TURBULENT FLAME ACCELERATION – MECHANISMS AND SIGNIFICANCE FOR SAFETY CONSIDERATIONS

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Abstract

Accidental unstationary combustion processes are the main issue of safety considerations in connection with hydrogen technology. The overpressure loads produced by detonations but as well those imposed upon structures by fast, turbulent deflagrations are easily of sufficient strength for serious damage. Since an accidental combustion process is most likely to start as a slow deflagration, detailed knowledge of the mechanisms of flame acceleration leading to high speed reaction fronts is of vital importance for design guidelines and safety analysis. In this paper the parameters influencing turbulent flame acceleration processes, i.e. initial conditions and geometry of the combustion volume, are discussed and a brief outlook for necessary future research activities is provided.

1. INTRODUCTION

Unstationary combustion processes are characterized by traveling reaction fronts after ignition of the combustible gas mixture. The danger potential inherent to unstationary flames results from the temperature increase due to the exothermic reaction as well as from the local overpressure of the flame front. However, the temperature increase usually presents no serious threat because the flame front travels comparatively fast and the structures have a high heat capacity and absorb the surplus heat very quickly. Therefore the overpressure of the flame front has to be dealt with in safety analysis.

Generally it can be said that the higher the speed of the reaction front, the higher the maximum overpressure in the combustion zone. It should be noted however, that the load imposed on structures by an unstationary reaction front is not only determined by the maximum overpressure, but also depends on the time this overpressure is present, i.e. the integral of the pressure over time. Most accident scenarios predict an accidental combustion being initiated by a weak ignition source, e.g. a spark of an electric discharge. Starting from the ignition point at very low speeds, the flame can strongly be accelerated under the influence of turbulence inducing obstacles in the flame path. Thus an initially slowly propagating flame front can reach very high speeds well above the speed of sound with pressure waves causing serious damage to facilities, buildings etc.. Therefore the phenomenon of flame acceleration is of vital importance for safety analysis. In this paper the current understanding of the mechanisms and the parameters influencing flame acceleration as well as their significance are outlined and areas of lacking knowledge are pointed out.

2. COMBUSTION MODES AND THEIR DANGER POTENTIAL

Before the actual problem of flame acceleration is discussed extensively, a brief introduction into the different modes of combustion and the corresponding pressure profiles shall be given. Basically in unstationary combustion two different modes can be distinguished: deflagration and detonation. However, when dealing with safety, an unstable type of combustion, referred to as supersonic flame (or fast deflagration), has to be considered.

Deflagration

A deflagrative flame front is made up of two zones, the preheat zone and the reaction zone, separated by the point of ignition. The propagation results from heat transfer by thermal conduction and diffusion from the hot reaction zone to the preheat zone. In laminar flames, the propagation or burning velocity is limited by the heat transfer rates and typical

values of the burning velocity in hydrogen air mixtures are between 0,5 m/s and 3 m/s [2], depending on the hydrogen concentration and initial temperature of the mixture. If the heat transfer is enhanced by turbulence, the resulting burning velocities increase significantly reaching values of more than one order of magnitude higher than the laminar burning velocity (i.e. [3]).

Depending on geometry, i.e. degree of confinement, form of obstacles, obstructions, mixture composition and thermodynamic initial conditiones very fast deflagrations propagating at speeds far beyond the speed of sound are possible. In this case the deflagration front is characterized by by a leading pressure wave that increases pressure and temperature behind it, followed by a highly turbulent flame. This type of flame front is referred to as supersonic flame. Overpressures up to 15 times the initial pressure have been observed in experiments.

