The need to calculate detonation pressure profiles and use them as a source term in FE calculations to quantify the response of the containment subjected to detonations

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Outline of talk

- Introduction
- For which p_{det}-scenarios seems the corresponding mechanical load p_{stat} to be clear
- For which p_{det}-scenarios is the corresponding mechanical load p_{stat} not yet clear
- What do experiments suggest
- Why are systematic experiments difficult
- Simple analytic approach („breathing mode“) to quantify radial displacement of wall in dependence of duration of detonative pressure pulse
- What is our hope concerning the mechanical load p_{stat} brought about by detonative pressure pulses
- What might help to answer the open questions with regard to mechanical load p_{stat}

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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 of the explosion diagram**

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

for all possible scenarios of p_{det} and for all possible geometries of the containment.

- stable detonation
- reflection of stable detonation
- DDT in „infinitely“ long pipes
- DDT short before reflection
- precompression
- „surface detonations“

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

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Reminder: Definition of „*static equivalent pressure*“

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

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

- Experimental finding so far for steels with 200 $N/mm^2 \le R_{p0.2} \le 250\ N/mm^2$:

$$p_{stat} = \alpha * p_{det} \quad \text{with } \alpha < 1$$

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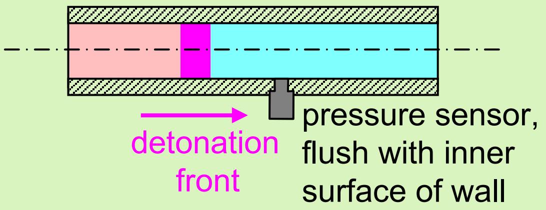
Scenario I: Side-on pressure of a stable Detonation in a pipe

(i. e. in plane perpendicular to shockfront)



$p_{det} = p_{initial} * P_{CJ\_r}$

P_{CJ_r} : denotes the *Chapman-Jouguet-pressure ratio* of the explosive gas mixture evaluated at the temperature the mixture had at the moment of igniton

$p_{initial}$: the pressure of the mixture at the moment of ignition

$\mathbf{p_{stat} = \alpha_{stab\_deto\_side-on} * p_{det}}$

with $\alpha_{stab\_deto\_side-on} = 0.6$

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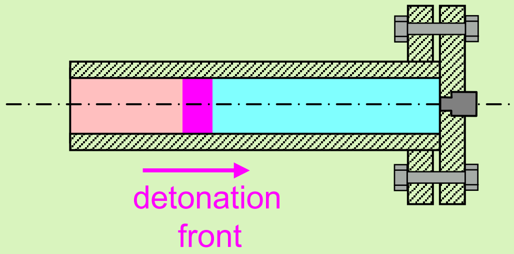
Scenario II: Reflected pressure of a stable Detonation in a pipe

(i. e. in plane parallel to shockfront, e. g. at blind flange)



$$p_{det} = p_{initial} * P_{CJ\_r} * F_{reflec}$$

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

$$p_{stat} = \alpha_{stab\_deto\_reflected\_pressure} * p_{det}$$

with $\alpha_{stab\_deto\_reflected\_pressurre} = 0.6$

Important:
Furthermore it should be born in mind that the shock reflected at the blind flange propagates backwards into the taylor expansion fan of the detonation front that had arrived at the blind flange just before. Close to the blind flange the side-on pressure of the reflected shock is about twice the side on pressure of the original detonation. When the reflected shock has propagated backwards over a distance equal to the width of the taylor expansion fan, the side-on pressure it exerts on the wall has dropped to the value of the side-on pressure of the original detonation.

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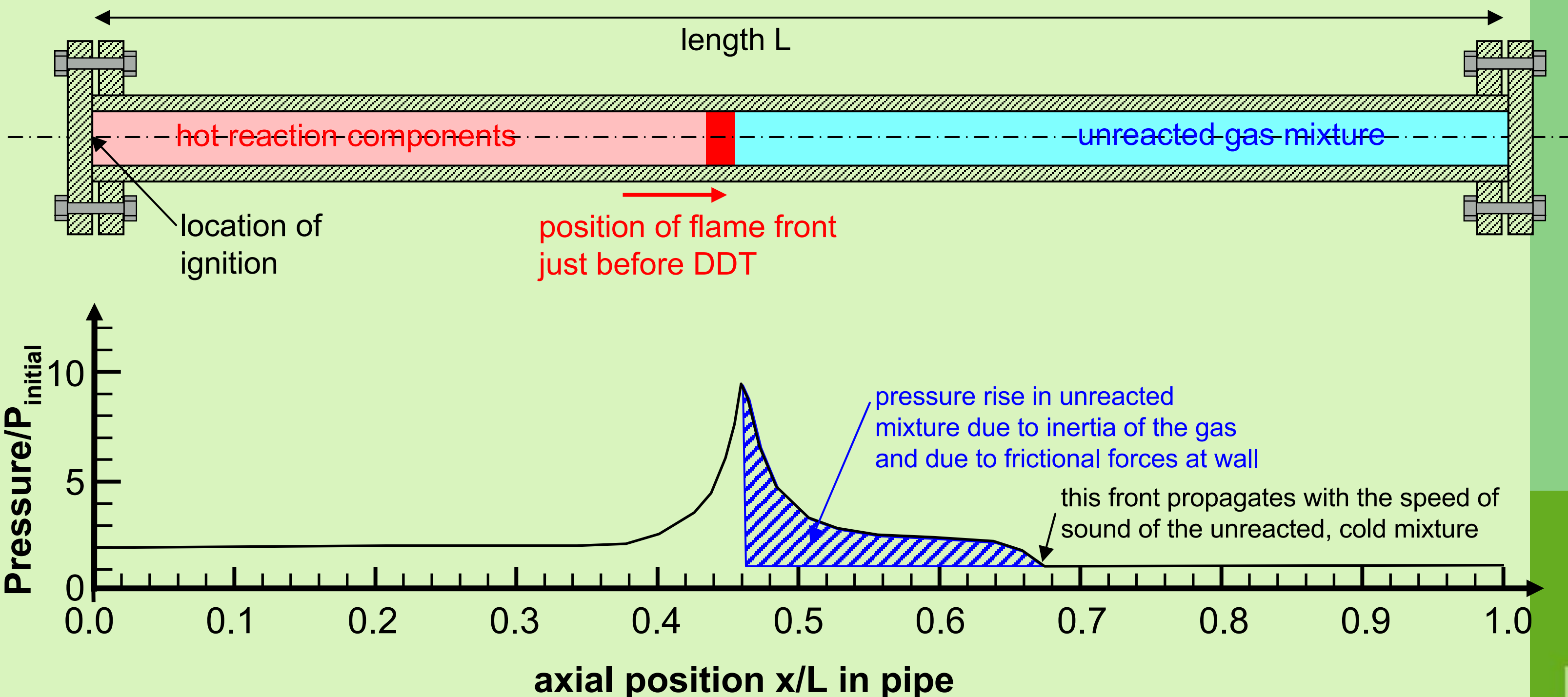
Scenario III: Side-on pressure in a long pipe at the location where the DDT occurs

<u>meaning of „long“:</u> pressure waves send out during initial deflagrative stage of explosion have not yet reached the blinded end of the pipe at the moment when the DDT occurs and will even not arrive at the blinded end before the detonation does.

<u>Qualitative sketch of this scenario (just before DDT happens):</u>



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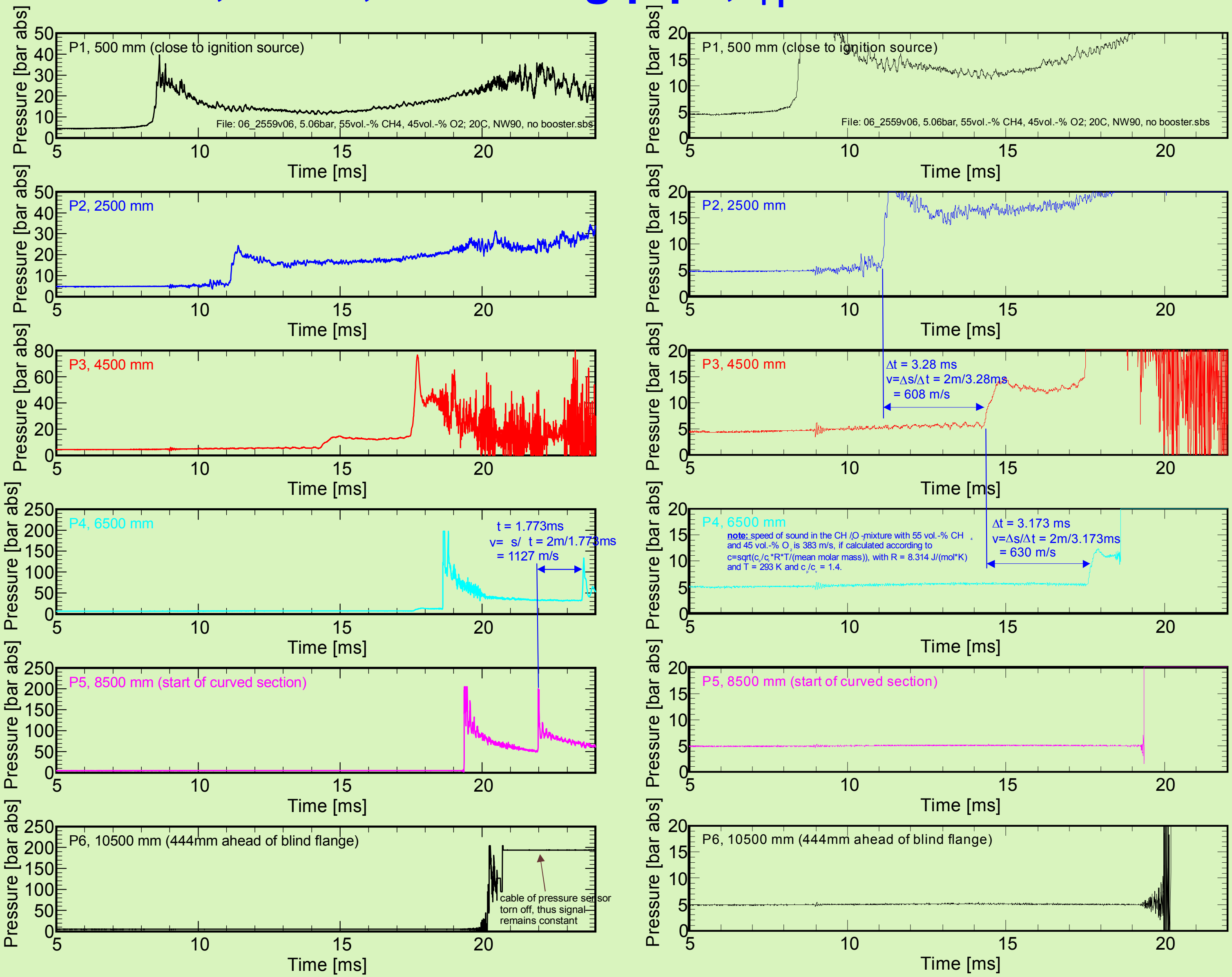
Example for scenario III: DDT in CH_4:O_2=55:45 mol:mol, 5 bar abs, 20°C, 11 m long pipe, ϕ_i = 86 mm



at 17.7 ms DDT is just before completion, here in a region where unburned gas, which has an inertia, was present at about twice it's initial pressure because it got accelerated by the expanding reaction gases

here the detonation is established

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

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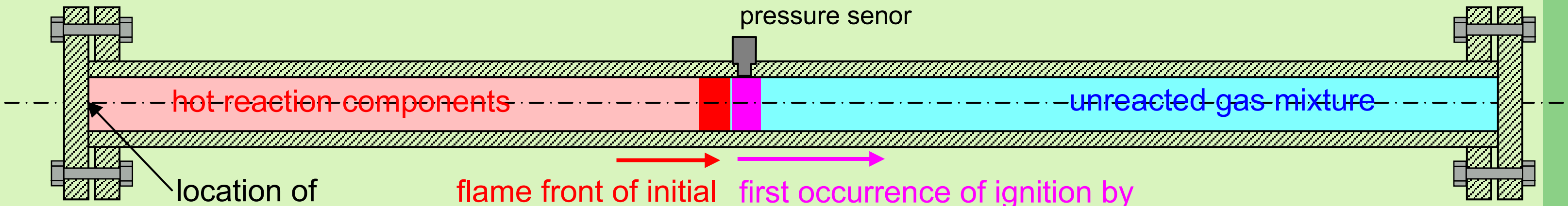
Scenario III: Side-on pressure in a long pipe at the location where the DDT occurs (continued)



$p_{det} = p_{initial} * P_{CJ\_r} * F_{DDT}$

F_{DDT} = ? (some people assume a factor of about 8)

$\mathbf{p_{stat} = \alpha_{DDT\_long\_pipe} * p_{det}}$

$\mathbf{\alpha_{DDT\_long\_pipe} = ?}$

Limited number of experiments suggest that p_{stat} at the DDT in a long pipe is not larger than 1.75 times the value of p_{stat} for the stable detonation.
If this were generally true and if F_{DDT} were really 8, then $\alpha_{DDT\_long\_pipe}$ would be 1.75 * 0.6/8 = 0.13

