

VOL. 48, 2016



DOI: 10.3303/CET1648042

Copyright © 2016, AIDIC Servizi S.r.I., ISBN 978-88-95608-39-6; ISSN 2283-9216

Guest Editors: Eddy de Rademaeker, Peter Schmelzer

Gas-Phase Detonations in Pipes: the 8 Possible Different Pressure Scenarios and their Static Equivalent Pressures Determined by the Pipe Wall Deformation Method (part 2)

Hans-Peter Schildberg

BASF SE, D-67056 Ludwigshafen, Germany hans-peter.schildberg@basf.com

The abstract of the second part of this paper is included in the abstract of part 1.

4.1.1 Long pipes

A pipe shall be defined as "long" when the detonation front arrives at the blind flange of the pipe <u>before</u> the pressure wave generated by the initial deflagrative stage does. When plotting the maximum pressure ratios attained in a long pipe at each axial position during the course of an explosion with transition from deflagration to detonation, a diagram as displayed by figure 5b is obtained. Here, four discrete detonative pressure scenarios exhibiting different maximum pressures can be distinguished. The following statements explain this in more detail:

- a) At the location of the DDT a very large pressure is generated (scenario 1) which is due to the fact that the bump of unreacted mixture that was compressed directly ahead of the accelerating piston suddenly autoignites. Neither the dependence of the height of this pressure peak nor the dependence of its exact duration on the mixture composition, the initial pressure and the initial temperature are quantitatively understood. Experiments suggest that the duration be less than about 20 μs.
- b) In the region between the location where the DDT occurred and the position of the pressure front propagating slightly faster than the speed of sound, the detonation propagates in a mixture having a higher pressure than at the moment of ignition. This is the region where the detonation is usually termed "unstable detonation" or "overdriven detonation" (scenario 2).
- c) The final stage of detonation propagation is always the propagation in the unreacted gas mixture which is still present in the pipe at the initial temperature and the initial pressure, i.e. at the values valid at the moment of ignition. When this stage is reached, the detonation is termed "stable detonation" (scenario 3). The pressure/time trace of the stable detonation is well understood (see figure 7). The peak height is given by the product of p_{initial} and the so-called Chapman-Jouguet pressure ratio, the width of the Taylor expansion fan is about 25% of the time interval over which the detonation has propagated, but in very long pipes it will not become larger than 25% of the time needed to propagate over a distance of 70 to 120 pipe diameters (Edwards 1970, Ligon 2015).
- d) In case that the pipe has a blinded end, the propagation of the stable detonation, which consists of a leading shock front being directly followed by the reaction zone, ends at the blind flange. The shock front gets reflected and propagates backwards through the hot reaction products. The side-on pressure at the point of reflection is about a factor of 2.4 larger than the side-on pressure of the stable detonation (scenario 4).
- e) In highly reactive gas mixtures which have a large flame speed right from the start, the region of unstable detonation no longer appears, because the flame front already overtakes the pressure wave caused by the initial deflagrative stage of the explosion before the DDT occurs. For hydrocarbon/O₂/N₂ mixtures this happens for O₂-concentrations exceeding about 30 vol.-%, for self-decomposing Acetylene this happens (Schildberg 2014) for initial pressures larger than about 15 bar abs (note that the decomposition speed of Acetylene increases substantially with increasing initial pressure as it does for all other decomposable

substances). In such cases scenario 2 will be missing, but the other scenarios 1, 3 and – in case that a blinded pipe end being present – scenario 4 will occur as for the not so reactive gas mixtures.

f) Since scenario 2 always follows scenario 1 in space and time, and since the location of the DDT is not exactly determined even if the location of the ignition source were known, the pipe region, where the DDT can be expected and which must hence be designed to cope with scenario 1, will usually always include the region where scenario 2 occurs. Since the static equivalent pressures (p_{stat}) occurring in scenario 2 are less than p_{stat} of scenario 1, scenario 2 is irrelevant with regard to detonation pressure proof pipe design.



