)

a) Huygens principle. Phil.Trans.R.Soc. A **370**, 625 (2012)

b) Anisotropic gas. CTM **18**, 261 (2014)

c) Nonmonotonisity and Σ model. CTM **20**, 798 (2016)

C) DDT in unconfined space. C&F **175**, 307 (2017)

A) 1D Fanno Model.

I. Brailovsky & G. Sivashinsky (1998) CTM **2**, 429.

consists of next equations:

continuity and state, $\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \qquad P = \rho T,$

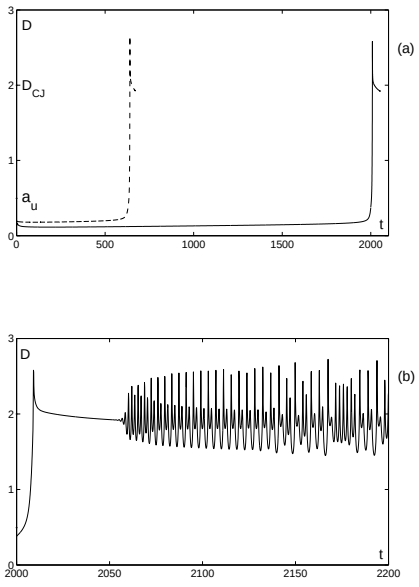
momentum, $\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\gamma}\frac{\partial P}{\partial x}\right) = \frac{4}{3}Pr\varepsilon\frac{\partial^2 u}{\partial x^2} + F,$

heat, $\rho\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x}\right) = \left(\frac{\gamma-1}{\gamma}\right)\left(\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x}\right)$
$+\varepsilon\frac{\partial^2 T}{\partial x^2} + (\gamma-1)Pr\varepsilon\left(\frac{\partial u}{\partial x}\right)^2 + (1-\sigma)\Omega$

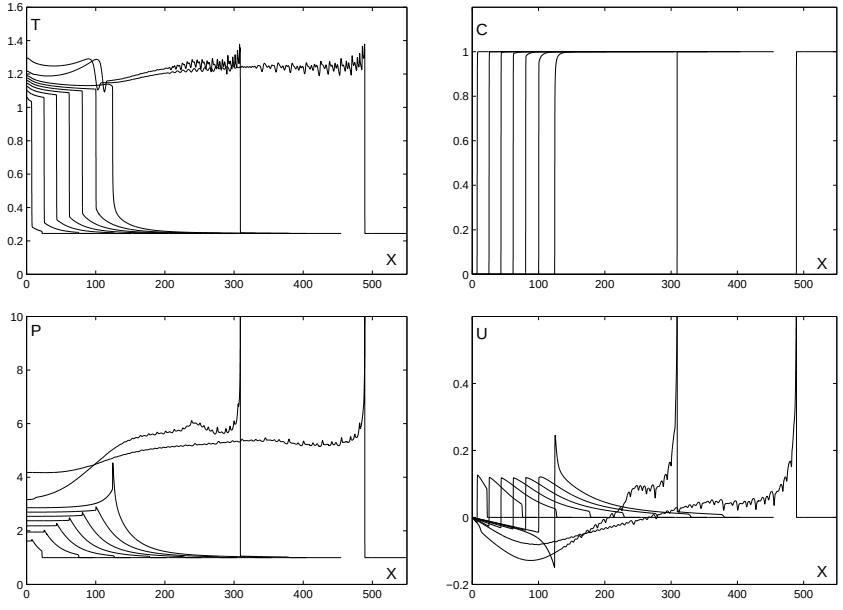
concentration, $\rho\left(\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x}\right) = \frac{1}{Le}\varepsilon\frac{\partial^2 C}{\partial x^2} - \Omega$

$\Omega = AC\rho^n \exp\left(-E/T\right)$ - Arrhenius kinetics of n-order. $n = 1, 2$.
$F = k|u|^m u$- friction (hydraulic resistance), $m = 0$ or $m = 1$

Results of Numerical Simulations of Fanno Model.



