Auto-ignition of spontaneous hydrogen leaks

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Abstract

This paper is devoted to the study of the self-ignition of a hydrogen leak. In order to analyse this particular case and to understand the physical phenomena behind spontaneous ignition of sudden high-pressure hydrogen releases, analytical calculations and a CFD simulation were carried out. The modeling involved a shock tube where high-pressure hydrogen was separated from the atmospheric air by a rupture disk. It was concluded that due to the high-pressure difference, in the event of a sudden release, a shock wave could form inside the tube, mixing shock heated air with cold expanding hydrogen which could ignite in the presence of enough temperature and sufficient mixing. It was also found that if the downstream geometry of the hole is too long, the mixture will fade and there will be no ignition due to lean mixture. This is observable by the study of a tube with downstream geometry of 0.5 meters where 40 bar of high-pressure hydrogen was input. The temperatures reached were as high as 1200K, well above the spontaneous ignition of hydrogen, however due to the length of the tube the mixture fades and the necessary conditions for the mixture to ignite are not gathered. However, the same pressure was studied for smaller tube where, although the temperature reached wasn't as high as the previous case, the mixture stayed stoichiometric at the necessary temperature for spontaneous ignition, meaning that the conditions for spontaneous ignition were gathered.

Keywords: Hydrogen, Spontaneous ignition, High pressure, Shock wave, CFD

1. Introduction

With the increase usage of hydrogen in several industries throughout the last 100 years, several issues concerning safety have made it very difficult to progress and expand its usage as a clean fuel. These safety issues include its transportation, storage and usage. Since it is a very volatile gas and can be very explosive as it combusts with just one-tenth of the energy required for gasoline, the safety concerns turn to avoid combustion at all costs. On top of explosive issues, hydrogen is odorless and colorless.

When handling high-pressure hydrogen, improper use of valves, damage to the ducts/reservoirs or embrittlement can lead to high velocity leaks that can ignite with minimal effort, whether it is a spark, static electricity or even just a hot surface. Many have been the reported accidents involving high-pressure flammable gas with spontaneous ignition, for that reason many studies have been made around the subject of hydrogen auto-ignition.

Over the last century, several combustion incidents have been reported due to high-pressure hydrogen leaks without a determined cause. A platform called HIAD [2], Hydrogen Incident and Accident Database, is a free access database that keeps track of all the accidents related with hydrogen worldwide. To this day there is a total of 364 accidents involving hydrogen that transitioned into jet fire or explosions. While most of them have an associated cause (about 86%), about 14% of the accidents registered have no known cause.

Diffusion ignition was first studied in 1972 by Wolański and Wójcicki [12]. What they meant by "diffusion ignition" was the ignition produced by the discharging jet, when the fuel expanding through a shock tube came into contact with an oxidizing atmosphere heated by the shock wave. The reason why it was named diffusion ignition is because they identified diffusive mixing. It was predicted that ignition would be achieved once an upstream pressure of 39 bar, was obtained causing a shock-wave mach number of 2.8 or higher leading to a temperature of 575K. In 1990 Chaineaux et al. [5], coined the term "spontaneous ignition", which they used after achieving it by discharging high pressurized hydrogen at approximately 100 bar through a 12mm hole extended by a tube with 120mm of length and 15mm inside diameter producing a sort of CD nozzle.

Mogi et al. [10], studied the effect of the downstream tube length from the rupture disk, by varying it from 3 to 300mm, using 5 and 10mm nozzle diameters. They were able to get jet fire ignition at a approximately 60 bar with a 185mm tube and a 5 mm diameter nozzle. In the same year Golub et al.[8] made a very similar experimental study, accompanied with CFD work. From the experimental part, ignition was achieved using a very similar configuration as Mogi et al. with the same pipe length and nozzle diameter but this time ignition was achieved with just 40 bar of high-pressurized hydrogen. They concluded that the reason for the possible spontaneous ignition was "the heating by the primary shock wave of the surrounding oxidizer, resulting in gas ignition on the contact surface". Still in 2007, Dryer et al.[6] released a paper where more than 200 experiments were done using several downstream geometries (downstream of the burst disk) and several burst pressures concluding that for a downstream geometry of 127mm of length and 4mm diameter ignition would be certain from hydrogen pressures of 22.4 bar up, with a possible ignition at a minimum pressure of 20.6 bar. With the work presented it was possible to conclude that "within the storage and pipeline pressures used today and/or contemplated in the future for hydrogen, transient shock processes associated with rapid pressure boundary failure have the capacity to produce spontaneous ignition of the compressed flammable released into air, providing sufficient mixing is also present".

