The need for research in the field of gas phase detonation as seen by BASF

Dr. Hans-Peter Schildberg
BASF SE
GCT/S - L511
D-67056 Ludwigshafen
Email: hans-peter.schildberg@basf.com
Tel: +49 (0) 621 60-56049

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Need to quantify the mechanical load associated with gas phase detonations

persistent efforts to increase productivity necessitate access to process parameters (P, T, gas phase composition) even in hitherto uncommon ranges

steadily increasing standards on process safety are to be heeded.

Process engineering has a vital interest to quantifiy the mechanical load associated with gas phase detonations as precise as possible

<u>for all possible effects</u> and <u>for all possible geometries</u>.

for all possible effects:
- DDT
- Reflection
- Taylor expansion fan
- precompression
- „surface detonations“

for all possible geometries:
- long pipes
- short pipes
- vessels
- vessel with attached pipes
- dry packings
- irrigated packings
- columns (alternating: packing - free space)
- bubble columns

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Outline of talk

- Design basis for detonation pressure proof pipes
  (already shown in Talk of 41st UKELG meeting)
- Side-on pressure at point of DDT: how large really compared to side-on pressure of stable detonation?
- Reflected shock wave: how long has to be the enforced pipe end?
- Static equivalent pressure: which value, in particular for high-strength materials?
- Is the scenario „DDT directly ahead of a blind flange" realistic?
- Under what circumstances can there be a DDT in bubble columns in case of injection of pure O_2 into the organic liquid?

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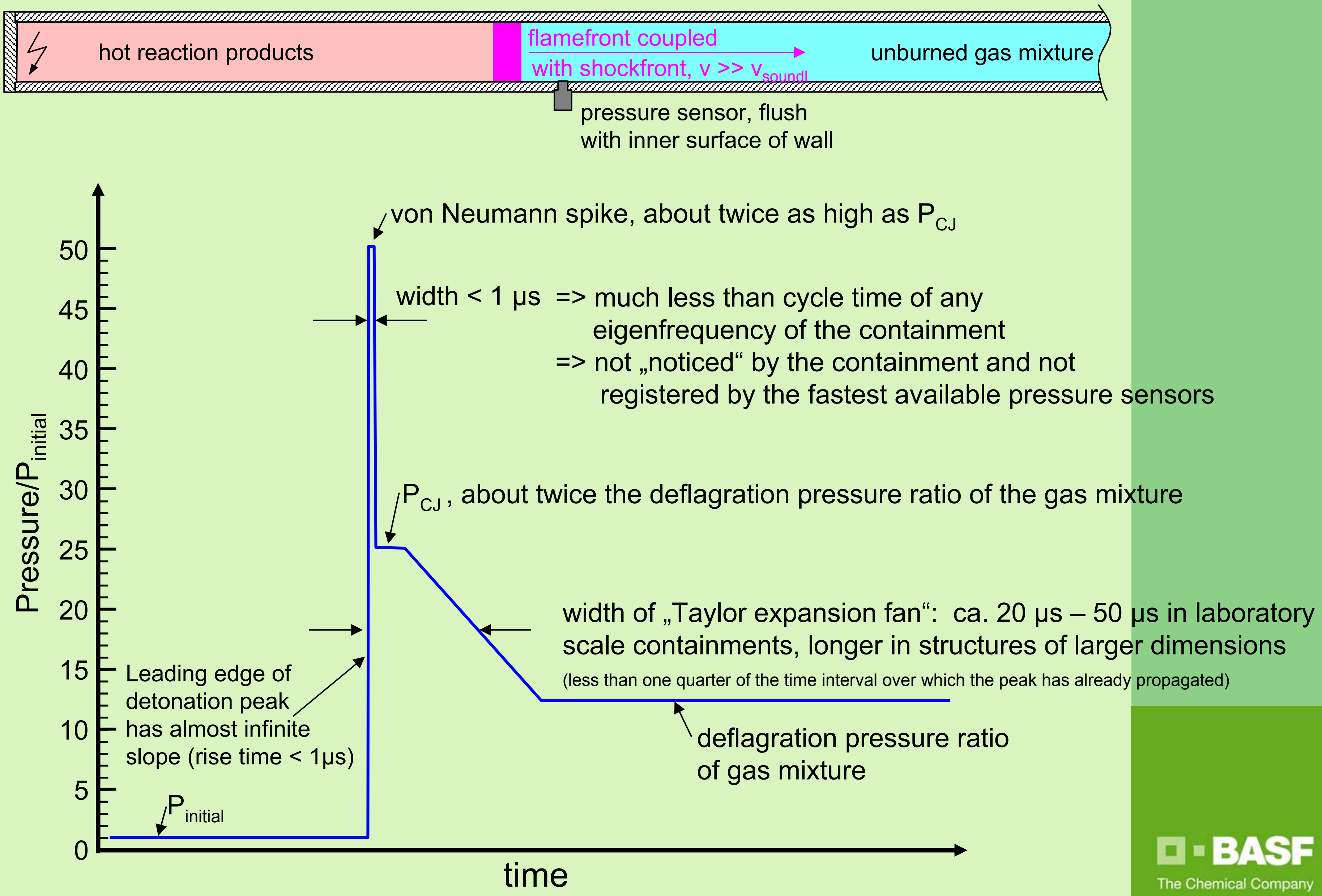
Schematic pressure-time trace of a detonative pressure pulse



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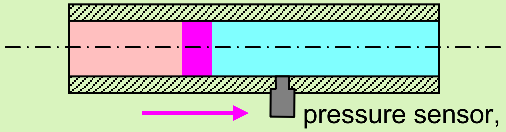
Detonation pressures P_{det} in long pipes ($L >> L_{predet}$, no precompression)

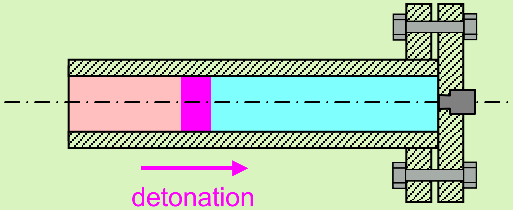
● **Stable Detonation, side-on pressure (i. e. in plane perpendicular to shockfront)**



$$P_{det} = P_{initial} * P_{CJ}$$

P_{CJ} is the so-called
Chapman-Jouguet-pressure ratio
of the explosive gas mixture

● **Stable Detonation, reflected pressure (i. e. in plane parallel to shockfront, e. g. blind flange)**



$$P_{det} = P_{initial} * P_{CJ} * F_{reflec}$$

$$2 \leq F_{reflec} \leq 2.5$$

Important:
The pipe directly ahead of the blind flange experiences the reflected pressure as well. The length of this section corresponds to the axial extension of the taylor expansion fan.
(In lab-scale equipment of up to 5 m length a section of about 3 pipe diameters from the blind flange back into the pipe is affected, in longer pipes this section increases).

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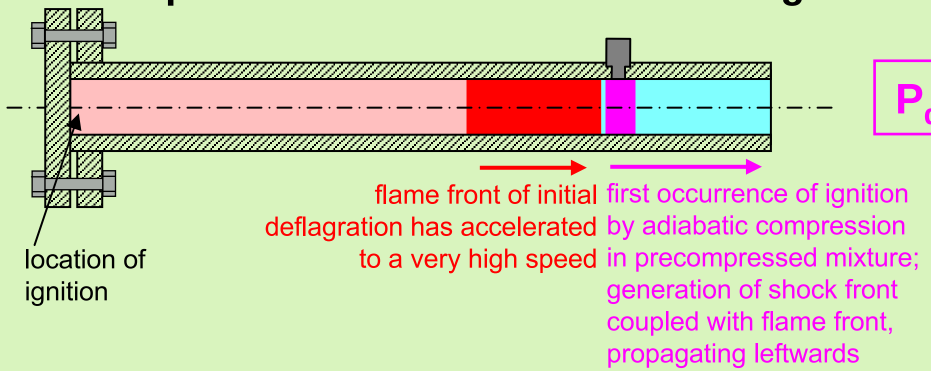
Detonation pressures P_{det} in long pipes ($L >> L_{predet}$, no precompression) (continued)

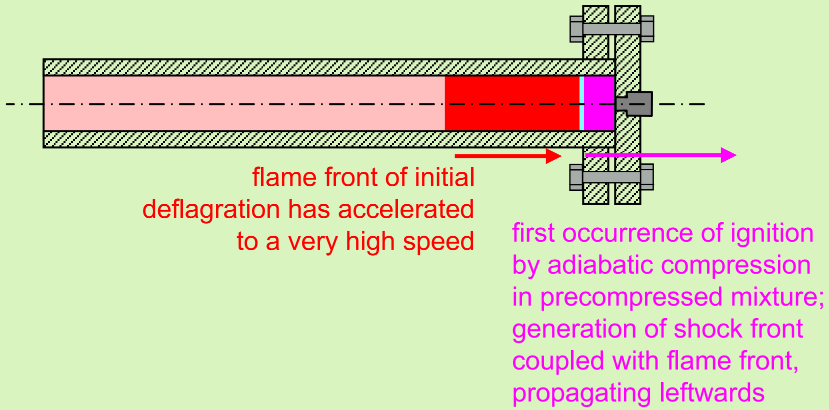
● **Side-on pressure at location where Deflagration-to-Detonation transition (DDT) occurs**



$$P_{det} = P_{initial} * P_{CJ} * F_{DDT}$$

$$1.5 \le F_{DDT} \le 2$$

● **Reflected pressure, if DDT occurs directly in front of blind flange (a very rare case!)**



$$P_{det} = P_{initial} * P_{CJ} * F_{DDT} * F_{reflec}$$

$$1.5 \le F_{DDT} \le 2$$

$$2 \le F_{reflec} \le 2.5$$

Important:
The pipe directly ahead of the blind flange experiences the reflected pressure as well. The length of this section corresponds to the axial extension of the taylor expansion fan.
(In lab-scale equipment of up to 5 m length a section of about 3 pipe diameters from the blind flange back into the pipe is affected, in longer pipes this section increases).

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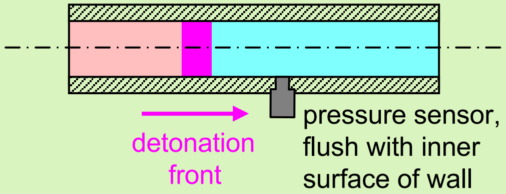
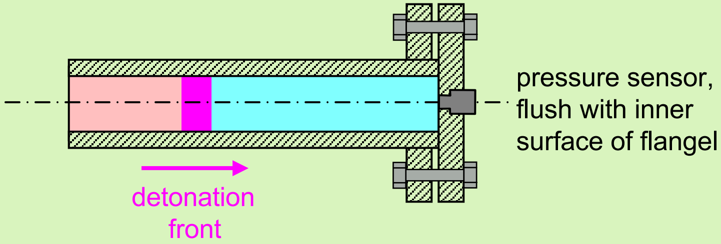
Detonation pressures P_{det} in pipes with precompression (1/2)

● **Side-on pressure (i. e. in plane perpendicular to shockfront)**



$$P_{det} = P_{initial} * P_{CJ} * F_{precomp} * F_{temp}$$

● **Reflected pressure (i. e. in plane parallel to shockfront, e. g. blind flange)**



$$P_{det} = P_{initial} * P_{CJ} * F_{reflec} * F_{precomp} * F_{temp}$$

Important:
about 3 pipe diameters from the blind flange back into the pipe this higher pressure also acts on the wall of the pipe!

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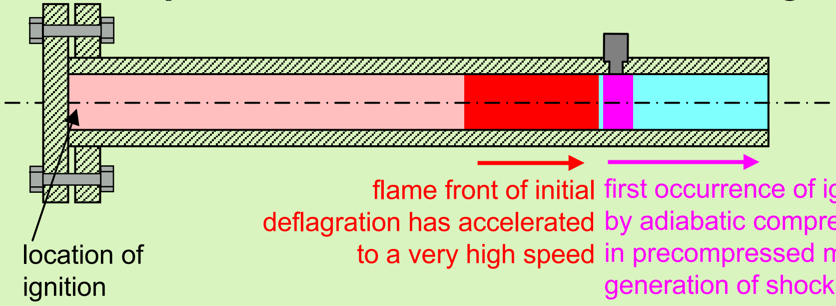
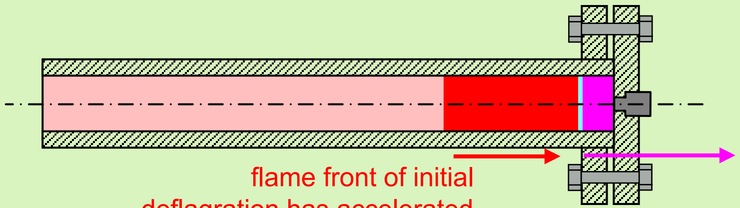
Detonation pressures P_{det} in pipes with precompression (2/2)

- **Side-on pressure at location where Deflagration-to-Detonation transition (DDT) occurs**



$$P_{det} = P_{initial} * P_{CJ} * F_{DDT} * F_{precomp} * F_{temp}$$

- **Reflected pressure, if DDT occurs directly in front of blind flange (a very rare case!)**



$$P_{det} = P_{initial} * P_{CJ} * F_{DDT} * F_{reflec} * F_{precomp} * F_{temp}$$

Important:
about 3 pipe diameters from the blind flange back into the pipe this higher pressure also acts on the wall of the pipe!