Figure 7: Left picture: schematic sketch of the pressure/time trace of the side-on pressure of a stable detonation. The von Neumann spike is too short to be recorded by a piezoelectric pressure sensor and also too short to be noticed by the walls of the containment (its duration is at least one or two orders of magnitude less than the cycle time of the fundamental oscillation modes). Right picture: examples for typical approximations of detonative pressure peaks used in FE-calculations. If the stable detonation is to be approximated, p_{det} equals the Chapman-Jouguet pressure, FWHM equals the width of the Taylor expansion fan and p_{∞} equals 0.5 p_{det} .

4.1.2 Short pipes

A pipe is defined as "short" when the detonation front arrives at the blind flange of the pipe <u>after</u> the pressure wave generated by the initial deflagrative stage did.

When plotting the maximum pressure ratios attained in a short pipe at each axial position during the course of an explosion with transition from deflagration to detonation, a diagram as displayed by figure 6b is obtained. Three new pressure scenarios with different maximum pressures are obviously distinguishable, and there is even a fourth new one not drawn in figure 6b: it is given by the coalescence of DDT and reflection. The following statements explain the short pipe scenarios in more detail:

- a) There has not yet emerged a consistent terminology when referring to detonations in short pipes. Alternative terms are "detonation in a precompressed gas mixture" or "detonation with precompression".
- b) There is nowhere a region where the detonation propagates as stable detonation. Between the location, where the DDT occurs, and the blinded pipe end the detonation propagates as "overdriven" or, alternatively, "instable" detonation.
- c) The reflection of the detonation at the blind flange always occurs in a gas mixture having been influenced by the incoming and the reflected pressure wave. Consequently, the loads on the pipe for scenario 7 will be higher than generated by scenario 4.
- d) For the status of the unreacted mixture at the location of the DDT there are two possibilities in the short pipe:
 - I: the reflected pressure wave has not yet reached this location at the moment when the DDT occurs. This is illustrated schematically by the curve labelled "t_{0,1}" in figure 6a. The load generated by the DDT in this case is hence still the same as in the long pipe configuration.

II: the reflected pressure has already passed this location at the moment of DDT occurrence ("t_{0,2}" in figure 6a). The load generated by the DDT in this case will hence be higher than in the long pipe configuration. Both cases are really found in the experiments (Schildberg 2013, 2015). With regard to detonation pressure proof pipe design one always has to assume the occurrence of the more severe case II (as it was also done in the sketch of figure 6b). Therefore it is justified to define the new scenario 5 for the DDT load in the short-pipe configuration.