In 2010, Bragin et al.[4] validated a LES model by comparing the results with the results printed from Mogi [10]. The paper had the objective of studying the "physical phenomena underlying the spontaneous ignition of hydrogen following a sudden release from high-pressure storage and transition to sustained jet fire" creating a LES model for engineering design of pressure relief devices.

The objective of this paper is to study what exactly happens inside the hole that leads to a possible ignition. Since the behaviour inside a hole is similar to a shock tube, the problem is portrayed as a shock tube like geometry where the driver is designed as the high-pressured reservoir and the driven section as the atmosphere.

2. Background

In order to better understand the physical and chemical phenomena behind spontaneous ignition through diffusive ignition, an analytical approach is required to complement the numerical study. In order to do so an overview of the theoretical component that involves shock tube theory and what happens inside it, is studied.

2.1. Overview of the shock tube theory

2.1.1 The Shock tube

The shock tube is composed of two parts which are denoted as the driver section and the driven section presented in figure 1. The driver section contains high-pressure gas at pressure P_4, while the driven section contains low-pressure gas at pressure P_1, which are separated by a diaphragm designed to burst at a certain pressure.

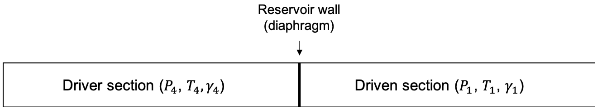

Figure 1: Diagram illustrating the driver and driven sections of a shock tube(at t=0), similar to the model used numerically.

Once the designed pressure is achieved the diaphragm bursts releasing the high-pressure gas, very rapidly, through the driven section creating a shock wave moving in the same direction. In the driver section, rarefaction waves (taken from Shapiro [11]) move in the opposite direction of the shock wave due to the expansion of the high-pressured gas. Once the diaphragm is ruptured, two additional regions appear as regions 2 and 3. Region 2 is located behind the shock wave and region 3 is right behind it separated by the contact surface as shown in figure 2.

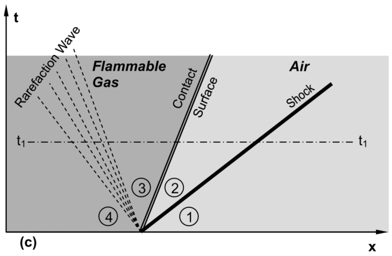

Figure 2: Position of contact surface in a shock environment as a function of time. (From Shapiro, 1954.[11])

Since hydrogen and methane are going to be tested in the driver section, a lot of properties that lead to the calculations, are different. Although the initial temperatures, both in the driver and driven sections, are the same (300K), the species in both regions are different with different gas constants which leads to different speed of sound values in both sections of the shock tube. For that, the speed of sound for each species can be calculated as,

$$a = \sqrt{\gamma R T} \tag{1}$$

where γ is the adiabatic exponent of the gas at 300K and R is the universal gas constant.

Pressure

A shock tube works by implementing a big pressure difference. With the burst of the diaphragm, the high-pressured gas is released into the low pressured zone. This being said pressure is the key for a shock tube to work. Since pressure in the driver section and in the driven section is known (regions 4 and 1 respectively), it is possible to design a pressure profile along the tube length using the following equations from Liepmann et al. [9].

$$\frac{P_4}{P_1} = \frac{P_2}{P_1}\left[1 - \frac{(\gamma_4-1)(a_1/a_4)(P_2/P_1-1)}{(\sqrt{2\gamma_1})(\sqrt{2\gamma_1+(\gamma_1+1)(P_2/P_1-1)}}\right]^{\frac{-2\gamma_4}{\gamma_4-1}} \tag{2}$$

$$\frac{P_3}{P_4} = \frac{P_2/P_1}{P_4/P_1} \tag{3}$$

These equations allow the construction of the pressure profile in figure 3.

