Numerical investigation of a mechanical device subjected to a deflagration-to-detonation transition

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Introduction

- Investigation of the effects of the combustion of a stoichiometric mixture of hydrogen-air on a mechanical device (long tube, $L = 7$ m, $D = 0.245$ m, filled with an irregular set of obstacles of different shape).

- Amongst the most dangerous regimes
  - deflagration-to-detonation transition (DDT);
  - detonation initiation due to shock reflection.

- Concerning a DDT, there is some uncertainty regarding the time and the location of the transition. It depends on
  - nature of the mixture;
  - shape and nature of the obstacles;
  - roughness of the wall.

Introduction (2)

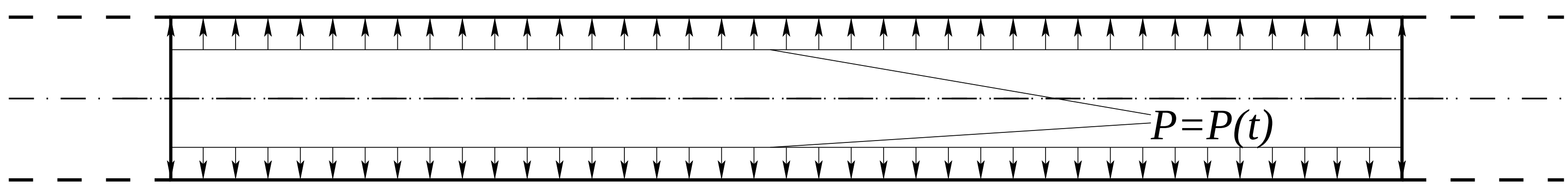
- Detailed numerical simulation of DDT and of the run-up distance requires:
  - capability of dealing with flows at all speeds (from low Mach number to fast flows);
  - detailed chemical model;
  - correct representation of the wall roughness and of the obstacles, and to perform fluid structure interaction;
  - capability of computing boundary layer.
  - ...

- Since we are not able to perform such computations, we have followed a different strategy (research for a regime more dangerous than the possible one).

Introduction (3)

- Three stages.
  1. We consider different 1D combustion regimes:
     - steady flames;
     - DDT at the flame;
     - detonation initiated by the shock reflection.

  2. To select the most dangerous regime, we apply $P = P(t)$ to an infinite cylinder in axisymmetric deformation with the same radius and the same material properties as the mechanical device.