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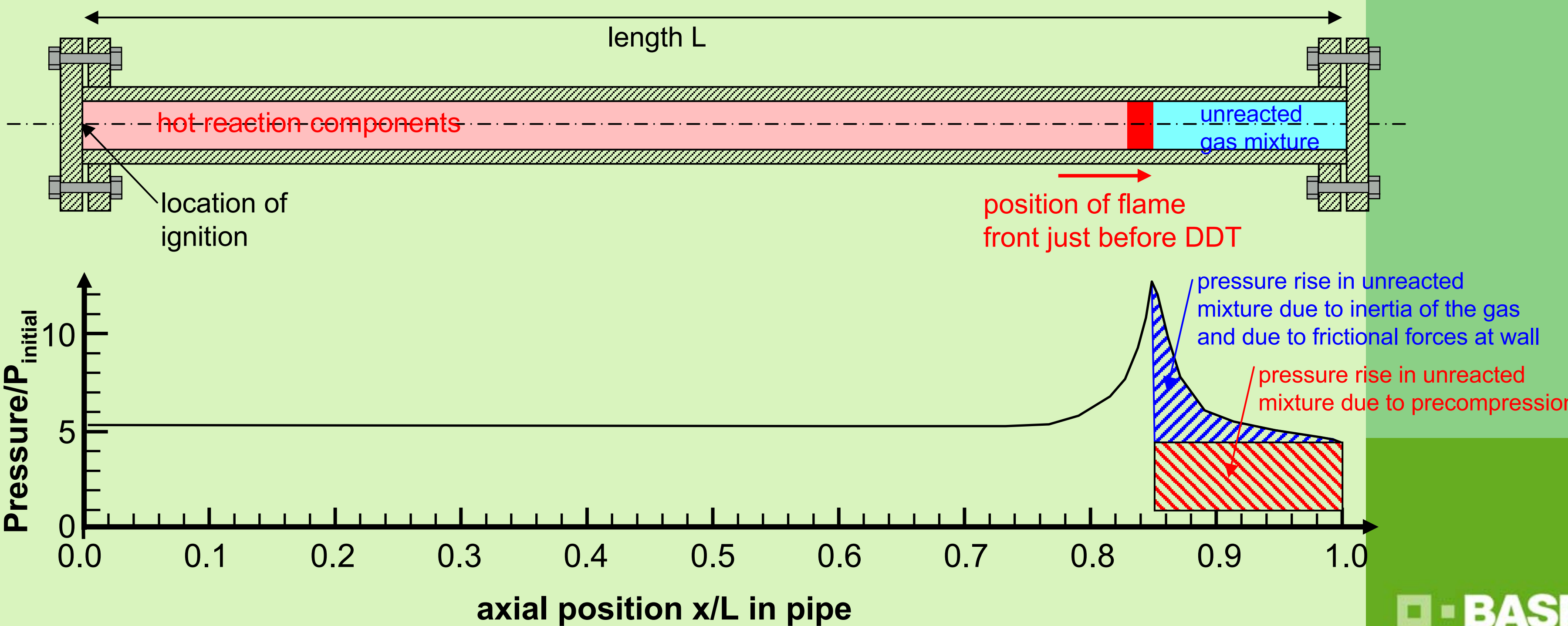
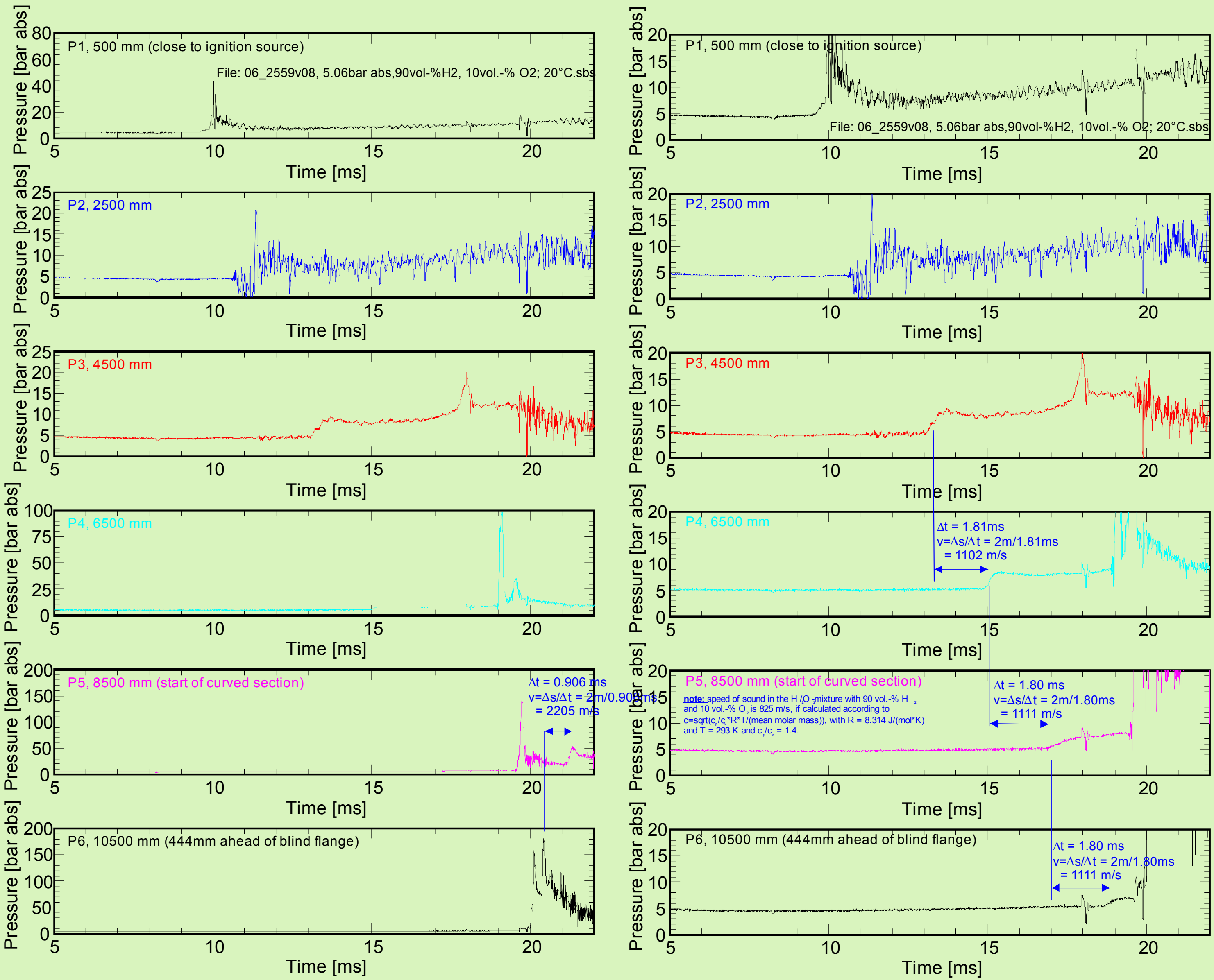
Scenario IV: Side-on pressure in a pipe at location where DDT occurs in case that the pressure waves sent out during initial deflagrative stage of the explosion have already reached the blinded end

Note:
This scenario is usually referred to as „DDT in precompressed mixture“.
The contribution to the pressure rise in the unreacted mixture due to precompression can vary between 0 and $P_{initial}$ * (deflagration pressure ratio).

Qualitative sketch of this scenario (just before DDT happens):



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

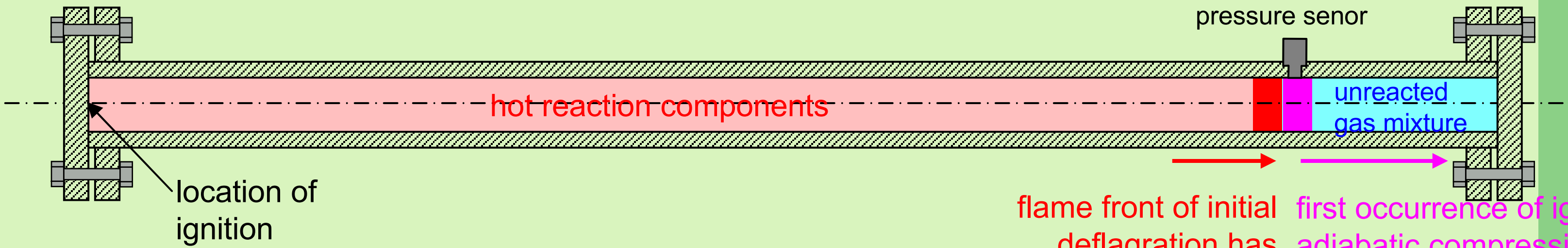


at 18.0 ms DDT starts to emerge in a region where unburned gas, which has an inertia, was present at about twice it's initial pressure because it got accelerated by the expanding reaction gases

DDT has occurred

here detonation has not yet overtaken the pressure wave caused by the very initial deflagrative stage of the reaction. Presumably it will not overtake it in the last 500 mm of the pipe.

Scenario IV: Side-on pressure in a pipe at location where DDT occurs in case that the pressure waves sent out during initial deflagrative stage of explosion have already reached the blinded end. (continued)



Tentative equations:

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

with $F_{precomp}$ and F_{temp} as defined in talk at 41st UKELG-meeting

$$p_{stat} = \alpha_{DDT\_short\_pipe} * p_{det}$$

$\alpha_{DDT\_short\_pipe}$ = ?

Open questions and problems:

- If the pressure front that propagates with the speed of sound arrives at the blind flange, is reflected and propagates backwards, how will it influence the DDT?
- Can one use $F_{precomp}$ and F_{temp} as defined in talk given at 41st UKELG-meeting?
- Can we use the same value of F_{DDT} as in scenario III or will F_{DDT} depend on $F_{precomp}$ and F_{temp} ?
- What will be the final relation between p_{stat} and p_{det} , i. e what will be $\alpha_{DDT\_short\_pipe}$?
- If for a given geometry and a given mixture it can not be excluded that scenario IV will happen instead of scenario III and since the point where the DDT occurs can never be predicted exactly, one might always have to assume the maximum value for $F_{precomp}$, i. e. the deflagration pressure ratio.

Comment to scenario IV

- Scenario IV will be rare in **pipes**, because they are usually much longer than the predetonation distance.
  This means that in most cases scenario III occurs and not scenario IV.

- However, if a DDT occurs in an empty **vessel**, scenario IV will occur in most cases instead of scenario III, because typical vessel diameters are of the order of the predetonation distance.

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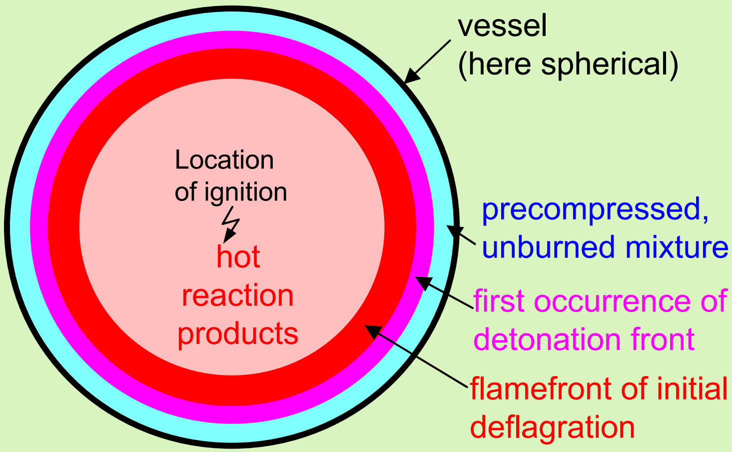
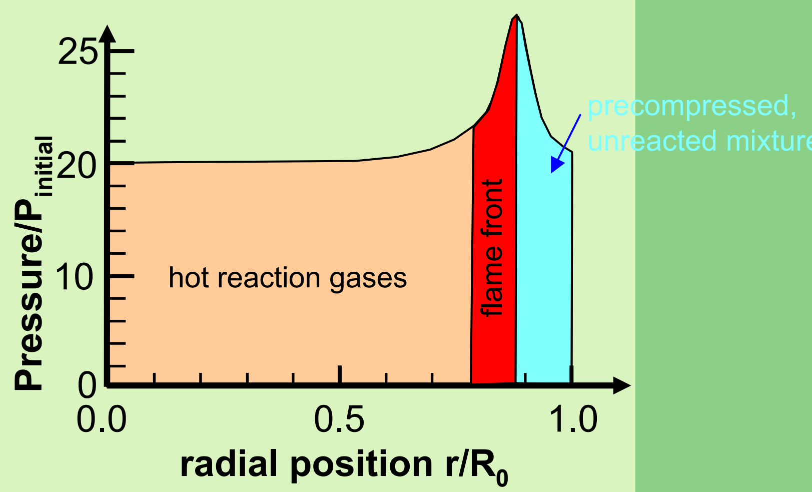
Example for scenario IV : DDT in a 20 l sphere

Gas mixture: Propene = 38 vol.-%, O_2 = 62 vol.-%, $P_{initial}$ = 5 bar abs, $T_{initial}$ = 25°C, ignition in center, deflagration pressure ratio = 22 (see talk given at 41st UKELG-meeting)

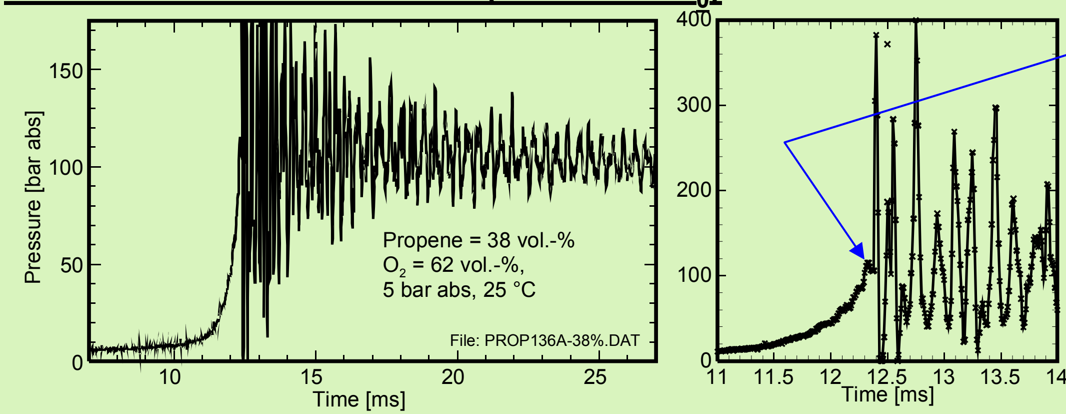
Qualitative sketch of spacial distribution of gases inside sphere at the moment of DDT



Qualitative sketch of radial pressure distribution directly before DDT occurs



Pressure measured in wall (i. e. at r = R_0)



precompression by factor 20. This is almost equal to the deflagration pressure ratio of this mixture, which is 22.