248

- e) The location where the DDT occurs is always rather close to the blind flange. Otherwise the fast (1600 2500 m/s) detonation peak would have overtaken the slow (ca. 350 m/s) pressure wave and it would have been a detonation in a "long" pipe. The largest distance between a DDT, which had been influenced by the reflected pressure wave, and the blind flange found by the author in pipes with inner diameters of φ_i = 43.1 mm and φ_i = 107.1 mm was about 50 ·φ_i.
- f) The mixture in the section between the location of the DDT and the blind flange has in any case been influenced over the entire length by the initial pressure wave which brought about a pressure rise by a factor of about 2. In analogy to what was discussed in point d) the reflected pressure wave influences only part of this section or the entire section. From the point of view of safety, one has to assume the latter case, and therefore the pressure of scenario 6 in this section will be larger than the pressure of scenario 2.
- g) Since scenario 6 always follows scenario 5 in space and time and since the location of the DDT is not exactly determined even if the location of the ignition source were known, the pipe region, where the DDT can be expected (in a short pipe this is an approximately 50 φ_i long section upstream of the blind flange) and which must hence be designed to cope with scenario 5, will usually always include the region where scenario 2 occurs. Since the static equivalent pressures (p_{stat}) occurring in scenario 6 are less than p_{stat} of scenario 5, scenario 6 is irrelevant with regard to detonation pressure proof pipe design.
- h) Scenario 8, which represents the coalescence of scenario 5 and scenario 7 under omission of scenario 6 generates the largest load of all detonative pressure scenarios in long and short pipes.
- i) When a pipe, which must be regarded as "short" under the given conditions (composition of gas mixture, pipe diameter, pipe length, initial temperature, initial pressure), shall be designed detonation pressure proof, the end of the pipe must always be designed for the worst case scenario 8, since the location of the DDT is to some extent stochastic and, in all practical applications, variations of the composition of the mixture must be assumed. Since the DDT itself affects the pipe wall in the axial direction only over a distance of not more than about 2 pipe diameters, it will suffice when a short pipe section in front of the blind flange (not longer than 3 pipe diameters) is enforced to withstand scenario 8. The rest of the pipe only has to be able to withstand the load of the other scenarios.
- j) As already mentioned when discussing the detonative pressure scenarios in long pipes (see statement e in chapter 4.1.1), for highly reactive mixtures the region of unstable detonation no longer appears, because the flame front already overtakes the pressure wave caused by the initial deflagrative stage of the explosion before the DDT occurs. In such a case it is conceivable that the DDT does not necessarily always occur well ahead of the blind flange (as tacitly assumed in statement e), but also directly at the blind flange. When strictly adhering to the definition of "long pipe", such a special situation would be a new long pipe scenario. Actually, it resembles the short pipe scenario 8. The static equivalent pressures at the pipe end can be expected to be less than the static equivalent pressures that would have occurred if a mixture having the same Chapman-Jouguet pressure ratio had undergone an "ordinary" scenario 8. So far, the author could not yet generate such a pressure scenario with highly reactive gas mixtures in an experiment.
- k) It has to be born in mind that the short pipe scenarios do not only occur in closed pipes whose overall length is a bit larger than the predetonation distance and where ignition occurs at one end (this was the underlying geometry of figure 6), but may also occur in cases of very long pipes having one blinded end, if the ignition

Type of pressure scenario			State of knowledge regarding the detonative pressure profile		Scenario relevant for detonation
no.	pipe	name	p_{det} (peak height)	FWHM (width at half maximum)	pressure proof pipe design
1	ong pipe	DDT	estimates	estimates	yes
2		instable detonation	estimates	estimates	no
3		stable detonation	$p_{det_stable} = p_{CJ_r} \cdot p_{initial}$	known	yes
4		reflected stable detonation	2.4 • p _{det_stable}	known	yes
5	short pipe	DDT	unknown	unknown	yes
6		instable detonation	unknown	unknown	no
7		reflected instable detonation	unknown	unknown	yes
8		coincidence of DDT and reflection	unknown	unknown	yes

Figure 8: Summary of the different proposed pressure scenarios and pipe types. Furthermore the state of knowledge concerning the detonative pressure profiles of the different scenarios is summarized. p_{CJ_r} denotes the Chapman-Jouguet pressure ratio of the detonable gas mixture.

source is located at a distance slightly larger than the predetonation distance from the blinded end of the pipe. In the section between ignition source and blinded end the short pipe scenarios will occur, whereas on the other side of the ignition source the long pipe scenarios are found. This is explained in more detail by Schildberg (2013).

I) Note that for the sake of easier and better illustration, the axial positions of the scenarios in figures 5b and 6b do not correspond to what would be expected from figures 5a and 6a, respectively.

Figure 7 summarizes the proposed scenarios and the proposed differentiation between the both pipe types. Also included is the present state of knowledge concerning the detonative pressure/time profiles (or pressure/space profiles) of the different scenarios.