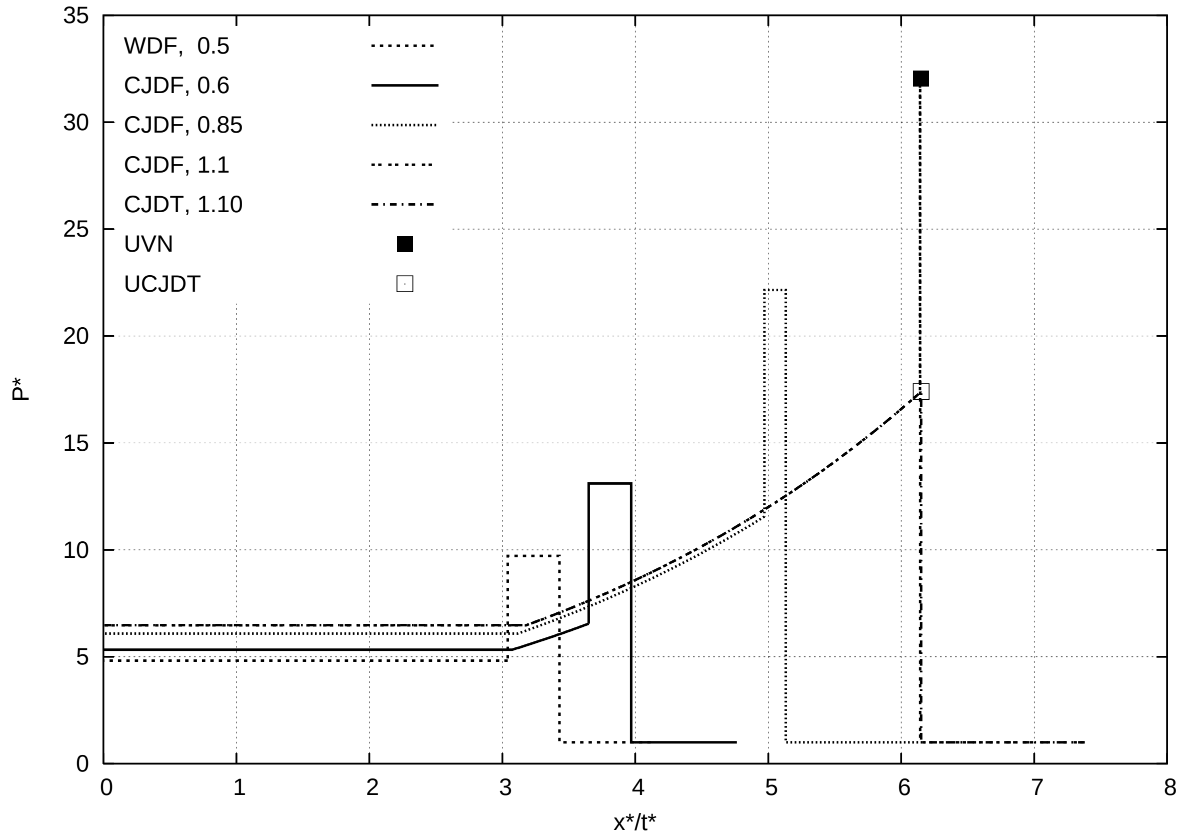


Introduction (4)

3. For the most critical combustion regime in the step 2, we compute the flow inside the mechanical device and evaluate stress and strain.

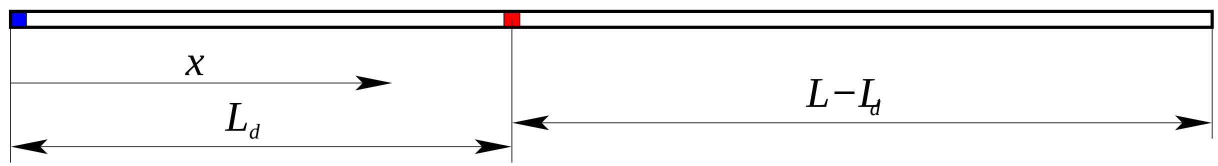
Steady deflagrations

- 1D constant speed deflagrations.
- Before the interaction with the wall, the non-dimensional solution is a function of $x/(t\sqrt{R_u T_0}), K_0/\sqrt{R_u T_0}$



Stoichiometric H_2-air. Ambient conditions. $\sqrt{R_u T_0} = 300$ m/s.