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Calculation of the rise in volume of the expanding reaction gases and rise of pressure inside sphere <u>during</u> the deflagrative explosion inside the sphere

Calculation of precompression of the unreacted gas mixture in the 20 l sphere in dependence of the percentage of the overall mols that have undergone the explosion reaction which is assumed to start in the center of the sphere

8	Total Volume of reactor	0,02	m3
9	Initial temperature in mixture = Propene/O2 (in degree Celsius)	20	°C
10	Initial temperature in mixture = Propene/O2 (in degree Kelvin)	293	K
11	initial Pressure in mixture (in bar abs)	5	bar abs
12	initial Pressure in mixture (in Pascal)	500000	Pascal
13	Universal Gas constant R	8,314	J/(mol*K)
14	Value of gamma = cp/cv	1,3	
15	Number of mols in reactor	4,16	
16	Propene concentration in Propene/O2-mixture	38	vol.-%
18	Explosion pressure ratio at 20°C for this concentration	22	
19	Explosion pressure ratio at actual feed gas temperature	22,000	
20	Pressure after explosion in Total volume	110,000	[bar abs]
21	Temperature of reaction gases (in degree Celsius)	6173	°C (since we neglected the mole number increase, the temperature is higher than in reality to reproduce the oberved pressure rise)
22	Temperature of reaction gases (in degree Kelvin)	6446	K
23	mean cp-value of reaction gases	48,314	J/(mol*K) (was assumed constant over the entire temperature range)
24	mean cv-value of reaction gases, cv = cp - R	40	J/(mol*K)

Ro von 20 l = 16,838903 cm

Note 1: internal energy of ideal gas dQ = cv*M*dT +p*dV; in case of adiabatic expansion is cv*M*dT = -p*dV (see Gerthsen, p. 218, p. 221)

	B: Percentage of original number of mols that are going to react [%]	C: original volume V1 of mixture that is going to react [m3]	D: absolute number of moles that react	E: remaining volume V2 of gas mixture that is going to be compressed adiabatically [m3]	F: remaining number of mols of unreacted mixture	G	H: Assumption for V2-compressed [% of V2]	I: V2-compressed [m3]	J: work done to compress unreacted mixture from V2 to V2-compressed [J]	K: pressure in volume V2-compressed containing the unreacted mixture [bar abs]	L: temperature in compressed unreacted mixture [°C]	M: explosion pressure ratio of the compressed unreacted mixture, i.e. at its acutal temperature	N: explosion pressure that would be measured if compressed mixture explodes in deflagrative manner and does not expand backwards to the reactor head [bar abs]	O: Temperature decrease deltaT in mixture of reaction gases required to release this work [K]	P: Temperature of reaction gases after cooling down by deltaT [°C]	Q: Volume V1-expanded available for reaction gases [m3]	R: Pressure in Volume V1-expanded available for reaction gases [bar abs]	S: Difference between pressure in reacted and pressure in compressed mixture (should be 0 if solver did work properly) [bar]	T: Zielwert [bar]	Radius of V1 expanded divided by Ro [-]	Pressure divided by initial pressure inside containment [-]	Volume of expanded reaction gases divided by total volume [-]
29	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20			
32	0,03	0,0000	0,00	0,01999	4,1583		99,47	0,0198889	-52,71	5,03	20,46	21,97	110,59	1056,08	5116,92	0,0001	5,03	0,00	0	0,17708645	1,0069	0,00555336
33	0,07	0,0000	0,00	0,01999	4,1566		98,78	0,0197429	-122,50	5,08	21,08	21,92	111,37	1061,83	5121,17	0,0003	5,08	0,00	0	0,23424619	1,0160	0,01285339
34	0,1	0,0000	0,00	0,01998	4,1554		98,27	0,0196350	-174,45	5,11	21,53	21,89	111,96	1048,46	5124,54	0,0004	5,11	0,00	0	0,26327424	1,0229	0,01824841
35	0,3	0,0001	0,01	0,01994	4,1471		95,02	0,0189478	-512,77	5,34	24,52	21,68	115,84	1027,30	5145,70	0,0011	5,34	0,00	0	0,37470266	1,0686	0,05260904
36	0,5	0,0001	0,02	0,01990	4,1388		92,02	0,0183120	-837,90	5,57	27,40	21,48	119,68	1007,19	5165,81	0,0017	5,57	0,00	0	0,43864819	1,1142	0,08440128
37	1	0,0002	0,04	0,01980	4,1180		85,40	0,0169101	-1599,51	6,14	34,20	21,03	129,08	961,34	5211,66	0,0031	6,14	0,00	0	0,53658643	1,2277	0,15449665
38	2	0,0004	0,08	0,01960	4,0764		75,02	0,0147046	-2941,14	7,26	46,38	20,27	147,22	883,85	5289,15	0,0053	7,26	0,00	0	0,64212815	1,4529	0,26476778
39	3	0,0006	0,12	0,01940	4,0348		67,20	0,0130373	-4094,59	8,38	57,10	19,64	164,63	820,32	5352,68	0,0070	8,38	0,00	0	0,70347477	1,6765	0,34813331
40	4	0,0008	0,17	0,01920	3,9932		61,07	0,0117248	-5102,99	9,49	66,72	19,11	181,44	766,76	5406,24	0,0083	9,49	0,00	0	0,7451604	1,8987	0,41376077
41	5	0,0010	0,21	0,01900	3,9516		56,10	0,0106598	-5995,32	10,60	75,47	18,66	197,75	720,67	5452,33	0,0093	10,60	0,00	0	0,77584455	2,1198	0,4670078
42	6	0,0012	0,25	0,01880	3,9100		52,00	0,0097753	-6792,08	11,70	83,51	18,26	213,64	680,37	5492,63	0,0102	11,70	0,00	0	0,79960066	2,3401	0,51123364
43	7	0,0014	0,29	0,01860	3,8684		48,53	0,0090268	-7508,41	12,80	90,97	17,91	229,15	644,68	5528,32	0,0110	12,80	0,00	0	0,81865555	2,5596	0,54866042
44	8	0,0016	0,33	0,01840	3,8268		45,56	0,0083836	-8155,81	13,89	97,92	17,59	244,34	612,73	5560,27	0,0116	13,89	0,00	0	0,8343487	2,7785	0,58082162
45	9	0,0018	0,37	0,01820	3,7852		42,99	0,0078237	-8743,29	14,98	104,45	17,30	259,24	583,88	5589,12	0,0122	14,98	0,00	0	0,84754192	2,9968	0,60881251
46	10	0,0020	0,42	0,01800	3,7436		40,73	0,0073312	-9278,04	16,07	110,62	17,04	273,87	557,63	5615,37	0,0127	16,07	0,00	0	0,85881845	3,2146	0,63343798
47	11	0,0022	0,46	0,01780	3,7020		38,73	0,0068937	-9766,32	17,16	116,46	16,80	288,28	533,62	5639,38	0,0131	17,16	0,00	0	0,86859454	3,4321	0,65531677
48	12	0,0024	0,50	0,01760	3,6604		36,94	0,0065022	-10212,21	18,25	122,01	16,58	302,46	511,48	5661,52	0,0135	18,25	0,00	0	0,87715813	3,6491	0,67489107
49	13	0,0026	0,54	0,01740	3,6188		35,34	0,0061493	-10620,06	19,33	127,30	16,37	316,44	490,99	5682,01	0,0139	19,33	0,00	0	0,88473645	3,8658	0,69253506
50	15	0,0030	0,62	0,01700	3,5356		32,57	0,0055374	-11334,78	21,49	137,21	16,00	343,85	454,17	5718,83	0,0145	21,49	0,00	0	0,89757873	4,2982	0,72313213
51	20	0,0040	0,83	0,01600	3,3276		27,43	0,0043883	-12644,48	26,87	158,93	15,25	409,71	379,98	5793,02	0,0156	26,87	0,00	0	0,92074641	5,3749	0,78058483
52	25	0,0050	1,04	0,01500	3,1197		23,85	0,0035770	-13433,61	32,23	177,44	14,66	472,55	322,96	5850,04	0,0164	32,23	0,00	0	0,93642725	6,4468	0,8211493
53	30	0,0060	1,25	0,01400	2,9117		21,19	0,0029671	-13829,98	37,58	193,66	14,19	533,00	277,07	5895,93	0,0170	37,58	0,00	0	0,94787843	7,5160	0,85164367
54	35	0,0070	1,46	0,01300	2,7037		19,14	0,0024881	-13914,21	42,90	208,16	13,79	591,52	238,94	5934,06	0,0175	42,90	0,00	0	0,956683	8,5804	0,87559682
55	40	0,0080	1,66	0,01200	2,4957		17,49	0,0020993	-13741,14	48,22	221,31	13,45	648,41	206,47	5966,53	0,0179	48,22	0,00	0	0,96371003	9,6434	0,89503319
56	45	0,0090	1,87	0,01100	2,2878		16,14	0,0017759	-13350,11	53,52	233,36	13,15	703,89	178,31	5994,69	0,0182	53,52	0,00	0	0,96947934	10,7044	0,91120412
57	50	0,0100	2,08	0,01000	2,0798		15,01	0,0015014	-12770,54	58,82	244,51	12,89	758,15	153,51	6019,49	0,0185	58,82	0,00	0	0,97432235	11,7636	0,92492815
58	54	0,0108	2,25	0,00920	1,9134		14,23	0,0013094	-12186,58	63,05	252,87	12,70	800,77	135,64	6037,36	0,0187	63,05	0,00	0	0,97768155	12,6099	0,93452787
59	57	0,0114	2,37	0,00860	1,7886		13,71	0,0011787	-11684,73	66,22	258,86	12,57	832,31	123,21	6049,79	0,0188	66,22	0,00	0	0,97995579	13,2440	0,94106464
60	60	0,0120	2,50	0,00800	1,6638		13,22	0,0010578	-11131,96	69,39	264,62	12,44	863,52	111,51	6061,49	0,0189	69,39	0,00	0	0,98205052	13,8777	0,94711234
61	64	0,0128	2,66	0,00720	1,4974		12,63	0,0009097	-10320,88	73,61	272,00	12,29	904,65	96,92	6076,08	0,0191	73,61	0,00	0	0,98460244	14,7219	0,95451492
62	67	0,0134	2,79	0,00660	1,3727		12,23	0,0008073	-9660,45	76,77	277,32	12,18	935,15	86,66	6086,34	0,0192	76,77	0,00	0	0,9863692	15,3546	0,95963326
63	70	0,0140	2,91	0,00600	1,2479		11,86	0,0007115	-8967,95	79,93	282,47	12,08	965,38	76,91	6096,09	0,0193	79,93	0,00	0	0,98799806	15,9868	0,96442458
64	74	0,0148	3,08	0,00520	1,0815		11,40	0,0005928	-7959,44	84,15	289,09	11,95	1005,27	64,65	6108,35	0,0194	84,15	0,00	0	0,99002151	16,8293	0,97036224
65	77	0,0154	3,20	0,00460	0,9567		11,08	0,0005097	-7166,59	87,30	293,89	11,85	1034,90	55,94	6117,06	0,0195	87,30	0,00	0	0,9914316	17,4608	0,97451441
66	80	0,0160	3,33	0,00400	0,8319		10,78	0,0004313	-6337,94	90,46	298,55	11,77	1064,29	47,62	6125,38	0,0196	90,46	0,00	0	0,99275961	18,0919	0,97843572
67	83	0,0166	3,45	0,00340	0,7071		10,50	0,0003571	-5475,02	93,61	303,09	11,68	1093,46	39,65	6133,35	0,0196	93,61	0,00	0	0,99401333	18,7227	0,98214728
68	86	0,0172	3,58	0,00280	0,5823		10,24	0,0002866	-4579,24	96,77	307,51	11,60	1122,41	32,00	6141,00	0,0197	96,77	0,00	0	0,99519953	19,3532	0,98566761
69	88	0,0176	3,66	0,00240	0,4991		10,07	0,0002417	-3964,44	98,87	310,40	11,55	1141,60	27,08	6145,92	0,0198	98,87	0,00	0	0,9959558	19,7733	0,9879164
70	90	0,0180	3,74	0,00200	0,4160		9,91	0,0001982	-3335,98	100,97	313,23	11,50	1160,70	22,28	6150,72	0,0198	100,97	0,00	0	0,99668631	20,1934	0,99009184
71	91	0,0182	3,79	0,00180	0,3744		9,83	0,0001769	-3016,72	102,02	314,63	11,47	1170,22	19,92	6153,08	0,0198	102,02	0,00	0	0,99704237	20,4034	0,99115334
72	94	0,0188	3,91	0,00120	0,2496		9,60	0,0001152	-2039,39	105,17	318,77	11,40	1198,64	13,04	6159,96	0,0199	105,17	0,00	0	0,99807581	21,0331	0,99423863
73	95	0,0190	3,95	0,00100	0,2080		9,53	0,0000953	-1707,21	106,21	320,13	11,37	1208,07	10,80	6162,20	0,0199	106,22	0,00	0	0,99840924	21,2430	0,9962363
74	96	0,0192	3,99	0,00080	0,1664		9,46	0,0000757	-1371,90	107,26	321,47	11,35	1217,48	8,59	6164,41	0,0199	107,26	0,00	0	0,99873739	21,4528	0,99621695
75	97	0,0194	4,03	0,00060	0,1248		9,39	0,0000563	-1033,48	108,31	322,81	11,33	1226,87	6,40	6166,60	0,0199	108,31	0,00	0	0,99906041	21,6626	0,99718388
76	98	0,0196	4,08	0,00040	0,0832		9,32	0,0000373	-692,01	109,36	324,14	11,30	1236,24	4,24	6168,76	0,0200	109,36	0,00	0	0,99937843	21,8724	0,99813645
77	99	0,0198	4,12	0,00020	0,0416		9,25	0,0000185	-347,50	110,41	325,45	11,28	1245,60	2,11	6170,89	0,0200	110,41	0,00	0	0,99969159	22,0821	0,99907504
78	99,9	0,0200	4,16	0,00002	0,0042		9,19	0,0000018	-34,88	111,35	326,63	11,26	1254,00	0,21	6172,79	0,0200	111,35	0,00	0	0,99996937	22,2709	0,99990811

