Comparison OF TNT-Equivalency Approach, TNO Multi-Energy Approach and a CFD Approach in Investigating Hemispheric Hydrogen-Air Vapor Cloud Explosions

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Outline

- Introduction

- Approaches and related problems
  - Point explosion
  - TNT approach
  - 1D point-symmetrical deflagration
  - TNO multi-energy approach
  - CFD approach

- Test problem and its solution

- Approaches analysis on the test problem

- Summary, conclusion and future work

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Introduction

- CEA is working in the design of Generation IV Nuclear Power Plants.
- Part of the heat produced by the Very High Temperature Gas Reactor is used for hydrogen production.

Introduction (2)

- We have an accident, with the **formation of a cloud** of hydrogen and air.
  - If the combustion occurs, which is the safety distance for the buildings?
  - Which is the safety distance for general public?

- **Problem.** How to evaluate the pressure load as function of time and space in real configurations?
  - In open environment, the interesting domain can be huge.
  - There are several complex obstacles.
  - ...

  3D Computational Fluid Dynamics (**CFD**) is not always possible.

- There exist **criteria** involving the **overpressure** and the **positive impulse** in the **free field**.

Introduction (3)

- **Purpose of this work**.
  We analyze three simple approaches for investigating (hydrogen-air) 1D point-symmetric vapor cloud explosions (VCE), i.e.
  - TNT-equivalency approach,
  - TNO-multi energy approach,
  - 1D CFD approach,

  which provide maximum overpressure and positive impulse.

- **Hypotheses.**
  - We deal with ideal gases (calorically or thermally perfect).
  - We suppose that the flame is infinitely thin.
  - We only consider one global irreversible reaction.
  - We neglect the viscosity, the species diffusion and the thermal diffusion (⇒ the Euler equations).

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Point explosion

- The flow generated by a **TNT explosion on the ground** is similar to the one generated by a **point explosion** with the released energy

$$E = 2 \cdot m_{\mathrm{TNT}} \cdot 4.2\mathrm{MJ/kg}$$

- In the case of a calorically perfect gas, the solution depends on

Variable	SI units	Meaning
r	m	distance from the center
t	s	time
P_0	J/m^3	“unperturbed” pressure
c_0	kg/m^3	“unperturbed” sound speed
E	J	released energy
γ		specific heat ratio

Point explosion (2)

- The non-dimensional solution can be expressed as function of

  $$r/r_{\mathrm{ref}}, \quad t/t_{\mathrm{ref}}, \quad \gamma$$

  where

  $$\begin{aligned} r_{\mathrm{ref}} &= \left(\frac{E}{P_0}\right)^{\frac{1}{3}} && \text{(energy-based length)} \\ u_{\mathrm{ref}} &= c_0 && \text{(unpert. sound speed)} \\ t_{\mathrm{ref}} &= \frac{r_{\mathrm{ref}}}{u_{\mathrm{ref}}} \end{aligned}$$

- The **overpressure at the first shock** and the **positive impulse** can be expressed as

  $$\begin{aligned} \frac{DP_{\mathrm{max}}}{P_0} &= f\left(\frac{rP_0^{1/3}}{E^{1/3}};\gamma\right) \\ \frac{I^+}{P_0\left(\frac{E}{P_0}\right)^{\frac{1}{3}}}c_0 &= f\left(\frac{rP_0^{1/3}}{E^{1/3}};\gamma\right) \end{aligned} \qquad (1)$$

Point explosion and TNT explosion

- In TNT experimental diagrams we find similar expression like (1), but

$$E \to m_{\mathsf{TNT}}$$

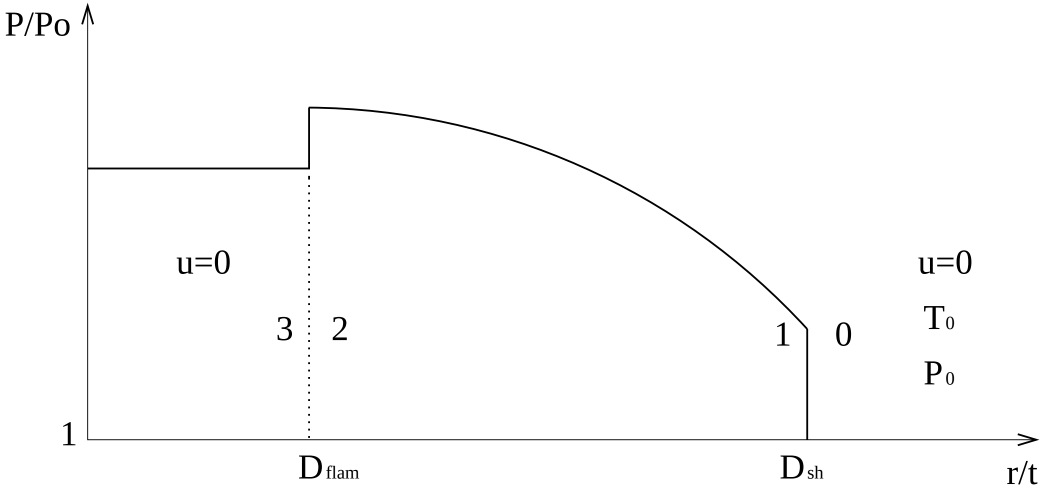
- In the **TNT equivalency approach** for VCE

$$m_{\mathsf{TNT}}(\mathsf{kg}) = \alpha \cdot E/(4.2\mathsf{MJ})$$

  where
  - E is the chemical energy inside the cloud,
  - $\alpha \in (0,1)$ is an **efficiency factor**.

Homogeneous 1D-point symmetrical defl.

- We consider a 1D-point symmetrical flame propagating at constant velocity in a homogeneous medium.
- Problem solved by [Sedov 1959], [Kuhl 1973]
- The solution is self similar (it depends on r/t).



$$D_{\mathsf{flam}} = \frac{\rho_2}{\rho_3} K_0 = \sigma K_0, \quad D_{\mathsf{sh}} > c_0, \quad u_2 = D_{\mathsf{flam}} - K_0$$

- The lower the flame speed, the larger the ratio $D_{\mathsf{sh}}/D_{\mathsf{flam}} \approx c_0/D_{\mathsf{flam}}$.

TNO-multi energy approach

- We restrict our attention to hemispheric VCE.

- There exist **abacuses** which give the non-dimensional maximum overpressure, the positive impulse (or the positive duration time) and the shape of the wave as function of the energy-scaled distance and a **strength** index arising from 1 (weak deflagration) to 10 (detonation)

- These abacuses have been obtained by computing the **decaying of the** flow generated by the **1D point-symmetric steady flame** as the combustion is finished, using the FCT scheme.

- There exist tables which help in the choice of this index.

TNO-multi energy approach (2)

Table 1. Guidance for Selecting Charge Strengths for the TNOME Method.

Type of Flame Expansion [b]	Mixture Reactivity [c]	TNOME Method Charge Strength [a]		
		Obstacle Density [d]		
		High	**Medium**	**Low**
1-D	High	10	10	10
	Medium	9 – 10	9	7 – 8
	Low	9 – 10	7 – 8	4 – 5
2-D	High	9	7 – 8	6
	Medium	7 – 8	6 – 7	2 – 3
	Low	6	5 – 6	1 – 2
3-D	High	6	3	1
	Medium	3 – 4	2	1
	Low	3	2	1

From [Roberts 2004]

CFD approach

- The Reactive Euler Equations are solved via an operator splitting technique:
  non-reactive Euler equations + reactive source term.

- The non-reactive Euler equations for thermally perfect gases are solved using
  - a FV conservative approach;
  - a first-order discretization explicit in time;
  - TVD-type reconstruction (a second-order reconstruction on density, velocity, pressure, mass fractions using a minmod-type limiter);
  - the shock-shock Riemann-type solver.

- In the particular case of 1D-geometry, the source term is treated to determine the quantity of gas burnt per time unit

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \rho_{u,\mathsf{fl}} K_0 S_f .$$

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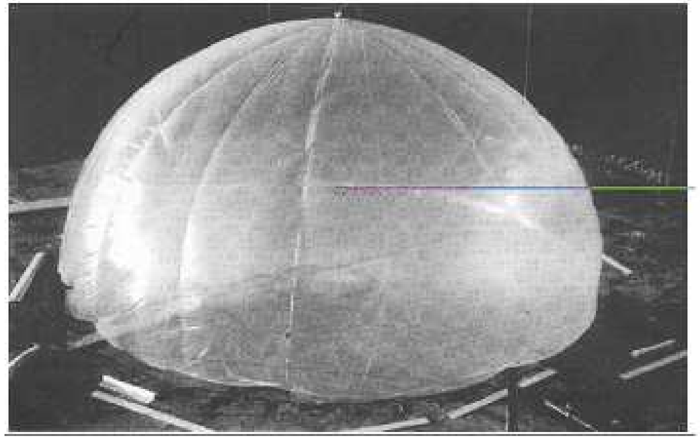
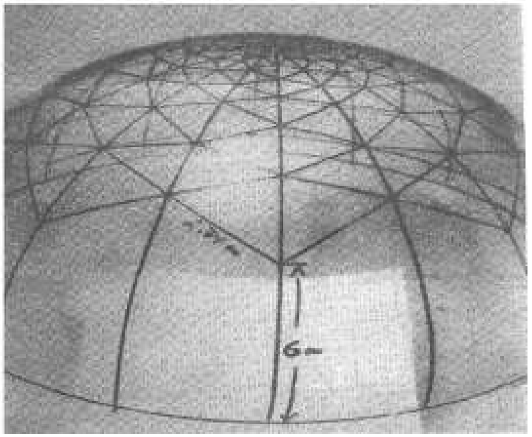
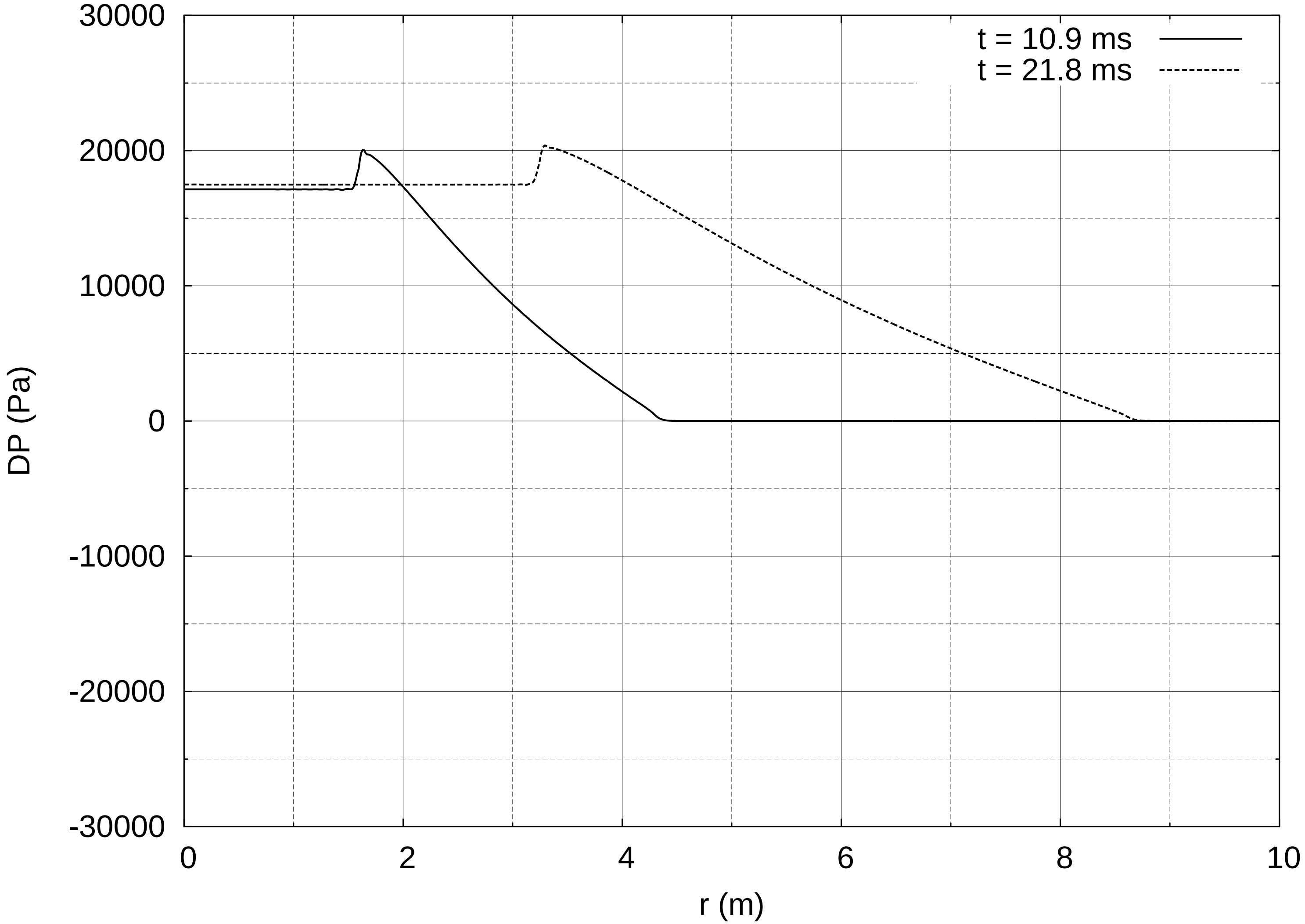
Test problem