DDT at the flame

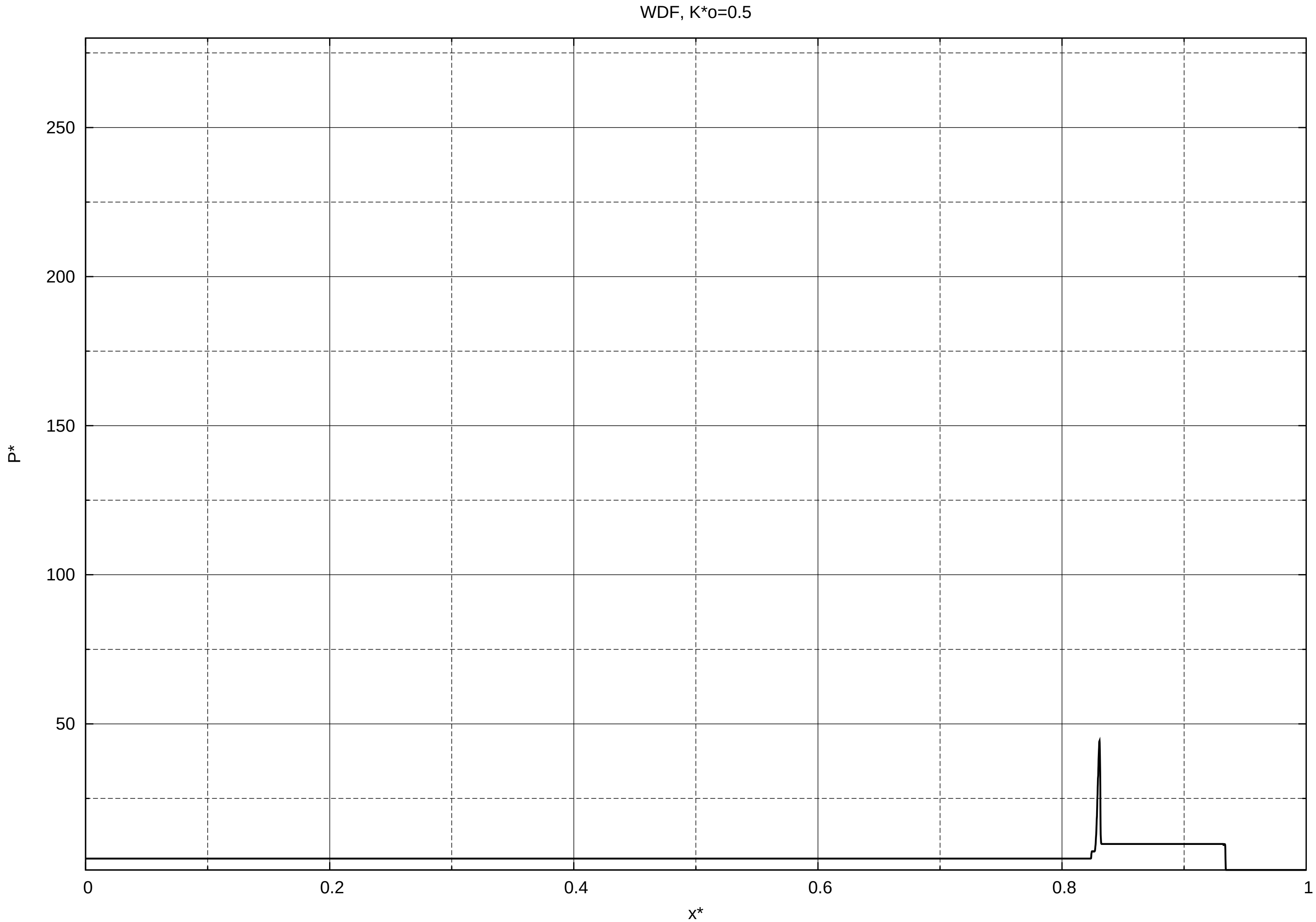


- **Simple model :** the DDT occurs at the flame of a steady deflagration.

- Two non-dimensional parameters:

$$\frac{L_d}{L}, \frac{K_0}{\sqrt{R_u T_0}}$$

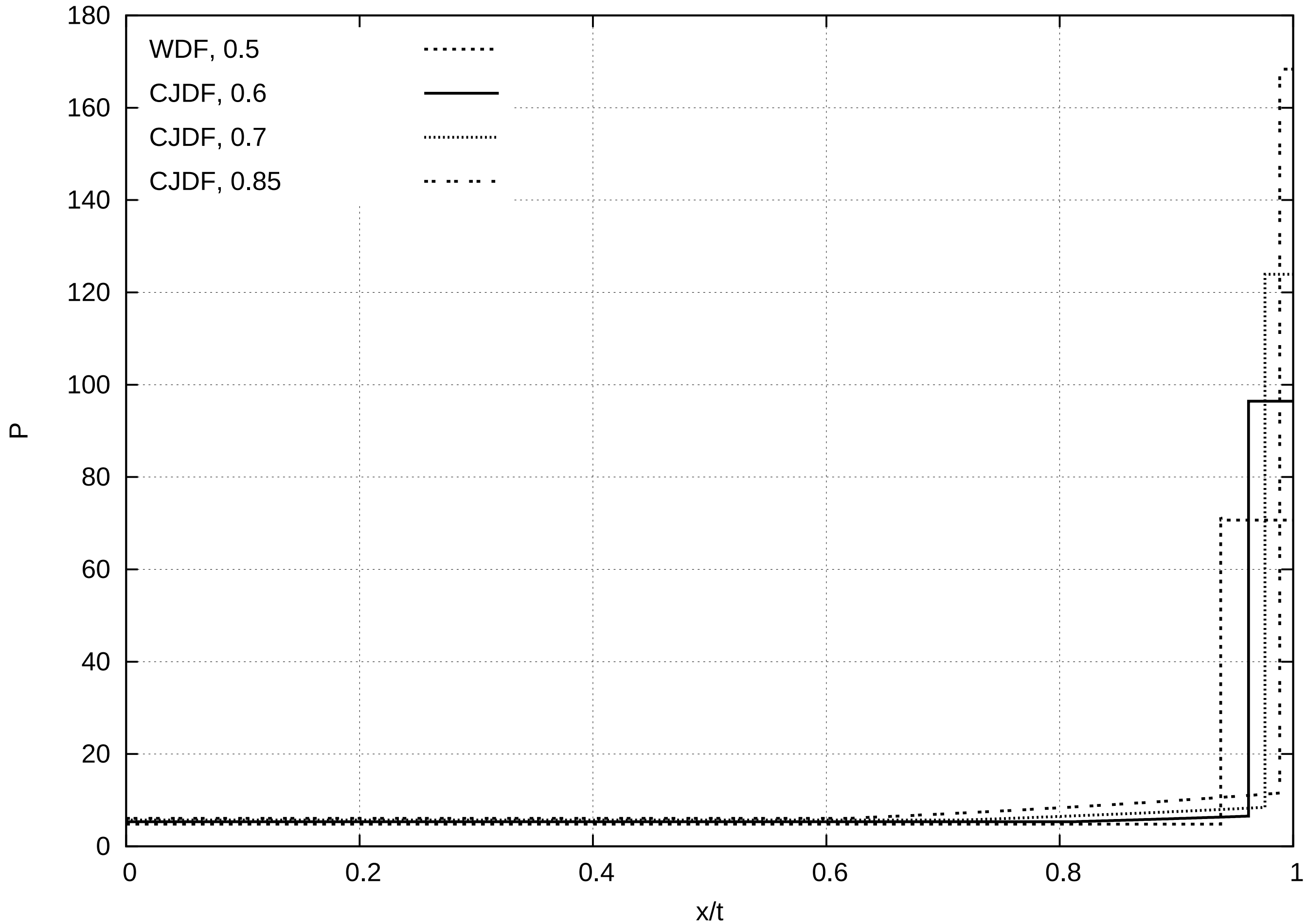
DDT at the flame. Fast flame (2)



Detonation caused by the shock reflection

- The non-dimensional solution is function of K_0^* only.
- Three stages.
  1. Before the interaction of the wall, we have a steady deflagration.
  2. The interaction of the precursor shock with the wall generates a left-travelling detonation, moving in a right travelling unburnt gas (CJDT or SDT).
  3. The interaction of the right travelling flame with the left travelling detonation wave generates a non reactive flow (everything is already burnt) consisting in left and right travelling shock waves.