This column is important (column I)

This column is important (column N)

Solv

von Zeile 32 bis Zeile 78

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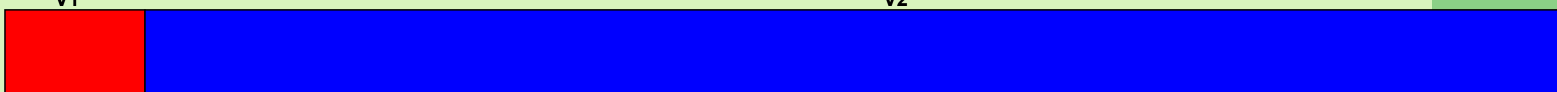
Some explanations to the calculations

Sketch for understanding what is meant with V1, V1-expanded, V2 and V2-compressed

1. step: V1 and V2 contain the same explosive mixture. There is no membrane between V1 and V2. In a Gedankenexperiment we let only V1 react, but do not yet allow expansion of the reaction gases. V1 now contains the hot reaction gases at high pressure, V2 still contains the unreacted mixture at the initial pressure and temperature

V1 **V2**



2.step: Now we allow V1 to expand at the expense of V2 until pressure equilibrium is attained, which means that the pressure in the expanded volume V1 (labelled "V1-expanded") is equal to the pressure in the adiabatically compressed volume V2 (labelled "V2-compressed")

V1-expanded **V2-compressed**

(temperature of reaction gases has dropped slightly due to expansion, i.e. the work that had to be brought up for compressing V2)

(temperature of the yet unreacted mixture in V2-compressed has risen slightly due to the adiabatic compression brought about by the expansion of the reaction gases in Volume V1-expanded)

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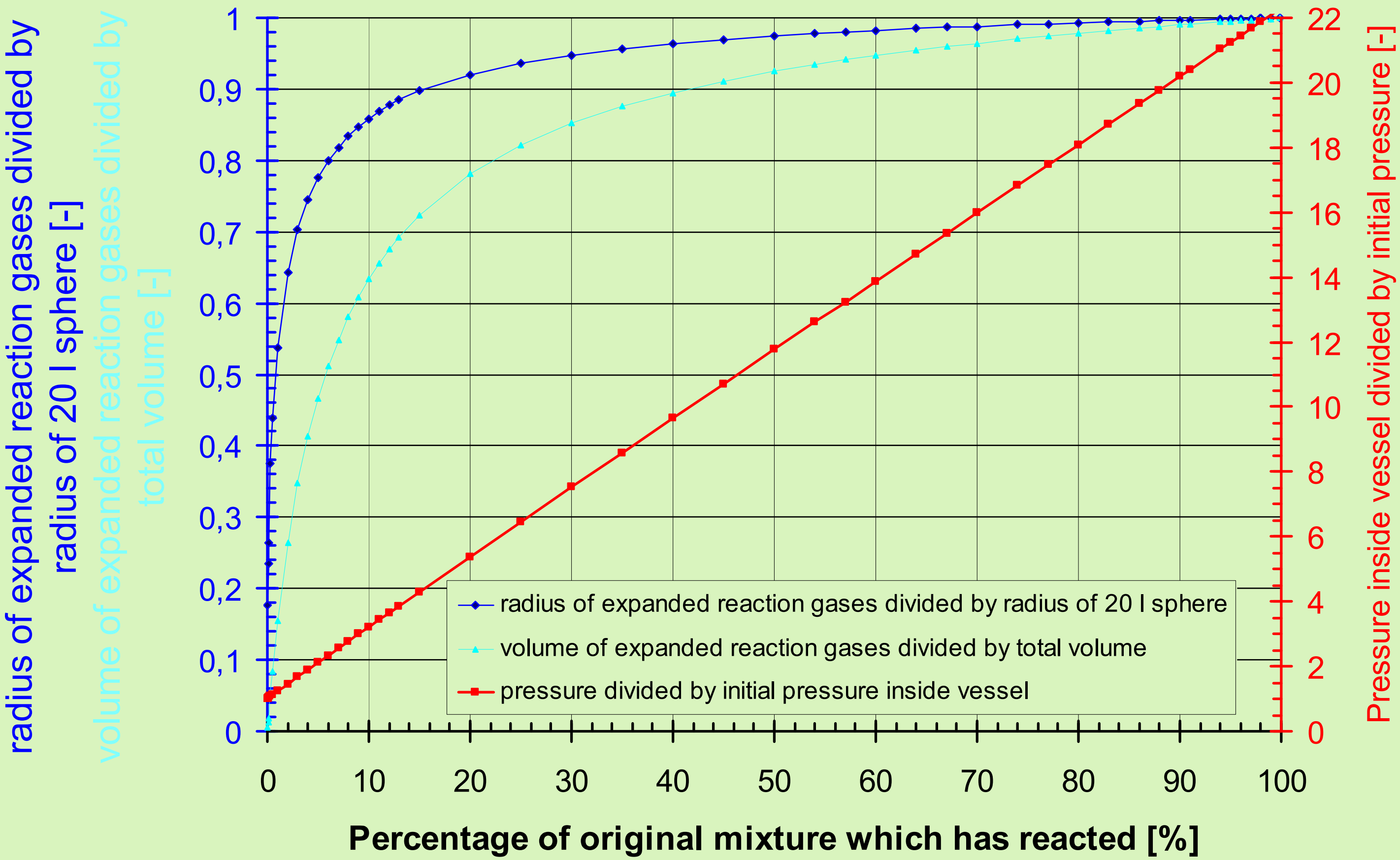
Further information to DDT in 20 l sphere: Rise in volume of the expanding reaction gases and rise of pressure inside sphere during the deflagrative explosion inside the sphere

Gas mixture: Propene = 38 vol.-%, O_2 = 62 vol.-%, $P_{initial}$ = 5 bar abs, $T_{initial}$ = 25°C, ignition in center, deflagration pressure ratio = 22 (see talk given at 41st UKELG-meeting)



Note. When precompression has reached a factor of 20, the shell of unreacted precompressed mixture is extremely thin in radial direction. The DDT probably does not happen over an entire spherical surface at the same instant, but only over a sub-surface. So there is a good chance that the first pressure peak „seen" by the pressure sensor is not the detonation peak but the reflected shock wave comming from the detonation that hit the wall elsewhere.

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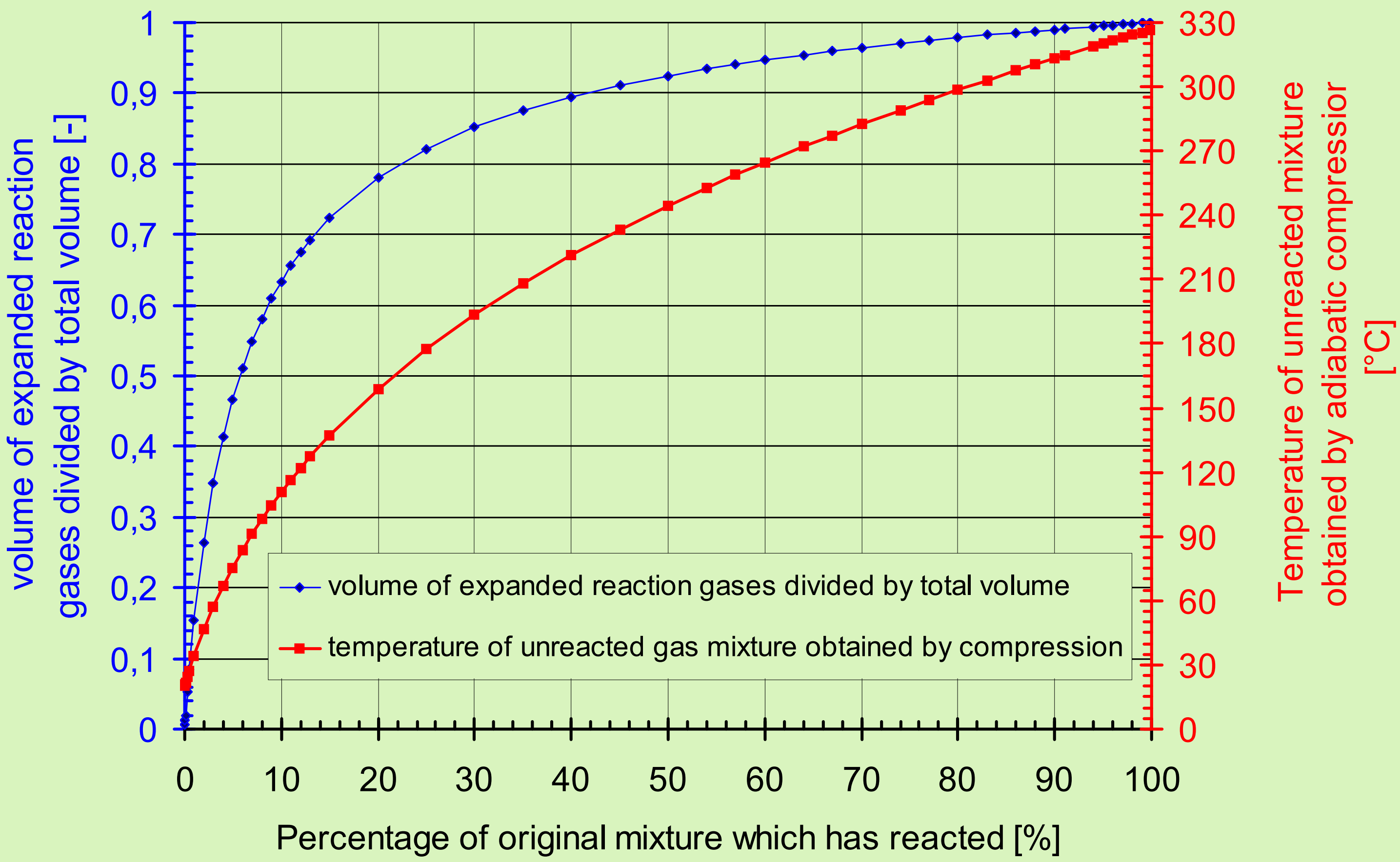
Further information to DDT in 20 l sphere: Rise in volume of expanded reaction gases and rise of temperature in the unreacted mixture during the deflagrative explosion inside the sphere

Volume of expanded reaction gases divided by total volume of vessel and temperature in unreacted mixture obtained by adiabatic compression (Data for Propene:O_2 = 38 vol.-% : 62 vol.-%, $P_{initial}$ = 5 bar abs and $T_{initial}$ = 20°C in 20 l sphere, = 1.3)



Further scenarios which are unclear

- Scenario IV with reflection:

  If the detonation established in scenario IV hits the blind flange and gets reflected, what will be p_{stat} at the blind flange?

  (since p_{stat} will presumably decrease when the detonation propagates from the point, where it came into being, to the blind flange, p_{stat} at the blind flange will most likely depend on the distance between the DDT point and the blind flange. However, because the location of the DDT is not excatly predictable, one would have to assume the worst-case scenario, which is the DDT directly ahead of the blind flange. This means maximum precompression).