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Detonation pressure P_{det} acting on the wall of a vessel (almost always with precompression)

P_{det} = Initial pressure in vessel at moment of ignition ($P_{initial}$)

x Chapman-Jouguet pressure ratio of the mixture at the temperature the mixture exhibits at the moment of ignition (P_{CJ})

x Precompression factor ($F_{Precomp}$)

x Temperature factor (F_{Temp})

x Factor accounting for reflection of stable detonation at wall (F_{reflec})

x Factor accounting for extra pressure if DDT happens directly before wall (F_{DDT}), otherwise factor is 1

$P_{det} = P_{initial} * P_{CJ} * F_{precomp} * F_{temp} * F_{reflec} *$ (F_{DDT} or 1, depending on where DDT happened**)**

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Example: Detonative pressure pulses P_{det} acting on the wall of a 20 l sphere in case of Propene/O_2/N_2, $P_{initial}$ = 5 bar abs, $T_{initial}$ = 25°C

$$P_{det} = 5 bar abs \cdot 20 \cdot 10 \cdot \left(\frac{1}{10}\right)^{(1.4-1)/1.4} \cdot 2.25 \cdot 1.75 = 2039 bar abs$$

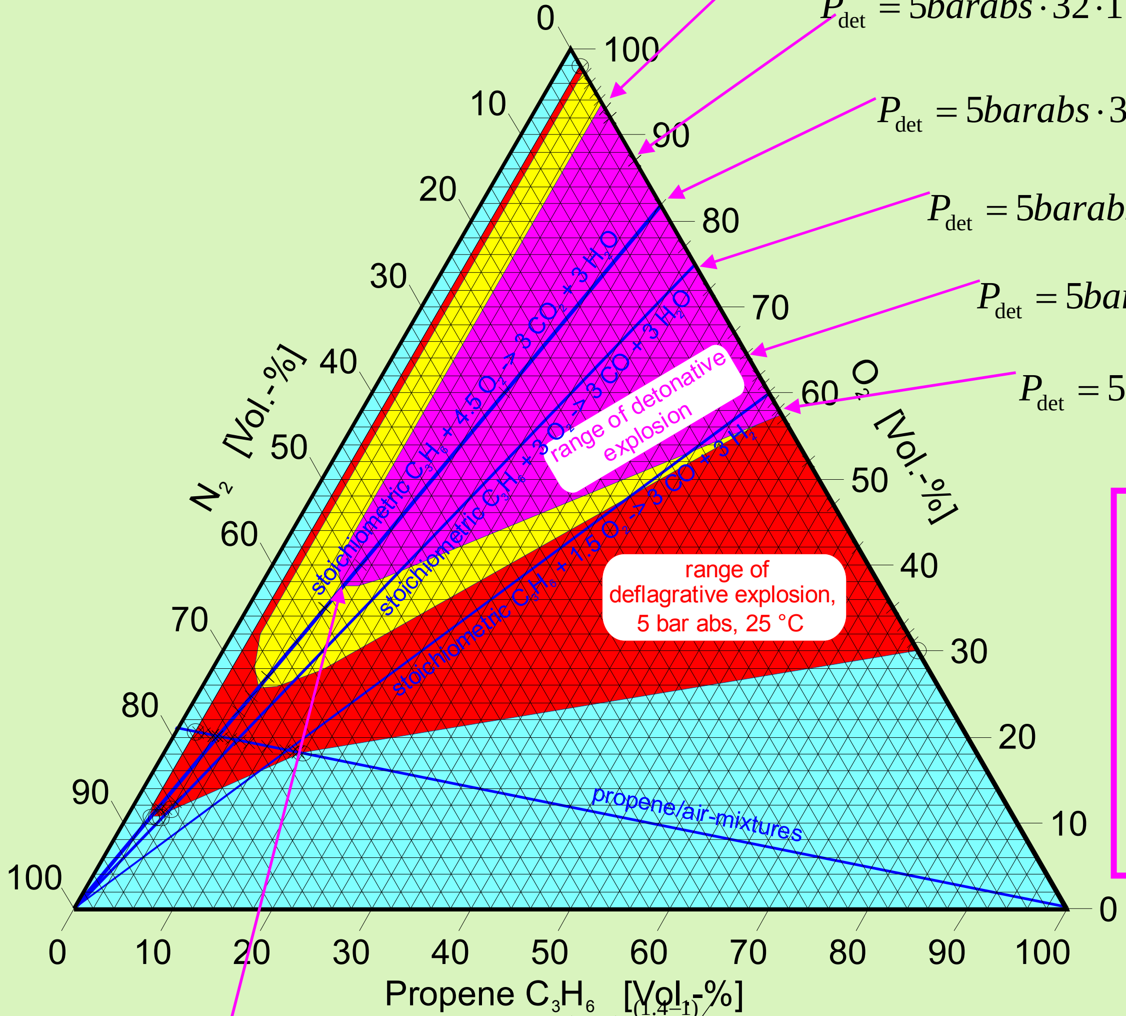
$$P_{det} = 5 bar abs \cdot 32 \cdot 1.1 \cdot \left(\frac{1}{1.1}\right)^{(1.4-1)/1.4} \cdot 2.25 \cdot 1 = 385 bar abs$$

$$P_{det} = 5 bar abs \cdot 37 \cdot 1 \cdot \left(\frac{1}{1}\right)^{(1.4-1)/1.4} \cdot 2.25 \cdot 1 = 416 bar abs$$

$$P_{det} = 5 bar abs \cdot 44 \cdot 1 \cdot \left(\frac{1}{1}\right)^{(1.4-1)/1.4} \cdot 2.25 \cdot 1 = 495 bar abs$$

$$P_{det} = 5 bar abs \cdot 47 \cdot 4 \cdot \left(\frac{1}{4}\right)^{(1.4-1)/1.4} \cdot 2.25 \cdot 1 = 1627 bar abs$$

$$P_{det} = 5 bar abs \cdot 40 \cdot 20 \cdot \left(\frac{1}{20}\right)^{(1.4-1)/1.4} \cdot 2.25 \cdot 1.75 = 6692 bara$$



$$P_{det} = 5 bar abs \cdot 27 \cdot 13 \cdot \left(\frac{1}{13}\right)^{(1.4-1)/1.4} \cdot 2.25 \cdot 1.75 = 3320 bar abs$$

Pressure at border line of detonative range about factor 6 to 17 larger than in center because of precompression.

The highest value attainable by $P_{det}/P_{initial}$ is about 1300 !!

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- Design basis for detonation pressure proof pipes
  (already shown in Talk of 41st UKELG meeting)
- Side-on pressure at point of DDT: how large really compared to side-on pressure of stable detonation?
- Reflected shock wave: how long has to be the enforced pipe end?
- Static equivalent pressure: which value, in particular for high-strength materials?
- Is the scenario „DDT directly ahead of a blind flange“ realistic?
- Under what circumstances can there be a DDT in bubble columns in case of injection of pure O_2 into the organic liquid?

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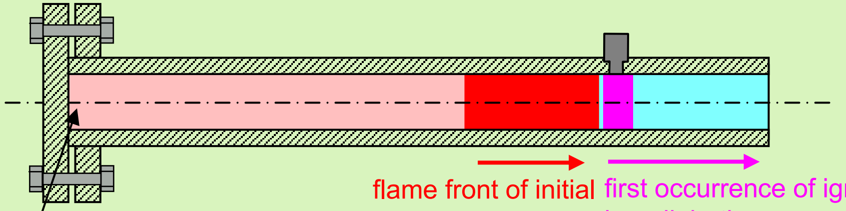
Present estimate for side on pressure at location of DDT



$P_{det} = P_{initial} * P_{CJ} * F_{DDT}$

$1.5 \leq F_{DDT} \leq 2$

Side-on pressure at location where Deflagration-to-Detonation transition (DDT) occurs is by a factor 1.5 to 2 larger than side-on pressure of stable detonation

Problem: data base still very unsatisfactory

- Nowhere reliable quantification of side-on pressure at location of DDT
- Rare number of documented cases where deformation was observed in a pipe which could be associated with the DDT. These cases suggest $1.5 \leq F_{DDT} \leq 2$
- Own (but also rare) indirect experience with pipe deformation technique is compatible with $1.5 \leq F_{DDT} \leq 2$.
  („indirect“ means: initial pressure of gas mixture in detonation tests successively increased until first deformation in front of the blinded pipe occurs. In these cases no deformation could be found somewhere else in the pipe => side-on pressure at DDT seems to be less than reflected pressure)
- Reliable quantification only seems to be possible with pipe deformation technique, since pressure sensors are never positioned at point of highest load and even if so, the measured pressure values exhibit large error bars.

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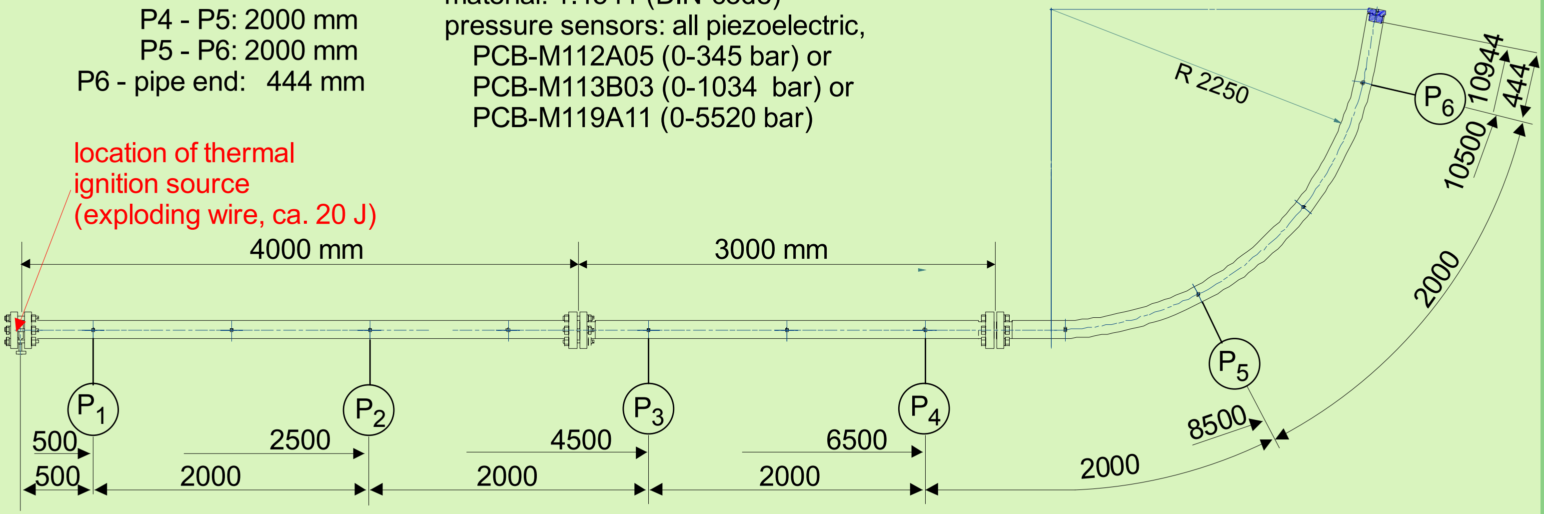
Experimental setup for examples 1 and 2 related to side-on pressure at point of DDT

Distances:

ignition source - P1: 500 mm
P1 - P2: 2000 mm
P2 - P3: 2000 mm
P3 - P4: 2000 mm
P4 - P5: 2000 mm
P5 - P6: 2000 mm
P6 - pipe end: 444 mm

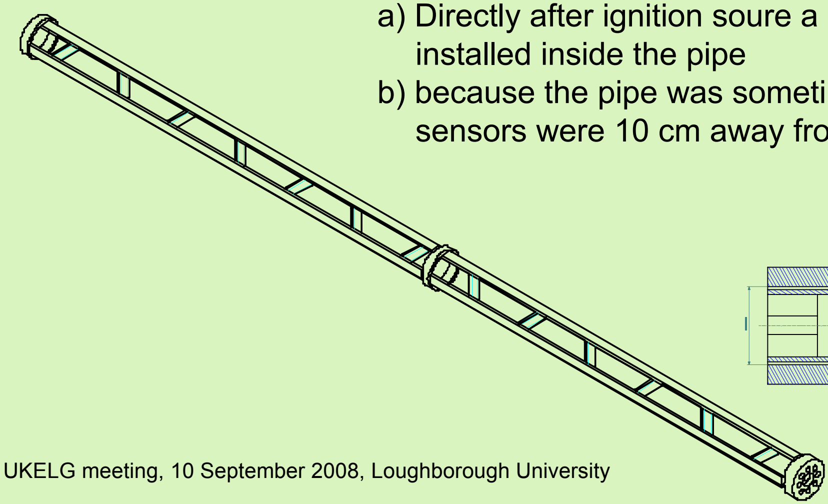
Pipe and pressure sensors:

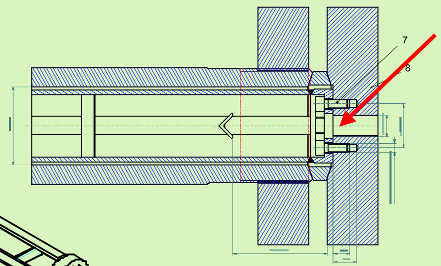
total length of pipe: 10.944 m
individual segments: 4m, 3m and 3.944m
inner and outer diameter: ϕ_i = 86 mm, ϕ_o = 127 mm
material: 1.4541 (DIN-code)
pressure sensors: all piezoelectric,
PCB-M112A05 (0-345 bar) or
PCB-M113B03 (0-1034 bar) or
PCB-M119A11 (0-5520 bar)



Note:

a) Directly after ignition soure a 2 m long turbulence enhancer was installed inside the pipe
b) because the pipe was sometimes heated to 220 °C, pressure sensors were 10 cm away from inner wall, access via a 6x1 pipe





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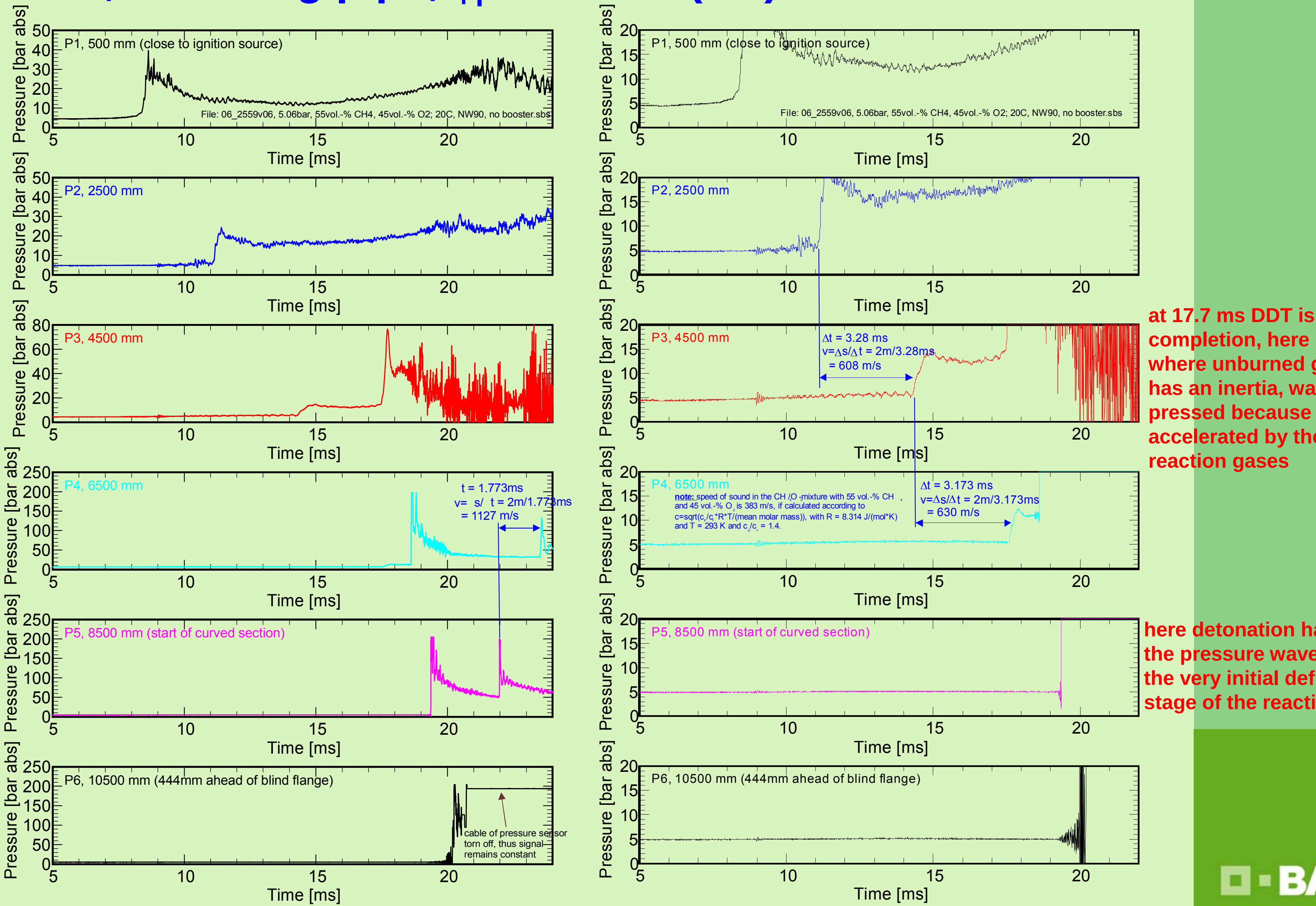
Example 1: DDT in $CH_4:O_2$=55:45 mol:mol, 5 bar abs, 20°C, 11m long pipe, ϕ_i = 86 mm (1/2)



at 17.7 ms DDT is just before completion, here in a region where unburned gas, which has an inertia, was precompressed because it got accelerated by the expanding reaction gases

here detonation has overtaken the pressure wave caused by the very initial deflagrative stage of the reaction

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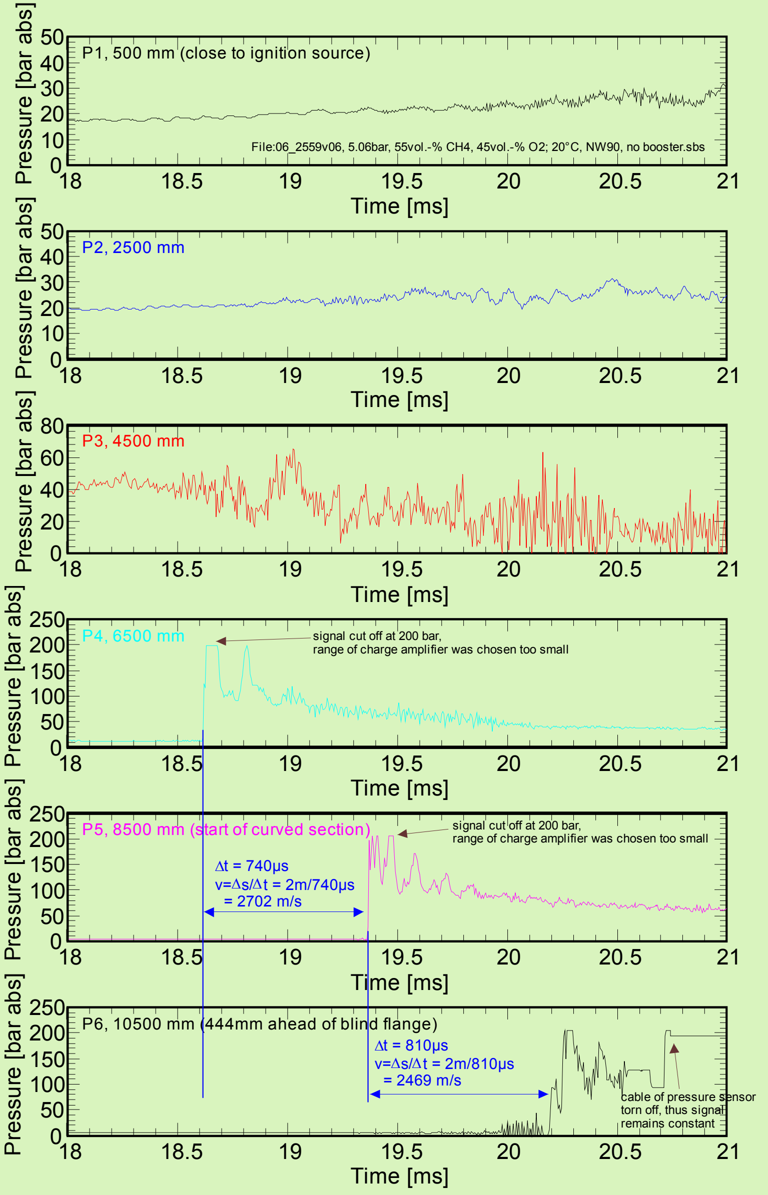
Example 1: DDT in CH_4:O_2=55:45 mol:mol, 5 bar abs, 20°C, 11m long pipe, ϕ_i = 86 mm (2/2)



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Remarks concerning pressure/time recordings of CH_4/O_2-mixture of example 1

- No retonation peak seen ?!?

- Do we have to assume that F_{DDT} is by a factor of 2 larger than otherwise because the DDT occurs in a mixture precompressed by a factor of 2?

- Can the precompressed region be understood in terms of Jukowsky pressure?

Jukowsky pressure Δp in a medium with density ρ, whose speed of sound is c and which undergoes a change in speed of Δv, is given by:

$$\Delta p = \rho * c * \Delta v$$

For the methane/O_2 mixture in the pipe which was at rest under 5 bar abs and which is accelerated by the expanding reaction gases generated while the flame propagated through the turbulence enhancer, one finds:

$\Delta p = \rho * c * \Delta v = 5*0.963 \text{ kg/m}^3 * 383 \text{ m/s} * \Delta v$

If we also assume that Δv = 383 m/s, one finds:

Δp = 5*0.963 kg/m3 * 383 m/s * 383 m/s = 0.706 MPa = 7 bar

This would fit the experimental observation

(Note: Density of $CH_4:O_2$=55:45 mol:mol mixture at 20 °C and 1 bar abs is 0.963 kg/m^3, speed of sound in this mixture at 20°C is 383 m/s)

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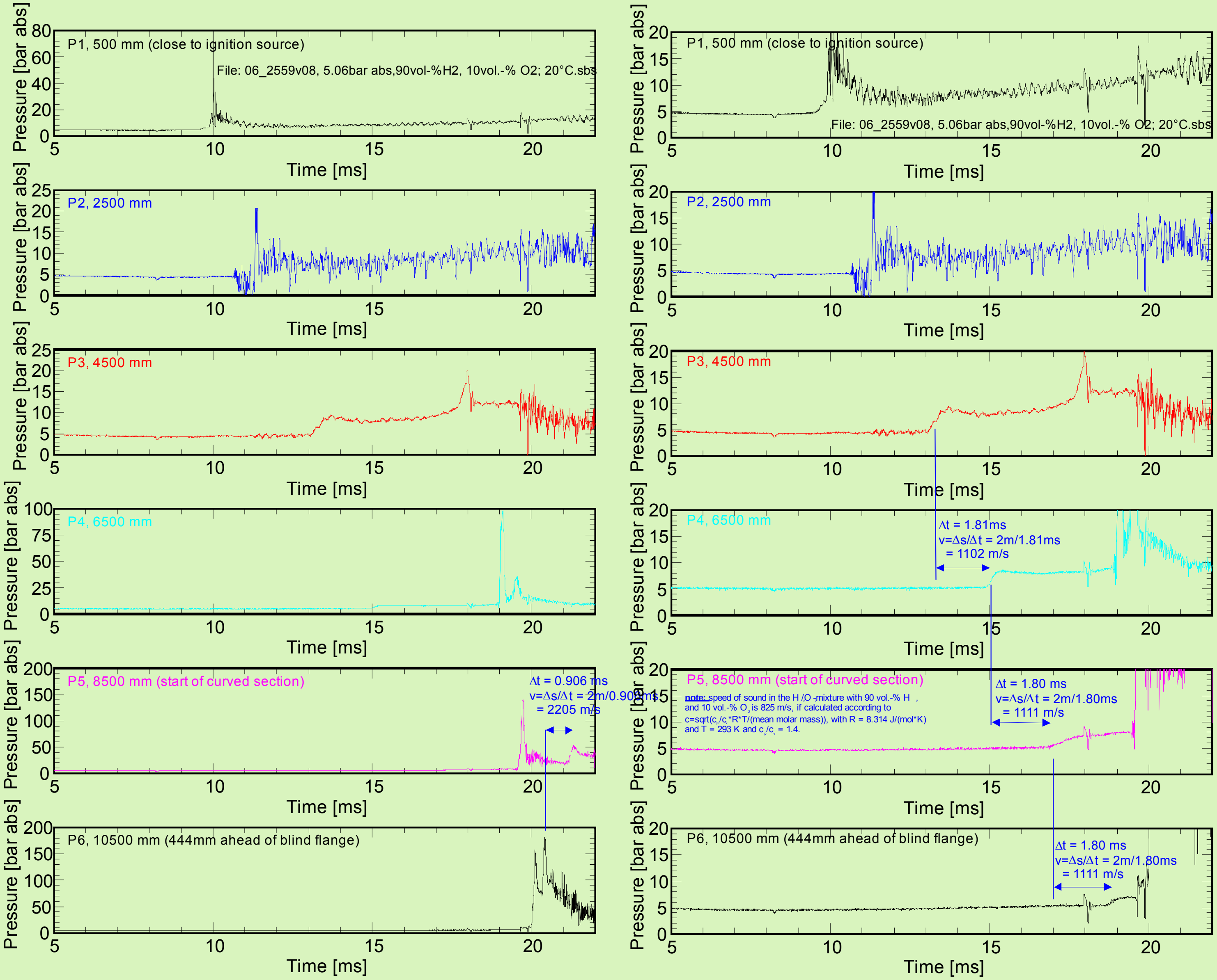
Example 2: DDT in H_2:O_2=90:10 mol:mol, 5 bar abs, 20°C, 11m long pipe, ϕ_i = 86 mm (1/2)



at 18.0 ms DDT starts to emerge, here in a region where unburned gas, which has an inertia, was precompressed because it got accelerated by the expanding reaction gases

here detonation has not yet overtaken the pressure wave caused by the very initial deflagrative stage of the reaction