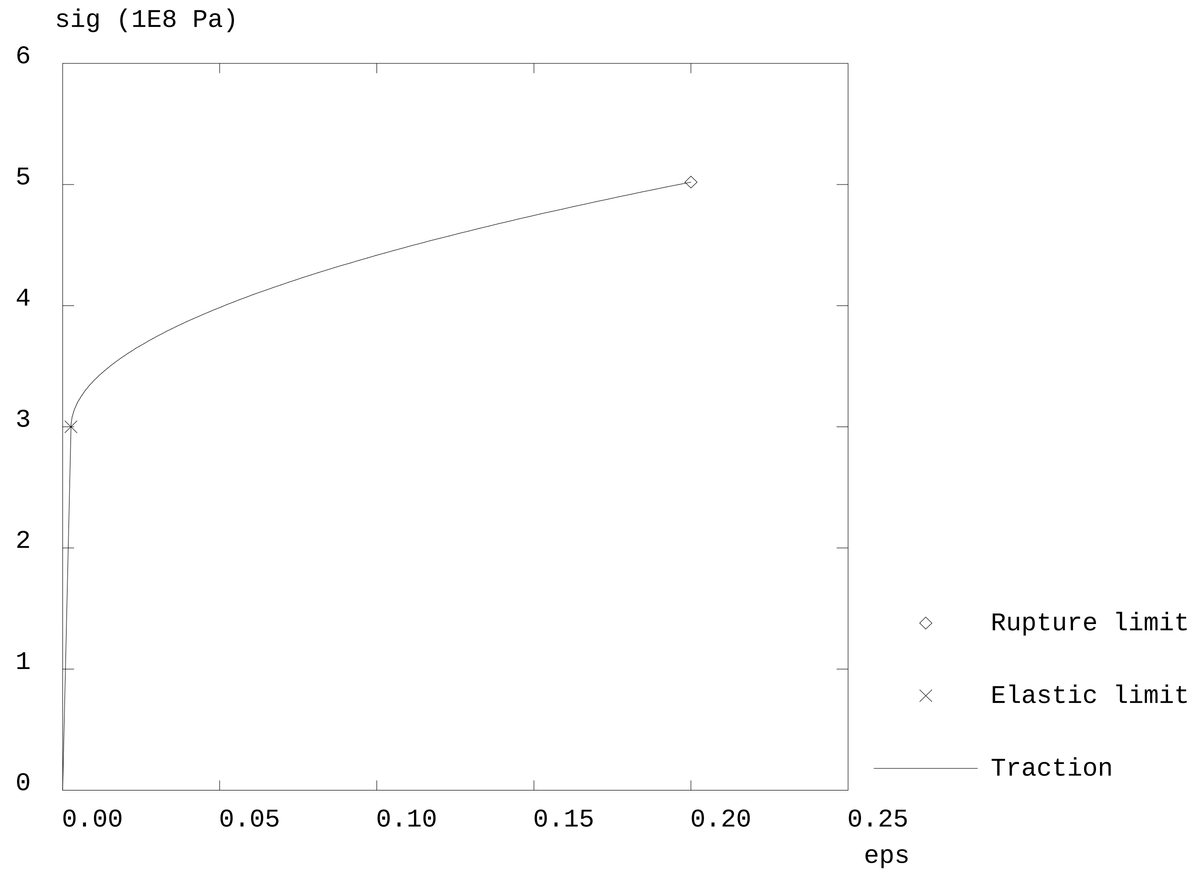
Detonation caused by the shock reflection. Stage 2



- For $K_0^* = 0.5$, CJDT pressure is 71.2 pressure behind the Taylor wave is 70.7.
- For $K_0^* > 0.6$ we have strong detonation

Infinite cylinder investigation

- We suppose that the material obeys to a isotropic von Mises low.



- For the infinite cylinder, we have the maximum strain (around 3.5 %) in case of deflagration-to-detonation transition at the flame, K_0^* between 0.5 and 0.7.

Mechanical device investigation

- We use the CEA EUROPLEXUS code, with the Reactive Discrete Equation Method for the reactive flow computation (on a Arbitrary Lagrangian Eulerian mesh) and a Lagrangian Finite Element approach for the discretization of the mechanical device.
- We take as initial solution, the steady deflagration with $K_0 = 0.5$, just before the interaction of the precursor shock with the wall
- We initiate the detonation at the flame
- In this case we obtain a strain lower than 4%, apart from a little region in which it reaches the value of 19%

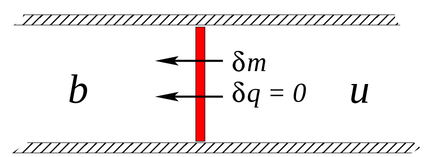
Conclusion and future work

- In order to investigate if a (long) mechanical device can afford a combustion of hydrogen-air, we have used a simplified model.
- Using this model, we have considered the case of DDT at the flame and detonation initiation due to shock reflection.
- Once established the most critical situation, we have performed a Fluid-Structure interaction computation.
- Material model should be improved by taking into account the strain time variation.

DDT at the flame. Slow flame

- If the flame velocity is negligible with respect to the flame speed, non-dimensional solution depends on L_d/L only. Low Mach number approximation: **thermodynamic pressure** $P = P(t)$.

- Two stages
  1. Slow deflgration. We suppose that in the burnt and unburnt region we have constant states. The flame behaves like a permeable piston.



  2. Detonation at the flame

DDT at the flame. Slow flame (2)

- Equation of state $P = \rho_u R_u T_u = \rho_b R_b T_b$.