- detonation in columns (alternating: packing - free space)

- detonation in bubble columns

- „surface detonations“

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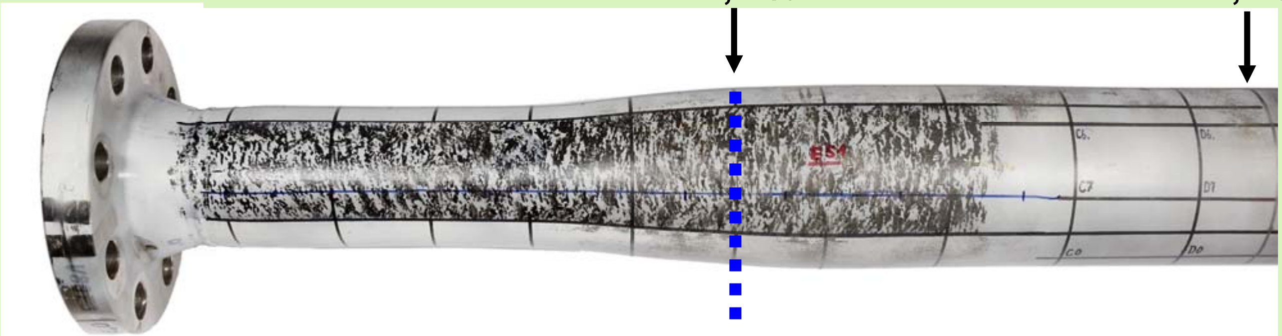
Example 1: DDT and stable detonation (W. Stadtmüller)

Parameters of 114.3 x 6.02 pipe made out of 1.4541:
- wall thickness s = 6.02 mm
- inner diameter ϕ_i = 102.26 mm
- yield strength $R_{p0.2}$ = 230 N/mm^2 at 25°C (sample cut out of the wall)
- ultimate tensile strength R_m = 590 N/mm^2 at 25°C (sample cut out of the wall)
- pressure generating a hoop stress equal to $R_{p0.2}$: $P_{Rp0.2} = 2*s*R_{p0.2}/\phi_i$ = 270.8 barg
- burst pressure in a hydraulic test: 519 bar

Conditions for detonation test:
80 vol.-% H_2:O_2=2:1, 20 vol.-% N_2, initial pressure 70 bar, 20°C, P_{CJ} = 1470 bar, $P_{CJ}/P_{initial}$ = 21

Increase of diameter: 37,1 % 31,4 %



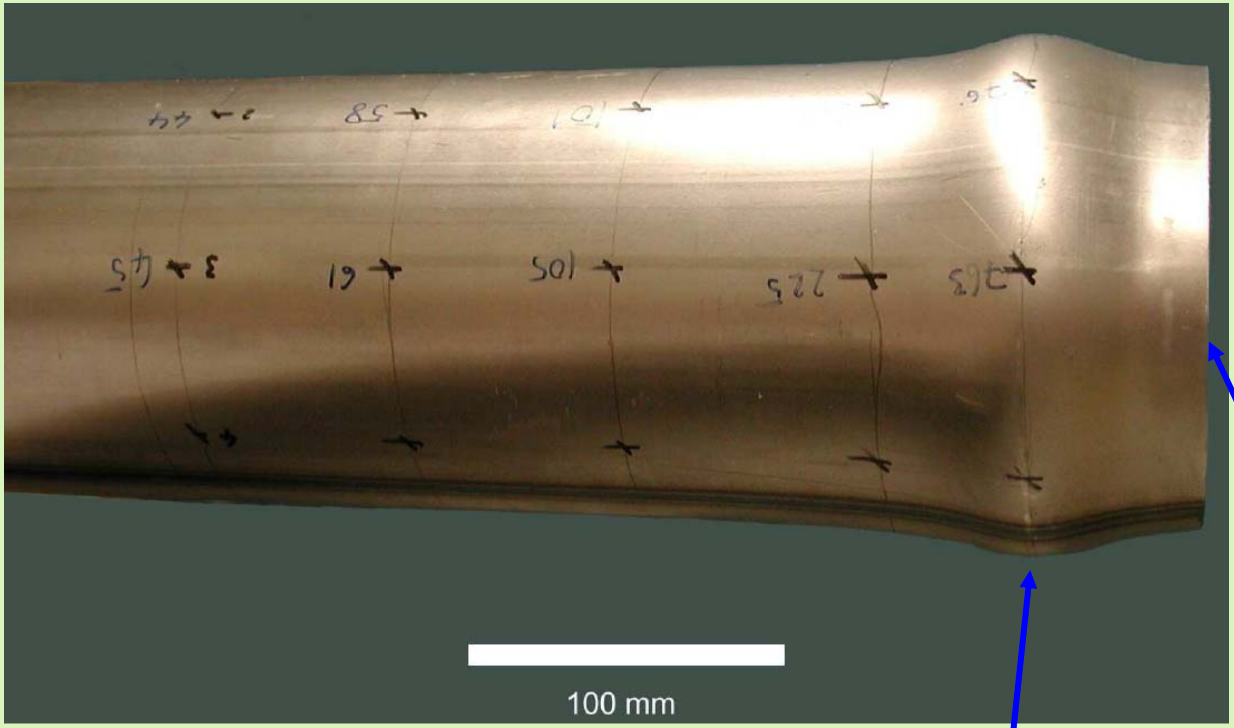
Flange on the ignition side

DDT in 520 mm distance from the ignition

Since detonative pressure at DDT is much larger than P_{CJ}, the ratio between the static equivalent pressure p_{stat} and the detonative pressure p_{det} at the DDT is much less than 519/1470 = 0.353

Reference:
W. Stadtmüller, E. Roos, S. Offermanns, Materialprüfungsanstalt University Stuttgart, private communication within the scope of the reactor safety research of the German Federal Ministry of Economics and Technology (BMWi). Parts of the research work will be published at the *International Conference on Structural Mechanics in Reactor Technology SMiRT 20 – Conference*, August 09-14, 2009, Helsinki, Finnland

Example 2: DDT short before blind flange (J.E. Shepherd)



The peak pressure measured at the end was approximately 500 bar according to Shepherd

15% plastic deformation

Tube parameters:

- wall thickness s = 1.5 mm
- inner diameter ϕ_i = 129 mm
- yield strength $R_{p0.2}$ = 305 N/mm^2 (AISI1010 steel)
- pressure generating a hoop stress equal to $R_{p0.2}$: $P_{Rp0.2} = 2*s*R_{p0.2}/\phi_i$ = 70.9 barg

Since static pressure yielding 15% deformation is of the order of 1.5*$P_{Rp0.2}$, the ratio between the static equivalent pressure p_{stat} and the detonative pressure p_{det} at the DDT is about (1.5*70.9)/500 = 0.21

Reference:

J.E. Shepherd, "*STRUCTURAL RESPONSE OF PIPING TO INTERNAL GAS DETONATION*", Proceedings of PVP2006-ICPVT-11, 2006 ASME Pressure Vessels and Piping Division Conference, July 23-27, 2006, Vancouver BC, CANADA

Example 3: DDT directly ahead of blind flange (BASF) (1/2)

picture of reactor used for the tests:

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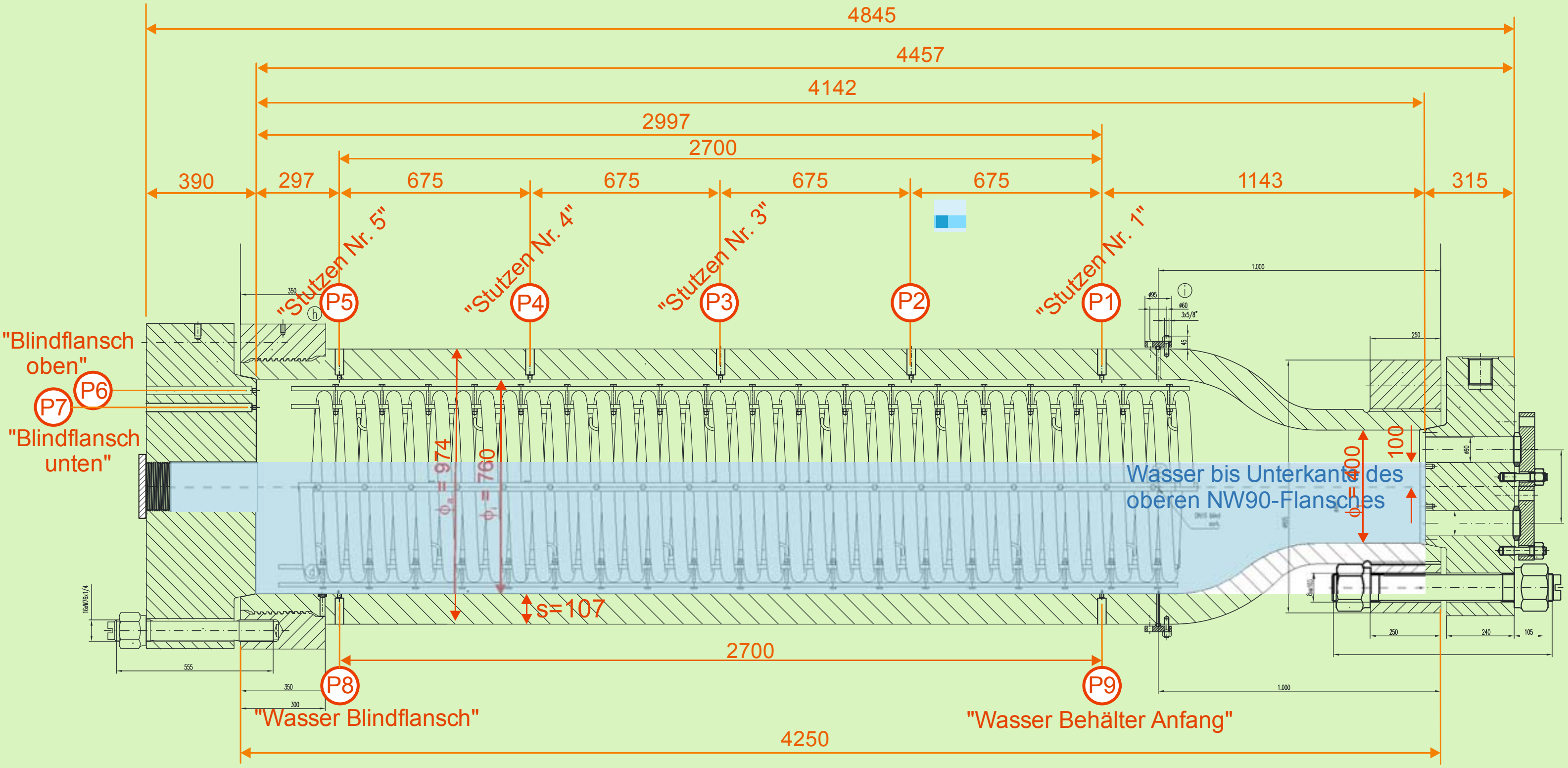
Example 3: DDT directly ahead of blind flange (BASF) (2/2)

Parameters of 974 x 107 pipe reactor:

- wall thickness s = 107 mm
- inner diameter ϕ_i = 760 mm
- wall material Ce36, $R_{p0.2}$ = 506 N/mm², R_m = 691 N/mm² at 25°C
- pressure generating a hoop stress equal to $R_{p0.2}$: $P_{Rp0.2} = 2 * s * R_{p0.2} / \phi_i$ = 1424 barg

Conditions for detonation test:

15 bar C_2H_2, 20°C, $P_{CJ}/P_{initial}$ = 20 at 20 °C, ignition at position of pressure sensor P3, DDT occurred between P5 and left blind flange, mixture was precompressed to at least 110 bar, pressure recording of P6 und P7: 5300 bar



Oberservation: no deformation of blind flange or wall, not even lift-off of blind flange

Summary

Although at the DDT the value of p_{det} is presumably much larger than the value of p_{det} of the stable detonation, the static equivalent pressure at the DDT is presumably not by the same factor larger than the static equivalent pressure of the stable detonation.

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Difficulties with experiments for clearifying the load in scenarios III and IV

- Information about p_{stat} can only be obtained by conducting experiments at such high initial pressures that permanent deformations are generated in the pipe wall.
  Since repeated detonative loads at the limit of or even beyond the elastic range of the wall material changes its mechanical parameters (strain-hardening („Kaltverfestigung“) and embrittelment („Versprödung“); see example with 100 l vessel), one would have to replace the test pipes at best after each detonation => very expensive and very time consuming.

- When trying to realize scenario IV in a test, the number of tests will be extremely large, because most tests will end up with scenario III or will not show a DDT at all.

- Even if scenario IV does occur in some experiment, it is not as well defined in the mechanical load as scenario III, because the degree of precompression can take any value between 0 and the deflagration pressure ratio.

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Example for embrittlement of the wall of vessels by repeated exposure to strong detonative loads

Vessel parameter:
V = 100 l, design pressure: 64 bar, ϕ_o = 355.6, ϕ_i = 327.2, s=14.2; Material of cylindrical section: St35.8 = 1.0305, $R_{p0.2}$=339 N/mm^2 , R_m = 453 N/mm^2 (tested was 1 pipe of the charge of 355.6 x 14.2 pipes), $P_{Rp0.2}$ = 294 bar

Conditions for the detonation tests:
- About 20 tests with stoichiometric Ethylene/O_2 at initial pressures of 2 to 8 bar abs. Then vessel was filled with Raschig-Rings 15 mm x 15 mm, s = 0.3 mm
- Test no. 19: $P_{initial}$ = 18 bar abs => 2 % diameter increase;
- Test no. 20: $P_{initial}$ = 20 bar abs => rupture (see picture below).
  An increase of 10% in $P_{initial}$ should not result in a transition from 2% diameter increase to vessel rupture unless the material had become brittle by all the preceding tests at rather high pressure loads.