Detonation

Provided a mixture composition sufficiently reactive in connection with a high degree of turbulence being generated a deflagration possibly undergoes a transition to a detonation. A detonative flame front consists of three zones, the leading shock, the induction zone and the reaction zone. Unlike in a deflagration there is no heat transfer involved in a detonation. It is rather the strong leading shock wave that is responsible for the start of the reaction. The shock wave is so strong, that the temperature behind it is high enough to cause self ignition in the combustible mixture. After a short induction time the exothermic reaction starts. Typical detonation velocities in hydrogen air mixtures are around 2 km/s, about three orders higher than the corresponding laminar burning velocities. Detonations show a very strong, distinct maximum overpressure in the leading shock, the von-Neumann-spike. This overpressure is very large, depending on the initial hydrogen concentration about twenty to thirty times the initial pressure.

At the authors' institute overpressure profiles were recorded in an explosion tube (fig. 1) for different hydrogen-air mixtures. Fig.3 shows typical pressure profiles for accelerated deflagrations, one of them traveling comparatively slowly, the other one propagating as a supersonic flame and a detonation obtained in H₂-air mixtures with 10, 16 and 26 vol.% H₂. Initial conditions were set to 1 bar total pressure and ambient temperature. The explosion tube (length 6m, diameter 66mm) was equipped with an turbulence inducing obstacle array consisting of orifice rings with a blockage ratio of 32% mounted in equidistance of 150 mm over the entire length of the tube (fig.2a). A spark plug was used as ignition source. The pressure profiles were recorded by two pressure transducers on of them mounted in the tube wall 4.8m from the ignition source (referred to as side-on) the other one in the end flange (head-on), to obtain the maximum overpressure in case of reflection of a pressure wave.

The deflagration in the mixture with 10 vol.% H₂ shows comparatively slow pressure build up and low peak overpressure (fig. 3a). It should be regarded however, that the overpressure of 0.4 bars measured here already suffices to impose serious damage to a building. The pressure profiles of a detonation show the very strong leading shock wave. It can be seen that the reflection of the shock at the end flange causes a peak overpressure of more than double the value of the corresponding side-on measurement. The pressure wave of the supersonic flame is not as high as the detonation shock, but it's duration is longer. Since the momentum, the integral of the pressure over time represented by the area underneath the pressure profiles in fig. 3b and c, is a relevant parameter for stability analysis for a given structure, a supersonic flame can impose a load of the same order as a detonation, i.e. the fact of lower peak pressures of a supersonic flame in comparison with a detonation is partially compensated by the longer duration resulting both from lower speeds of propagation and higher reaction front thickness. From this considerations it can be concluded that for safety analysis it is of minor importance if a flame front propagates as a supersonic flame or if a transition to a detonation actually occurs.

3. UNSTATIONARY COMBUSTION PROCESSES

As indicated in the introduction, an accidental unstationary combustion is most likely to start as a slow deflagration. The reaction front propagates in all (unconfined) directions from the point of ignition. Due to the energy release in the reaction front there is a strong

expansion of the gases. Since the gases behind the flame front are blocked, either by a geometric boundary or the burnt gases of the flame propagating in the opposite direction, an expansion flow is produced in the unburnt gas ahead of the flame front. If this flow encounters obstacles like tubes, staircases or rough surfaced walls turbulence is produced. This turbulence enhances the heat transfer in the combustion zone and therefore increases the reaction rate per unit area of the flame front surface. The increase in reaction rate, however, in turn causes an increase of the volumetric expansion and therefore induces a stronger expansion flow ahead of the flame. As long as the obstacles produce more turbulence in the unburnt gas, a positive feedback cycle is formed [4].

If an unstationary flame front propagates toward an obstacle with a small opening, such as a door or window in a wall, a highly turbulent jet through the opening is formed due to the expansion flow. When the flame front reaches the opening the high degree of turbulence present in the jet and it's shear layer causes a fierce flame acceleration. By this mechanism extremely strong flame acceleration can be achieved over very short distances.