- Equation of conservation of the total mass and total energy

$$L_d \rho_b + (L - L_d)\rho_u = L\rho_0$$

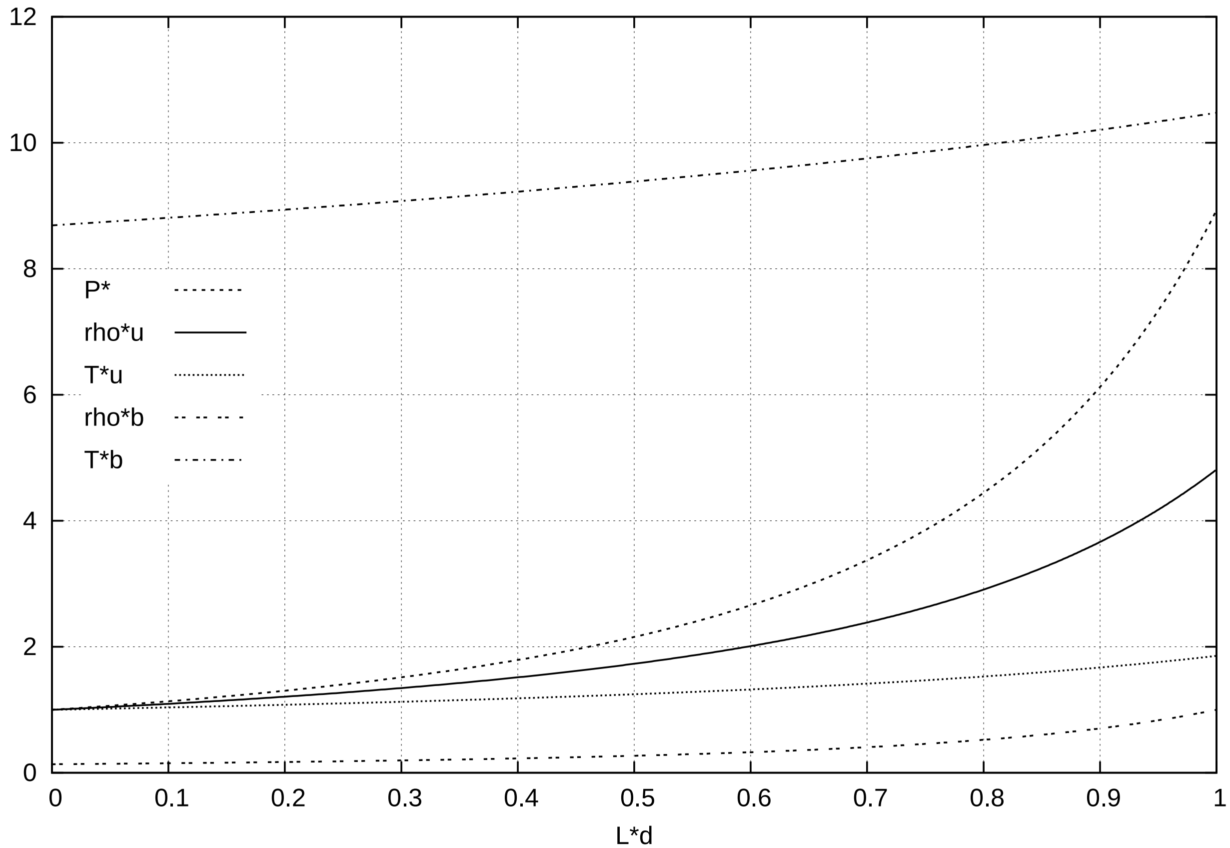
$$\left(L_d \rho_b \int_0^{T_b} \mathrm{d}\tau \left\{ c_{v,b}(\tau) \right\} \right) + \left((L - L_d)\rho_u \int_0^{T_u} \mathrm{d}\tau \left\{ c_{v,u}(\tau) \right\} \right) =$$
$$L\rho_0 \int_0^{T_0} \mathrm{d}\tau \left\{ c_{v,u}(\tau) \right\} + L_d \rho_b q.$$

- In the unburnt mixture an isentropic compression occurs, i.e.

$$0 = \delta q = c_{v,u}\mathrm{d}T_u - \frac{P}{\rho_u^2}\mathrm{d}\rho_u, \quad \text{i.e.} \quad 0 = \frac{1}{\gamma_u(T_u) - 1}\frac{\mathrm{d}T_u}{T_u} - \frac{\mathrm{d}\rho_u}{\rho_u}$$