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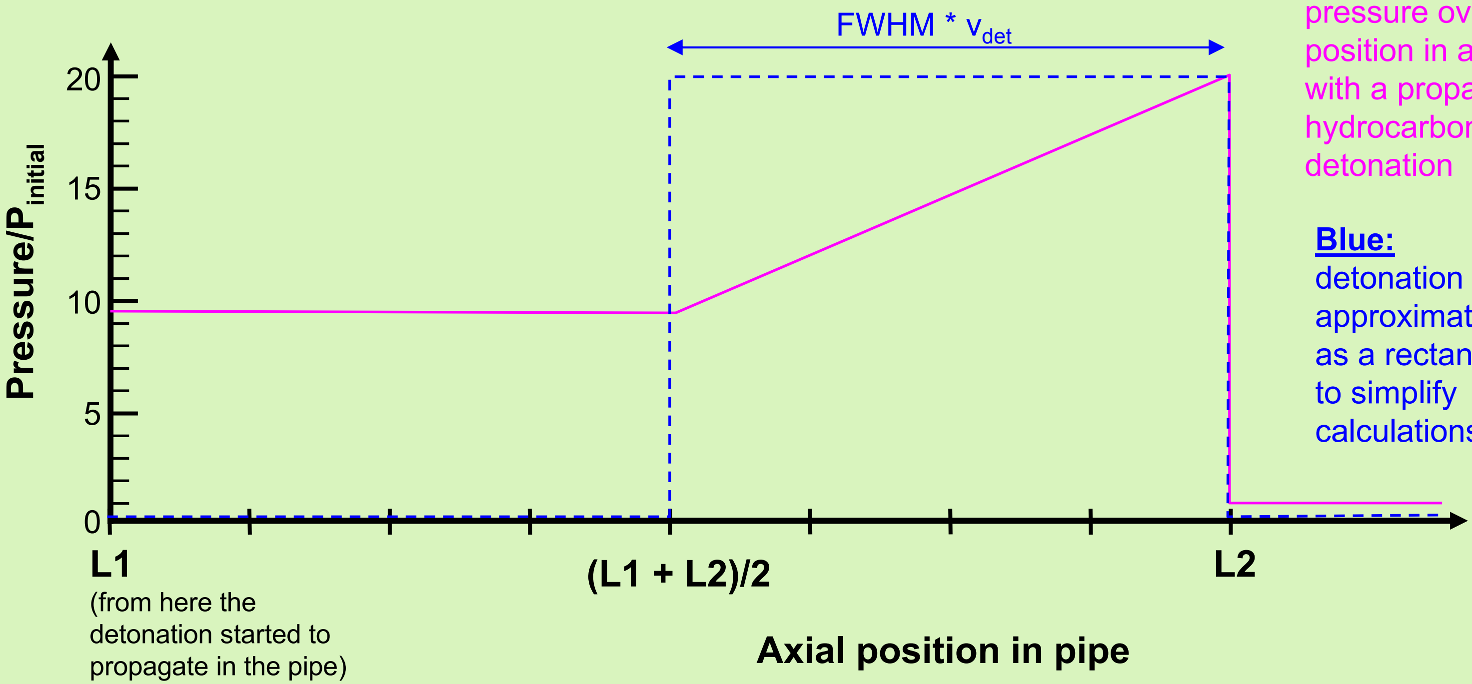
Approximation of detonative pressure pulse by rectangular peak of duration FWHM



Magenta:
pressure over axial position in a pipe with a propagating hydrocarbon/air detonation

Blue:
detonation peak approximated as a rectangle to simplify calculations

Note: Δs: distance the detonation has travelled

v_{det}: detonation speed

ϕ_i: inner pipe diameter

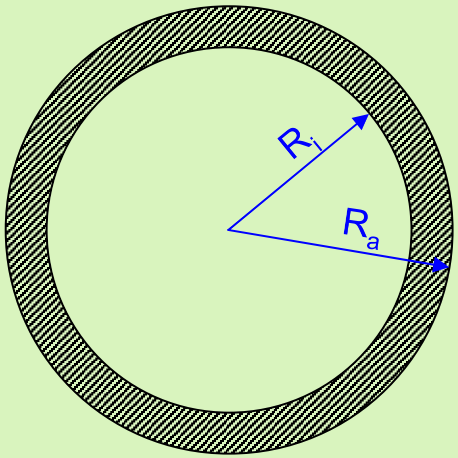
Approximately the following holds as long as $\Delta s < 70 * \phi i$: FWHM $\cong 0.5 * \Delta s / v_{det}$

For $\Delta s > 70 * \phi_i$ FWHM will usually no longer increase, i.e. constant pressure/space profile

Definition of parameters for calculating the pipe response to a detonative load with a simplified pressure/time profile

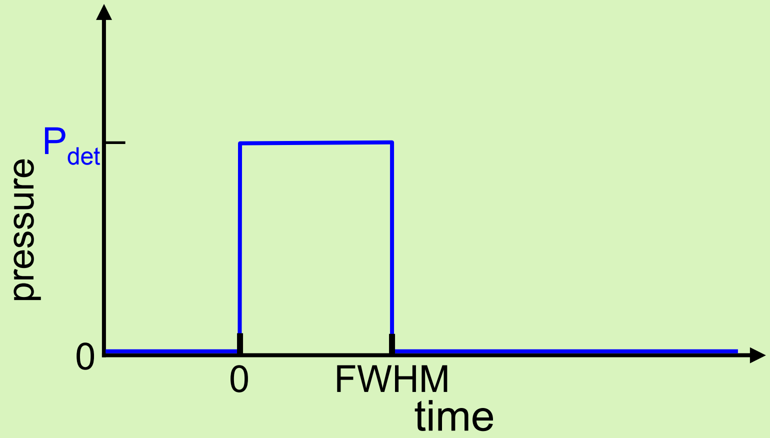
Parameters defining the pipe:

R_i = inner radius
R_o = outer radius
s = wall thickness = R_o - R_i
ρ= density of pipe material, typical 7800 kg/m^3
E = E-modulus of pipe material, typical 200000 N/mm^2
r(t) = displacement of the wall in radial direction from the position at rest, i.e. without pressure inside the pipe



Parameters defining the pressure pulse acting on the wall:

Overall shape of detonation peak is a rectangle;
Pressure is „switched on“ at t = 0;
P_{det} = height of detonation peak;
FWHM = full width at half maximum of peak;
Approximation that pressure acts over the entire length of the pipe at the same time.



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Solution for the time dependent displacement r(t) of the wall from the position of rest (fundamental radial oscillation mode)

Time range I: $t < 0$ $$r(t) = 0$$

Time range II: $0 \le t \le FWHM$ $$r(t) = \frac{K2}{K1} \cdot \left(1 - \cos(\omega \cdot t)\right)$$

Time range III: $t > FWHM$ $$r(t) = A \cdot \cos(\omega \cdot t) + B \cdot \sin(\omega \cdot t) = \sqrt{A^2 + B^2} \cdot \sin\left(\omega \cdot t + \arctan\left(\frac{A}{B}\right)\right)$$

$$\omega = 2 \cdot \pi \cdot \nu = \sqrt{K1}$$

$$\nu = \frac{1}{2 \cdot \pi} \cdot \sqrt{\frac{4 \cdot E}{\rho \cdot (R_o + R_i)^2}} = \frac{1}{2 \cdot \pi \cdot R_{mean}} \cdot \sqrt{\frac{E}{\rho}}$$

$$T = \frac{1}{\nu}$$

$$K1 = \frac{4 \cdot E}{\rho \cdot (R_o + R_i)^2} = \frac{E}{\rho \cdot R_{mean}^2}$$

$$A = \frac{K2}{K1} \cdot \left(\cos(\omega \cdot FWHM) - 1\right)$$

$$K2 = \frac{2 \cdot R_i \cdot P_{\det}}{\rho \cdot \left(R_o^2 - R_i^2\right)} \cong \frac{P_{\det}}{\rho \cdot s}$$

$$B = \frac{K2}{K1} \cdot \sin(\omega \cdot FWHM)$$

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Maximum displacements in case that FWHM ≥T/2

In time range II r(t) adopts at least once its maximum value, which is given by:

$$r_{maxII} = 2 \cdot \frac{K2}{K1} = \frac{(R_o + R_i) \cdot R_i}{s \cdot E} \cdot P_{\det} \cong \frac{2 \cdot R_{mean}^2}{s \cdot E} \cdot P_{\det} \qquad (20)$$

The largest displacement in time range III is given by:

$$r_{maxIII} = 2 \cdot \frac{K2}{K1} \cdot \sin\left(\pi \cdot \frac{FWHM}{T}\right) \qquad (21)$$

Obviously $r_{maxIII} \leq r_{maxII}$ and hence the largest displacement is given by the equation 20 for r_{maxII}.
Note that this is exactly twice the value that would have been obtained if the pressure had not been switched on suddenly but had been increased slowly from zero to P_{det} ($\sigma = P*\phi_i/(2*s) = P*2*R_{mean}/(2*s) = P*R_{mean}/s$;
$r(t)/R_{mean} = \varepsilon = \sigma/E$ => $r_{max} = P_{det} * R_{mean}^2 / (s * E)$).

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Maximum displacements in case that FWHM <T/2

In time range II r(t) increases monotonously with t, but never reaches the value given by eq. (20), because the pressure of the detonation peak which is the driving force for the wall displacement drops down to zero before r(t) would have attained its maximum displacement at t = T/2 for the first time. However, for a short period after the pressure dropped down to zero the outwardly directed movement of the wall continues due to the kinetic energy stored in the moving wall at time t = FWHM. The largest displacement is hence attained in time range III and is given by eq. (21):

$$r_{maxIII} = 2 \cdot \frac{K2}{K1} \cdot \sin\left(\pi \cdot \frac{FWHM}{T} \right) \qquad (21)$$

Obviously, the largest displacement in case that FWHM < T/2 is less than the largest displacement reached in case that FWHM ≥ T/2.

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Introduction of damping factor D in case that FWHM < T/2

Definition of D:

D is the ratio between the largest displacement in case that FWHM < T/2 („long“ detonative pressure pulse) and the largest displacement in case that FWHM > T/2 („short“ detonative pressure pulse).
Hence D quantifies the damping of the displacement of the wall due to the inertia of the wall material.

$$D = \sin\left(\pi \cdot \frac{FWHM}{T}\right)$$

Convenient procedure to simplify the „handling“ of D:

- Express FWHM as fraction of T, e. g. FWHM = T/α, α > 2

- Use approximation that sin(x) = x for small x

$$D = \frac{\pi}{\alpha}$$

Example:

If the width of the detonation peak is one twentieth of T (i.e. α = 20), one finds D = 0.157. Hence the maximum radial displacement and the corresponding circumferential stress only amount to 15.7% of the values both parameters would have attained if the width of the detonation peak had been longer than T/2.

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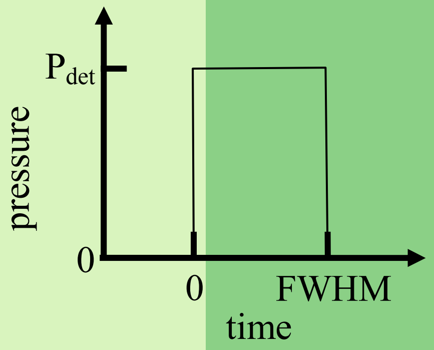
Example 1a: pipe 1080 x 130, P_{det} = 325 bar, FWHM = 1900µs



Parameters of the exciting detonative pressure pulse

detonative pressure pulse is approximated by a rectangular-shaped pressure-time trace (see sketch to the right)

height of the detonative pressure pulse Pdet	325	bar
width of the detonative pressure pulse FWHM	1900	µs

Parameters of the pipe exposed to the detonative pressure pulse

outer diameter of pipe ϕo	1080	mm	
inner diameter of pipe ϕi	820	mm	
wall thicknes s	130	mm	
outer radius of pipe Ro	540	mm	
inner radius of pipe Ri	410	mm	
mean radius of pipe Rmean	475	mm	
density ρ of wall material	7900	kg/m3	
E-modulus of wall material E	200000	N/mm2	(typical for all steels)
mass per length of pipe Ml	3065,095	kg/m	
inner volume per length	528,102	liter/m	
frequency ν o fundamental radial oscillation mode	1685,885	Hz	
cycle Time T of fundamental radial oscillation mode	0,59316023	milliseconds	
angular frequency ω	10592,7285	radian/s	
damping D	1		