Figure 3: Pressure profile along the length of the tube

Temperature

Due to rapid release of high-pressure flow with great velocity, a shock wave is formed, heating the low pressured gas as it travels through the driven section. On the other way around, flow of high-pressure driver gas expands through the driver section on the opposite direction of the shock wave, cooling it. Since the pressure profile was already designed and the results of the previous equations calculated, it is possible to construct a temperature profile with the following equations from Liepmann et al. [9].

$$\frac{T_3}{T_4} = \left(\frac{P_3}{P_4}\right)^{\frac{(\gamma_4-1)}{\gamma_4}} = \left(\frac{P_2/P_1}{P_4/P_1}\right)^{\frac{(\gamma_4-1)}{\gamma_4}} \tag{4}$$

$$\frac{T_2}{T_1} = \frac{1+\frac{\gamma_1-1}{\gamma_1+1}\frac{P_2}{P_1}}{1+\frac{\gamma_1-1}{\gamma_1+1}\frac{P_1}{P_2}} \tag{5}$$

This leads to a temperature profile inside the tube where, although temperature in region 4 and in region 1 is constant, in regions 2 and 3 the gas heats up and cools respectively. Therefore, the temperature profile is supposed to look like the following figure 4.

Density

Assuming ideal gas across the shock tube, $P = \rho RT$ is used for the calculation of density across the contact surface. Remembering that $P_3 = P_2$ it is possible to conclude that the density ratio is inversely proportional to the temperature ratio,

$$\frac{\rho_2}{\rho_3} = \left(\frac{R_2T_2}{R_3T_3}\right)^{-1} \tag{6}$$

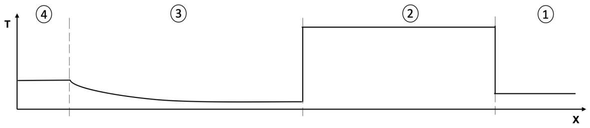

Figure 4: Temperature profile along the length of the tube

Mach number

Gaydon and Hurle [7] in 1963, developed equations for the relations between the initial pressure ratio with the shock Mach number and the ratio of temperatures across the shock wave with the shock Mach number, as seen in the following equations.

$$\frac{P_4}{P_1} = \frac{2\gamma_1 Ms^2-(\gamma_1-1)}{\gamma_1+1}\left[1 - \frac{\gamma_4-1}{\gamma_1+1}\frac{a_1}{a_4}\left(Ms - \frac{1}{Ms}\right)\right]^{\frac{-2\gamma_4}{\gamma_4-1}} \tag{7}$$

$$\frac{T_2}{T_1} = \frac{\left[2\gamma_1 Ms^2 - (\gamma_1 - 1)\right]\left[(\gamma_1 - 1)Ms^2 + 2\right]}{(\gamma_1 + 1)^2 Ms^2} \tag{8}$$

These simplified equations lead to the possibility of studying the critical pressure to which the flammable driver gas would auto-ignite. By knowing T_2, it is possible to calculate at what Mach number the gas would reach those temperatures and then calculate the minimum critical pressure to produce such shock wave. Using these equations and the information from the engineering toolbox [1] it was possible to calculate the critical ignition pressures for several common gaseous fuels and the Mach number produced by releases at these pressures, as it is possible to see from table 1.

Time

A shock wave is transient phenomena so it is time dependent as it is possible to understand through figure 2. As the shock Mach number increases, so does its speed and the lesser time the shock wave needs to travel through the length of the tube. The following equations explain just that.

$$Ms = \frac{cs}{a_1} \tag{9}$$

$$\Delta t = \frac{l}{cs} \tag{10}$$

Boundary layer influence

Although a lot of the properties behaviour in the shock tube are explained in the above sections, none of the governing equations take into account the viscosity present in the gas. With the appearance of a boundary layer near the wall, as the flow develops through the tube, the shock wave will reflect off of it leading to the appearance of oblique shocks, resulting in a bigger increase of temperature of the fuel/air mixtures formed in the contact region along with better mixing influenced by turbulent mixing.