4.2 Proposal for using static equivalent pressures to quantify the effective pressure experienced by a pipe wall when exposed to a detonative pressure scenario

As outlined in chapter 2, there are not yet any guidelines available to design a pipe explosion pressure resistant against the load brought about by gas-phase detonations. For two scenarios the pressure/time information is available, but translating this information into an effective load seen by the pipe wall is still a non-trivial procedure. For all the DDT-related pressure scenarios 1, 2, 5, 6, 7 and 8 not even this fundamental information is available, since a reliable theoretical understanding of these scenarios has not yet emerged. Even if it existed the experimental verification of the theoretical predictions of the pressures at the DDT would be extremely difficult.

As a way out of this problem we propose to determine the *static equivalent pressures* of the various detonative pressure scenarios. We define the static equivalent pressure as 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}. The static equivalent pressure can be determined by the so-called *pipe wall deformation method* in the following way:

- 1) A large number of test pipes is manufactured, preferably of one melt only.
- 2) For one pipe of each melt the dependence of the residual plastic deformation on the internal static pressure is determined by a hydraulic test in the range from about 1 % diameter increase up to rupture (rupture occurs, depending on the type of steel, typically between about 6 % and 35 % diameter increase).
- 3) Explosion tests using a thermal ignition source at one pipe end and producing a transition from deflagrative to detonative transition are conducted in the test pipes with the mixture whose static equivalent pressures are to be determined. The initial pressures are chosen high enough to generate residual plastic deformation. This means that in the pipe wall the residual plastic deformation is recorded as function of axial position with a resolution in axial direction of about one pipe diameter.
- 4) For the detonatively generated residual plastic deformation one determines on basis of the hydraulic tests carried through beforehand the static pressure that causes the same degree of deformation. This pressure is then regarded as *static equivalent pressure* of the detonative pressure scenario. (Actually, in the hydraulic tests one does not record the residual plastic deformation but the instantaneous deformation, which is the sum of the elastic component and the plastic component, the latter being usually termed "residual plastic deformation". Since the elastic component amounts to typically 0.1 percentage points only, it can be neglected against the residual plastic deformation over the entire range from about 1 % up to rupture.)

Once the *static equivalent pressures* of the various detonative load scenarios are known, the pipe can be designed explosion pressure resistant or explosion pressure shock resistant against the detonative pressure scenarios that have to be anticipated for the envisaged operating conditions by applying the established pressure vessel guidelines which can only cope with static loads.

This method has the following advantages:

- The knowledge of the height and the width of the DDT-related detonative peaks is not at all needed. This
 means we are no longer impeded by the lack of this fundamental knowledge which would be the "conditio
 sine qua non" for any successful application of FE calculations.
- 2) The method directly delivers the sought for correlation between the input parameters (mixture composition, p_{initial}, T_{initial}) and the desired final output values (static equivalent pressure), i.e. there are no more or less diffuse intermediate calculations and/or assumptions involved.
- 3) The effect of strain rate hardening is automatically included in the data. The tests conducted so far (Schildberg 2013, 2014, 2015, 2016) were done with RA2 (DIN steel number: 1.4541; corresponding ASTM grades: 321 or 304L stainless steel) as the most common representative of stainless steel and P235GH (DIN number: 1.0345; corresponding ASTM grades: A178 Grade A, A106 Grade A, A106 Grade B) as the most common representative of carbon steel employed in the pipework of process plants. Since the strain rate hardening of

250

steels with moderate $R_{p0.2}$ -values (200 N/mm² $\leq R_{p0.2} \leq$ 350 N/mm²) is very similar, the experiments cover a broad range of process relevant materials. Note, however, that high-strength steels usually do not exhibit the large increase in yield strength when going to strain rates of about 100 s⁻¹ being attained when pipes are exposed to internal gas-phase detonations.