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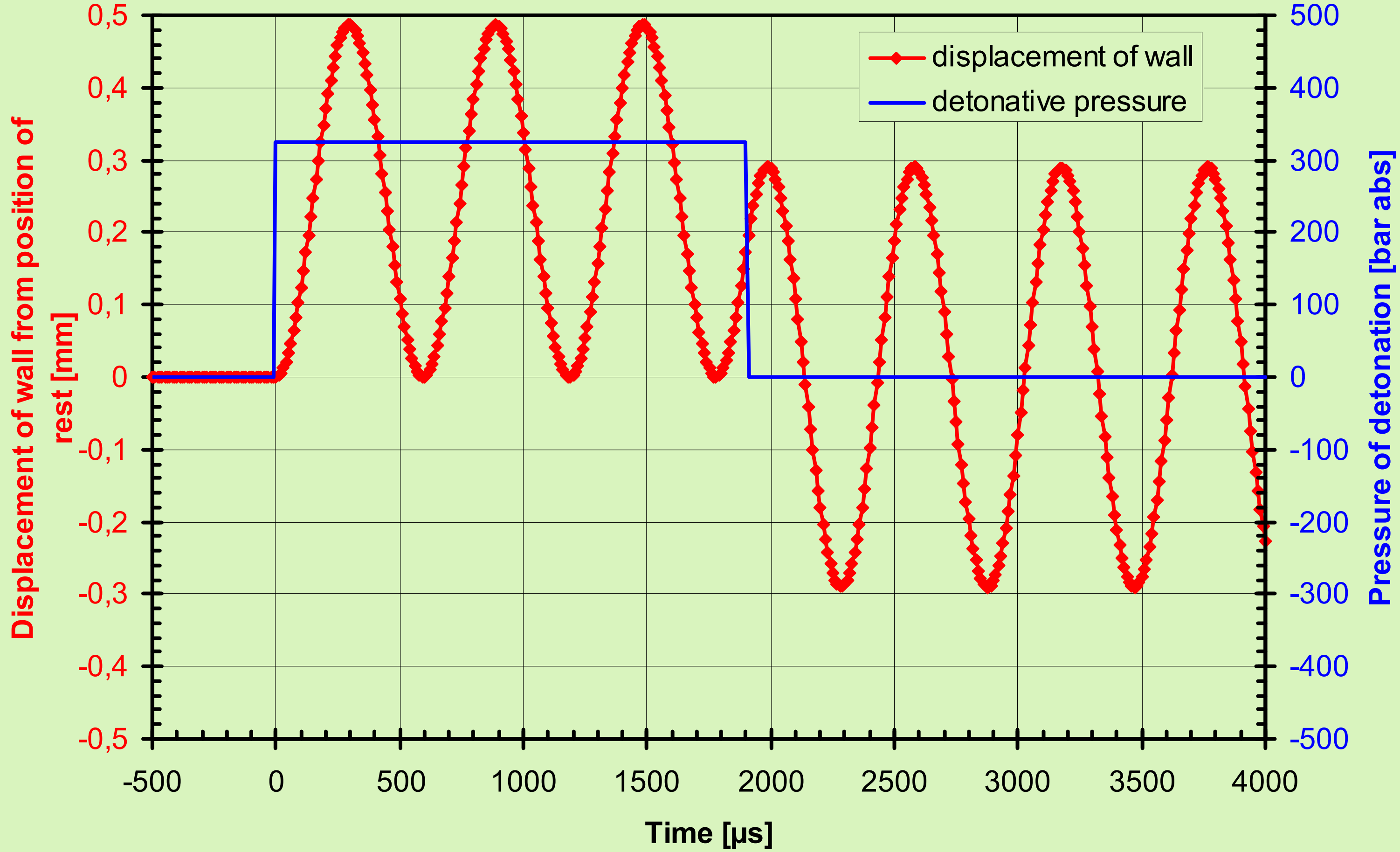
Example 1a: pipe 1080 x 130, P_{det} = 325 bar, FWHM=1900µs



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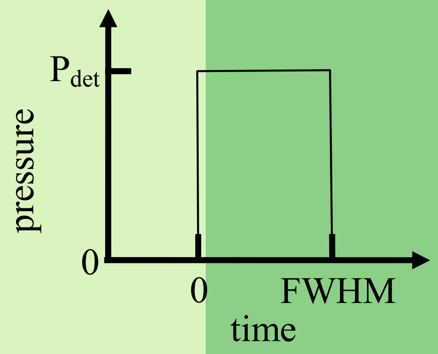
Example 1b: pipe 1080 x130, P_{det} = 325 bar, FWHM=94 µs

Parameters of the exciting detonative pressure pulse

detonative pressure pulse is approximated by a rectangular-shaped pressure-time trace (see sketch to the right)



height of the detonative pressure pulse Pdet	325	bar
width of the detonative pressure pulse FWHM	94	µs

Parameters of the pipe exposed to the detonative pressure pulse

outer diameter of pipe ϕo	1080	mm	
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cycle Time T of fundamental radial oscillation mode	0,59316023	milliseconds	
angular frequency ω	10592,7285	radian/s	
damping D	0,47754487		

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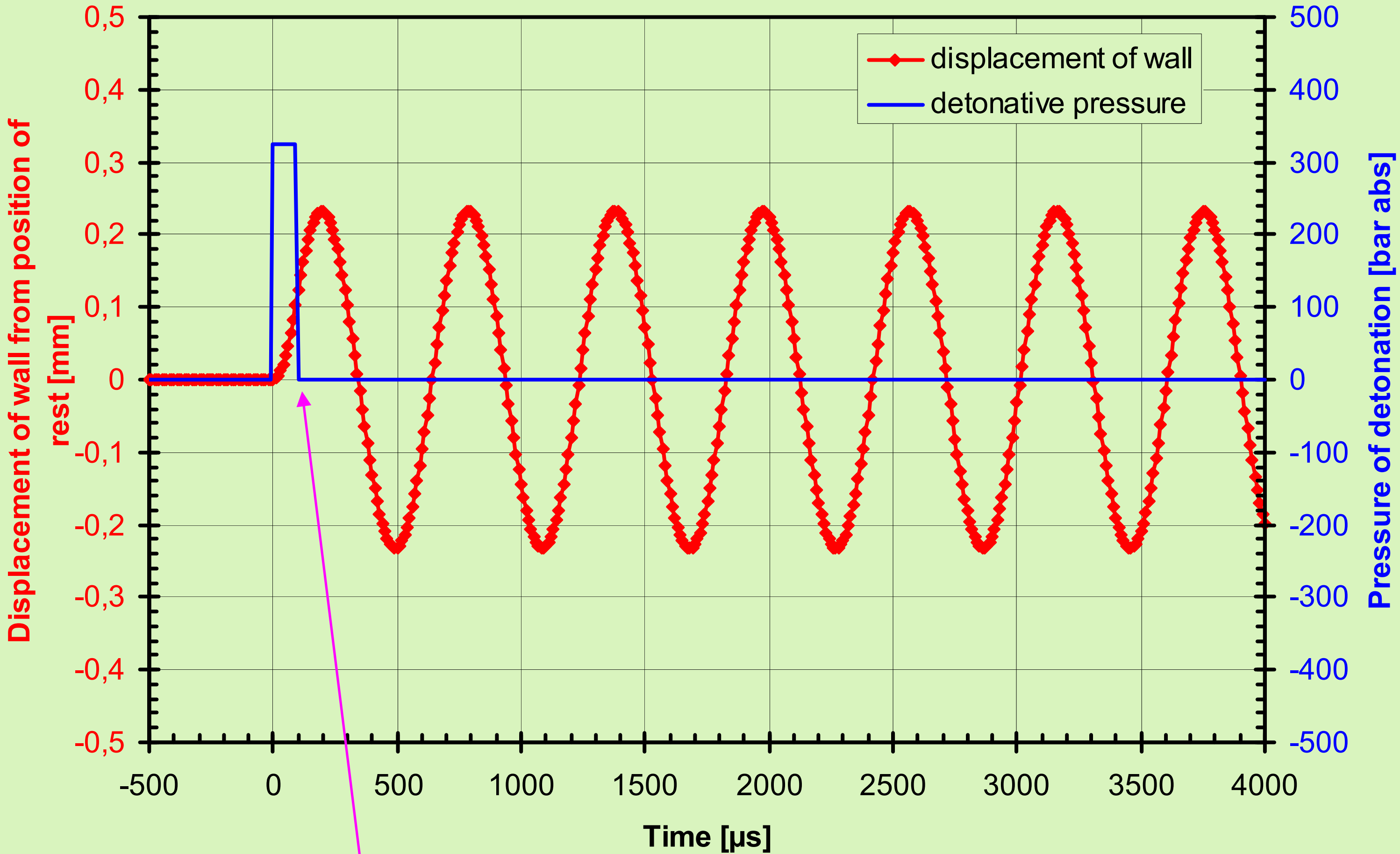
Example 1b: pipe 1080 x130, P_{det} = 325 bar, FWHM=94 µs

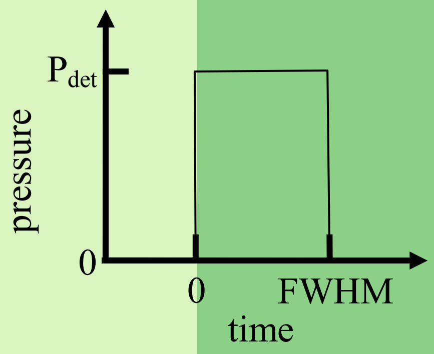


Width of detonative pressure FWHM is less than T/2
=> Pressure drops to zero **before** wall has undergone half an oscillation cycle
=> Maximum displacement is less than in case that FWHM ≥ T/2

Example 2a: pipe 114.3 x 6.02, P_{det} = 200 bar, FWHM = 100 µs

Parameters of the exciting detonative pressure pulse

detonative pressure pulse is approximated by a rectangular-shaped pressure-time trace (see sketch to the right)



height of the detonative pressure pulse Pdet	200	bar
width of the detonative pressure pulse FWHM	100	µs

Parameters of the pipe exposed to the detonative pressure pulse

outer diameter of pipe ϕo	114,3	mm	
inner diameter of pipe ϕi	102,26	mm	
wall thicknes s	6,02	mm	
outer radius of pipe Ro	57,15	mm	
inner radius of pipe Ri	51,13	mm	
mean radius of pipe Rmean	54,14	mm	
density ρ of wall material	7900	kg/m3	
E-modulus of wall material E	200000	N/mm2	(typical for all steels)
mass per length of pipe Ml	16,178	kg/m	
inner volume per length	8,213	liter/m	
frequency ν o fundamental radial oscillation mode	14791,197	Hz	
cycle Time T of fundamental radial oscillation mode	0,06760778	milliseconds	
angular frequency ω	92935,834	radian/s	
damping D	1		

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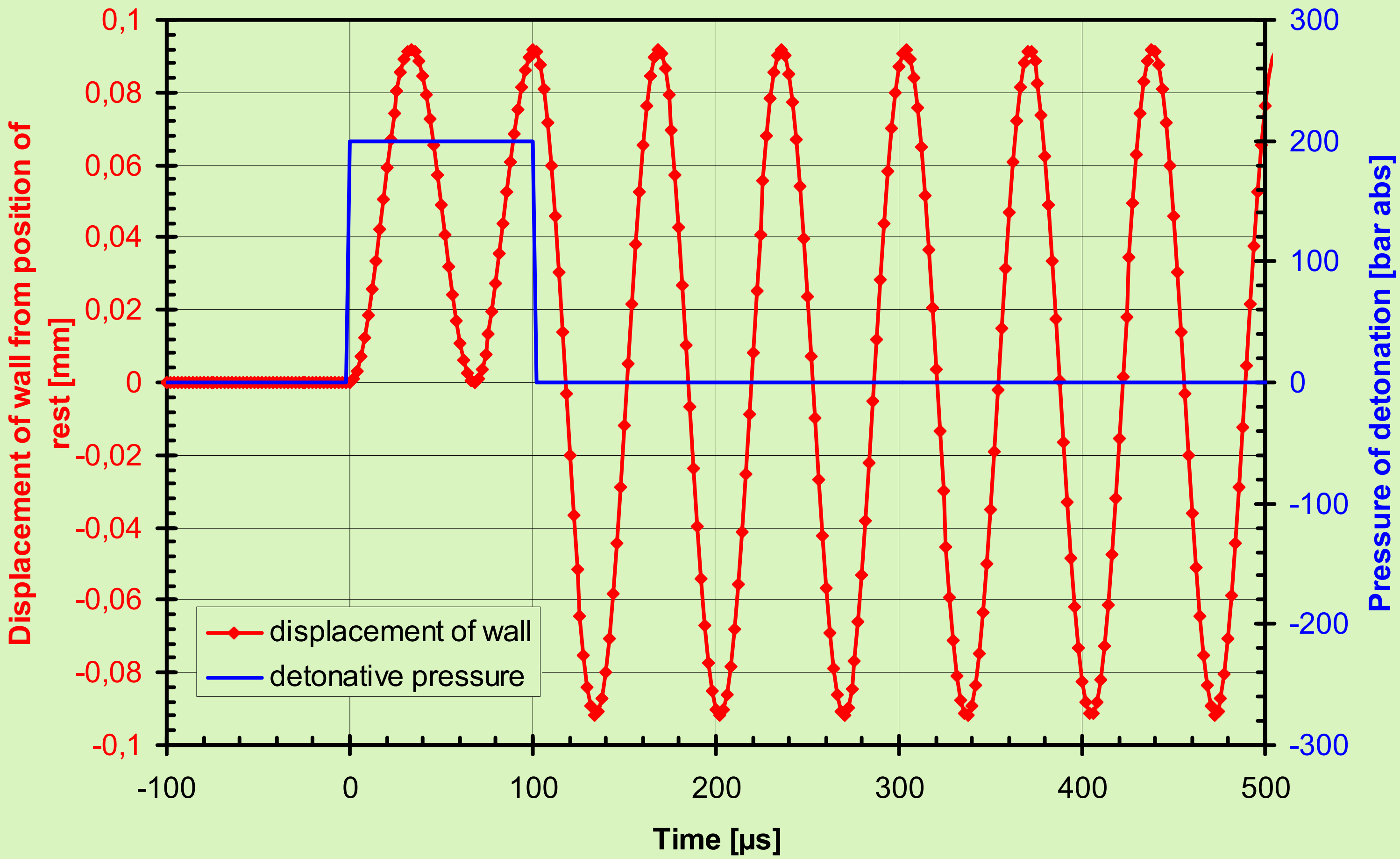
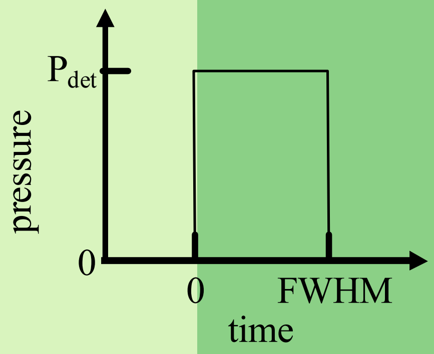
Example 2a: pipe 114.3 x 6.02, P_{det} = 200 bar, FWHM = 100 µs