- We have a 10 m radius hemispherical cloud.
- Inside the cloud, there is a stoich. mixture of H_2-air ($P_0 = 0.989$ bar, $T_0 = 283$ K, $m_{H_2} = 51$ kg, $E = 6.22E9$ J).
- Outside the cloud, we have air at the same conditions.
- The combustion is initiated in the center and occurs at constant speed.
- Experimental results exist (large scale deflagration at Fraunhofer Institute of Chemical Technology, with $D_{\text{flam,av}} = 65$ m/s)



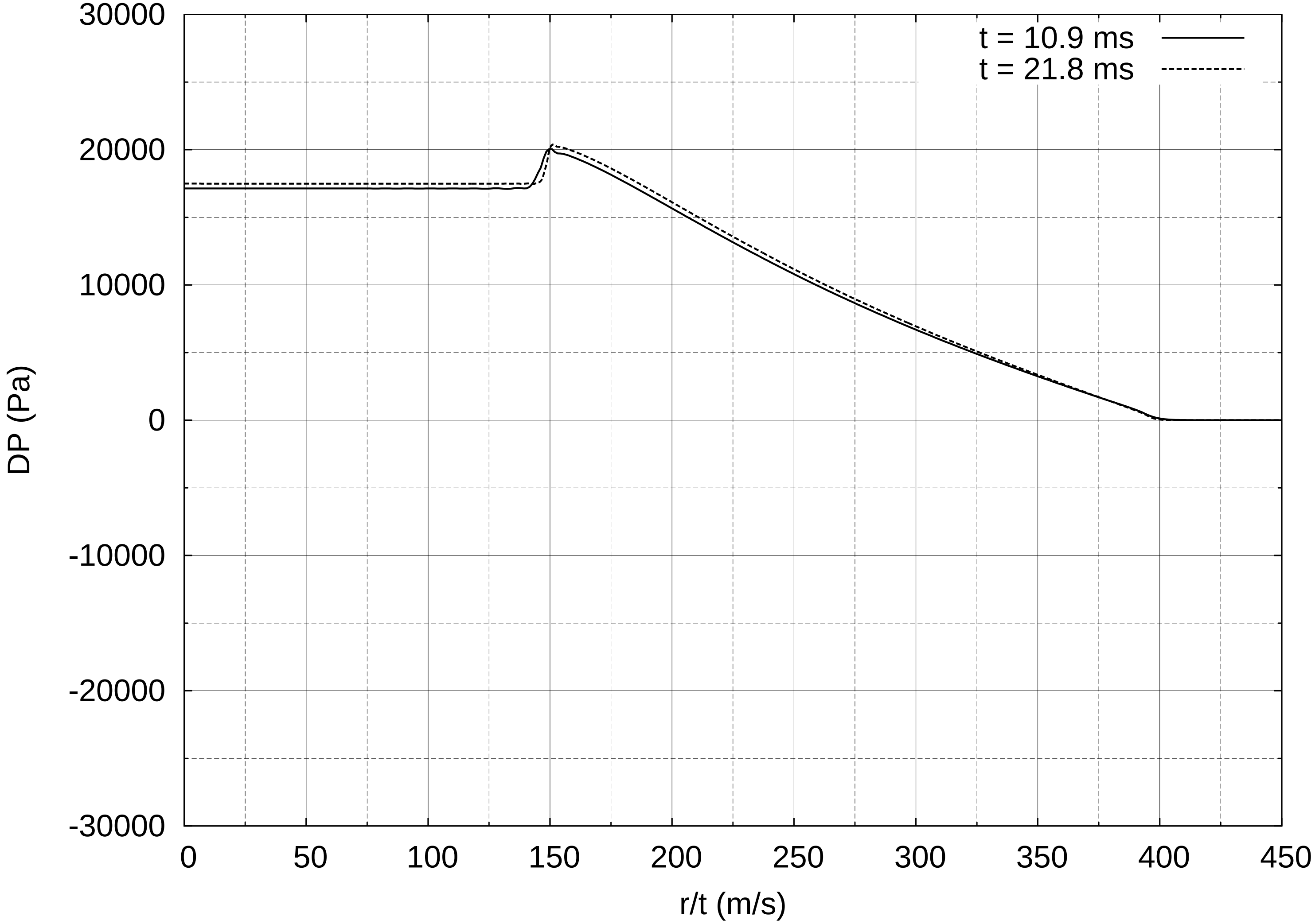


Test problem solution. Phase 1



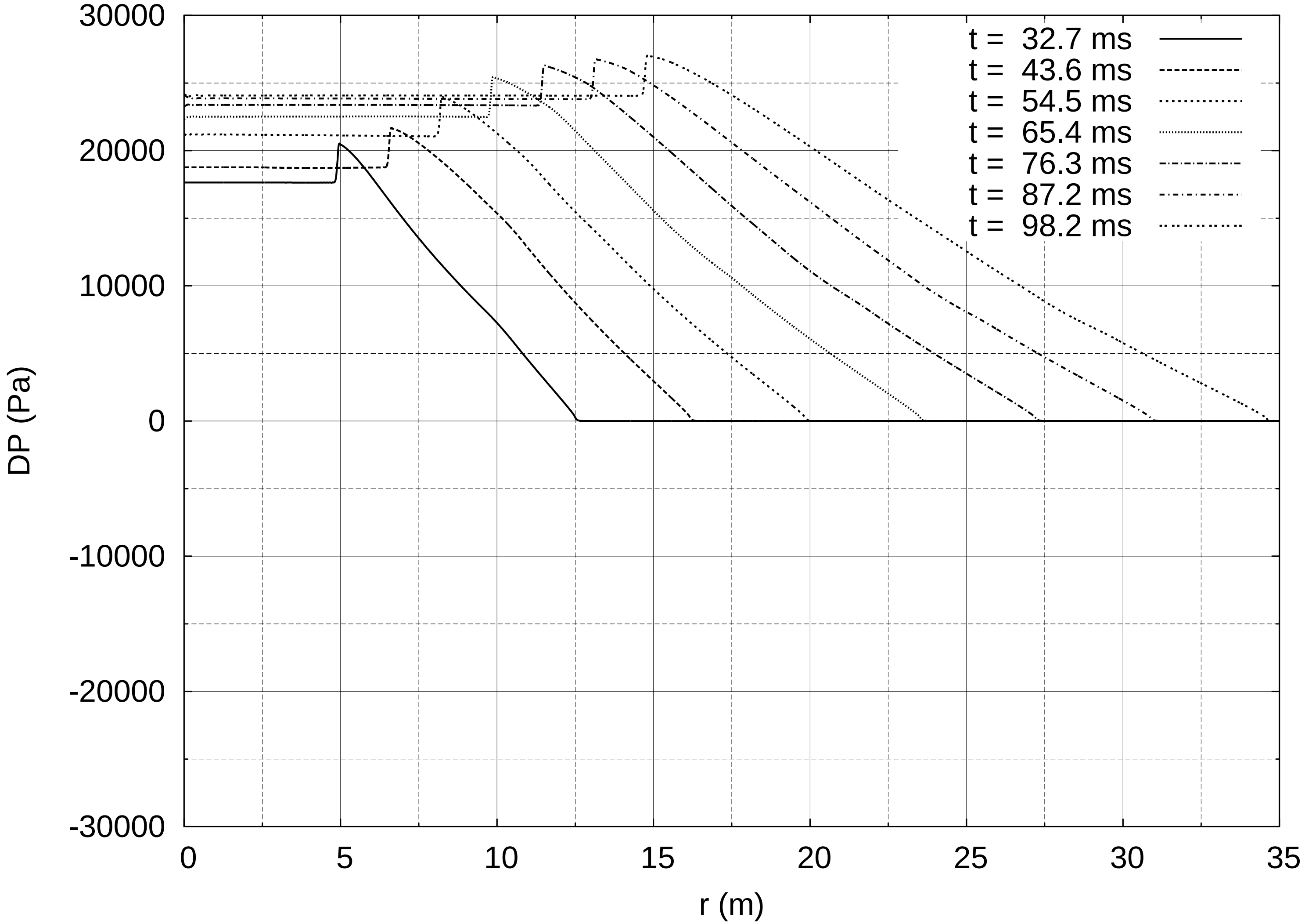
$K_0 = 22.6$ m/s, $D_{\text{flam}} \approx 160$ m/s, $D_{\text{flam}}/c_{0,\text{cloud}} \approx 0.4$

Test problem solution. Phase 1 (2)