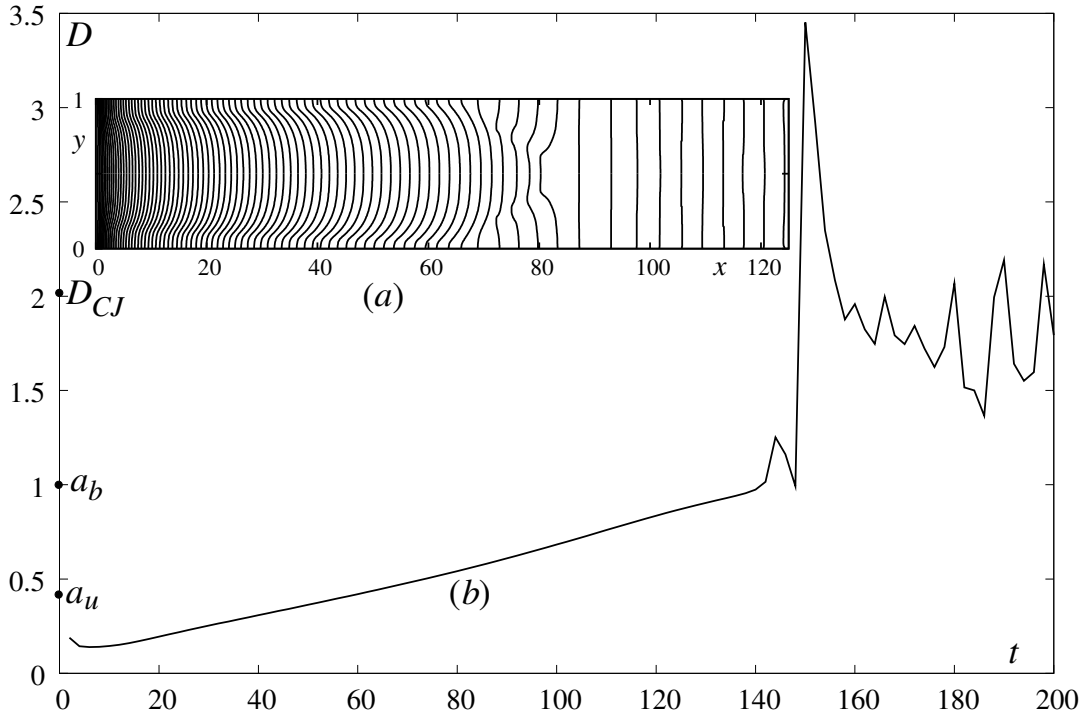
Flame velocity for several k, deflagration-to-detonation transition.