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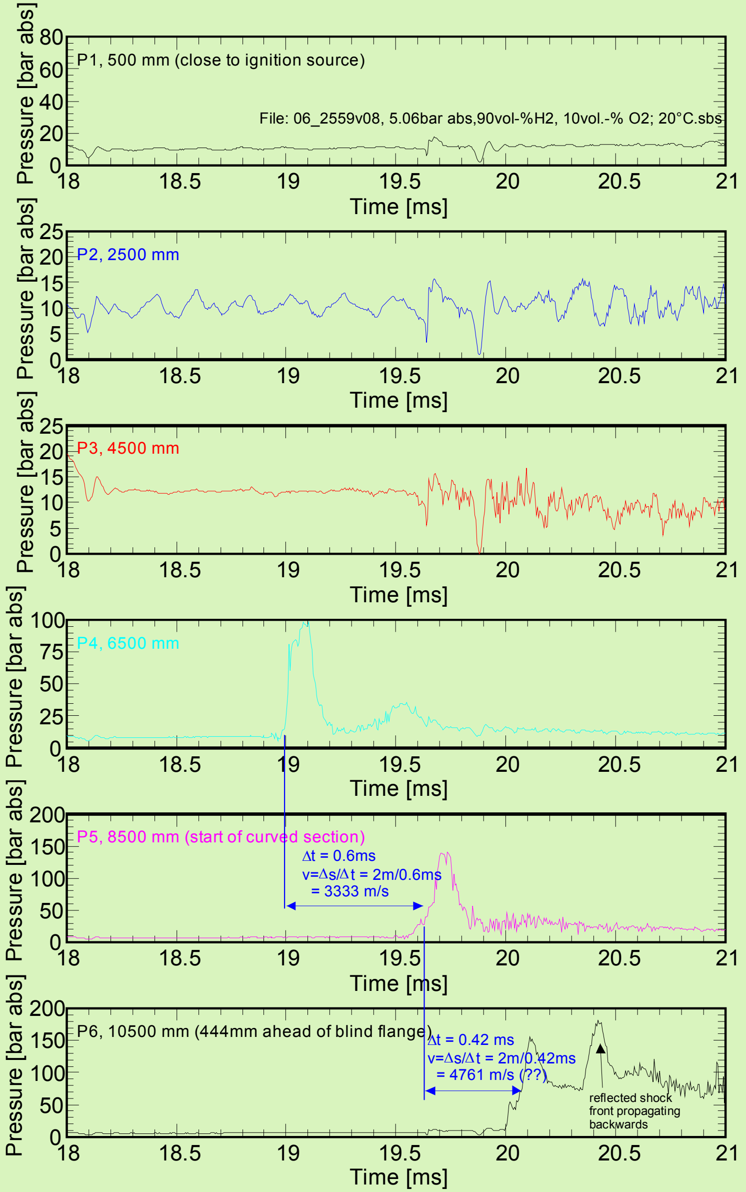
Example 2: DDT in H_2:O_2=90:10 mol:mol, 5 bar abs, 20°C, 11m long pipe, ϕ_i = 86 mm (2/2)



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Remarks concerning pressure/time recordings of H_2/O_2-mixture of example 2

- No retonation peak seen ?!?

- Do we have to assume that F_{DDT} is by a factor of 2 larger than otherwise because the DDT occurs in a mixture precompressed by a factor of 2?

- Can the precompressed region be understood in terms of Jukowsky pressure?

Jukowsky pressure Δp in a medium with density ρ, whose speed of sound is c and which undergoes a change in speed of Δv, is given by:

$\Delta p = \rho * c * \Delta v$

For the H_2/O_2 mixture in the pipe which was at rest under 5 bar abs and which is accelerated by the expanding reaction gases generated while the flame propagated through the turbulence enhancer, one finds:

$\Delta p = \rho * c * \Delta v = 5*0.222\ kg/m^3 * 825\ m/s * \Delta v$

If we also assume that $\Delta v = 825$ m/s, one finds:

$\Delta p = 5*0.222\ kg/m^3 * 825\ m/s * 825\ m/s = 0.706\ MPa = 7\ bar$

This would almost fit the experimental observation

(Note: Density of $H_2:O_2$=90:10 mol:mol mixture at 20 °C and 1 bar abs: 0.222 kg/m^3, speed of sound in this mixture at 20°C is 825 m/s)

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Experimental setup for example 3 related to pressure at DDT

- Internal diameter ϕ_i = 76 mm, L = 7 m

- Pressure sensors 13 mm recessed from inner pipe wall, access via a 6 mm bore, bore was filled with silicon grease to protect membrane of sensors against melting

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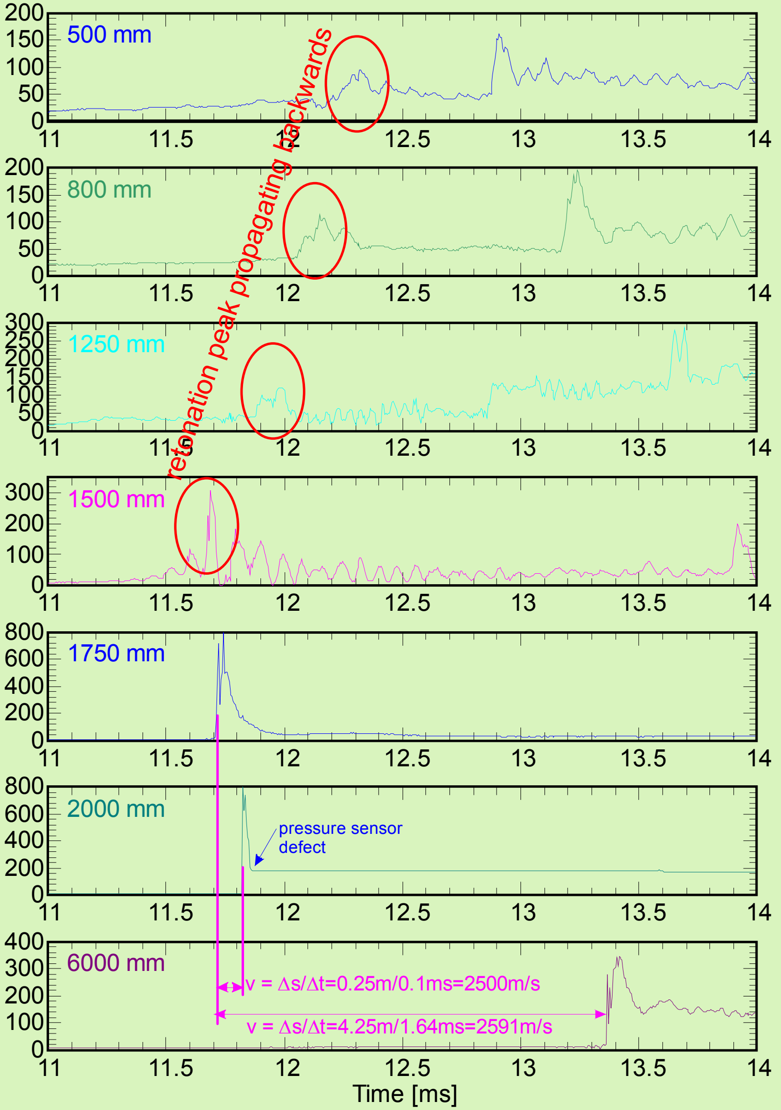
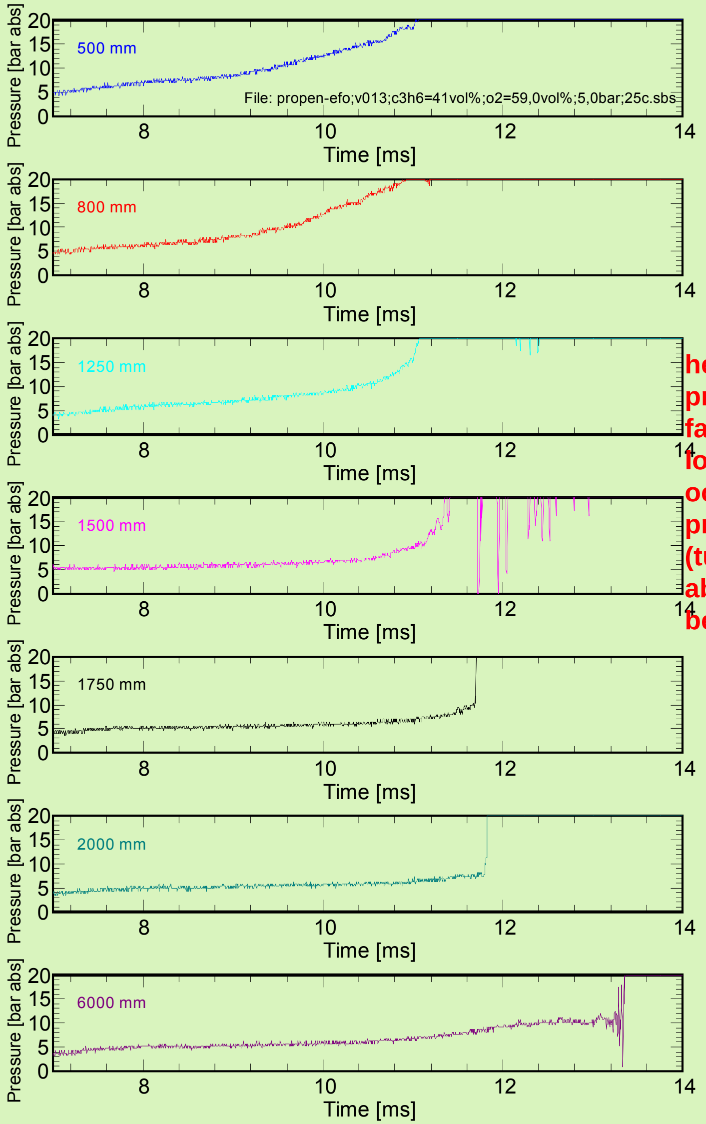
Example 3: DDT in Propene:O_2=41:59 mol:mol, 5 bar abs, 20°C, 7 m long pipe, ϕ_i = 76 mm (1/2)





here there is no pronounced pressure jump by about a factor of two ahead of the location where the DDT occurs as was seen in both previous examples (turbulence enhancer was absent in example 3. Can this be a reason?).

Remarks concerning pressure/time recordings of Propene/O_2-mixture of example 3

- Here there is no pronounced pressure jump by about a factor of two ahead of the location where the DDT occurs as was seen in both previous examples.
  (Turbulence enhancer was absent in example 3. Can this be a reason?).

- Will the ratio between the side-on pressure at point of DDT and the side on pressure at stable detonation be less than in examples 1 and 2 ?

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Research topics pertaining to quantifying the side-on pressure at point of DDT

- How large is side-on pressure at the point of DDT really in comparison to the side-on pressure of the stable detonation?

- Does this ratio increase when mixture gets less reactive (mixture must get compressed more to achieve higher temperatures to compensate for decreasing reactivity)?

- Will this ratio be higher for combustible gases with larger ignition temperature?
  (alkanes and alkenes with more than about 6 C-atoms have ignition temperatures of about 210± 10°C at 1 bar abs, shorter molecules exhibit higher values)

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- Design basis for detonation pressure proof pipes
  (already shown in Talk of 41st UKELG meeting)
- Side-on pressure at point of DDT: how large really compared to side-on pressure of stable detonation?
- Reflected shock wave: how long has to be the enforced pipe end?
- Static equivalent pressure: which value, in particular for high-strength materials?
- Is the scenario „DDT directly ahead of a blind flange“ realistic?
- Under what circumstances can there be a DDT in bubble columns in case of injection of pure O_2 into the organic liquid?