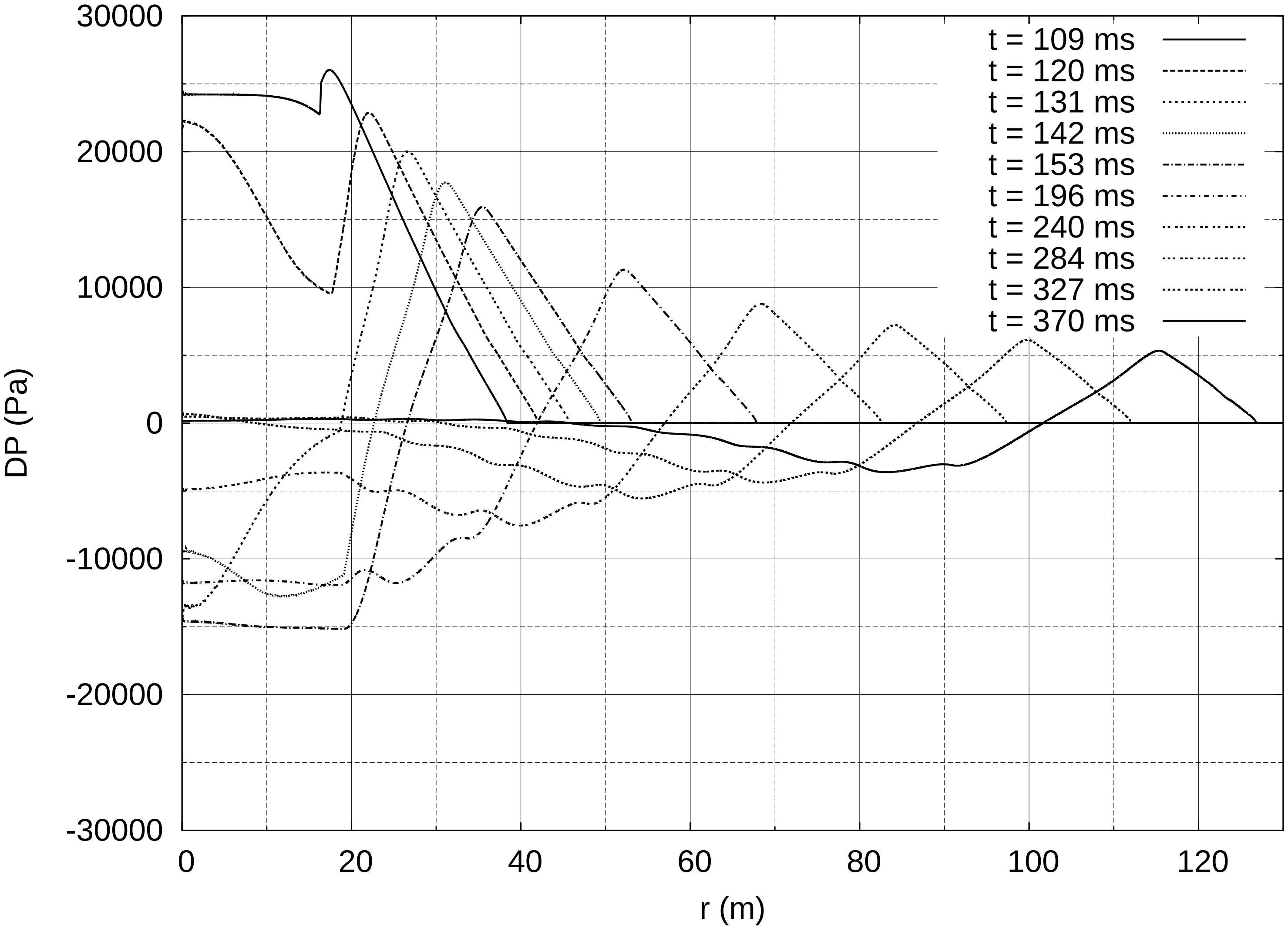
$K_0 = 22.6$ m/s, $D_{\text{flam}} \approx 160$ m/s, $D_{\text{flam}}/c_{0,\text{cloud}} \approx 0.4$

Test problem solution. Phase 2



$K_0 = 22.6$ m/s, $D_{\text{flam}} \approx 160$ m/s, $D_{\text{flam}}/c_{0,\text{cloud}} \approx 0.4$

Test problem solution. Phase 3



$K_0 = 22.6$ m/s, $D_{\mathrm{flam}} \approx 160$ m/s, $D_{\mathrm{flam}}/c_{0,\mathrm{cloud}} \approx 0.4$

Test problem solution. Characteristic scales

- For slow flames, once the combustion stop, the dimension of the cloud is

$$r'_{\mathsf{surf}} \approx r_{\mathsf{surf}} \sigma^{1/3}$$

Then the combustion time is

$$t_{\mathsf{combustion}} = r'_{\mathsf{surf}} / D_{\mathsf{flam}}$$

- For slow flames, once the combustion stop, the distance last by the precursor shock is

$$r_{\mathsf{acoustic}} \approx \left(\frac{c_0}{D_{\mathsf{flam}}} \right) r'_{\mathsf{surf}}$$

- The lower D_{flam}, the larger r_{acoustic}, the larger $t_{\mathsf{combustion}}$

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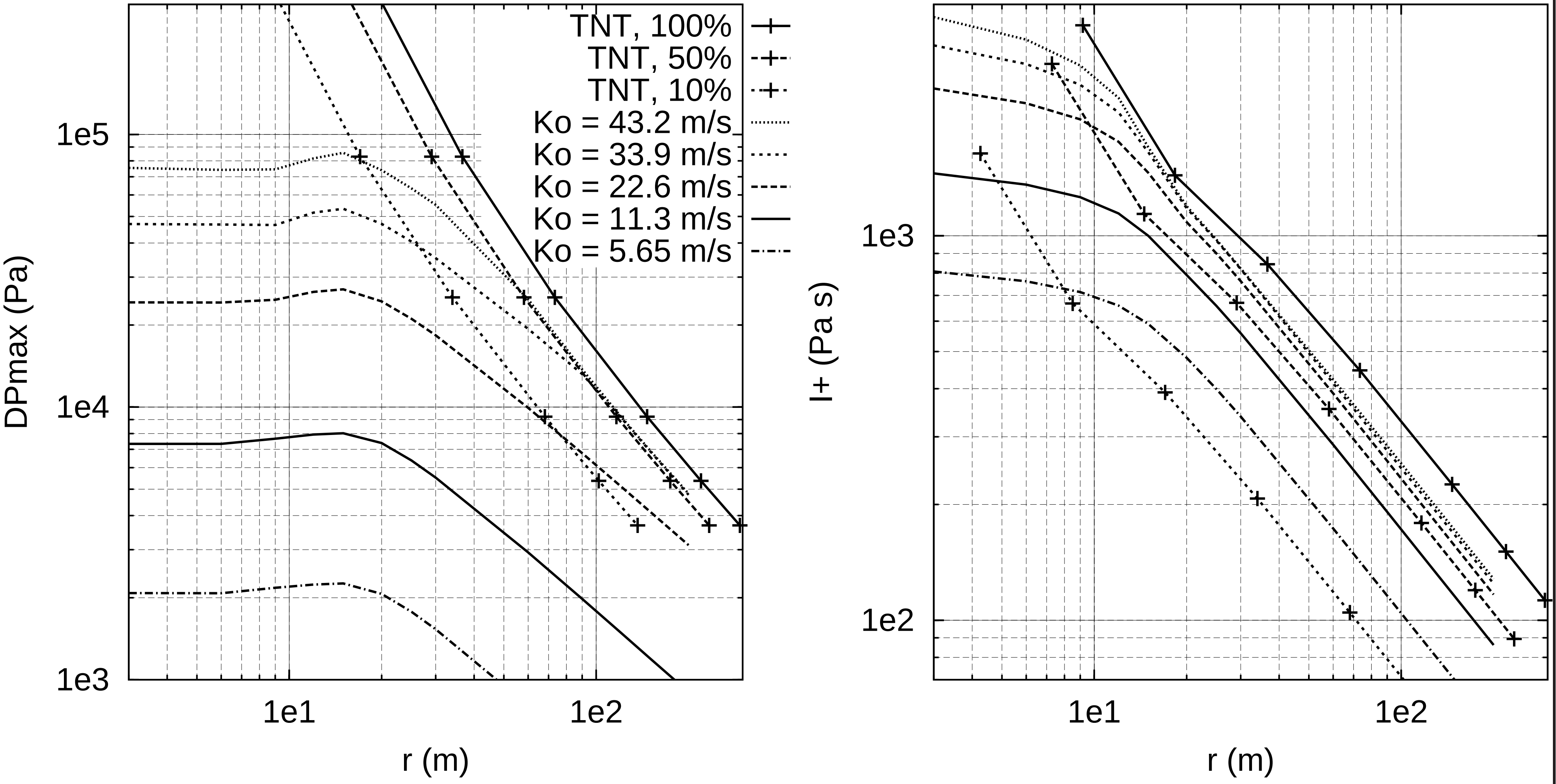
Approaches analysis

- TNT-equivalency versus CFD



$K_0 = 5.65,\ 11.3,\ 22.6,\ 33.9,\ 43.2$ m/s

$D_{\text{flam}}/c_{0,\text{cloud}} = 0.1,\ 0.2,\ 0.4,\ 0.6,\ 0.8$

Approaches analysis (2)