Profiles. Precursor shock, hydraulic resistance, precompression, preheating

B) Two Dimensional Model

L. Kagan & G. Sivashinsky, (2003) C&F **134** 389

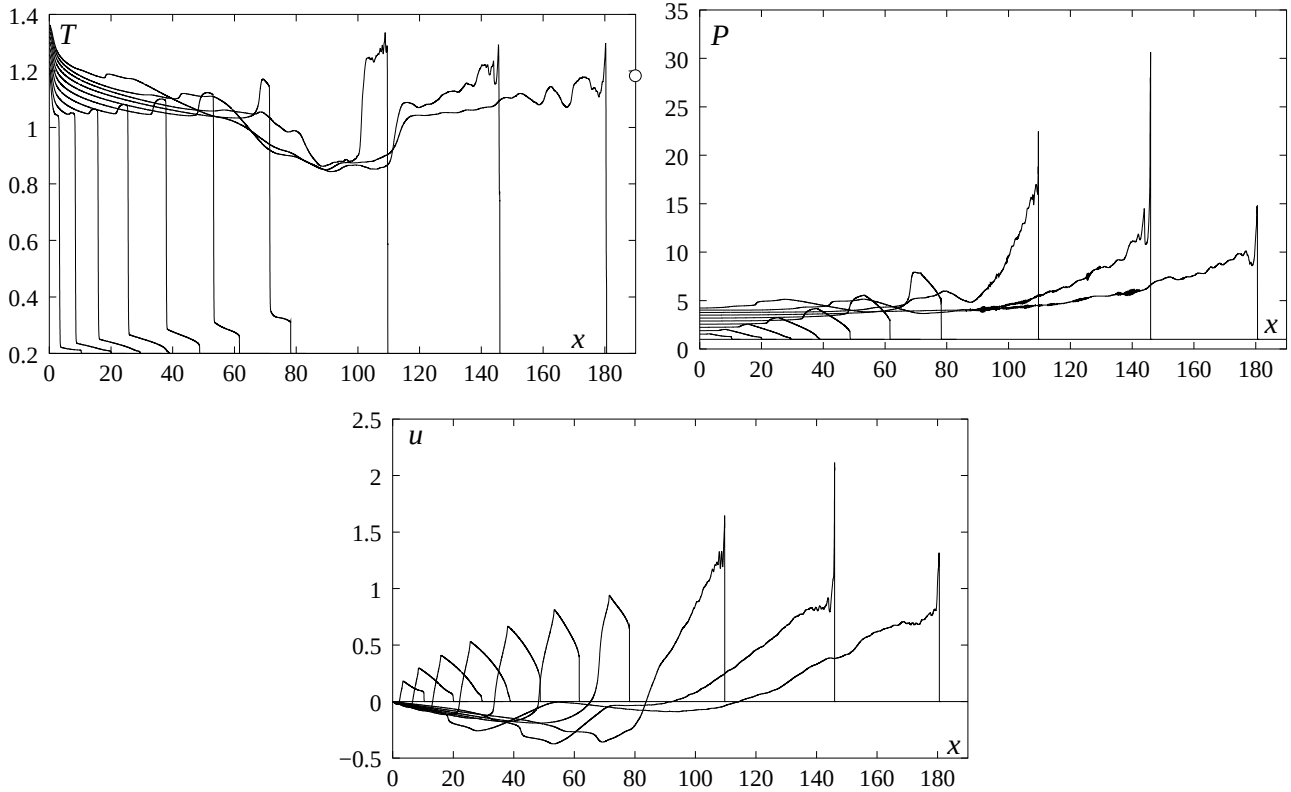


Flame velocity and flame fronts for DDT simulation. First order Arrhenius kinetics.

Hydraulic resistance introduced with the help of the slip boundary condition, with no half-empiric F function. DDT starts at the walls where impact of wall friction is maximal.