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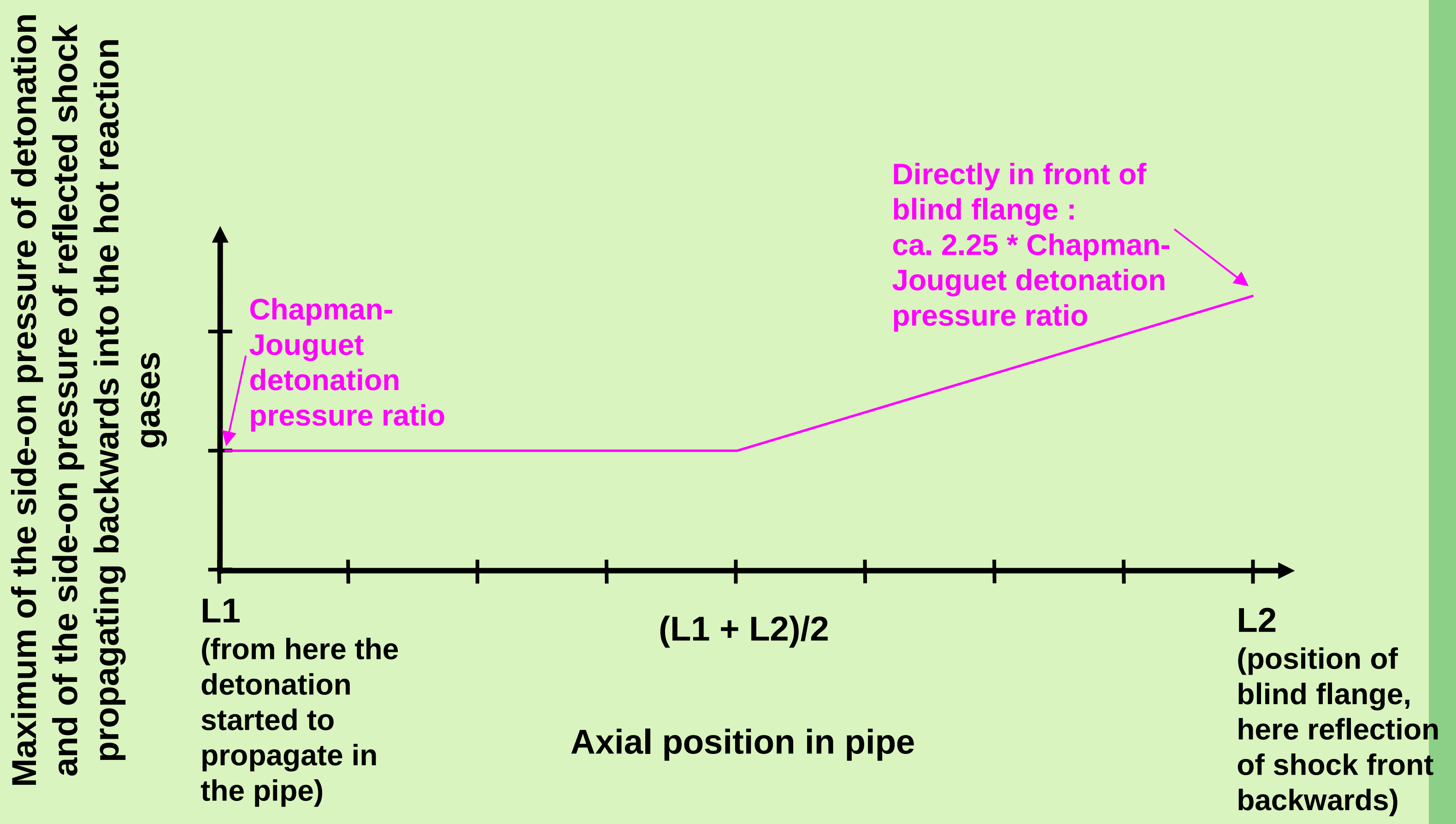
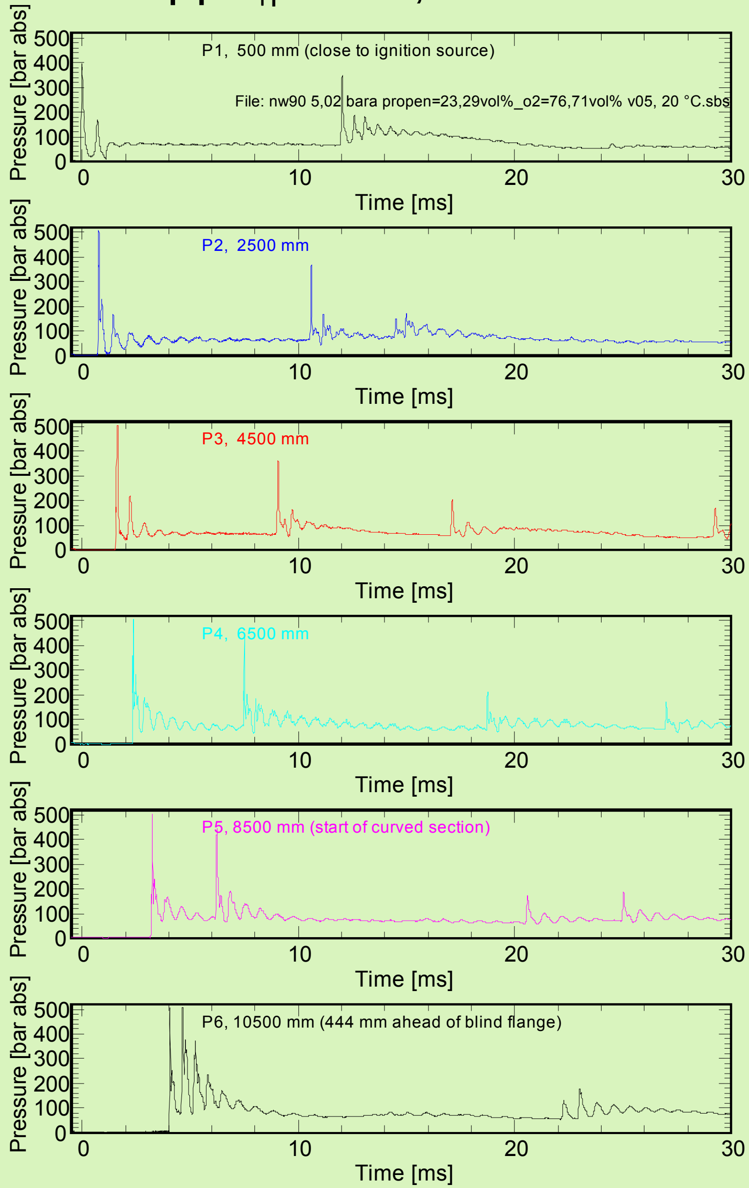
Coarse approximation of maximum side-on pressure in a pipe with reflection of detonation front at blind flange

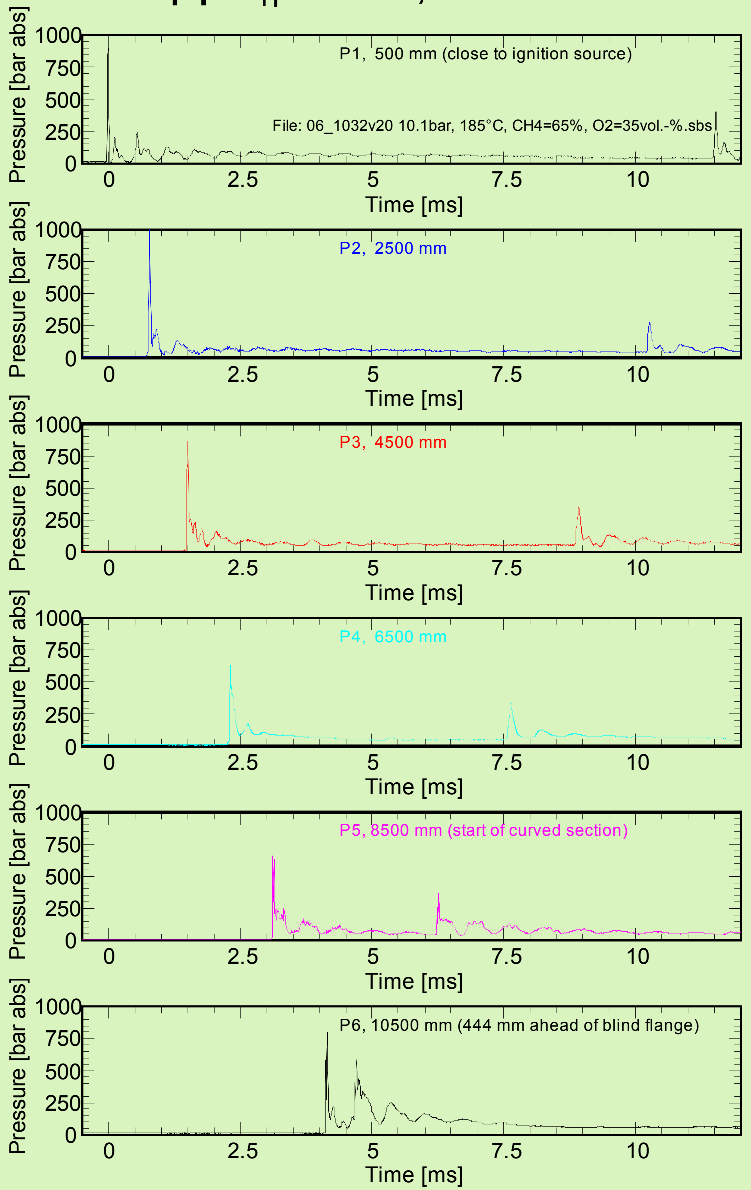


Examples for pressure caused by reflected shock in ϕ_i = 86 mm pipe, l = 10.944 m (1/2)

Propene:O_2=23mol:77mol, 5 bar abs, 20 °C, pipe: ϕ_i = 86 mm, L = 10.944 m



Methane:O_2=65mol:35mol, 10 bar abs, 185 °C, pipe: ϕ_i = 86 mm, L = 10.944 m



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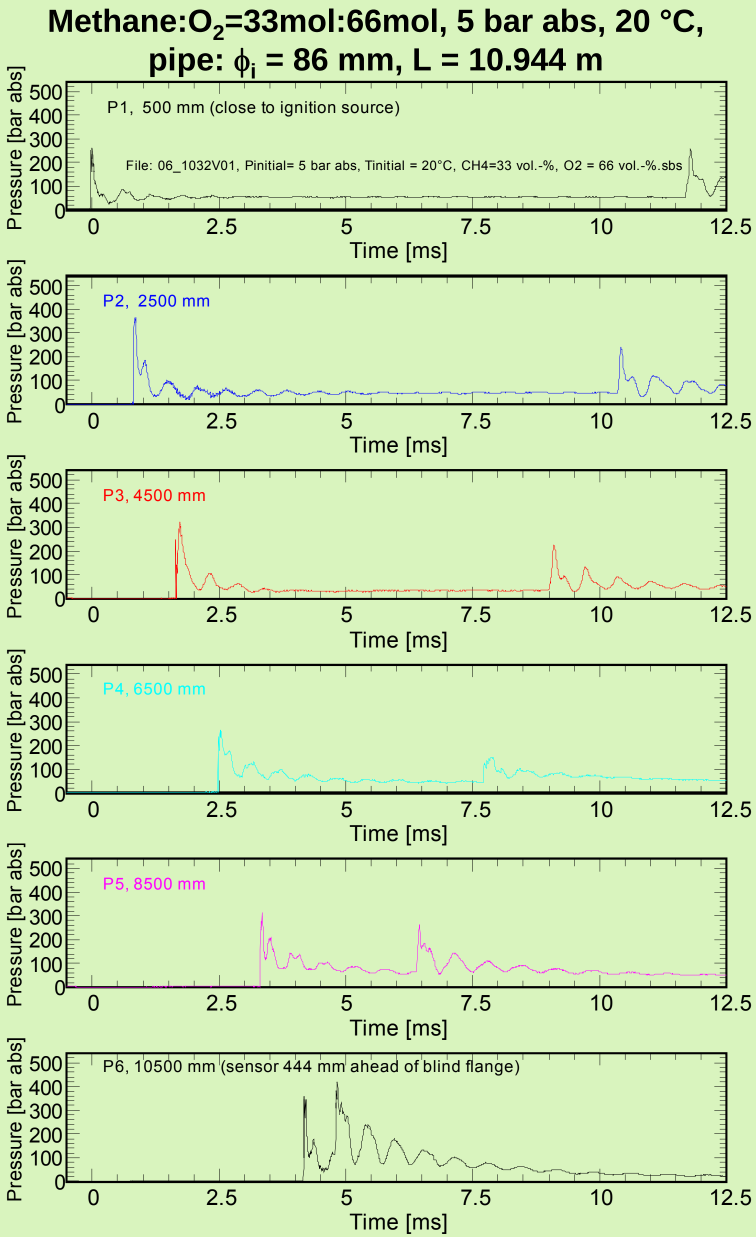
Examples for pressure cause by reflected shock in ϕ_i = 86 mm pipe, l = 10.944 m (2/2)



Remarks to examples in ϕ_i = 86 mm pipe

- Even though the absolute pressure values indicated by the piezoelectric pressure sensors are prone to errors, the ratio between the pressure signal caused by the incoming detonation and by the reflected shock propagating backwards in the hot reaction gases should be reliable.