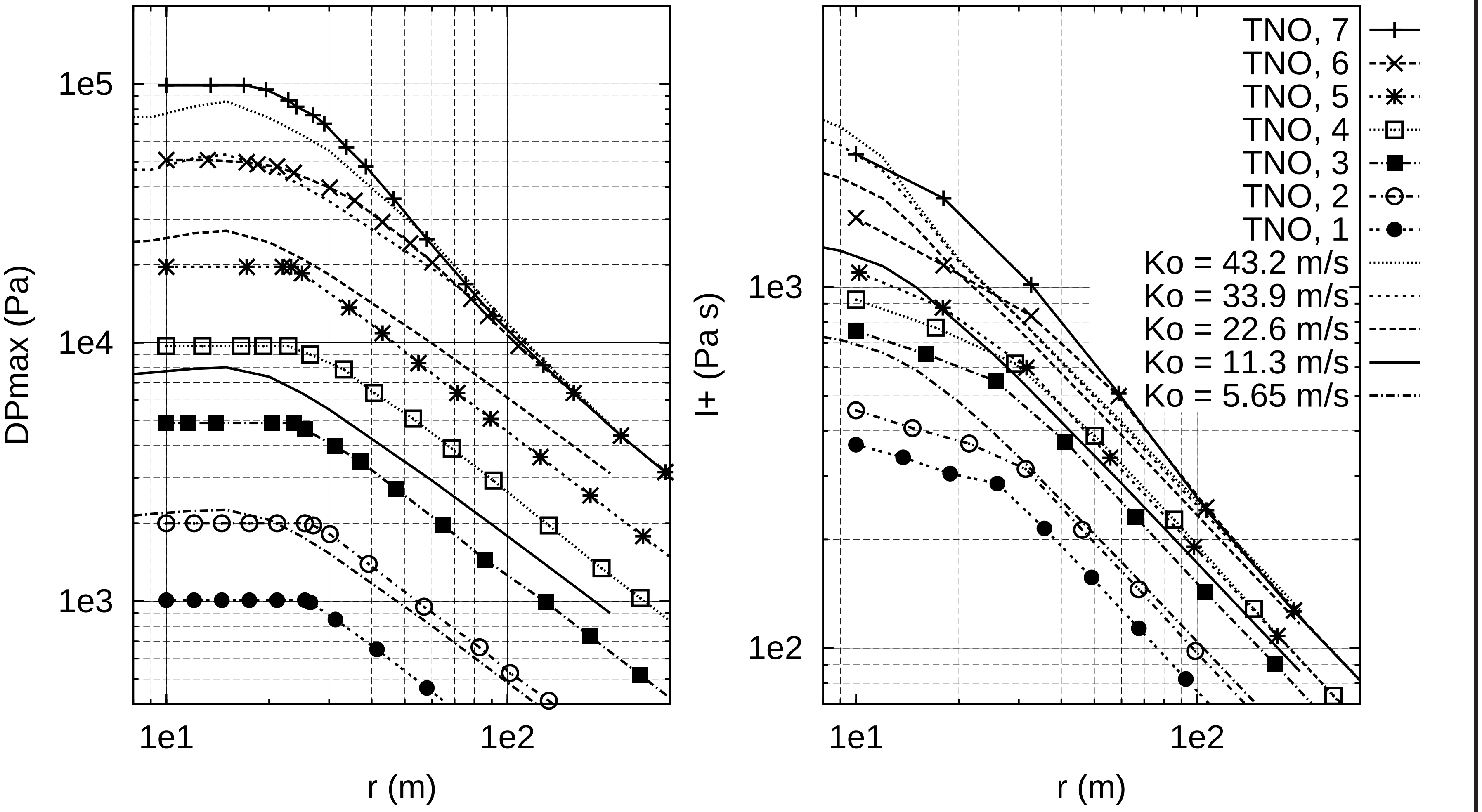
- The two physical phenomena behave in a different way.
  - A TNT explosion immediately releases all the energy in one point.
  - In a 1D-point symmetrical deflagration the energy is released in a finite time and, at the end of the combustion, the variation of energy involves a large area (which both vary with the flame speed)

- Because of different decay of the overpressure, it is impossible to link K_0 and a costant value of α.

- Even if α were a function of r, it is impossible to link α and K_0 to fit both overpressure and positive impulse curves.

Approaches analysis (3)

- TNO-multi energy versus CFD



$K_0 = 5.65,\ 11.3,\ 22.6,\ 33.9,\ 43.2$ m/s

$D_{\text{flam}}/c_{0,\text{cloud}} = 0.1,\ 0.2,\ 0.4,\ 0.6,\ 0.8$

Approaches analysis (4)

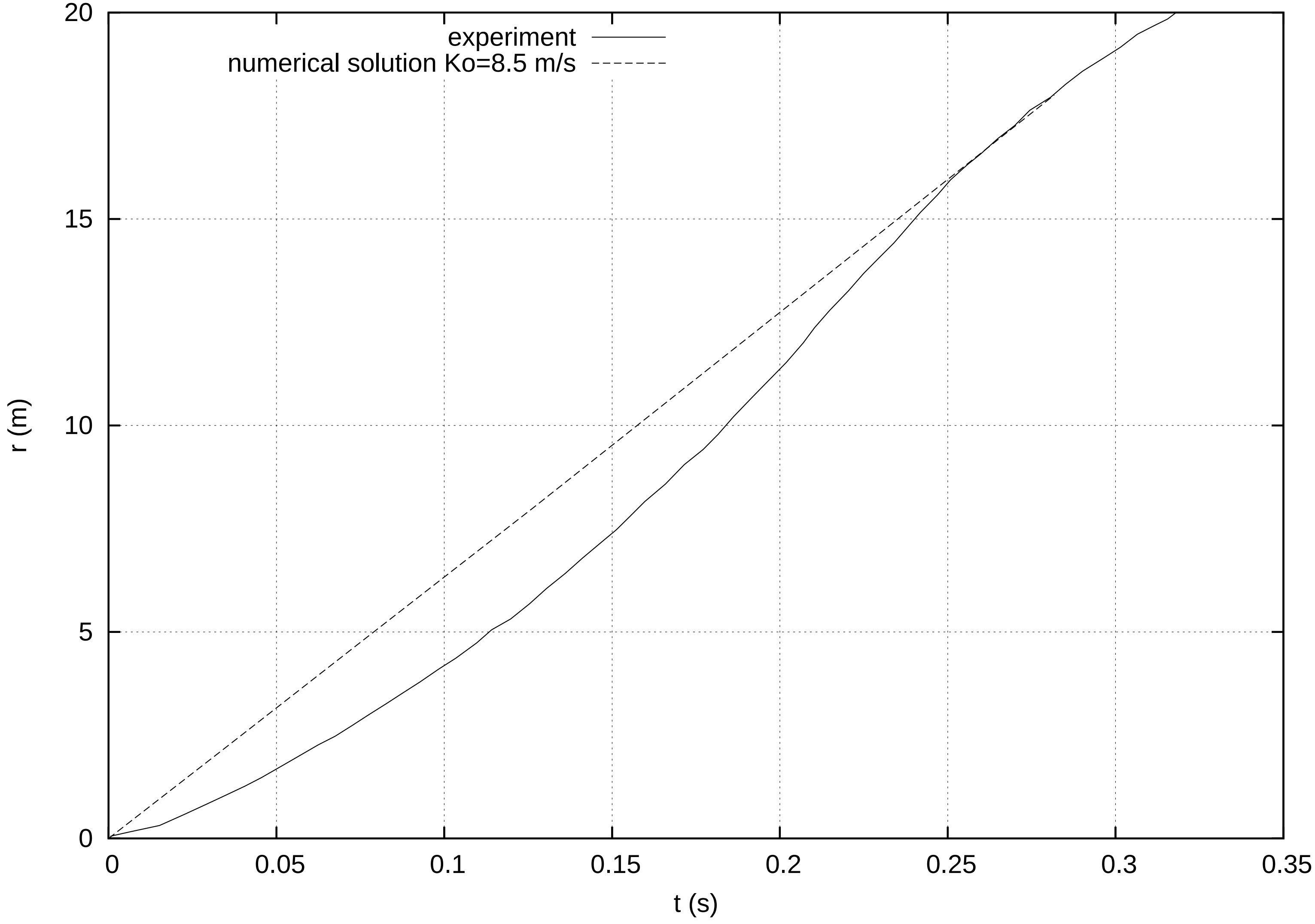
- TNO-multi energy method and CFD are comparable approaches.
  (TNO-multi energy data have been built using exact and numerical solutions!)

- TNO-multi energy does not correctly reproduce the "phase 2".
  Indeed, it does not involve any information concerning the physical properties of the cloud but its chemical energy.

- It is possible to establish a correlation between the strength index of the TNO-multi energy method and K_0.

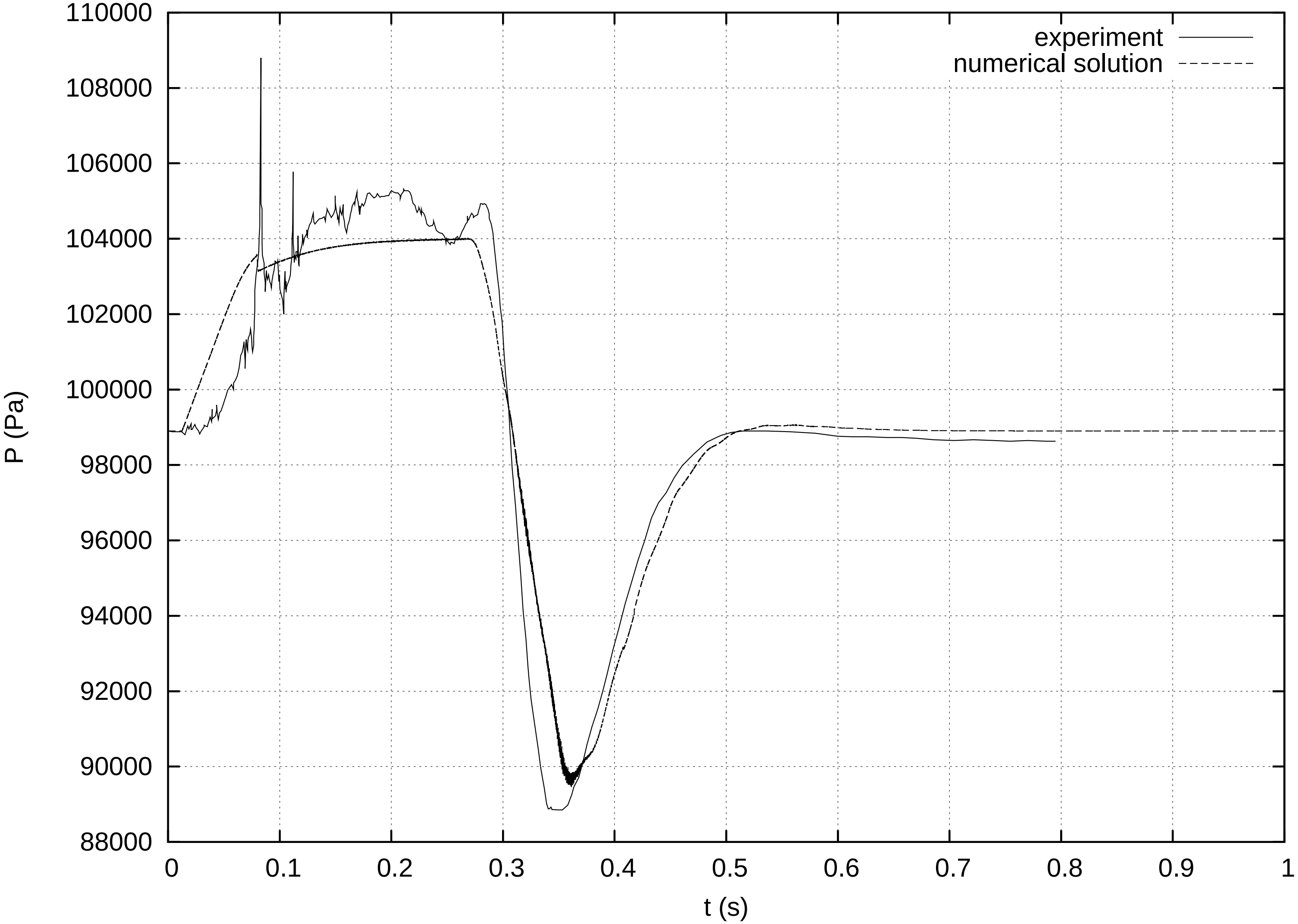
Approaches analysis (5)

- Experiment versus CFD ($K_0 = 8.5$ m/s)