As long as the flame speed is below the velocity of sound the combustion process produces the expansion flow ahead of the flame with a leading pressure wave that moves away from the flame front traveling at sound velocity. Therefore the combustion is influenced by the history of the overall process starting from the time of ignition. As soon as the flame front reaches the local velocity of sound the previous events lose importance, since the flame front with the leading shock wave travels faster than any pressure disturbances. This is true both for supersonic flames and detonations. Therefore for safety aspects from the general behaviour and the resulting overpressure impact supersonic flames and detonations have to be treated similarly. It should be kept in mind, however, that supersonic flames can not sustain themselves steadily without repeated obstacles. An established detonation on the other hand can propagate steadily as long as the mixture conditions allow it.

In order to get experimental information about the general flame behaviour, quasi-one-dimensional experiments were carried out in the explosion tube already described before. By measuring the time the flame arrives at a certain distance from the ignition end, the local flame speed can be obtained. This measurements are taken by means of a photodiode system (see fig.1). In the first half (3 m) of the tube various obstacle configurations are installed. Fig. 4 to 6 show typical profiles of the flame velocity along the length of the tube, each time with a different set of boundary conditions representing typical parameters.

In fig. 4 the initial hydrogen concentration was kept constant at 16 vol.% H_2 and the spacing between two successive obstacles consisting of orifice rings (fig.2) was equally 150 mm for both runs. The blockage ratio, that is the ratio of the blocked area to the full cross section of the tube, was 32% and 69%. The lower blockage ratio causes flame acceleration mainly by turbulence in the expansion flow, the higher blockage ratio causes a jet stream accelerated combustion. It can clearly be seen, that the flame is accelerated within a much shorter distance in the obstacle array with the higher blockage ratio. It should be noted here that there is no distinct value for the blockage ratio separating the regimes of turbulence and jet stream induced flame acceleration, at intermediate blockage ratios both mechanisms are effective.

Fig. 5 shows another very important effect of various blockage ratios. All parameters are identical to those of fig. 4, except the initial hydrogen concentration, which was set to 11 vol.% H₂. As with 16 vol.% H₂, the flame front is initially accelerated to higher speeds in the obstacle array with the higher blockage ratio. However, after a short distance, the mixing becomes so intense, that the flame is eventually quenched. In the array with a blockage ratio of only 32% the flame is accelerated to a much lower degree, but it does burn all the way through the obstacle array without being quenched. Therefore it can not be generally concluded that higher blockage ratios mean a higher danger potential.

Fig. 6 shows cumulative the typical flame front behaviour with the different modes of combustion for different hydrogen concentrations. For this example the obstacle array with the blockage ratio of 69% and an obstacle spacing of 490 mm was used. At a hydrogen concentration of 10 vol.% H₂ the flame is initially accelerated very strongly, but is eventually

quenched. At 16 vol.% H₂ the flame is accelerated to a speed of 1250 m/s within the obstacle array, a typical supersonic flame. However, as soon as the flame exits the obstacle array, the flame speed drops down rapidly because the supersonic flame cannot sustain itself without turbulence inducing obstacles. A detonation occurs at hydrogen concentrations above hydrogen concentrations of 22 vol.% H₂. Within the obstacle array the velocity does not reach the actual detonation velocity. This fact is due to the energy losses at the obstacles which are significant when the high blockage ratio is considered. As soon as the flame front exits the obstacle array, however, the detonation fully develops and travels with a speed of almost 2000 m/s.

4. PARAMETERS FOR FLAME ACCELERATION

Accidental combustions may occur after any release of hydrogen into the atmosphere. This release may be due to several reasons such as opening of a safety valve, leaks due to material fatigue or some type of mechanical accident. Even for a given geometrical arrangement many unknown parameters have to be taken into account. Primarily the amount of hydrogen released, the time and location of ignition and the gas flow induced by the released gas are important yet unknown parameters beforehand. Therefore for safety analysis the goal has to be a set of giudelines for the construction of systems involving hydrogen which minimizes the risk of a severe accident due to an accidental combustion with strong flame acceleration. As a first step it would already be useful to establish criteria for the localization and eventual elimination of the most critical spots in a system. In the following paragraphs the parameters influencing the course of an accidental combustion are outlined and discussed as far as this is possible at the moment. These parameters can be summarized in the the areas of mixture concentration, initial thermodynamical and fluidmechanical conditions and geometrical configuration.