Example 2b: pipe 114.3 x 6.02, P_{det} = 200 bar, FWHM = 10 µs

Parameters of the exciting detonative pressure pulse

detonative pressure pulse is approximated by a rectangular-shaped pressure-time trace (see sketch to the right)



height of the detonative pressure pulse Pdet	200	bar
width of the detonative pressure pulse FWHM	10	µs

Parameters of the pipe exposed to the detonative pressure pulse

outer diameter of pipe ¬o	114,3	mm	
inner diameter of pipe ¬i	102,26	mm	
wall thicknes s	6,02	mm	
outer radius of pipe Ro	57,15	mm	
inner radius of pipe Ri	51,13	mm	
mean radius of pipe Rmean	54,14	mm	
density ¬of wall material	7900	kg/m3	
E-modulus of wall material E	200000	N/mm2	(typical for all steels)
mass per length of pipe Ml	16,178	kg/m	
inner volume per length	8,213	liter/m	
frequency ¬o fundamental radial oscillation mode	14791,197	Hz	
cycle Time T of fundamental radial oscillation mode	0,06760778	milliseconds	
angular frequency ¬	92935,834	radian/s	
damping D	0,44813601		

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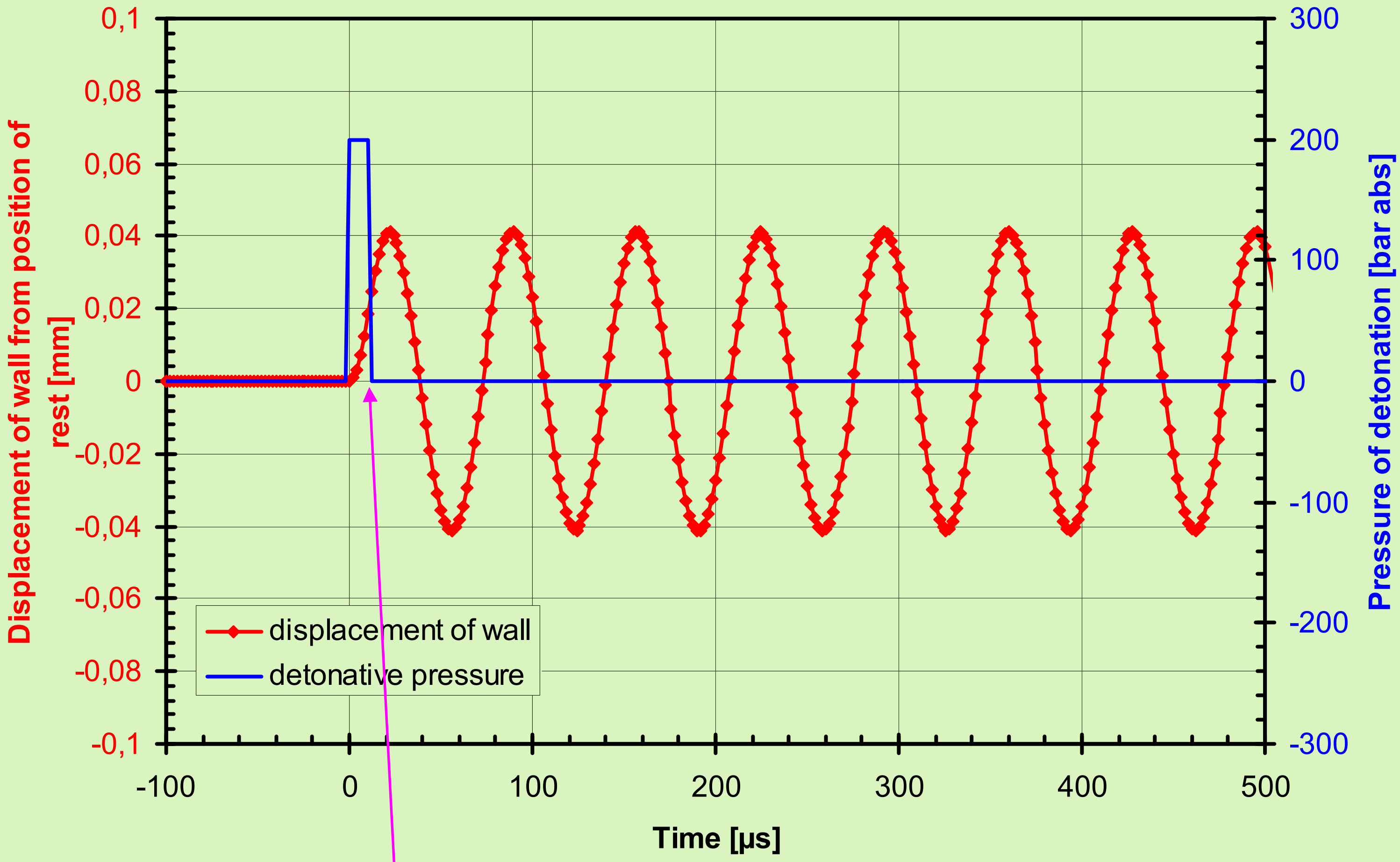
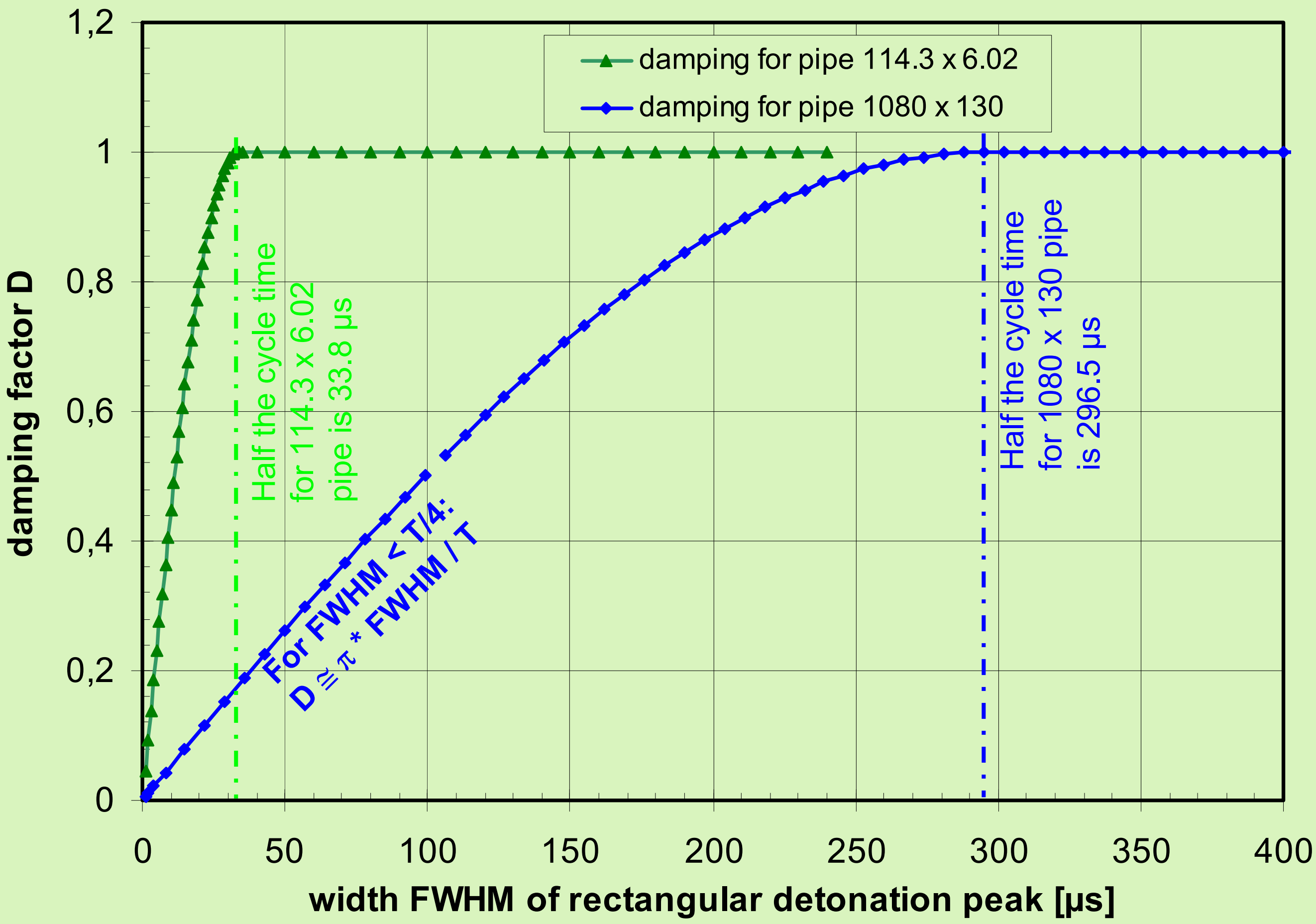
Example 2b: pipe 114.3 x 6.02, P_{det} = 200 bar, FWHM = 10 µs



Width of detonative pressure FWHM is less than T/2
=> Pressure drops to zero **before** wall has undergone half an oscillation cycle
=> Maximum displacement is less than in case that FWHM ≥ T/2

Damping of the displacement of the wall in case of detonation peaks short compared to the cycle time of the fundamental radial oscillation mode

$$\text{Damping factor D} = \frac{\text{Maximum displacement of wall obtained for actual value of FWHM}}{\text{Maximum displacement of wall obtained for FWHM} > T/2}$$



What is all missing in this simple model

- Actually the detonative pressure pulse is not present over the entire length of the pipe at the same time, but travels through. For certain propagation speeds there will be some nasty positive feedback effects between the detonation and flexural waves in the pipe wall.
- Higher order breathing modes not considered. (Will they be excited at all?)
- Bending modes not considered. (Will they be excited at all?)
- Potential mode coupling effects not considered.
  (Breating modes of cylindrical pipe are orthogonal to each other, coupling can not occur. But how about bending and breathing modes?)
- Effect of flange connections on oscillation behaviour not considered.
- Deviations from perfect cylindrical geometry not considered.

  Ovality can be neglected. Deviations of wall thickness over circumference can be neglected as far as this is due to the manufacturing process, but corrosive attack might reduce wall thickness at bottom of horizontally mounted pipes by up to 15%). Welding seams can be neglected

References for real pipe geometries:

DIN EN ISO 1127 „Stainless steel tubes, Dimensions, Tolerances and conventional masses per unit length

DIN EN 10217 “Welded steel tubes for pressure purposes – Technical delivery conditions”, parts 1, 2, 3, 5, 7

Public Available Specification PAS 1057 „Pipe classes for process plants”

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- Introduction
- For which p_{det}-scenarios seems the corresponding mechanical load p_{stat} to be clear
- For which p_{det}-scenarios is the corresponding mechanical load p_{stat} not yet clear
- What do experiments suggest
- Why are systematic experiments difficult
- Simple analytic approach („breathing mode“) to quantify radial displacement of wall in dependence of duration of detonative pressure pulse
- What is our hope concerning the mechanical load p_{stat} brought about by detonative pressure pulses
- What might help to answer the open questions with regard to mechanical load p_{stat}

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What is our hope?

Hope 1:
At the location where the DDT occurs and also closely downstream of it the duration of the detonation peak should be extremely short.

If this were true:
Although the height of the peak may be a factor of 4 to 8 larger than the height of the peak of the stable CJ-Detonation, the damping factor D will be much less than 1 and thus p_{stat} is only a factor 1.5 to 2 larger than in those regions where the stable CJ detonation propagates.

Hope 2:
Neither higher order modes nor mode coupling play a relevant role.

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The (hopefully) ultimate solution

- Calculate **reliable** pressure profiles $p_{det}(x)$* at the moment of DDT and in the short time intervals afterwards when the detonation still propagates through the region where the mixture got compressed by it‘s inertia and by frictional forces with the wall.
  If possible the calculation should also include the various degrees of precompression and the reflection of the detonative peak.

- Use these pressure profiles as a source term in FE calculations to quantify the response of the containment (pipes and vessels) subjected to these events. These calculations should include:

  a) interference effects of the different vibration modes of the pipe
  b) potential mode coupling effects
  c) decay of vibration modes due to energy dissipation
  d) critical propagation speeds of the detonation (interaction between propagating detonation and flexural waves in the wall)
  e) effects of elbows, flange connections, blind flanges
  f) realistic deviations from cylindrical symmetry of the wall material

*: let x denote the axial position in the pipe

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