Two Dimensional Model II

L. Kagan & G. Sivashinsky, (2003) C&F **134** 389

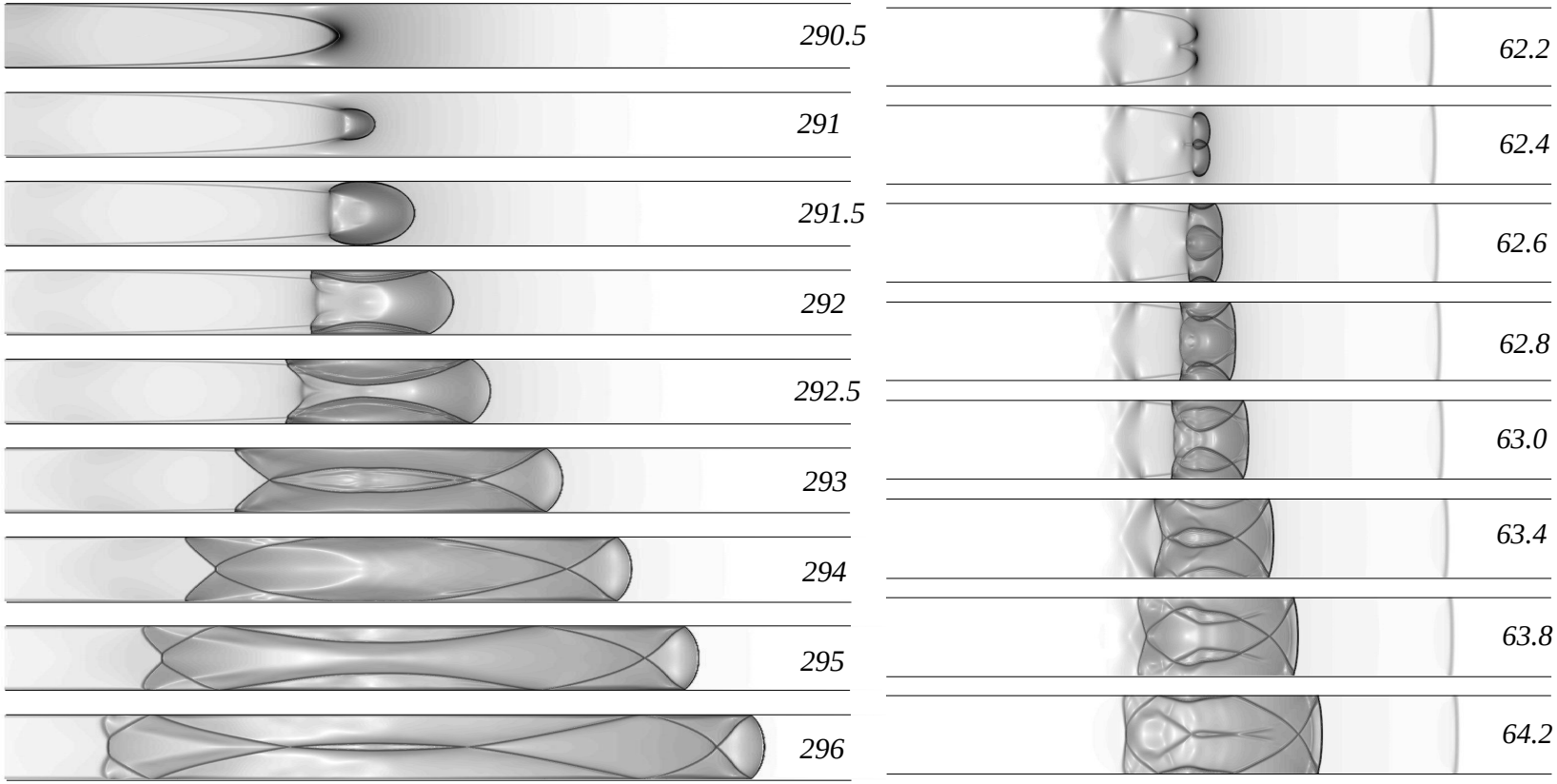


(T), pressure (P) and gas velocity (u) along channel centerline for several equidistant times.

Hydraulic resistance $\rightarrow$ precompression $\rightarrow$ preheating $\rightarrow$ explosion.

1) Bimolecular reaction: Isotherm vs adiabatic walls

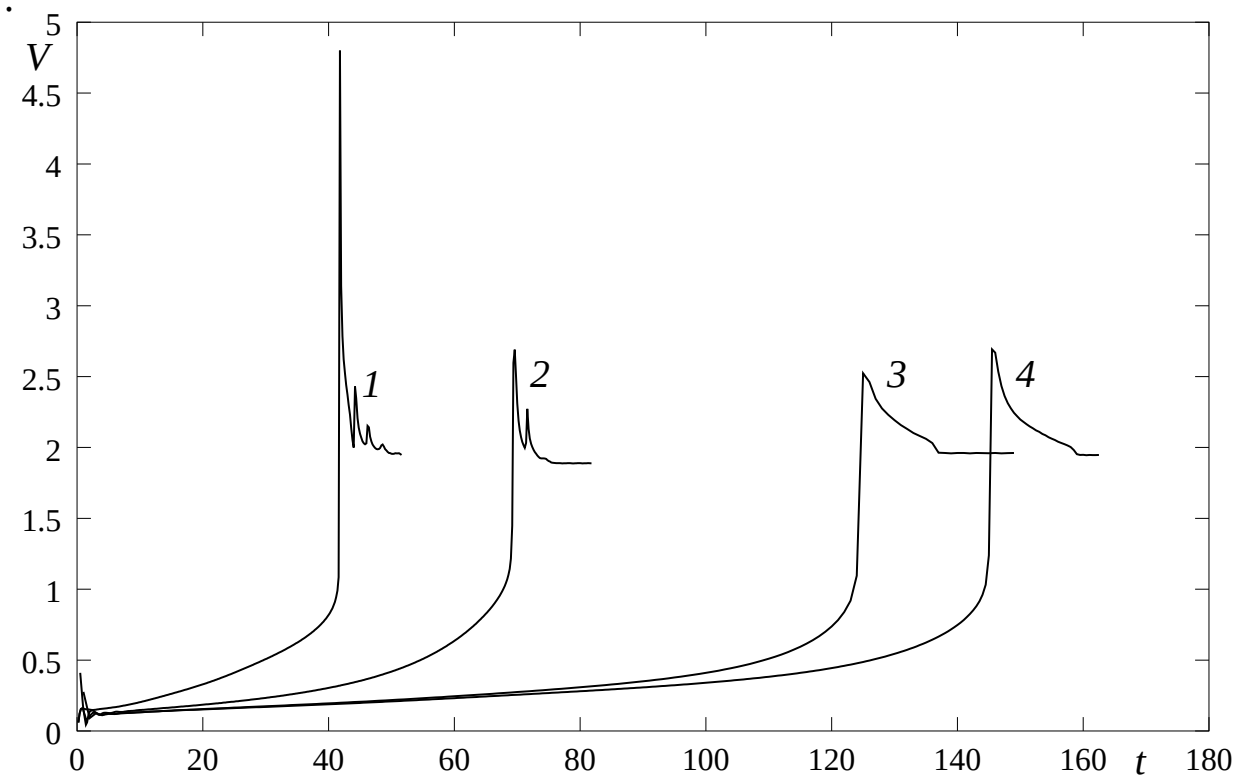
Flow Turbulence Combust. **84** 423 (2010)



(*a*) (*b*)

Pressure gradient norm at several consecutive instants of time (marked on the right). Stronger shading corresponds to higher pressure gradient.