4.3 Generalisation of the measured data

Figure 9 presents an example for the static equivalent pressures of stoichiometric Ethylene/air mixtures at 20 °C. Other data can be found in Schildberg (2014, 2015, 2016). It is most convenient to express the static equivalent pressures as multiples of the static equivalent pressure of the most simple detonative pressure scenario, which is scenario 3, i.e. the stable detonation. This scenario generates the smallest static equivalent pressure of all scenarios. The following can be said about the variation of the static equivalent pressures with mixture composition, T_{initial} and p_{initial}:

- The equation for scenario 3 can be regarded to be universally valid, as long as the correct value for p_{CJ_r} is used, which varies with mixture composition, initial temperature and also slightly with initial pressure. The Chapman-Jouguet pressure ratio can be calculated on basis of fundamental thermodynamic data of the mixture, see for example Schildberg (2014).
- 2) The equation for scenario 4 can also be regarded to be universally valid. The factor 2.4 accounts for the pressure rise upon reflection of a detonation at a blind flange and can be derived theoretically.
- 3) The equation for scenario 1 only holds for the investigated mixture. This means that the factor 4.9 will be different if the composition of the mixture changes or T_{initial} or P_{initial} changes. If the reactivity of the mixture increases, for example by changing the composition of ternary mixtures of type combustible/O₂/N₂ along the stoichiometric line to higher O₂ concentrations, the factor will drop, because the unburned mixture compressed ahead of the piston of expanding reaction gases does not need so high temperatures (and consequently less pressure) in order to bring the ignition delay time into the range of a few microseconds. Increasing T_{initial} should also reduce this factor. With an increase of p_{initial} the factor should also drop because the autoignition temperatures get less with increasing initial pressure.
- 4) The equations for scenarios 5, 7 and 8 describe DDT-related pressure scenarios. Hence, for these scenarios the same applies as for scenario 1.

The experimental data collected so far allows putting forward a proposal for estimating the static equivalent pressures of the short pipe scenarios on basis of scenario 1 and scenario 3 (see figure 10). This estimate is based on the following assumptions and approximations:

- 1) the pressure rise brought about by the reflection of <u>any</u> detonative pressure peak at a blinded pipe end is the same as the pressure rise derived theoretically for the reflection of the stable detonation at a blinded pipe end, i.e. 2.4.
- 2) for the pressure rise of the unburned mixture brought about by the pressure wave propagating with a speed slightly larger than the speed of sound we use the plateau-approximation discussed in chapter 3.

	Туре	e of pressure scenario	Static equivalent pressures for stoichiometric Ethylene/air mixtures at 20 °C
no.	pipe	name	
1	(D)	DDT	$p_{stat_DDT_long} = 4.9 \cdot p_{stat_stable}$
2	long pipe	instable detonation	(irrelevant)
3		stable detonation	$p_{stat_stable} = \alpha \cdot p_{CJ_r} \cdot p_{initial}$
4		reflected stable detonation	<i>p</i> _{stat_reflected_stable} = 2.4 • <i>p</i> _{stat_stable}
5	short pipe	DDT	$p_{stat_DDT_short} = 6.2 \cdot p_{stat_stable}$
6		instable detonation	(irrelevant)
7		reflected instable detonation	$p_{stat_reflected_instable} = 9.7 \cdot p_{stat_stable}$
8		coincidence of DDT and reflection	$p_{stat_coincidence_DDT_reflection} = 17.6 \cdot p_{stat_stable}$

Figure 9: Static equivalent pressures of stoichiometric Ethylene/air mixtures at 20 °C. ($p_{initial}$ denotes the variable initial pressure of the mixture; p_{CJ_r} denotes the Chapman-Jouguet pressure ratio of the mixture, which is about 19.5 at 1 bar abs and increases very slightly with initial pressure; the parameter α was determined empirically to 0.66 $\leq \alpha \leq$ 0.7 and mainly accounts for the effect of strain rate hardening).

Quantitatively, the experiments suggest a pressure rise by a factor of about 2 when the wave propagates in the quiescent mixture. Upon reflection at the blinded pipe end, the pressure rises further by a factor of 1.5. By applying this estimate, the experimental effort reduces to only determine the parameter R for the mixture under consideration. Such an experiment is rather simple to realize. The effort for experimental determination of the static equivalent pressures of the short pipe scenarios is substantially larger.