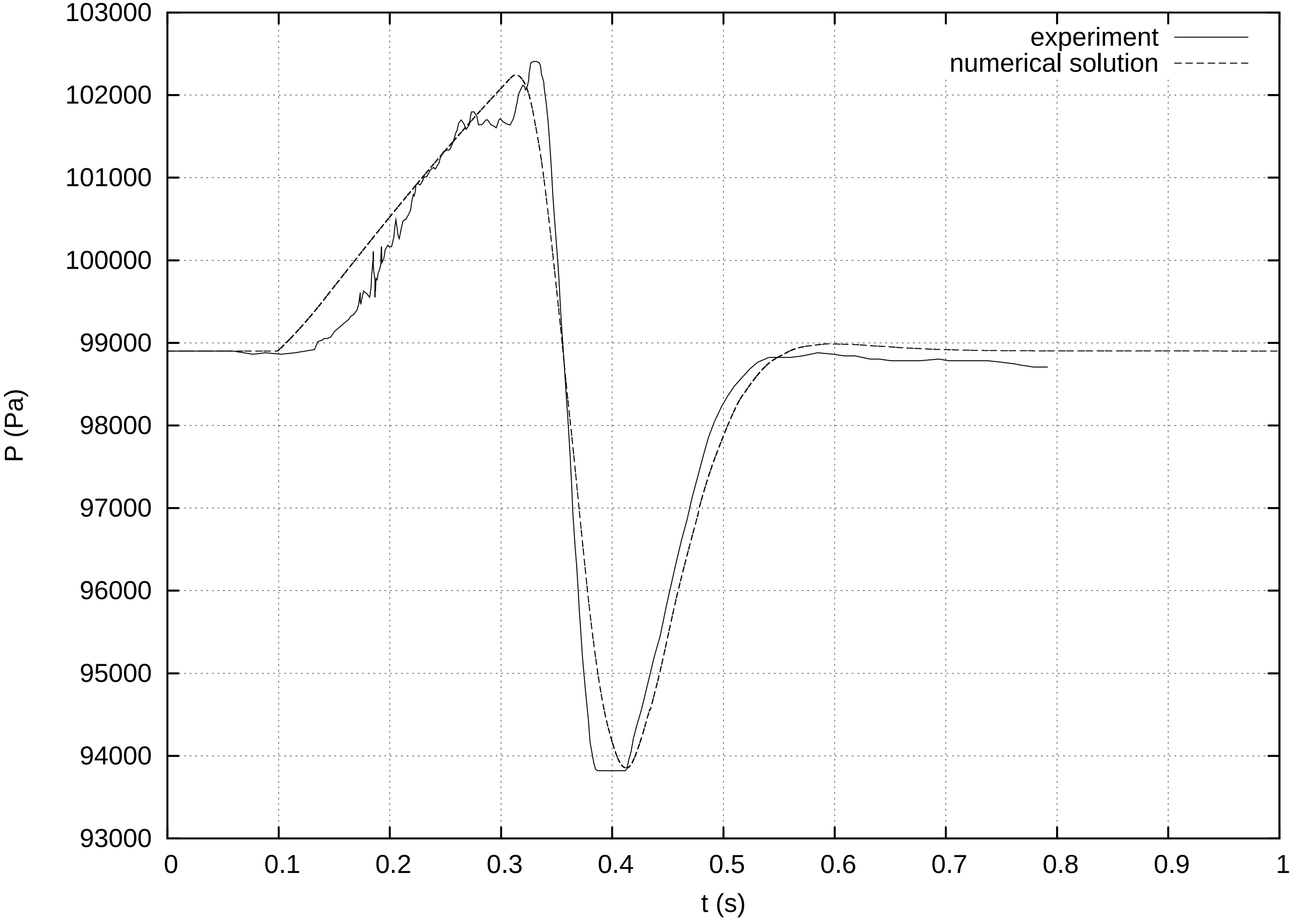
Approaches analysis (6)

- Experiment versus CFD ($K_0 = 8.5$ m/s, $r = 5$ m)



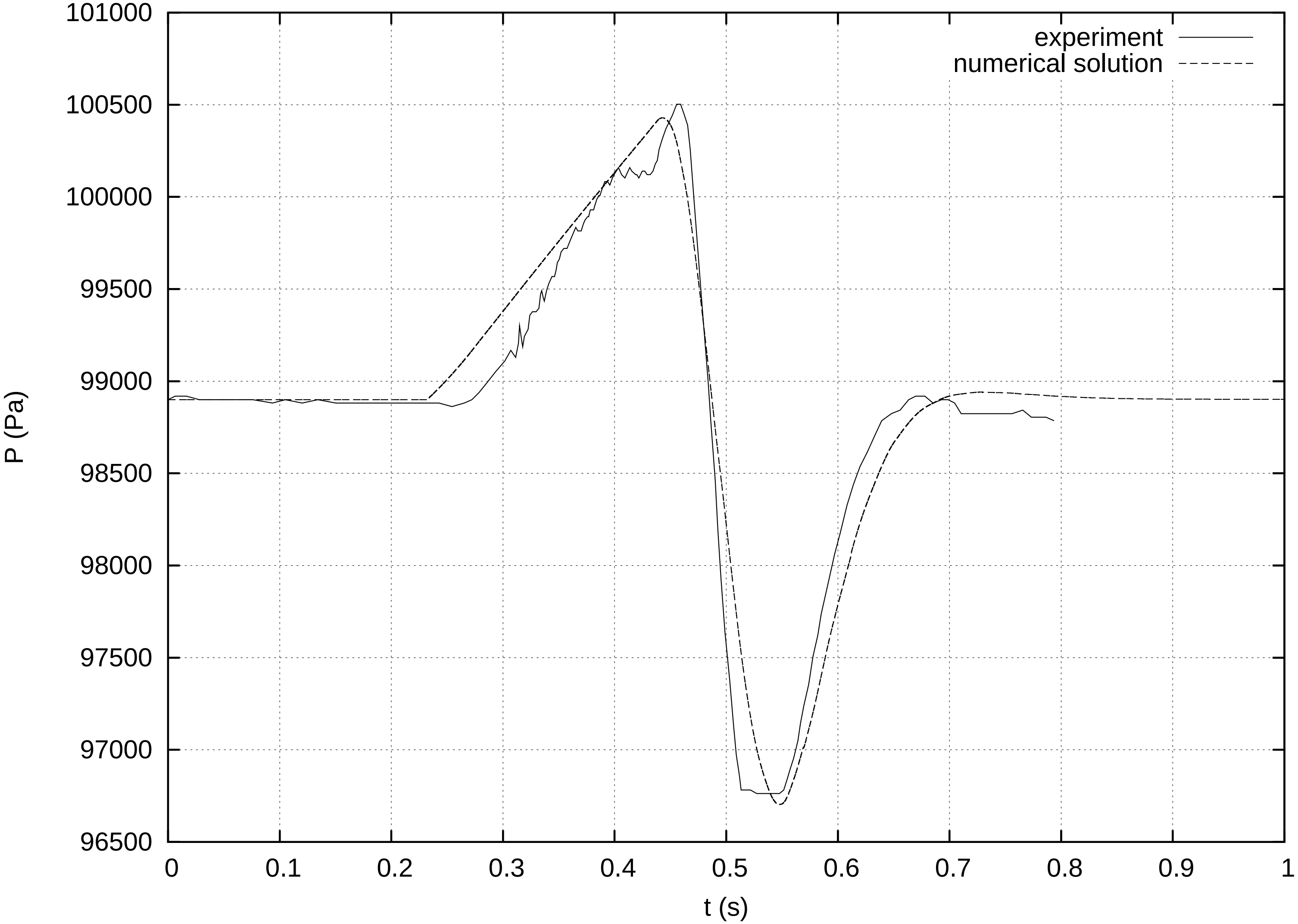
Approaches analysis (7)

- Experiment versus CFD ($K_0 = 8.5$ m/s, $r = 35$ m)



Approaches analysis (8)

- Experiment versus CFD ($K_0 = 8.5$ m/s, $r = 80$ m)



Approaches analysis (9)

- TNO-multi energy versus experiment
  - Following the TNO-multi energy approach, the index to take in this case is 1
  - CFD says that the fundamental velocity to take is 8.5 m/s, which corresponds to the index 3
  - It follows that TNO-multi energy approach underestimates the overpressure

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Summary and conclusion

- We have computed the solution of an hemispherical VCE.
- We have compared 3 existing approaches on this simple VCE.
- The TNT-equivalency approach is not a good candidate to evaluate the overpressure and the positive impulse in case of deflagrations.
- A part from a region close to the cloud, a correlation can be made between the TNO multi-energy strength factor and the fundamental flame speed.
- In this 1D problem, this 1D CFD approach gives good results if we take the correct value of the fundamental flame speed (the solution is very sensitive to its value).

Future work

- Maximum overpressure and positive impulse criteria are derived from tests with high explosives and can be applied **with confidence** only to steep rising shock waves [Galbraith 1998].

  Nevertheless we can use 1D CFD results as initial and boundary conditions for multi-dimensional CFD computations (analysis of isolated mechanical structures).