2) Channels vs tubes.
Flow Turbulence Combust. **84** 423 (2010)



Reaction wave velocity V (scaled) versus time t (scaled) for narrow ($d = 2$) tubes $(1, 2)$ and channels $(3, 4)$, for adiabatic $(1, 3)$ and cold $(2, 4)$ walls.

4) Nonmonotonisity and Σ model. CTM **20**, 798 (2016)

Parameters employed are specified as follows,

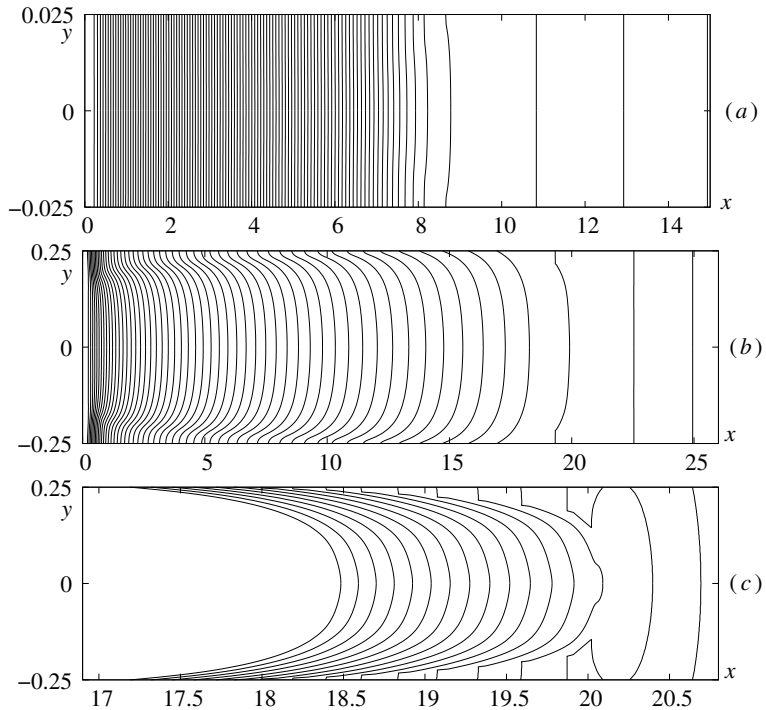
$$Pr = 0.75, \quad Le = 1, \quad \gamma = 1.3, \quad N_p = E/RT_p = 5,$$

$$\sigma_p = T_0/T_p = 0.125, \quad Ma_p = u_p/a_p = 0.05, \quad 1 < d/l_{th} < 20,$$

where d, $l_{th} = D_{th}/u_p$, channel and flame widths;

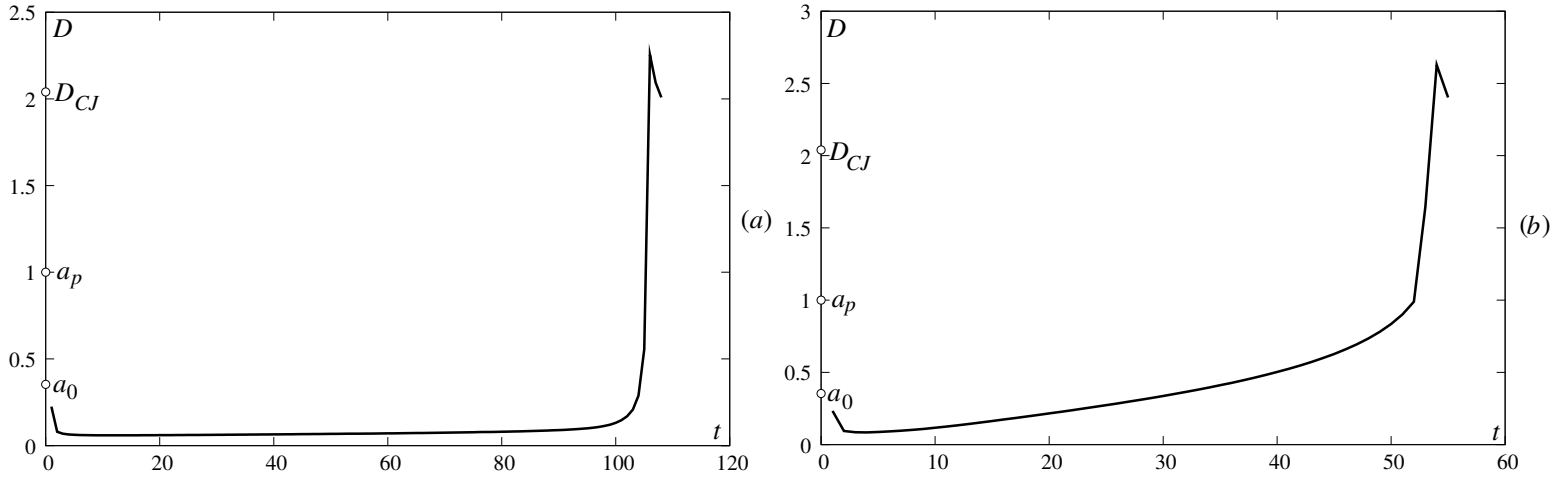
$a_p = 1000 m/s \quad \Rightarrow \quad u_p = Ma_p \cdot a_p = 50 m/s.$
Hence, the normal velocity of flame propagation
$u_n = \sigma_p \cdot u_p = 0.125 \cdot 50 m/s = 6 m/s.$