	Туре	e of pressure scenario	Static equivalent pressures for any detonable gas mixture
no.	pipe	name	(p _{CJ_r} of the mixture must be calculated, R must be determined experimentally)
1	0	DDT	$p_{stat_DDT_long} = \mathbf{R} \cdot p_{stat_stable}$
2	long pipe	instable detonation	(irrelevant)
3		stable detonation	$p_{stat_stable} = \alpha \cdot p_{CJ_r} \cdot p_{initial}$
4		reflected stable detonation	$p_{stat_reflected_stable} = 2.4 \cdot p_{stat_stable}$
5		DDT	$p_{stat_DDT_short} = 1.5 \cdot p_{stat_DDT_long}$
	short pipe		= 1.5 • R • p _{stat_stable}
6		instable detonation	(irrelevant)
7		reflected instable detonation	p _{stat_reflected_instable} = 1.5 • 2 • p _{stat_reflected_stable}
			= $1.5 \cdot 2 \cdot 2.4 \cdot p_{stat_stable}$
8		coincidence of DDT and reflection	$p_{stat_coincidence_DDT_reflection} = 2.4 \cdot p_{stat_DDT_short}$
			= $2.4 \cdot 1.5 \cdot p_{stat_DDT_long}$
			= 2.4 • 1.5 • R • p _{stat_stable}

Figure 10: Proposal for estimating the static equivalent pressures of scenarios 5, 7 and 8 on basis of scenario 1 and scenario 3. (*p*_{initial} denotes the initial pressure of the gas mixture, $0.66 \le \alpha \le 0.7$).

5. Conclusions

The different detonative pressure scenarios that can be expected when explosive gas mixtures undergo the transition from deflagration to detonation in pipes are specified. A procedure to quantify the effective load experienced by the wall of a pipe exposed to the different scenarios is proposed. Experiments conducted in the past 3 years proved that this procedure successfully delivers the values needed for detonation pressure proof pipe design. The final goal should be to extend the existing pressure vessel design guidelines to encompass the design rules for detonation pressure proof pipe design.

References

- Edwards D.H., Brown D.R., Hooper G., Jones A.T., 1970, "The influence of wall heat transfer on the expansion following a C-J detonation wave." Journal of Physics D: Applied Physics, pp. 365-376
- Ligon T.C., Pellman A.M., Minichiello J.C., 2015, "Experimental consideration of the detonation expansion wave limit", PVP2015-45969, Proceedings of ASME 2015 Pressure Vessels and Piping Conference
- Schildberg H.P., J. Smeulers, G. Pape, 2013, "Experimental determination of the static equivalent pressure of gas-phase detonations in pipes and comparison with numerical models", Proceedings of ASME 2013 Pressure Vessels and Piping Conference, Volume 5: High-Pressure Technology, ISBN: 978-0-7918-5569-0; doi: 10.1115/PVP2013-97677
- Schildberg H.P., 2014, "Experimental determination of the static equivalent pressure of detonative decompositions of acetylene in long pipes and Chapman-Jouguet pressure ratio", Proceedings of ASME 2014 Pressure Vessels and Piping Conference, Volume 5: High-Pressure Technology, ISBN: 978-0-7918-4602-5; doi: 10.1115/PVP2014-28197
- Schildberg H.P., 2015, "Experimental Determination of the Static Equivalent Pressures of detonative Explosions of Stoichiometric H₂/O₂/N₂-Mixtures in Long and Short pipes", Proceedings of the ASME 2015 Pressure Vessels and Piping Conference, Volume 5: High-Pressure Technology; doi: 10.1115/PVP2015-45286
- Schildberg H.P., 2016, "Experimental Determination of the Static Equivalent Pressures of detonative Explosions of CH₄/O₂/N₂-Mixtures and C₂H₄/O₂/N₂-Mixtures in Long and Short pipes", submitted for publication at the ASME 2016 Pressure Vessels and Piping Conference

252