- Pressures at P5 (8500 mm):

  In all tests pressure of reflected shock propagating in hot reaction gases is less than pressure of detonation

- Pressures at P6 (10500 mm):

  In some tests pressure of reflected shock at P6 is factor 1.5 to 2 larger than pressure of incoming detonation, in most tests pressure is less or equal than pressure of incoming detonation

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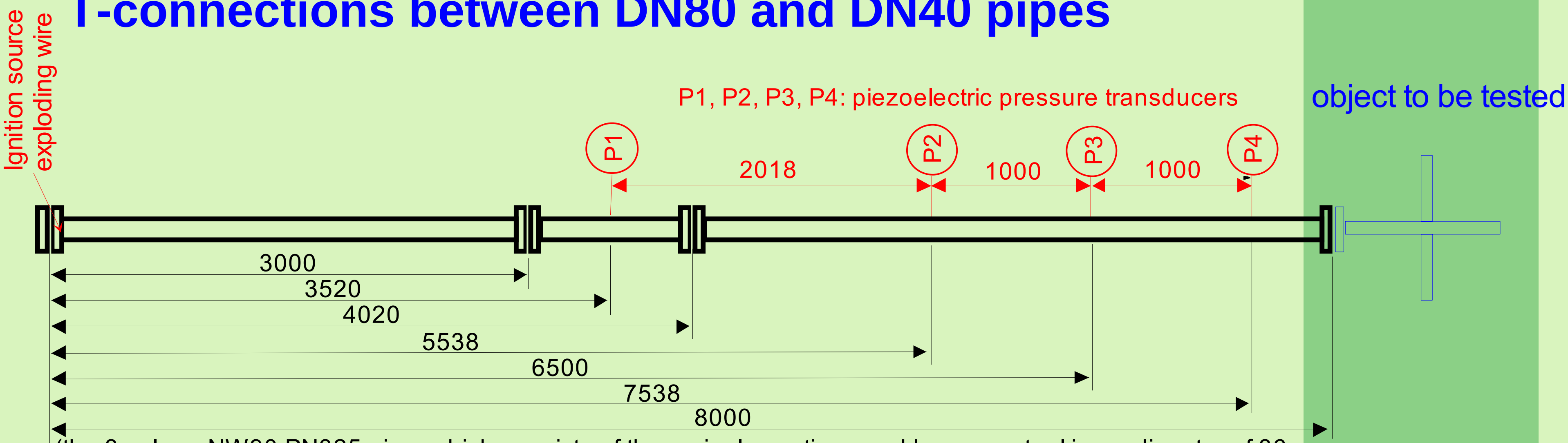
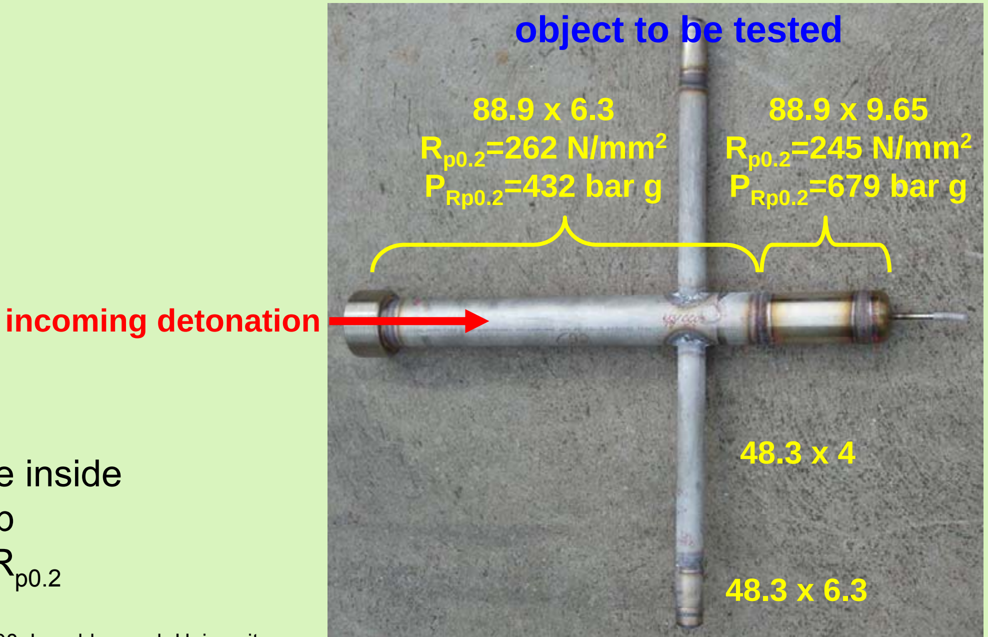
Experimental setup for testing the stability of welded T-connections between DN80 and DN40 pipes



(the 8 m long NW90 PN325 pipe, which consists of three single sections and has an actual inner diameter of 86 mm, serves to establish a stable detonation in the gas mixture. This stable detonation then propagates into the object whose mechanical stability is to be tested)



Note:

The pressure $P_{Rp0.2}$ is the pressure inside the tube which gives rise to a hoop stress equal to the yield strength $R_{p0.2}$

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Examples for pressure caused by reflected shock in ϕ_i = 76.3 mm pipe, l = 9 m

Three detonations in the following mixtures at 20 °C ($P_{det} = P_{inital} * (\gamma*M2+1)/(\gamma+1)$):

a) stoichiometric Ethylene/air (6.54 vol.-% ethylene) at $P_{initial}$ = 21 bar abs, v_{det}=1923 m/s, side-on pressure P_{det} = 372 bar abs

b) stoichiometric Ethylene/O_2 (25 vol.-% Ethylene) at $P_{initial}$ = 12.3 bar abs, v_{det} = 2631 m/s, side-on pressure P_{det} = 456 bar abs

c) stoichiometric Ethylene/O_2 (25 vol.-% Ethylene) at $P_{initial}$ = 15.2 bar abs, v_{det} = 2678 m/s, side-on pressure P_{det} = 584 bar abs, reflected pressure P_{reflec} ca. 2.25*584 bar = 1314 bar

Outer diameters (given in mm) after the three tests:

Pos. 1: 88.9 -> 91.3 = +2.7%

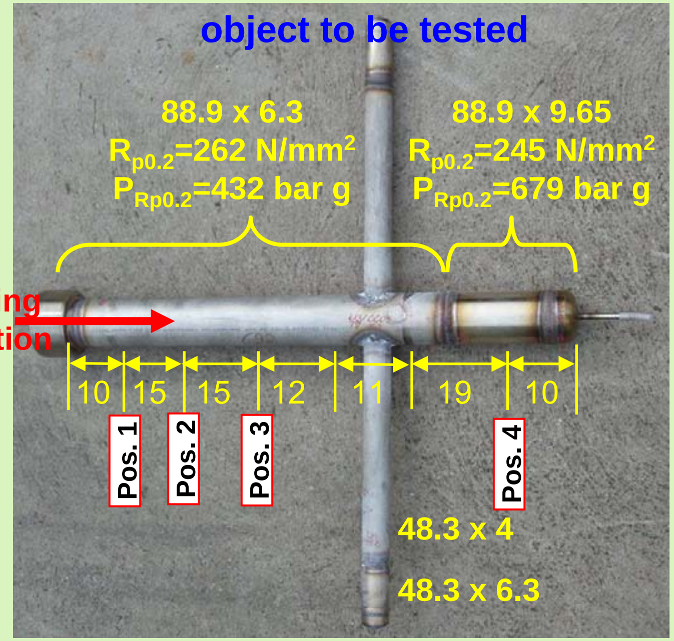
Pos. 2: 88.9 -> 92.3 = +3.8%

Pos. 3: 88.9 -> 93.9 = +5.6%

Pos. 4: 88.9 -> 91.3 = +2.7%

=> at position 1 the pressure of the reflected shock front has decayed already to 432/679 *100% = 63 % of the value present at position 4

incoming detonation



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Research topics pertaining to pressure cause by reflected shock propagating backwards into reaction gases

- **How long has to be the enforced section at the end of the pipe in front of the blinded end (or potentially closed valve)?**
  - What is the dependence of the length the detonation has already travelled?
  - Is it really independent on pipe diameter ?
  - for very long pipes (up to 5 km): is there a length of the enforced section that need not to be exceeded, irrespective of pipe length?

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- Design basis for detonation pressure proof pipes
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Definition of „*static equivalent pressure*“

- The „*static equivalent pressure*“ is the pressure P_{stat} applied in a hydraulic pressure test, which causes the same plastic deformation of the enclosure as a detonative pressure pulse, whose height is P_{det} (measured locally by e. g. piezoelectric pressure transducers)

- The *static equivalent pressure* is the basis for *explosion pressure resistant* or *explosion pressure shock resistant* design

- Experimental finding for steels with $200 \leq R_{p0.2} \leq 250$ N/mm^2: P_{stat} ca. $0.6 * P_{det}$

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Static equivalent pressure in case of deflagrative explosions

The static equivalent pressure is identical with the locally measured explosion pressure

(therefore one never talks about „static equivalent pressures“ in context with deflagrative explosions)

Reason:

- A deflagrative explosion is a slow process and represents an almost quasi-static load (i.e. strain rates $\Delta\varepsilon/\Delta t = \Delta l/l/\Delta t$ provoked in the enclosure by the deflagration are less than $10^{-2}\ s^{-1}$). Hence the $R_{p0.2}$-value as measured under standard conditions is relevant.

- The width of the deflagrative pressure peak at half maximum is orders of magnitude larger than the cycle time of the various vibrational modes of the enclosure. Hence no damping by the inertia of the wall material.

- At any given time the pressure is the same at any location in the volume affected by the deflagrative explosion. Hence the entire wall is exposed to the same pressure at any time.
  (exception: „pathological“ geometries like interconnected vessels)

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Possible reasons for P_{stat} being less than P_{det}

- **<u>For steels with low $R_{p0.2}$:</u>**

  Fast strain rate ($\Delta\varepsilon/\Delta t = \Delta l/l/\Delta t$) of about 100 s^{-1}, as it is caused by a detonative load, can increase the yield strength $R_{p0.2}$ by up to a factor 2

  (recording of stress/strain-curves with strain rates of only 10^{-4} s^{-1})

- **<u>For short pipes:</u>**

  Taylor expansion fan still short => axial extension of detonation front (i.e. zone of high pressure load) can be as short as a pipe diameter => stability of the affected wall segment is better described by the formula for spherical shells instead of the formula for cylindrical shells!

  (note that a spherical shell can sustain twice the pressure as a cylindrical shell of same wall thickness)

- **<u>For short cylindrical reactors (see introduction of this talk, L=4m, ϕ=1m):</u>**

  Damping of fundamental radial oscillation mode by inertia of wall
  (eigenfrequency only about 1 kHz, i. e. T/2 = 500 µs >> FWHM of detonation peak)

- **Other reasons ???**

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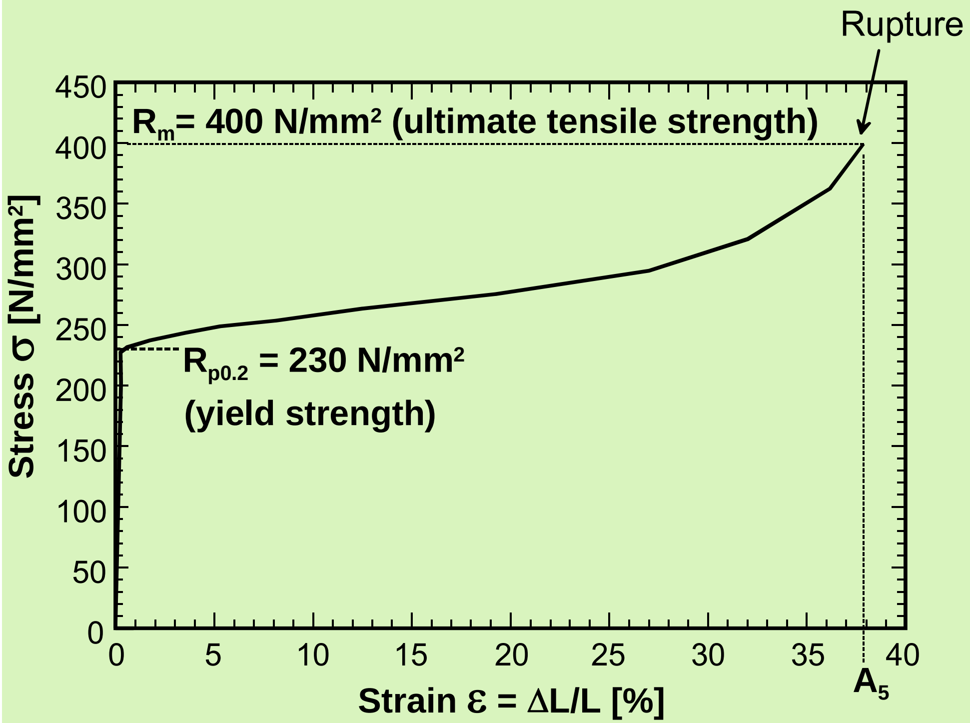
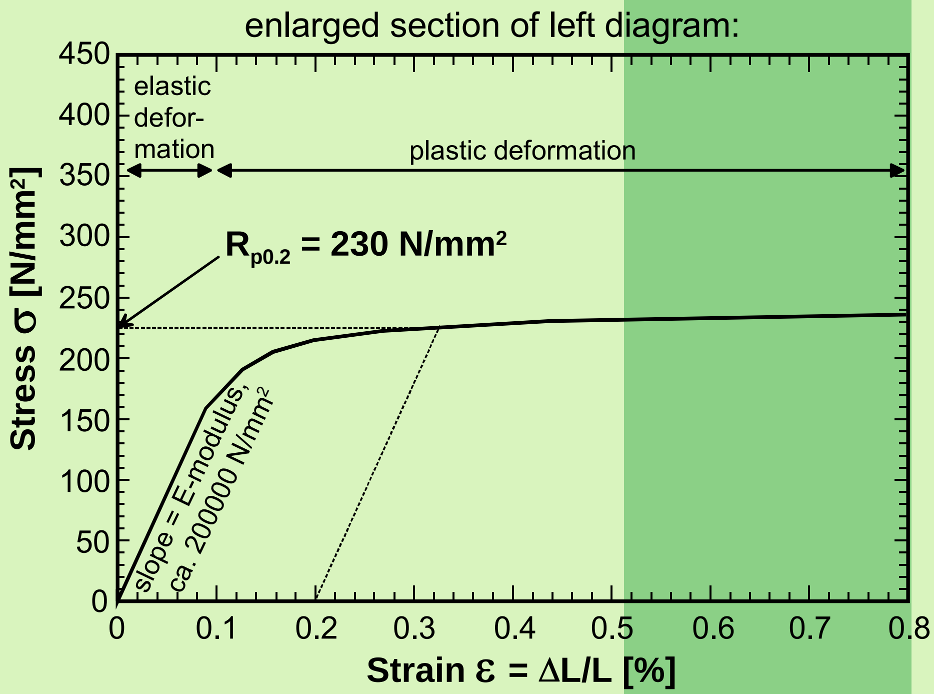
Stress-strain curve of standard steel at T = 20 °C (schematic)