4) Nonmonotonisity and Σ model. Results of Numerical Simulations



Reaction zone configurations ($\max W$) at several equidistant instants of time calculated for $d = l_{th}$ (a) and $d = 10 l_{th}$ (b, c-zoom). The transition occurs in two stages - first near the wall and thereupon at the centreline, reflecting the dual nature of the transition event.

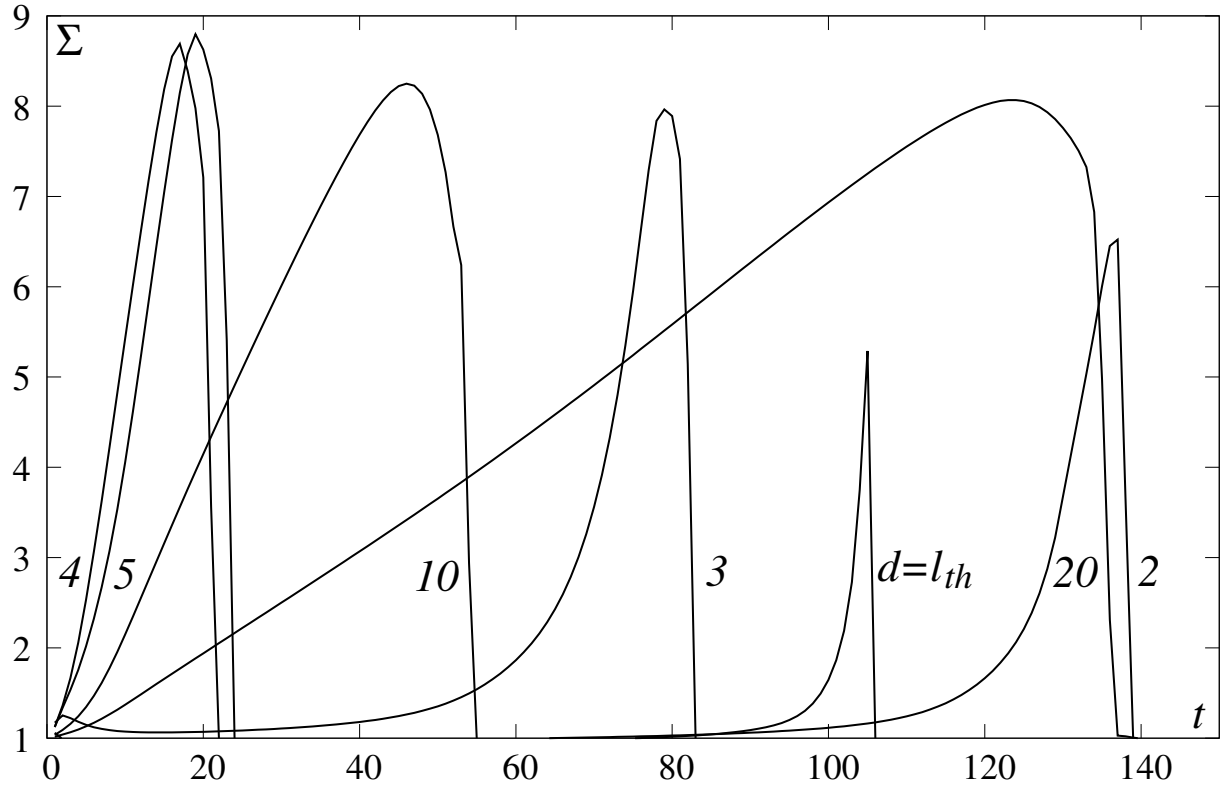
4) Nonmonotonisity and Σ model. Results of Numerical Simulations