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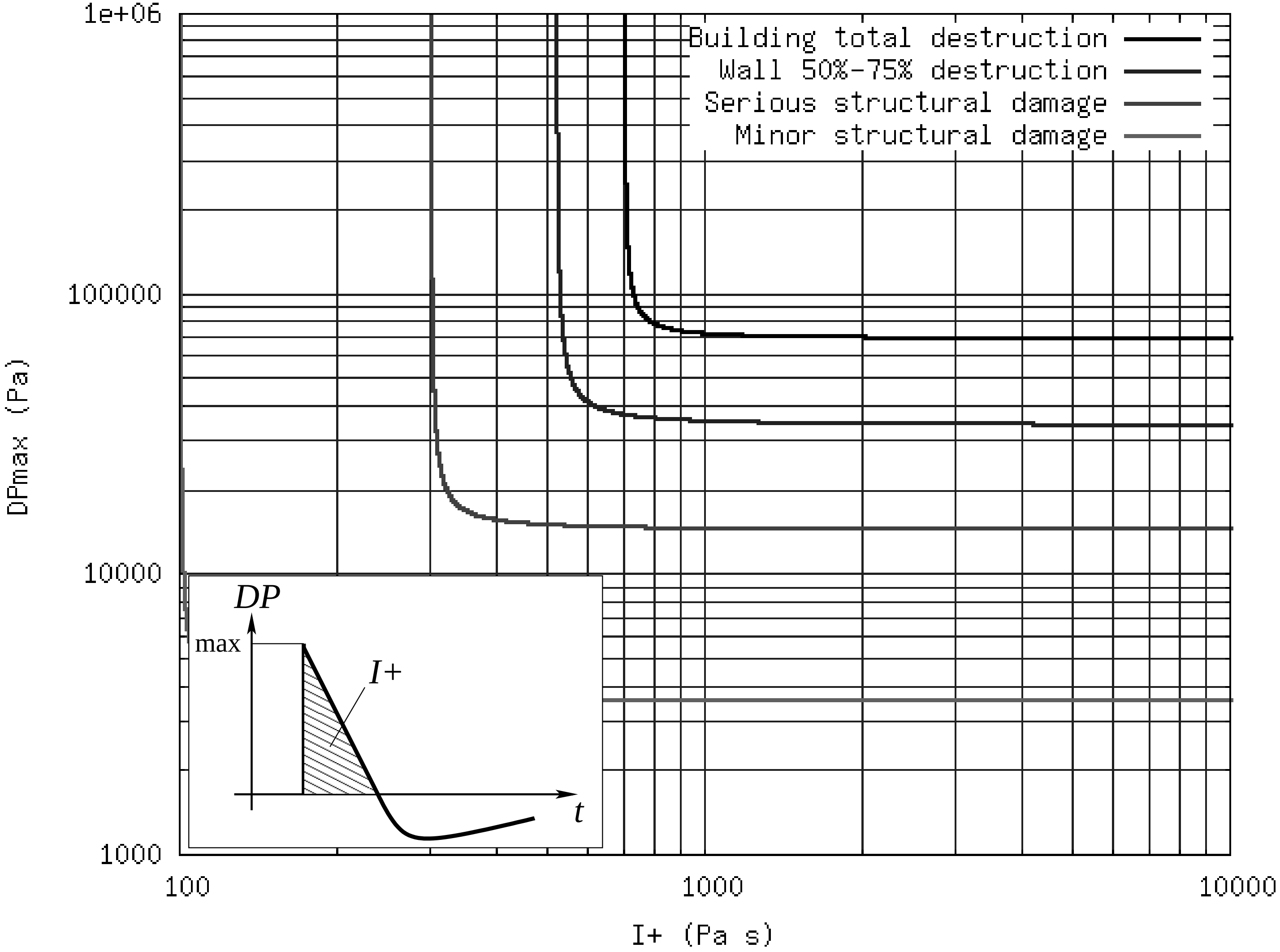
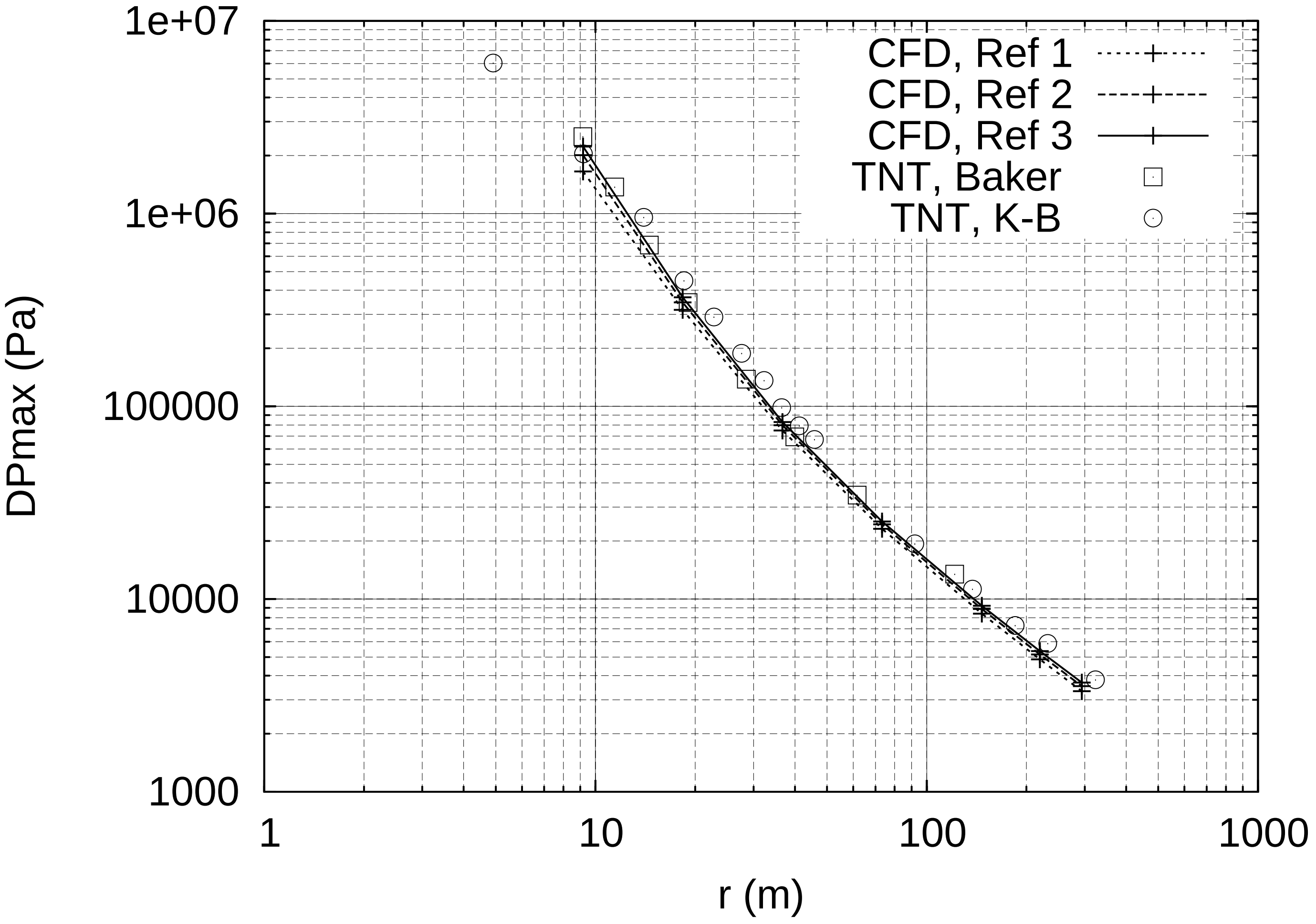
QUESTIONS

Criteria


Building total destruction
Wall 50%-75% destruction
Serious structural damage
Minor structural damage
1e+06
100000
10000
1000
DPmax (Pa)
100
1000
10000
I+ (Pa s)
DP
max
I+
t

Point explosion and TNT explosion (2)

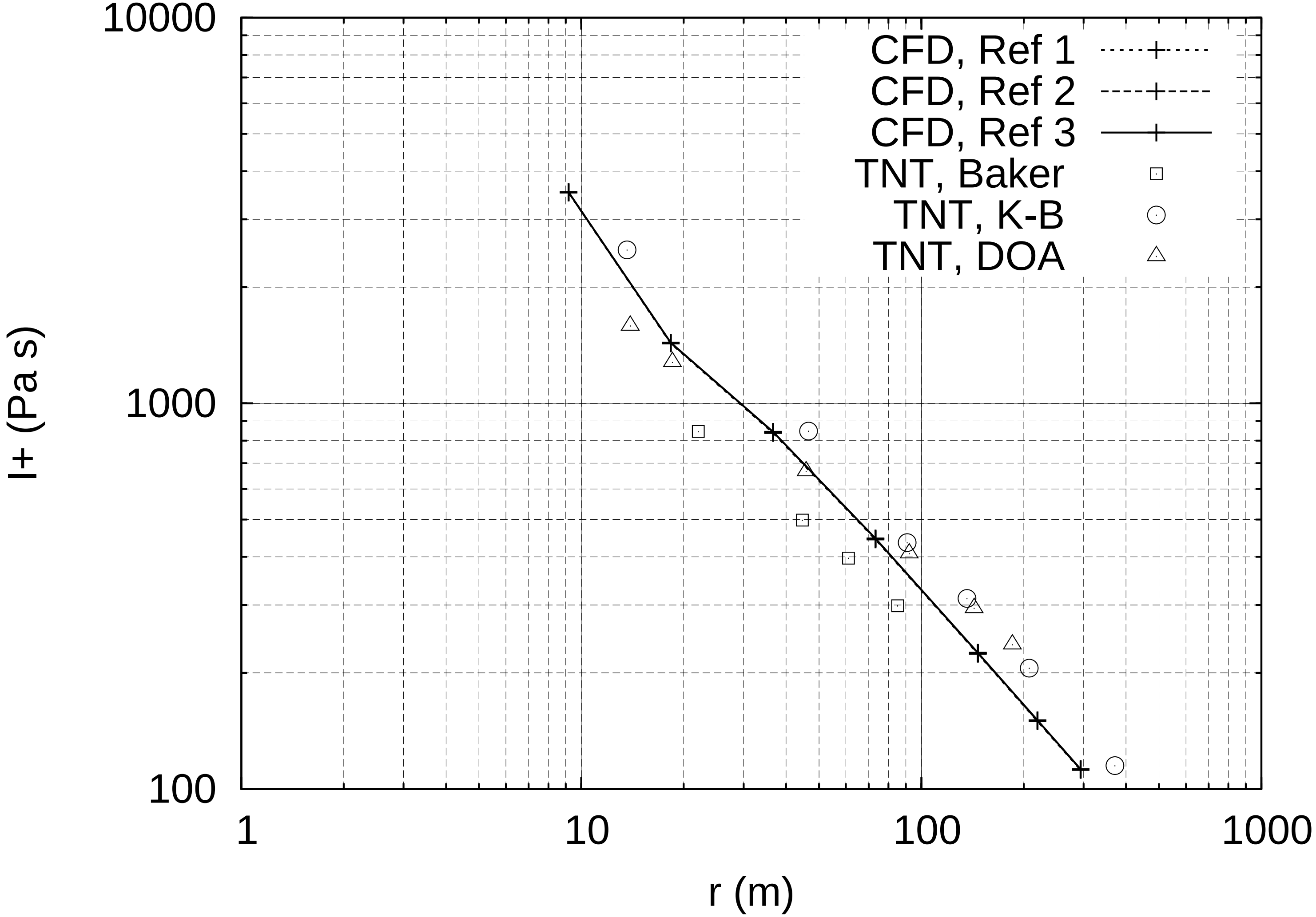


$E = 2 \cdot 6.29 \cdot 10^3\mathrm{MJ}$ (twice the chemical energy in the cloud)

Baker = [Baker 1983], K-B = [Kingery and Bulmash 1984],

$\Delta x_{\text{Ref i}} = \Delta x_{\text{Ref 1}}/2^{i-1}$

Point explosion and TNT explosion (3)



DOA = [DOA 1990]

Homogeneous 1D-point symmetrical deflagration

- We consider a 1D-point symmetrical flame propagating at constant velocity in a homogeneous medium.