Mixture concentration

The mixture concentration can generally not be assumed to be uniform throughout the entire combustion volume. Since the gas release is an unstationary process itself, and ignition may occur well before all of the hydrogen is released, the hydrogen distribution can not be estimated realistically. If influences like wind or larger moving objects such as cars or people are considered the situation becomes even more complex. Therefore some conservative estimates based on the expected maximum amount of gas released and possible locations of the release have to serve for safety guidelines. As far as the general hydrogen distribution is concerned it has to be assumed that the maximum concentration is around the location of the gas release. Around this location concentrations well above stoichiometry (29.6 vol.% H2 in air) can be expected, while points further away are rather below stoichiometry. In order to classify mixtures with regard to their potential safety hazard the experiments conducted in explosion tubes with regular obstacle arrangements are useful for conservative estimates. The flammability limits for hydrogen-air mixtures are 4 to 75 vol.% H₂ [1], but experiments show that at hydrogen concentrations between 4 and 8 vol. % H2 the combustion is generally incomplete [5]. Experiments in explosion tubes with obstacles show that up to 10 vol.% H2 the flame is quenched within the obstacle array or shortly afterwards. at higher blockage ratios the flames are. As a conservative estimate hydrogen concentrations up to 10 vol.% H₂ can be regarded as not dangerous. The same considerations apply to the combustion behaviour at the upper flammability limit. Here the conducted measurements have not been as extensive as at the lower concentrations, but mixtures over 70 vol.% H2 seem to be very sensitive for quenching. At this point it shall be pointed out, however, that a combustion in mixtures above stoichiometry may well result in multiple burns since there is not enough air to oxidize all the hydrogen present. Multiple burns are even more complex because both the mixture composition is changed by the first burn and the initial thermodynamic and fluiddynamic conditions are strongly influenced.

Initial Conditions

Three parameters have to be regarded as far as the initial conditions are concerned. The thermodynamic parameters are the pressure and the temperature, the fluiddynamic parameter is the degree of turbulence present in the unburnt mixture. The initial pressure is

not relevant since for most scenarios pressures near the atmospheric pressures can be assumed. Furthermore measurements in the explosion tube with different initial pressures showed no significant change in flame behaviour.

The initial temperature is of interest for two reasons. For one the accidents do not always occur at ambient temperature, especially if liquid hydrogen, is considered. On the other hand, if multiple burns are taken into account, the temperature after the first burn is well above the ambient temperature. At higher temperatures the reaction rate is increased resulting in higher laminar burning velocities [2]. In addition, the higher the temperature of the unburnt gas, the lower is the probability of quenching due to intense turbulent mixing. This has been shown in a tube burner in which stationary flames have been stabilized behind metal grid obstacles. Fig. 7 shows the minimum hydrogen concentration required to achieve a stable flame behind a grid with a blockage ratio of 55% over the approach velocity of the unburnt gas for different temperatures. For stationary flames the approach velocity of the unburnt gas is equal to the overall burning velocity. It can clearly be seen that the required hydrogen concentration decreases with the increasing initial temperature. Measurements of the length of the reaction zone, conducted in the same burner, exhibited a decrease in the length of the reaction zone with increasing temperature also indicating a higher reactivity of the gas. The influence of initial temperature on turbulent flame acceleration has been examined in the explosion tube for temperatures up to 300°C. Surprisingly, higher initial temperatures do not necessarily imply enhanced flame acceleration. This results mainly from a decrease of the expansion ratio of the gas at higher temperatures resulting in a slower expansion flow ahead of the flame. In obstacle arrays with low blockage ratios, i.e. turbulence induced flame acceleration, lower flow velocities mean less turbulence and therefore less flame acceleration. In arrays with high blockage ratios, on the other hand, flame acceleration is not limited as much by quenching. It can be concluded that with increasing initial temperature the geometry of the obstacles gains importance. The effect of initial temperatures below ambient temperature, which may be of interest when cryogenic hydrogen is released, has not been studied so far.