Time records of the reaction wave velocities $\hat{D}(\hat{t})$ (scaled), calculated for $d = l_{th}$ (a) and $d = 10l_{th}$ (b) along the channel centreline $y = 0$. Here $\hat{D}_{CJ}$ corresponds to the Chapman-Jouguet detonation, and $\hat{a}_0$, $\hat{a}_p$ - to the sonic velocities in fresh and burned gas, respectively.

In both cases one observes the transition from deflagrative to detonative burning. At $d = l_{th}$ the transition occurs practically without the incipient acceleration, while at $d = 10l_{th}$ the acceleration is quite pronounced.

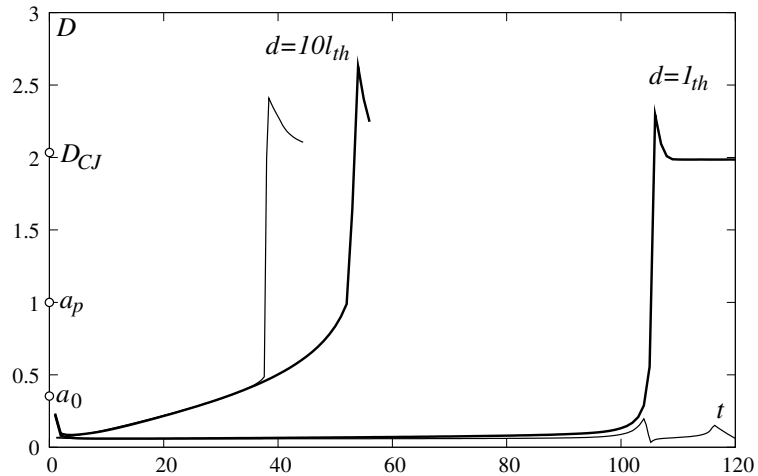
4) Nonmonotonisity and Σ model.



Time records of the folding ratio, Σ, calculated for several channel widths ($1 < d/l_{th} < 20$).

Folding Test. Σ-model

To elucidate the impact of folding a 1D *friction-free* version of the problem is considered, with the original reaction rate $\hat{W}$ replaced by, $\hat{W}_\Sigma = \Sigma^2 \hat{W}$, to ensure the overall mass flux through the flame $\hat{\rho}(\hat{D} - \hat{u})$ to be proportional to Σ.