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Mechanical properties of different steels as function of strain rate

Mechanical property		values of the mechanical properties of different steels at different strain rates [1/s]							
		St35.8; 1.0305 (typical unalloyed tube material)			30 CrNiMo 8; 1.6580 (high-strength, quenched and tempered material)			Inconel 718; 2.4668 (precipitation hardened Ni-based alloy)	
		ca. 10E-4	0.3	130	ca. 10E-4	12	130	ca. 10E-4	100
	yield strength $R_{p0.2}$ [MPa]	238	298	430	848	841	910	1100	1170
	ultimate tensile strength R_m [MPa]	380	409	466	998	1005	1040	1330	1350
	elongation at rupture A_5 [%]	40	28	25	-	13.7	16.4	16	17

The non high-yield strength steels exhibit an increase of the $R_{p0.2}$-value of up to 100% when increasing the strain rate to values as caused by detonative loads (ca. 100 s^{-1}) !

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Important: Damping of the displacement of the wall because of the combination of it's inertia and the short duration of the pressure pulse is in most cases not existing

The often claimed damping due to the combination of the inertia of the wall material and the short time period over which the detonative pressure acts onto the wall is not existing in pipes with ϕ_i < 500 mm (any length) and not in long pipes with ϕ_i > 500 mm.

Reason: full width at half maximum of the detonation peak is larger than half of the cycle time of the fundamental radial oscillation mode of the pipe wall.

This means that the wall experiences the full detonative pressure P_{det} and even responds with twice the displacement ("overshooting" because pressure is applied as step-function) than if applying a static pressure of height P_{det} !

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Design of pipes exposed to detonative gas phase explosions on the basis of the *static equivalent pressure*

1st step: Fixing the largest conceivable detonative pressure P_{det}

(worst case gas composition, largest conceivable initial pressure, initial temperature with largest ratio between P_{det} and $R_{p0.2}$, most unfavourable location of ignition with respect to precompression)

2nd step: Fixing the static equivalent pressure P_{stat}

($P_{stat} = 0.6 * P_{det}$ if $200\ N/mm^2 \leq R_{p0.2} \leq 250\ N/mm^2$ (at room temperature);
$P_{stat} > 0.6 * P_{det}$ if $R_{p0.2} > 250\ N/mm^2$ (at room temperature))

3rd step: Calculating the wall thickness s of a pipe with inner diameter ϕ_i

Explosion pressure shock resistant design: $s = \frac{P_{stat} \cdot \phi_i}{2 \cdot R_{p0.2}}$

Explosion pressure resistant design: $s = \frac{P_{stat} \cdot \phi_i}{2 \cdot R_{p0.2} / 1.5}$

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Research topics pertaining to static equivalent pressure

- **Highest priority:**
  Systematic work to <u>determine and understand</u> the ratio between P_{stat} and P_{det} for the most prevalent steel types in pipe design (i. e. materials with low $R_{p0.2}$: 200 N/mm^2 < $R_{p0.2}$ < 250 N/mm^2)

  Important:
  - Experiments should be done in very long pipes to find out whether the duration of impact (width of Taylor expansion fan increases with length of propagation) might also have an influence
  - material characteristics like $R_{p0.2}$, R_m, A_5 and A_v (yield strength, ultimate tensile strength, elongation at rupture, charpy impact strength) have to be determined from the same pipes that are lateron exposed to the detonative load in the test

- **Second priority:**
  Systematic work to determine and understand the ratio between P_{stat} and P_{det} for high-strength steels (250 N/mm^2 < $R_{p0.2}$ < 1000 N/mm^2)

  Presumably for steels with $R_{p0.2} \geq$ 250 N/mm^2: $0.6 * P_{det} \leq P_{stat} \leq 2*P_{det}$

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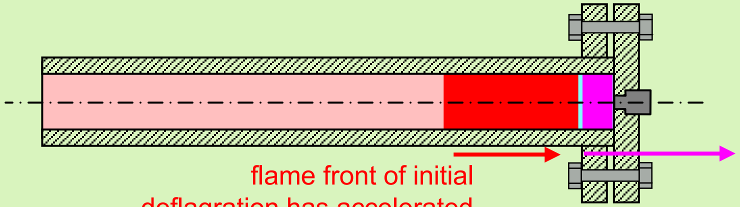
Detonation pressure P_{det} in long pipes ($L \gg L_{predet}$, no precompression) for the scenario „DDT in front of blind flange“

- **Reflected pressure, if DDT occurs directly in front of blind flange**



$$P_{det} = P_{initial} * P_{CJ} * F_{DDT} * F_{reflec}$$

$$1.5 \leq F_{DDT} \leq 2$$

$$2 \leq F_{reflec} \leq 2.5$$

Important:
The pipe directly ahead of the blind flange experiences the reflected pressure as well. The length of this section corresponds to the axial extension of the taylor expansion fan.
(In lab-scale equipment of up to 5 m length a section of about 3 pipe diameters from the blind flange back into the pipe is affected, in longer pipes this section increases).

If it could be shown, that this scenario will not happen, the wall thickness could be reduced by the factor F_{DDT}

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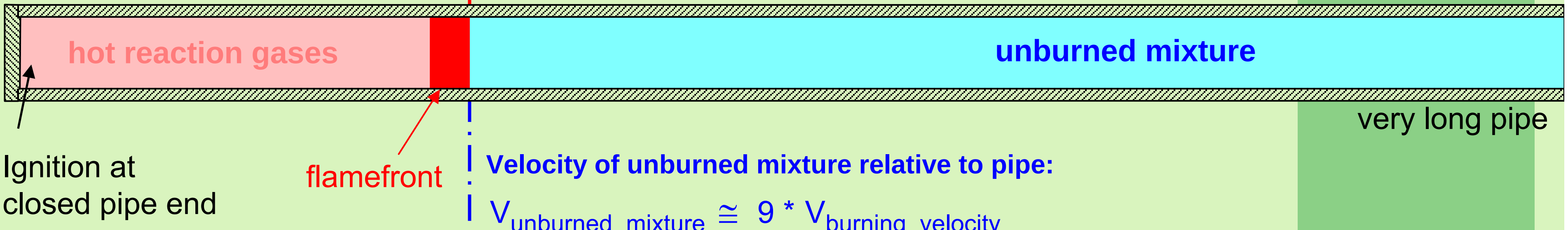
Flow velocity of unburned mixture and propagation velocities of the flame front at some stage during run-up to detonation <u>and flame far away from pipe end</u>

Velocity of flame relative to unburned mixture:

$V_{burning\_velocity} \geq V_{laminar\_burning\_velocity}$

Velocity of flame relative to pipe:

$V_{flame\_speed} \cong 10 * V_{burning\_velocity}$



Velocity of unburned mixture relative to pipe:

$V_{unburned\_mixture} \cong 9 * V_{burning\_velocity}$

Processes inside the pipe:

- The combustion transforms a „slice“ of unburned mixture with thickness d in axial direction into a roughly 10*d thick „slice“ of reaction gases.
- The expanding reaction gases act like a moving piston on the unburned mixture. The speed of the piston is $V_{unburned\_mixture} \cong 9 * V_{burning\_velocity}$

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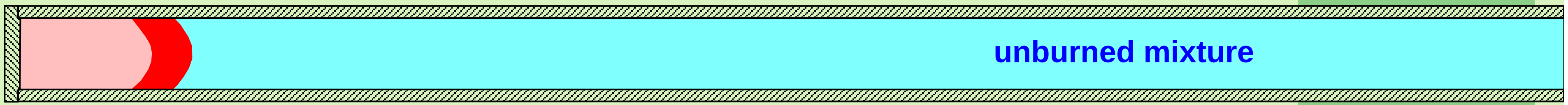
Acceleration of the flame

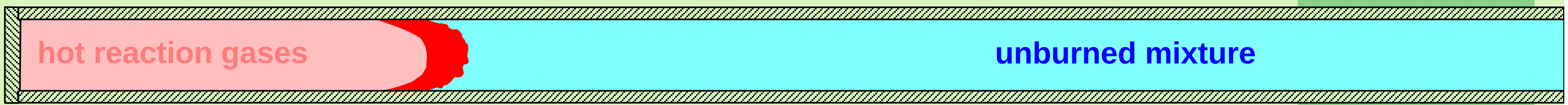
1. Phase: directly after ignition, flame spreads in quiescent unburned mixture

$V_{burning\_velocity} = V_{laminar\_burning\_velocity}$ $\qquad$ $V_{unburned\_mixture} \cong 9 * V_{burning\_velocity}$



2. Phase: flame propagates into the laminarly flowing unburned mixture

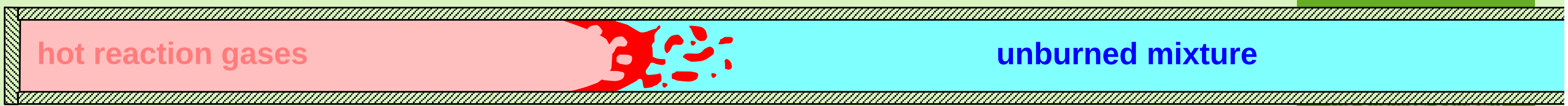
As time progresses, the surface of the flame becomes ever larger due to local instabilities („wrinkling of flame front“) → Increase of reaction rate (mass/time) → Increase of $V_{burning\_velocity}$ → Increase of $V_{unburned\_mixture}$ → Flow in unburned mixture becomes turbulent very soon



3. Phase: flow of unburned mixture has become turbulent, flame propagates in turbulent mixture

strong increase of the overall surface of all flame fronts → strong increase of the reaction rate (mass/time) → strong increase of $V_{burning\_velocity}$ → strong increase of $V_{unburned\_mixture}$ → strong increase of the degree of turbulence → (back to start)

positive feedback



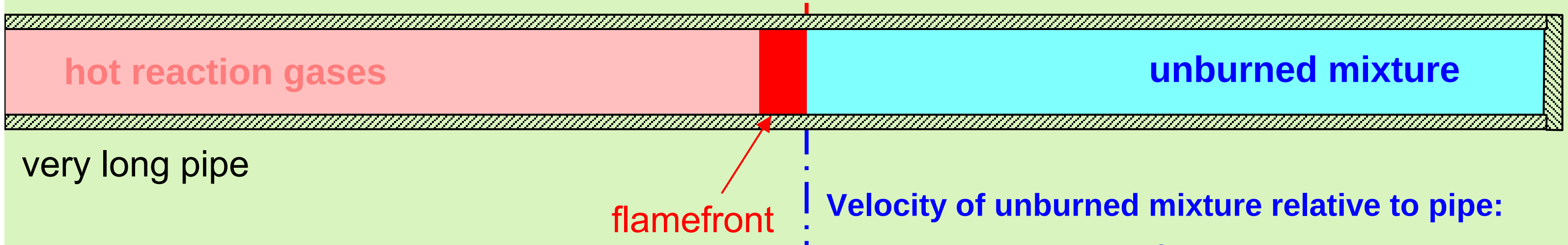
Flow velocity of unburned mixture and propagation velocities of the flame front at some stage during run-up to detonation <u>and flame is close to pipe end</u>

Velocity of flame relative to unburned mixture:

$V_{burning\_velocity} \geq V_{laminar\_burning\_velocity}$

Velocity of flame relative to pipe:

$V_{flame\_speed} \cong V_{burning\_velocity}$



Velocity of unburned mixture relative to pipe:

$V_{unburned\_mixture} \cong 0$

<u>Processes inside the pipe:</u>

- The combustion transforms a „slice“ of unburned mixture with thickness d in axial direction into a roughly 10*d thick „slice“ of reaction gases.
- The expanding reaction gases act like a moving piston on the hot reaction gases. The speed of the piston is $-9 \cdot V_{burning\_velocity}$, i. e. the piston moves backwards!