- Problem solved by [Sedov 1959], [Kuhl 1973]

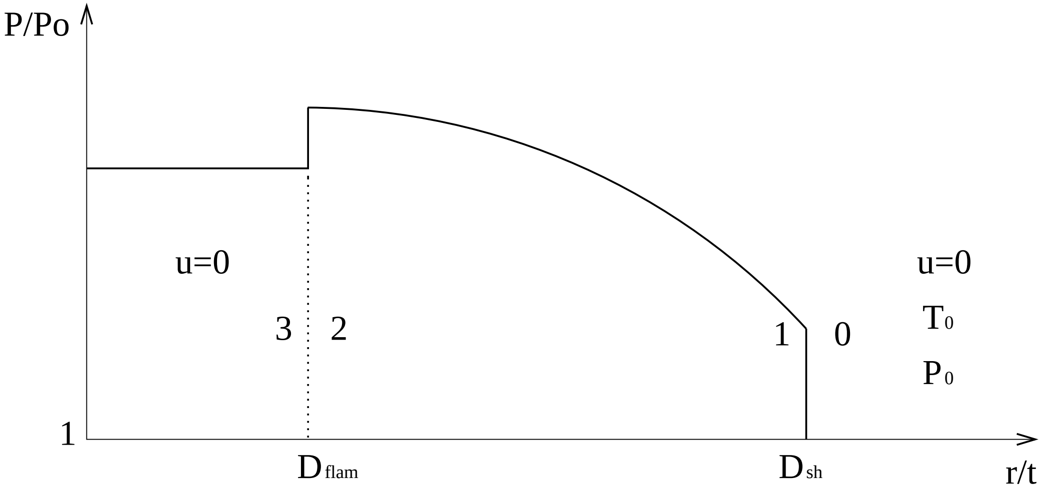
- In the case of calorically perfect gases, the solution depends on

Variable	SI units	Meaning
r	m	distance from the center
t	s	time
K_0	m/s	fundamental flame speed
P_0	J/m^3	“unperturbed” pressure
c_0	m/s	“unperturbed” sound speed
q	J/kg	released heat per unit mass
γ_u		specific heat ratio in unburnt region
γ_b		specific heat ratio in burnt region

Homogeneous 1D-point symmetrical defl. (2)

- We take as 3 reference quantities t, P_0 and c_0; it follows that the non-dimensional solution can be expressed as function of

$$\frac{r}{c_0 t},\ \frac{q}{c_0^2},\ \frac{K_0}{c_0},\ \gamma u,\ \gamma_b$$



$$D_{\text{flam}} = \frac{\rho_2}{\rho_3} K_0 = \sigma K_0, \quad D_{\text{sh}} > c_0, \quad u_2 = D_{\text{flam}} - K_0$$

- The lower the flame speed, the larger the ratio $D_{\text{sh}}/D_{\text{flam}} \approx c_0/D_{\text{flam}}$.

Test problem: dimensional analysis

- We have a 10 m radius hemisphere with inside a stoichiometric mixture of H_2-air at almost atmospheric conditions

$$P = 0.989 \text{ bar},\ T = 283 \ \text{ K}$$

- Inside the cloud (hemisphere)

$$(X_{\mathrm{H_2}}, X_{\mathrm{N_2}}, X_{\mathrm{O_2}}) = (0.296, 0.556, 0.148)$$

$$(Y_{\mathrm{H_2}}, Y_{\mathrm{N_2}}, Y_{\mathrm{O_2}}) = (0.0283, 0.745, 0.2267)$$

$$R = 398 \text{ J/kg/K},\ \rho = 0.879 \text{ kg/m}^3,\ c = 405 \text{ m/s}$$

$$m_{\mathrm{H_2}} = 52 \text{ kg},\ q_{\mathrm{H_2}} = 121 \cdot \text{MJ/kg (NIST)}$$

$$Q = 6.29 \cdot 10^3 \text{ MJ},\ q = 3.42 \cdot \text{MJ/kg}$$

- Outside the cloud

$$(X_{\mathrm{N_2}}, X_{\mathrm{O_2}}) = (0.79, 0.21)$$

$$(Y_{\mathrm{N_2}}, Y_{\mathrm{O_2}}) = (0.767, 0.233)$$

$$R = 288 \text{ J/kg/K},\ \rho = 1.21 \text{ kg/m}^3,\ c = 338 \text{ m/s}$$

Test problem: dimensional analysis (2)

- After an Adiabatic Isobaric Complete Combustion (AIBCC), using JANAF tables and supposing to deal with the one-global reaction only, we obtain

$$Y_{\mathrm{N_2}} = 0.745,\ Y_{\mathrm{H_2O}} = 0.255$$

	ρ	P (bar)	T	c	R	γ	$\bar{\gamma}$
Inside	0.878	0.989	283	405	398	1.41	1.42
AIBCC	0.116	0.989	2510	1030	339	1.24	1.29

(in SI units)

where

$$\gamma = \frac{\sum_i Y_i c_{p,i}}{\sum_i Y_i c_{v,i}}$$

$$\bar{\gamma} = 1 + \frac{P}{\rho \sum_i Y_i \int_0^T c_{v,i}(\xi)\mathrm{d}\xi}$$

Test problem: dimensional analysis (3)

- Characteristic scales for velocity

Meaning	Formula	Value
fundamental flame speed	K_0	^{a}
flame speed in the laboratory	$D_{\text{flame}} = \frac{\rho_u}{\rho_b} K_0$	^{a}
sound speed in the unburnt gas	c_{u}	405 m/s
sound speed in the burnt gas	c_{b}	1030 m/s
sound speed outside	c_{out}	338 m/s

[a] Example (Fraunhofer experiment)
$D_{\text{flame,av}} = 63,\ D_{\text{flame,max}} = 80,\ K_{0,\text{av}} = 8.5,\ K_{0,\text{max}} = 10.5$ m/s

Test problem: dimensional analysis (4)

- Characteristic scales for the distance

Meaning	Formula	Value
energy based length	$\left(\frac{2Q}{P_0}\right)^{1/3}$	50.3 m
initial sphere radius	r_{surf}	10.0 m
final sphere radius	$r'_{\text{surf}} = r_{\text{surf}} \left(\frac{\rho_u}{\rho_b}\right)^{1/3}$	19.6 m
acoustic distance	$r_{\text{acou}} \approx \frac{c_{\text{out}}}{D_{\text{flame}}} r'_{\text{surf}}$	105 m[b]

[b] For $D_{\text{flame,av}} = 63$ m/s, $c_{\text{out}}/D_{\text{flame,av}} = 338/63 = 5.37$

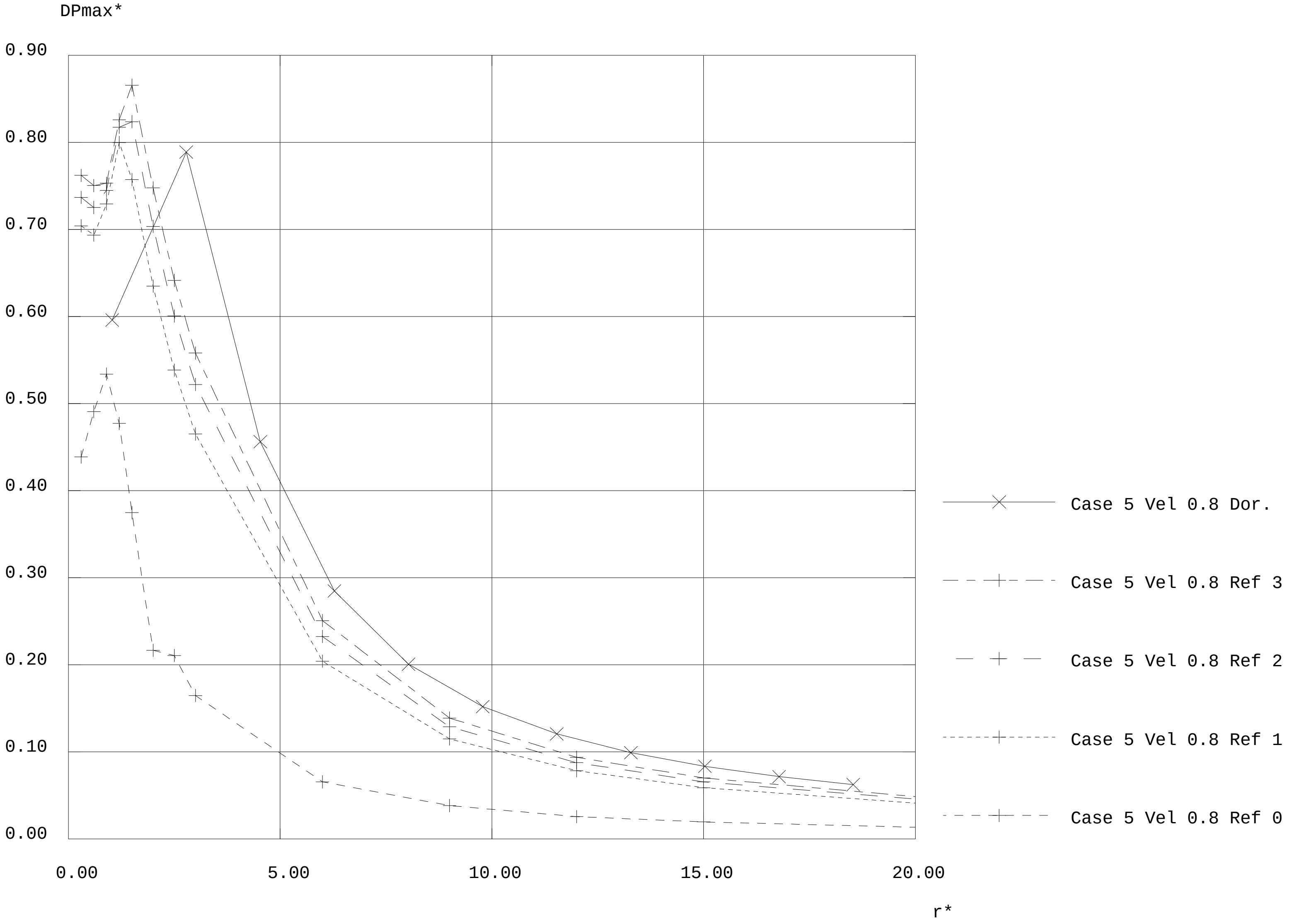
Test problem: Mesh refinement

- 4 regularly refined meshes.
  - 20 elements inside the cloud, 600 elements outside (in 3D $600^3 \approx$ 200E6 elements).
  - 200 elements inside the cloud, 6000 elements outside (in 3D $6000^3 \approx$ 200E9 elements).
  - 400 elements inside the cloud, 12000 elements outside (in 3D $12000^3 \approx$ 2E12 elements).
  - 800 elements inside the cloud, 24000 elements outside (in 3D $24000^3 \approx$ 10E12 elements).

- Because of operator splitting error, the results on the coarse mesh are very different from the others.

- CPU time consumption. 6h on a Linux PC for the finest mesh (500000 time steps).