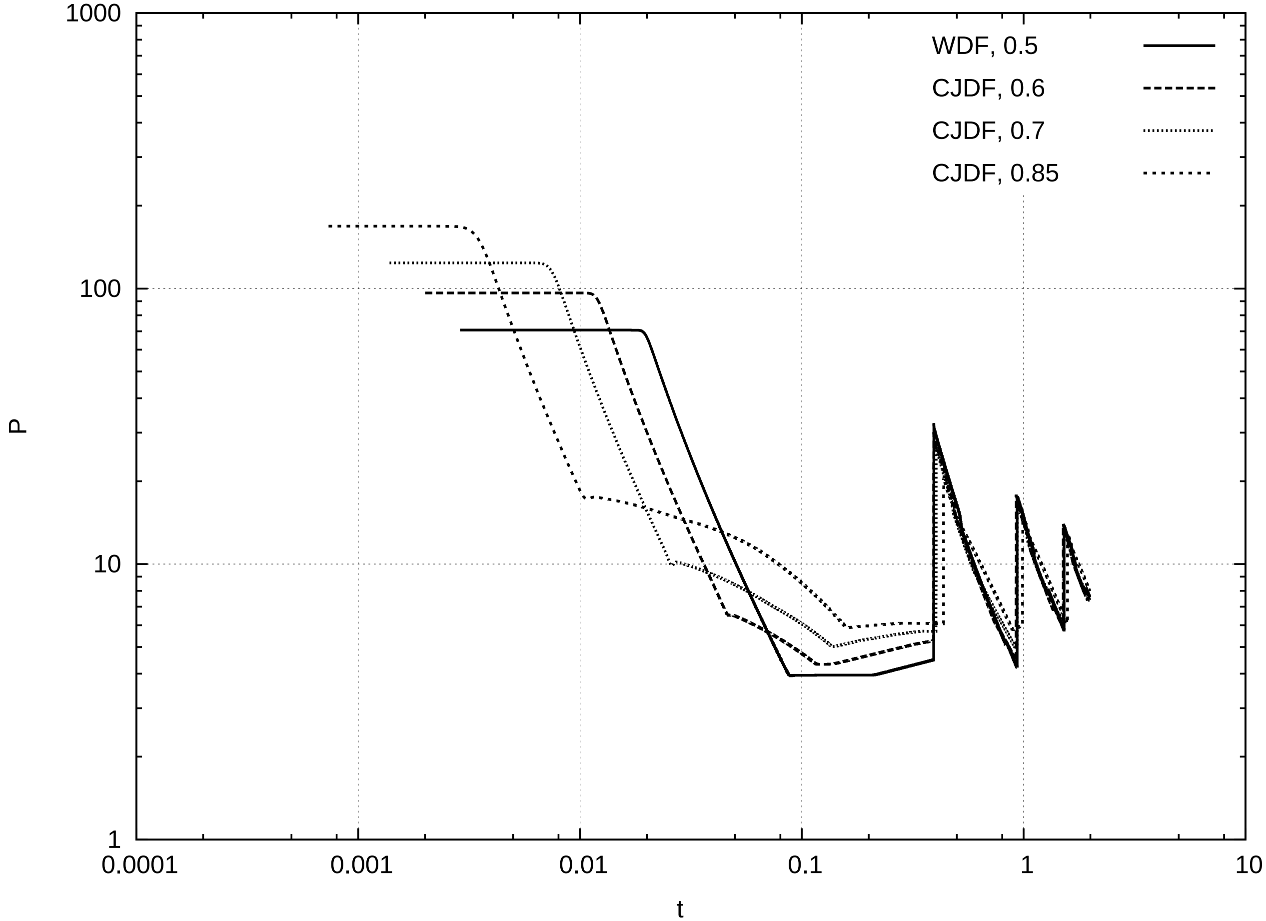
- Unknowns: P, ρ_u, T_u, ρ_b and T_b (five unknowns) as function of L_d.

DDT at the flame. Slow flame (3)



- If the DDT occurs at $L_d = 0$, we have a 1D detonation.
- If the DDT occurs at $L_d \approx 1$, we have a uniform pressurization of the mechanical device.

Detonation caused by the shock reflection. Stage 3



- The larger the flame speed, the larger the maximum value of P.
- The larger the flame speed, the lower the decreasing of the pressure in time.