The turbulence present in the unburnt mixture is generally expected to enhance the combustion process. However, the higher the induced turbulence and mixing due to obstacles, the less the importance of the initial turbulence.

Geometric Configuration

The geometry of the combustion volume is one of the most important, yet most complex parameters for flame acceleration. On the other hand, for accidents with unintentional combustion it is generally the only reliably known parameter. With respect to geometry, the experiments in explosion tubes can only show the phenomenology of flame behaviour because real geometries are much larger and in most real situations the obstacle arrangement does not show the regular pattern mostly used in explosion tubes. With respect to geometry three parameters are of relevance: the (relative) size of obstacles, the distance between successive obstacles and the degree of confinement of the combustion volume.

In experiments the size of the obstacles is usually defined in relation to the diameter of the combustion chamber and given as the blockage ratio, defined as the ratio of the value of the cross section area blocked by the obstacle and that of the entire chamber. The higher the blockage ratio, the higher is the gas velocity of the flow ahead of the flame in the free obstacle cross section and the more intense is the turbulent mixing in the area behind the obstacle. The effect of the blockage ratio has been explained extensively in the previous section. The distance between successive obstacles, in regular geometries termed spacing, is an important parameter for flame acceleration since a flame accelerated by one obstacle tends to slow down again if no more obstacles are encountered. The effect of obstacle spacing strongly interacts with the obstacle size. It can generally be said that for maximum flame acceleration the higher the blockage ratio, the longer the necessesary distance between succesive obstacles. Experiments in which the spacing of the obstacles has been varied have been carried out in an explosion tube. For comparison two types of orifice ring obstacles with blockage ratios of 29% and 69% were used and the hydrogen concentration was varied as the third parameter. Fig. 8 shows the maximum flame speed recorded for each case. From this diagram the

overall behavoiur of the flame for each run can not be seen. It does, however, show the maximum potential for flame acceleration in each case. For the high blockage ratio there is a distinct value of the spacing, almost independent of the hydrogen concentration, for which the maximum velocities are reached. If the spacing is above this value, the flame tends to slow down between the obstacles due to a lack of turbulence. If the spacing is below the value for maximum flame acceleration, the intense mixing processes lead to quenching effects and the pressure losses become significantly high. If the obstacle array with the lower blockage ratio is installed, the curves are shifted to lower spacing values, reaching their maximum at the lowest spacing tested. From the experiments it can not be said if the maximum flame velocity achieved at the lowest spacing value represents the absolute maximum for arrays with this blockage ratio, since there were no tests with lower spacings conducted.

In real geometries, the blockage ratio and obstacle spacing can not always be defined. To determine the blockage ratio a distinct value for combustion chamber size is required, which is not always obvious. In these cases it is necessary to determine a best estimate for the size of an imaginary combustion volume. However, in some cases there is still a strong lack of knowledge regarding the size of obstacles in combustion processes. Experiments investigating the effect of obstacle size, for example, in free gas clouds have not been carried out so far. As far as the spacing is concerned, usually very irregular arrangements are encountered. Only stairs or bundles of pipes etc. can be ragarded as regular arrays. Therefore, an important, yet not investigated parameter is the turbulence attenuation of flames accelerated by obstacles and subsequently propagating into areas without obstacles.