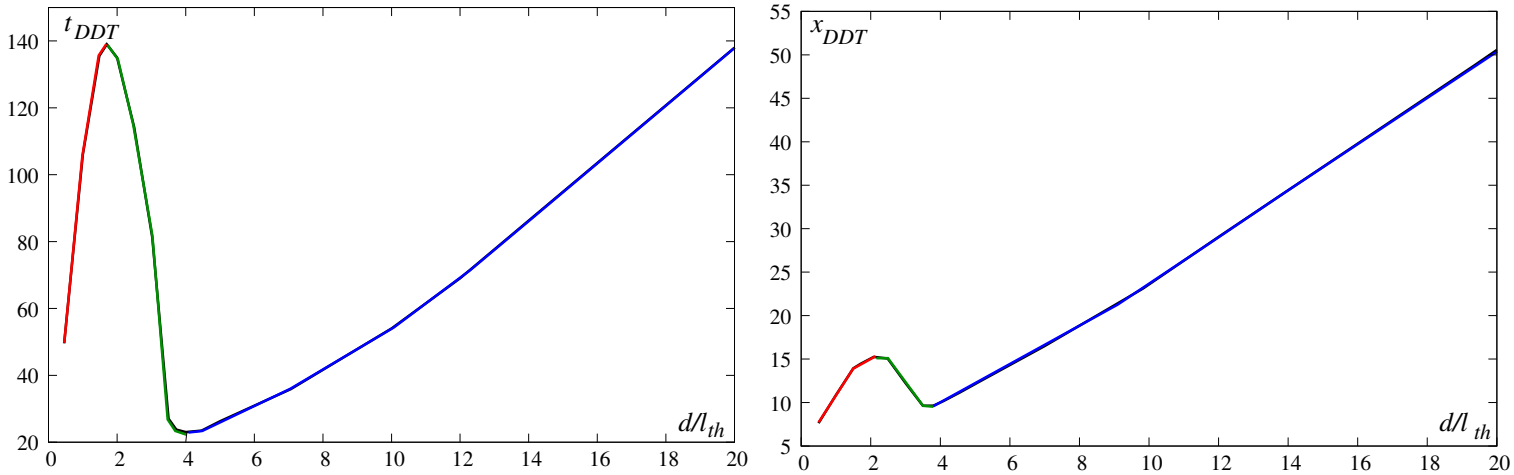


Time records of the reaction wave velocities $\hat{D}(\hat{t})$ for 1D Σ-models (solid lines) and for the associated 2D models (dashed lines), calculated for $d = 2l_{th}$ (a) and $d = 10l_{th}$ (b).

(a) In narrow channels ($d < 2l_{th}$) the developing level of folding is insufficient for triggering DDT. In this case the transition is caused by hydraulic resistance.

(b) In relatively wide channels ($d > 10l_{th}$) the transition may be induced by the folding alone.

4) Nonmonotonisity and Σ model. Conclusions

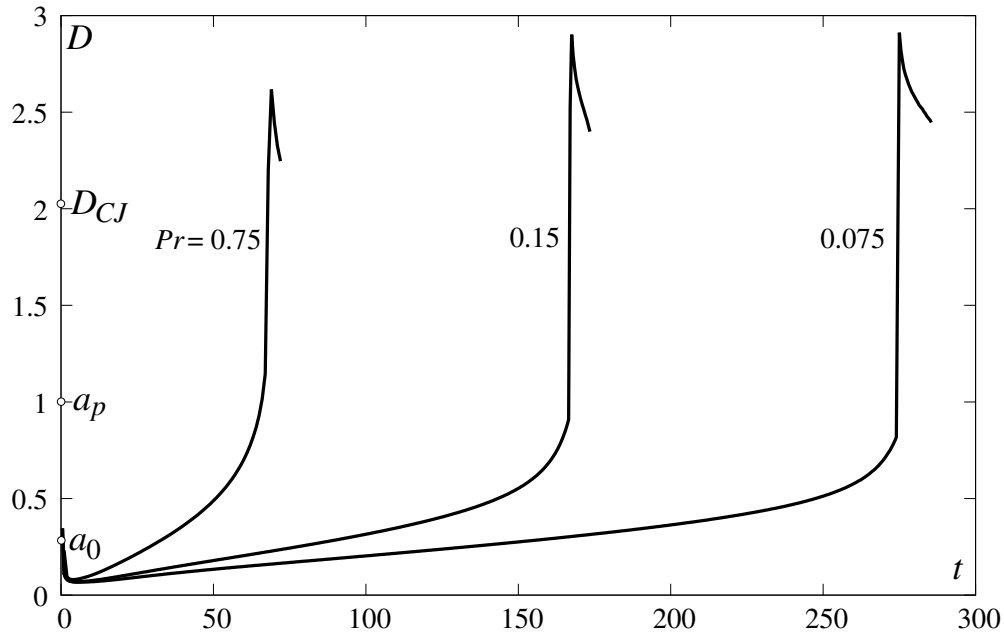


Run-up time ($\hat{t}_{DDT}$) and distance ($\hat{x}_{DDT}$) vs. normalized channel width d/l_{th}.

- Run-up time and distance depend on the channel width in a non-monotonic manner.
- The nonmonotonisity is likely to reflect different mechanisms for the transition:
  - In narrow channels the transition is caused by hydraulic resistance.
  - In relatively wide channels the impact of folding becomes important and perhaps even dominant. Yet in wide channels detonation generally nucleates in the boundary layer where the pressure buildup due to hydraulic resistance cannot be lightly dismissed.

4) Nonmonotonisity and Σ model. Prandtl number effect

In theoretical analysis the level of hydraulic resistance may be altered by changing the Prandtl number, other conditions being fixed.



Time records of the reaction wave velocity $\hat{D}(\hat{t})$ calculated for $d = 12 l_{th}$ at $Pr = 0.75, 0.15, 0.075$.

Reduction of the Prandtl number extends the pre-detonation time. This may be perceived as the influence of hydraulic resistance on the transition in wide channels.