Table 1: Theoretical critical pressure of ignition of common gaseous fuels

Gas	Known substance parameters			Calculated Values	
	Auto-ignition temperature (K)	Adiabatic exponent	Universal Gas constant	Mach number	Critical ignition pressure (bar)
Hydrogen	773	1.41	4124.2	2.91	22.5
Methane	853	1.32	518.28	3.15	187.9
Ethane	788	1.18	276.51	2.97	259.8
Propane	728	1.13	188.56	2.79	286.4
Butane	678	1.09	143.05	2.64	276.0

In figure 5, we see just that, where as the flow develops, the boundary layer near the tube, in light grey, grows influencing more as the shock travels the length of the tube.

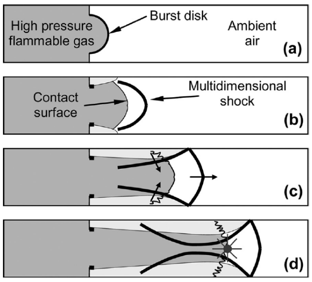

Figure 5: Development of a normal shock in a duct after the burst of a disk that was once separating a high-pressure flammable gas from the ambient air, by Dryer et. al[6]

3. Numerical model

In the present chapter the numerical implementation of the experiment will be approached. This chapter serves the purpose of showing and explaining the process behind the CFD work. Ansys Fluent was the program used to run the numerical model.

3.1. Implementation of the numerical model

Since this study consists of a real case, the use of Fluent must be as close to reality as possible. Just like mentioned before, in order to study what happens when a high-pressure gas spouts into the atmosphere, the best approach is to model a shock tube. This being said, a 2D rectangle separated in two equal sections (driver and driven) was designed in Fluent. Since there were two different cases being studied, several dimensions were studied. For the first case where the results were compared to those of the analytical approach, the dimensions used were 1 meter by 0.02 meters in order to vary only the initial pressure. On the second case, the initial pressure was fixed and the length varied as 0.36m, 0.42m and 0.48m with the driver and driven section each owning half of this length.

After designing the geometry, the next step was to mesh. Since the program used was the student version, it only permitted up to 512k nodes. Each one of the sections was face meshed with the quadrilateral symmetry and with a particular element size where after the refinement study the number of elements went from 120k to 501k in order to maximize the allowed number of nodes and to print out the best solution possible.

With the mesh done, all that is left to do is the setup and calculate the solution. In the setup tab, the solution was calculated using 4 solver processes with double precision for more accurate results. Using the density based-solver with transient time, energy equation on, and species transport the solution was run for both hydrogen/air and methane/air mixtures. Ideal gas, Sutherland viscosity and turbulent k-w standard flow with adiabatic conditions were used. Using implicit formulation with Roe-FDS and second order upwind discretization, the solution was initialized. For the first case the pressures studied were 5, 10, 20, 30 and 40 bar. For the second case, the solution was always initialized with 20 bar in order to only vary the length of the tube. Besides pressure, temperature was initialized both in driver and driven sections as 300K. The driven section was initialized with 1 atm of pressure. Mass fractions of both methane and hydrogen were set as 1 in the driver with 0.23 of O_2 and 0.77 of N_2 in the driven for the first case. For the second case only hydrogen was studied in the driver section. Finally, the solution was run with 2000 iterations consisting of 100 time steps of 20 iterations each, with a time-step calculated for each case. However, in order to achieve the best solution, the time-step used was calculated by trial and error.

4. Results

In this section, the results from both analytical and CFD approaches are going to be addressed while considering both cases studied in Fluent.

4.1. Analytical Results

Considering the equations 1 through 10, the properties studied inside the shock tube were pressure, temperature, density and the Mach number. Although the pressure profile is not the most important of the four properties to be studied, the initial pressure of the system prior to the burst disk rupture, is the most important and influential property as all the other properties depend on it. With equation 7, we have a direct relationship between the initial pressure ratio and the shock Mach number. This leads to the understanding that the bigger the ratio of pressures, the stronger the shock wave produced. Figure 6 shows the progression of the Mach number as a function of the initial pressure ratio for hydrogen, methane, ethane, propane and butane.