The third relevant geometric parameter is the degree of confinement. While in long channels with a comparatively small cross section the combustion process can be regarded as quasi-one-dimensional, partially or unconfined volumes lead to two or three-dimensional combustion processes. Beside the increasing complexity of more dimensional processes, the influence of the degree of confinement results from the dependence of the velocity of the expansion flow on the confinement. In fully confined geometries, like the explosion tubes or in real geometries rooms of buildings, the burnt gases can not escape from the channel and therefore induce a much stronger expansion flow than in partially confined geometries. Although no extensive testing of various arrangements with different degrees of confinment and more dimensional tests have been carried out so far, experiments in a long channel with 50% of one channel wall removed give an idea of the effect of confinement [6]. In the fully confined channel strong flame acceleration has been recorded at a hydrogen concentration of 25 vol. % H_2 without obstacles and at 15 vol. % H_2 with obstacles (blockage ratio = 33%). With 50% of the top cover removed, there was no significant flame acceleration without obstacles even at 28 vol. H2, close to stoichiometry. However, when the obstacles were installed, strong flame acceleration has been achieved at a hydrogen concentration of 20 vol.% H2. These results suggest that the lower the degree of confinement of the combustion volume, the lower the tendency toward flame acceleration. With obstacles, however, strong flame acceleration may well occur. As has already been mentioned, there has been no extensive testing regarding the degree of confinement yet.

5. CONCLUSION

Since an accidental combustion is assumed to start as a deflagration, turbulent flame acceleration, its mechanisms and parameters have to be analyzed in order to establish safety guidelines. The evaluation of the pressure profiles of the different modes of combustion showed that any flame reaching the velocity of sound builds up a shock wave yielding pressures that may pose a danger even to solid structures. As long as there are no reliable methods for calculations of gas distribution and subsequent combustion, the prevention of flame acceleration to supersonic speed can be regarded as a conservative limit. In order to analyze any given geometry for safety with respect to an accidental combustion, the mechanisms leading have to be understood and the influence of the relevant parameters has to be known quantitatively. Due to the complexity of real systems involving hydrogen in any use, experiments can only serve as indicators for typical flame behaviour under certain conditions. Some parameters like turbulence attenuation, influence of initial temperatures below ambient temperature or the effect of very low degrees of confinement have not been examined sufficiently yet. The

goal, however, has to be a much better overall understanding of unstationary combustion processes, especially the complex interactions of turbulent fluid dynamics and reaction kinetics, than it exists today. In order to obtain this understanding more basic research, preferably applying sophisticated, nonintrusive measuring techniques, is necessary.

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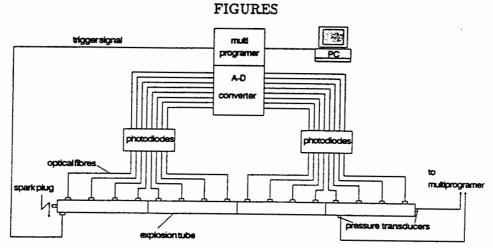


Fig. 1: Explosion tube: scheme of measuring arrangement for recording pressure profiles and photodiode system for flame speed measurements

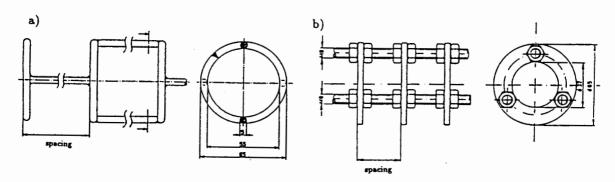


Fig. 2: Obstacle courses used for combustion experiments in the explosion tube: a) turbulence inducing obstacles, blockage ratio 32%, b) jet stream promoting obstacles, blockage ratio 69%