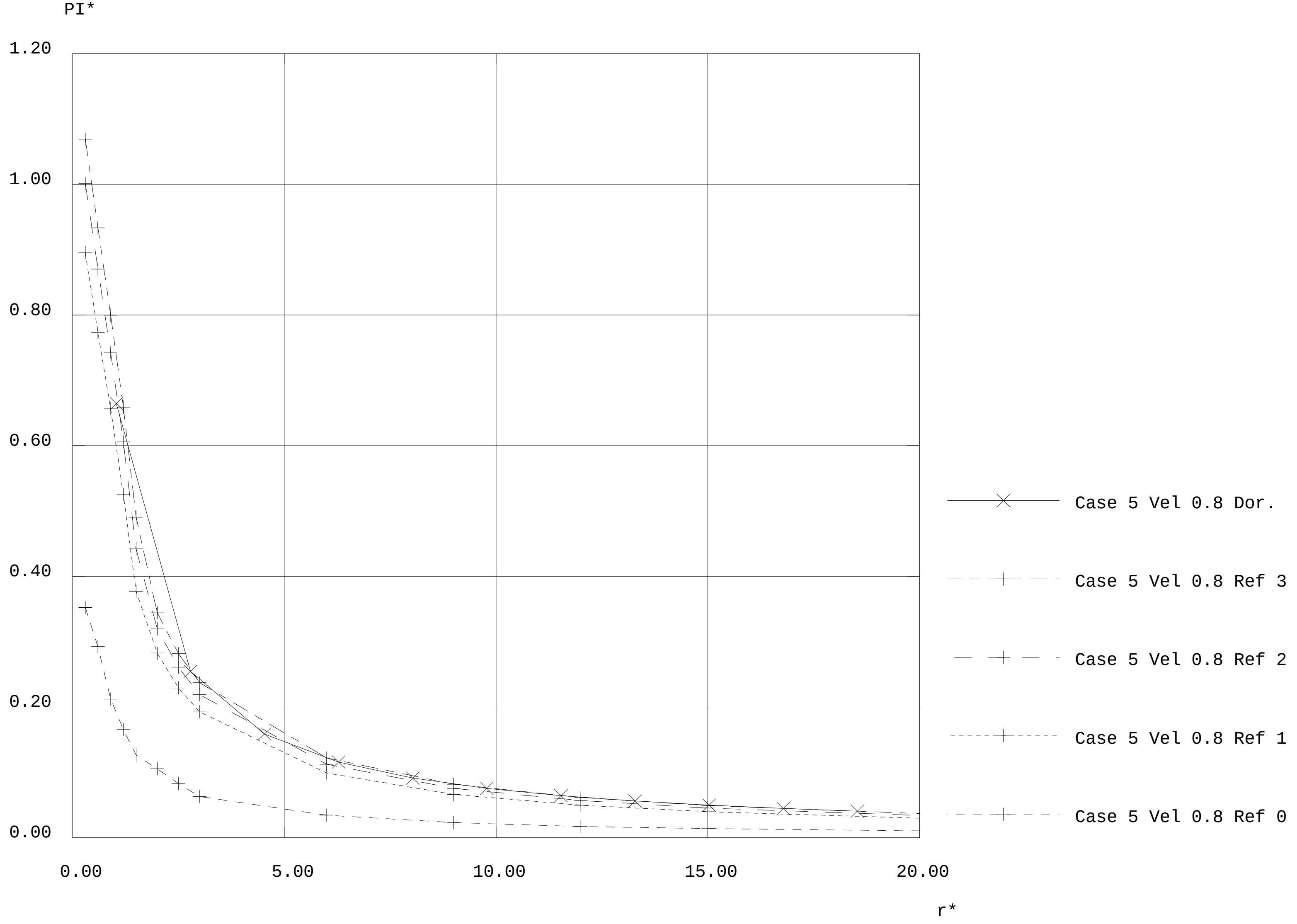
Test problem: Sensitivity analysis



$r^* = r/r_{\text{hemis}}$

$DP^*_{\text{max}} = DP_{\text{max}}/P_0$

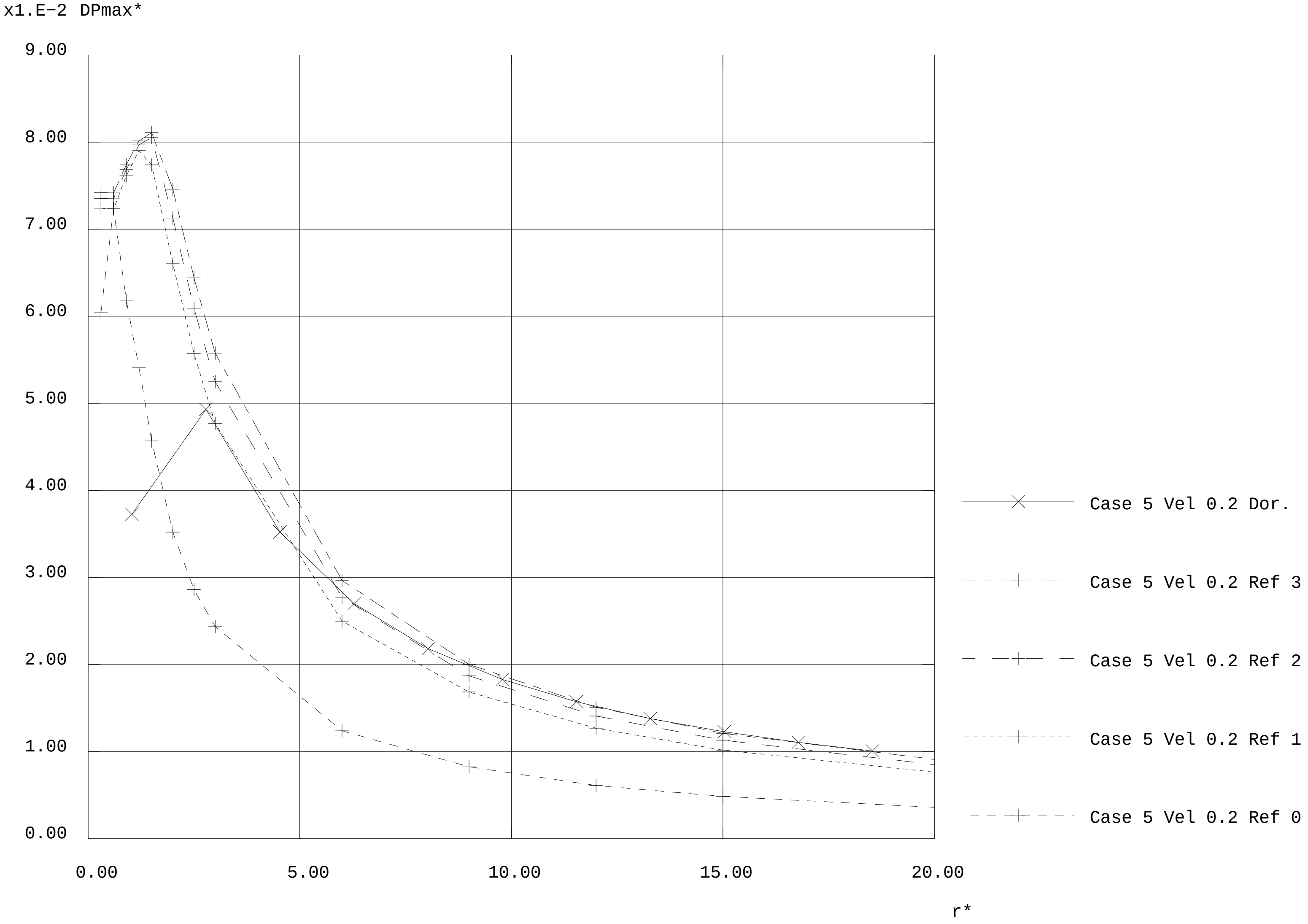
Test problem: Sensitivity analysis (2)



$r^* = r/r_{\text{hemis}}$

$PI^* = (I + c_0)/(r_{\text{hemis}} P_0)$

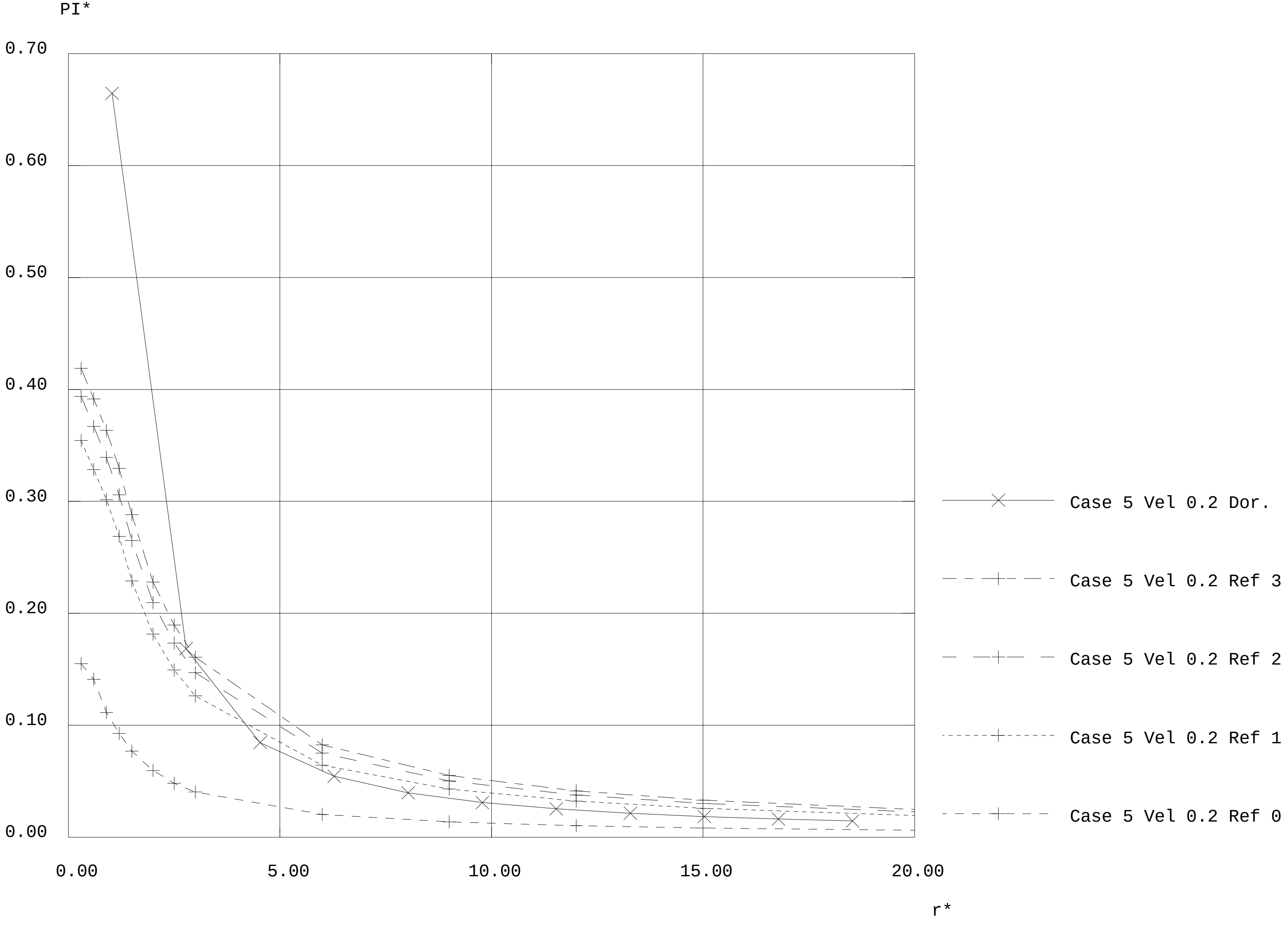
Test problem: Sensitivity analysis (3)



$r^* = r/r_{\text{hemis}}$

$DP^*_{\text{max}} = DP_{\text{max}}/P_0$

Test problem: Sensitivity analysis (4)



$r^* = r/r_{\text{hemis}}$

$PI^* = (I + c_0)/(r_{\text{hemis}} P_0)$

Test problem: Sensitivity analysis (5)