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Chain of arguments that renders the occurrence of a DDT in long pipes in front of a blind flange improbable

DDT had not occurred while the flame front was still far away from that end of the pipe to which the flame front was heading to and now flame is close to the blind flange

=> flow velocity in unburned mixture drops to zero, i. e. no longer turbulent flow

=> flame speed drops drastically

=> decrease in reaction rate

=> pressure in unburned gas directly ahead of flame front drops

=> temperature in unburned gas directly ahead of flame front drops

=> if DDT had not occurred before, it will occur now less than ever !!

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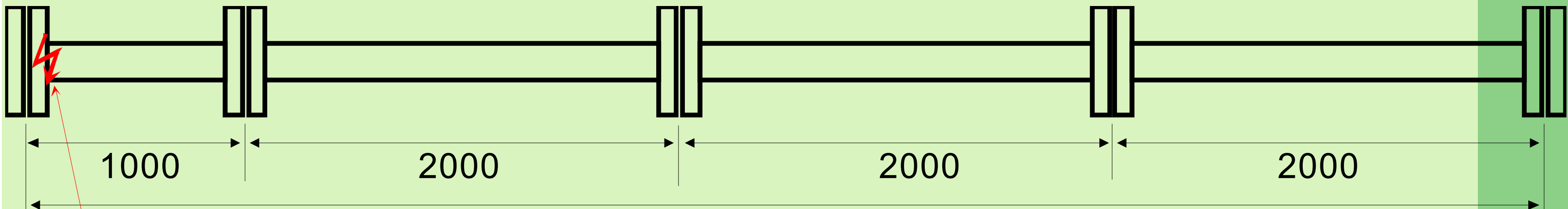
Own tests in a 7 m long ϕ_i = 76.3 mm pipe at $p_{initial}$ = 5 bar abs, 25°C

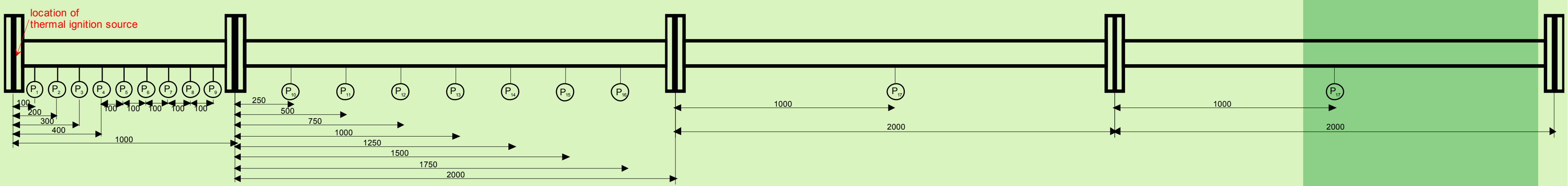


location of thermal ignition source

7000 mm, PN160, DN80, ϕ_o = 88.9 mm, ϕ_i = 76.3 mm, s = 6.3 mm

(the lengths of the tube segments are specified as from centre of gasket to centre of gasket, i. e. the actual tubes are slightly less than 1000 mm or 2000 mm, respectively)

Position of piezoelectric pressure sensors:



Tests conducted:

- Propene/O_2-mixtures, Propene content successively reduced until no longer detonation
- Propene/O_2-mixtures, Propene content successively increased until no longer detonation
- stoichiometric Propene/O_2/N_2-mixtures, O_2-content successively decreased until no longer detonation

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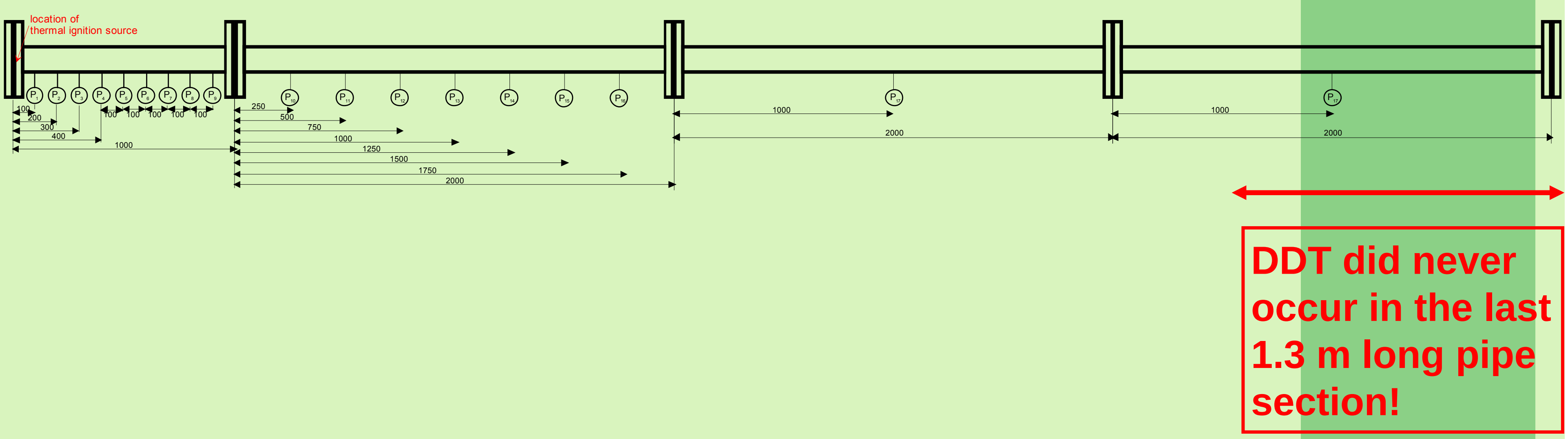
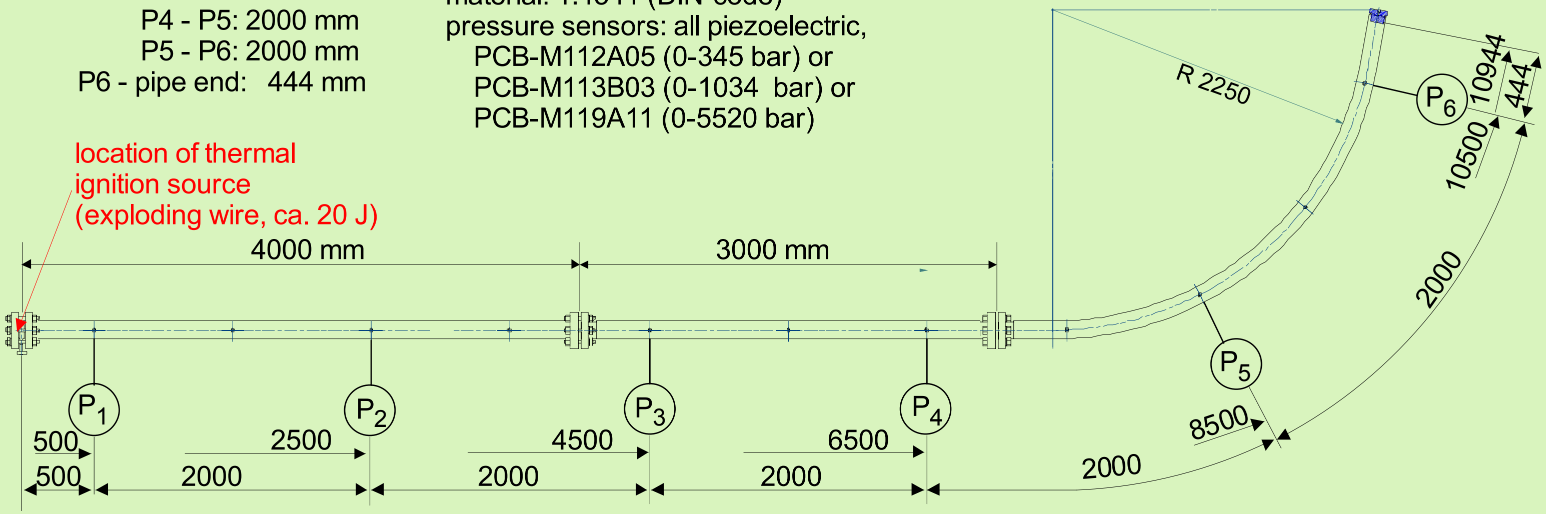
Oberservation in detonation tests with respect to the location of the DDT in the 7 m long, ϕ_i = 76.3 mm pipe



Own tests in a 11 m long, ϕ_i = 86 mm pipe

Distances:
ignition source - P1: 500 mm
P1 - P2: 2000 mm
P2 - P3: 2000 mm
P3 - P4: 2000 mm
P4 - P5: 2000 mm
P5 - P6: 2000 mm
P6 - pipe end: 444 mm

Pipe and pressure sensors:
total length of pipe: 10.944 m
individual segments: 4m, 3m and 3.944m
inner and outer diameter: ϕ_i = 86 mm, ϕ_o =127 mm
material: 1.4541 (DIN-code)
pressure sensors: all piezoelectric,
PCB-M112A05 (0-345 bar) or
PCB-M113B03 (0-1034 bar) or
PCB-M119A11 (0-5520 bar)



Tests conducted:

- H_2/O_2-mixtures, 5 bar abs, 20°C, H_2 content successively reduced until no longer detonation
- CH_4/O_2-mixtures, 5 bar abs, 20°C, CH_4 content successively increased until no longer detonation
- CH_4/O_2-mixtures, 10 bar abs, 180°C, CH_4 content successively increased until no longer detonation
- C_3H_6/O_2-mixtures, 5 bar abs, 20°C, C_3H_6-content successively increased until no longer detonation

Observation: DDT did never occur in the last 2.444 m long pipe section!

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Research topic pertaining to the location of the DDT in long pipes

- **Can DDT be directly ahead of blind flange or is there a „dead zone“ ahead of the blind flange which is „DDT-free“?**

- **By-product of such investigations:**
  As DDT gets closer to blind flange, how large is the precompression in the gas between DDT and blind flange?

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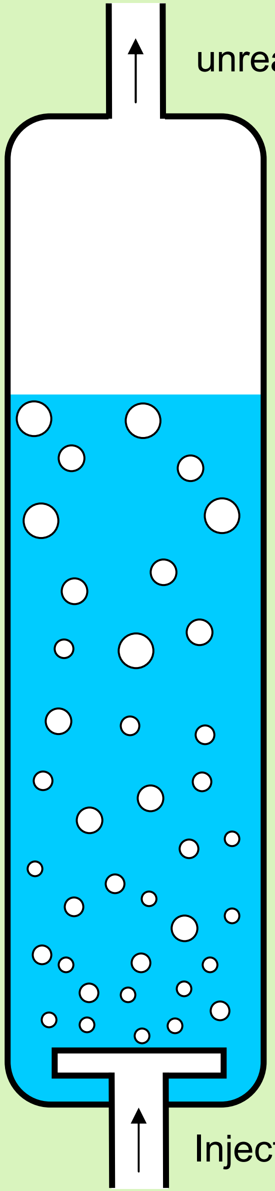
Principle of partial oxidation of organic liquids



Typical operating parameters:

1 bar abs ≤ P ≤ 20 bar abs

20°C ≤ T ≤ 200 °C

4 m ≤ height of bubble column ≤ 20 m

5 m^3 ≤ Holdup ≤ 200 m^3

10 % ≤ gas fraction ≤ 30 %

1 mm ≤ bubble diameter ≤ 30 mm

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Remarks concerning investigations of bubble columns

Last comprehensive study of bubble explosions:

„Shock induced bubble explosions in liquid cyclohexane“, K. Mitropetros, PHD-thesis, TU Berlin, April 2005 (can be downloaded from homepage of TU Berlin):

Deficits inherent to most investigations with bubble columns:

- **Number of bubbles per volume much less than in reality**

=>
- if bubbles explode, pressure at wall is negligible, i. e. tests not conservative
- Propagation of ignition from bubble to bubble will be difficult due to large average distances , i.e. tests are not conservative
- liquid with few bubbles is mechanically extremely stiff:

=>
Effect of explosion in gas phase of reactor with respect to igniting the explosive bubbles by adiabatic compresion will differ between a stiff and a soft bubble column

Effect of explosion of single bubbles with respect to igniting the other explosive bubbles by adiabatic compresion will differ between a stiff and a soft bubble column

- **Height of bubble column far less than in reality**

=> - The columns tested are mechanically stiffer than real columns

=> (same as above)

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Research topics pertaining to bubble columns

Tests with realistic height of column and realistic bubble concentrations and with O_2 or air as oxidants:

- Under what conditions (gas composition in gas space, gas composition in bubbles, volume fraction of bubbles, height of column) will an ignition of the gas space cause an ignition of the bubbles by adiabatic compression

- What pressure will develop in that case

- Under what conditions (gas composition in bubbles, volume fraction of bubbles, height of column) will the ignition of an individual bubble cause ignition of the other bubbles

- What pressure will develop in that case

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That's it

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