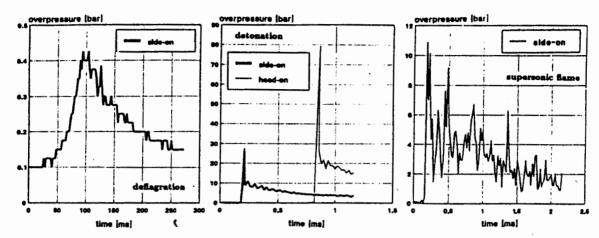
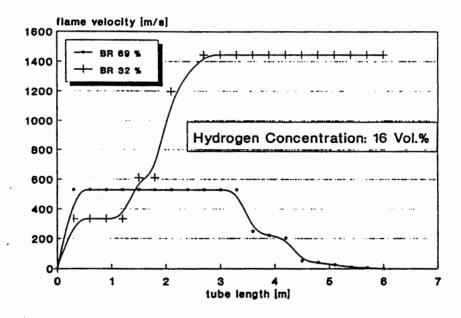


Fig. 3: Typical overpressure profiles for a comparatively slowly propagating deflagration (fig. 3a, left, 10 vol. % H₂), a detonation (fig. 3b, middle, 26 vol. % H₂) and a supersonic flame (fig. 3c, right, 16 vol. % H₂). The different scales for pressure and time should be regarded, especially for momentum considerations.



 $\frac{\text{Fig. 4:}}{\text{H}_2}$ Flame speeds recorded in an explosion tube at a hydrogen concentration of 16 vol.% $\frac{\text{Fig. 4:}}{\text{H}_2}$ for obstacle arrays with blockage ratios of 32% and 69% and a spacing of 150 mm.

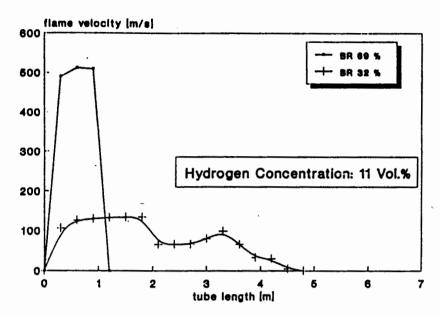


Fig. 5: Flame speeds recorded in an explosion tube at a hydrogen concentration of 11 vol.% H_2 for obstacle arrays with blockage ratios of 32% and 69% and a spacing of 150 mm.

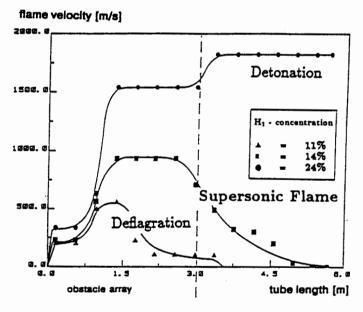


Fig. 6: Typical flame front behaviour with different modes of combustion as observed in an explosion tube with an obstacle array (blockage ratio 69%, spacing 490 mm).

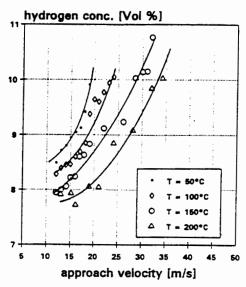


Fig. 7: Minimum hydrogen concentration required for a stable, stationary highly turbulent flame behind a metal grid (blockage ratio 55%) as a function of approach velocity of the unburnt gas and initial temperature. The approach velocity is equal to the overall burning velocity and proportional to the degree of turbulence induced by the grid.

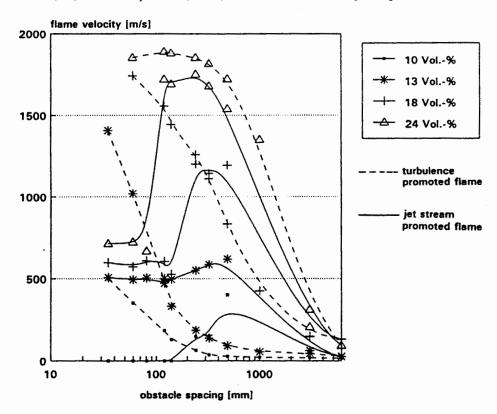


Fig. 8: Maximum flame speeds recorded in an explosion tube at various hydrogen concentrations for obstacle arrays with blockage ratios of 32% and 69% and different obstacle spacings.