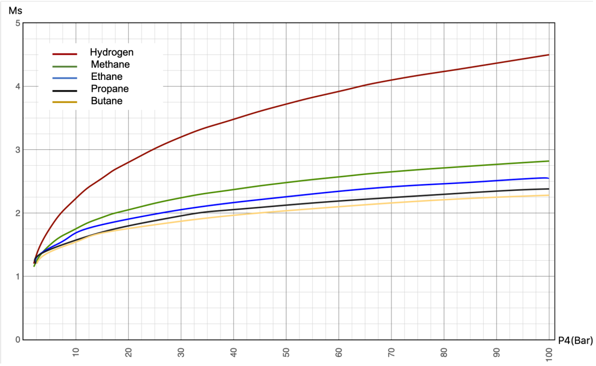

Figure 6: Shock wave Mach number(M_s) as a function of the driver pressure(P_4), using equation 7

As it is possible to observe for hydrogen, the Mach number produced increases a lot faster than the other gases presented in the figure 6. Using the results from equation 7, it is possible to print the ratio of temperatures across the shock wave as a function of the initial pressure ratio with equation 8. The results in figure 7 represent the temperature behind the shock wave, T_2 (as T_1 is constant at 300K), as a function of the initial pressure ratio of the system.

With the values from the engineering toolbox [1], only hydrogen will achieve high enough temperatures at "low pressure" leaks. While methane and hydrogen appear to be capable of reaching compression values of P_4 to cause ignition, ethane, propane and butane being liquefied gaseous fuels, are unable to reach the necessary driver pressures to do so, and so from now on the calculations presented will be on hydrogen and methane. From table 1, although the auto-ignition temperatures for the various gases does not vary much, the critical pressure of ignition is enlightening on how hydrogen can be very dangerous in the event of a leak.

Although the figures above show the calculation for ratios of pressure up to 100 bar, for comparing purposes with the results from Fluent, only the pressure ratios of 5, 10, 20, 30 and 40 bar were used for both mixtures of hydrogen and methane/air as they are more realistic.

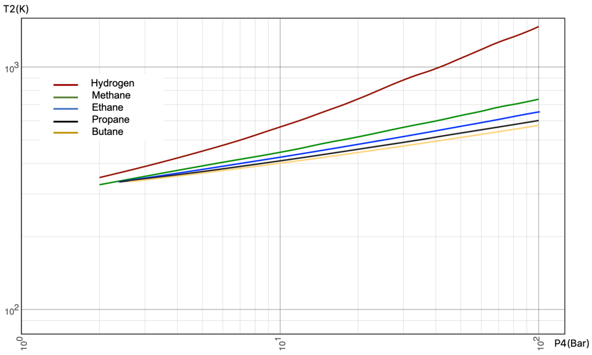

Figure 7: Temperature behind the shock wave(T_2) as a function of the driver pressure(P_4), using equations 7 and 8

4.2. Fluent Results for case 1

As previously said, Fluent was used to study 2 different cases. The first one had the objective of studying and comparing the results from the analytical approach. For this, using the assumptions described in the implementation section, Fluent was run for both hydrogen/air and methane/air mixtures for 5, 10, 20, 30 and 40 bar in order to compare the results. The values from pressure, temperature, density and velocity were compared.

4.2.1 Pressure

As said before, both mixtures were run in order to compare results from the governing equations. These presented similar graphs to figure 3. For this, since P_4 and P_1 are known, the only sections needed to be studied were P_2 and P_3, which as previously said, are assumed equal. In order to calculate P_2 equation 2 was used.

For the hydrogen/air mixtures, the values for P_2 extracted from Fluent are very similar to the results from the analytical approach. Calculating the percentile error between the two approaches, by assuming the results from Fluent as true, with the results from the last time step, we get a maximum error of 2%, allowing the conclusion that the assumptions made are correct. The same happens for the methane/air mixture although this time the maximum error calculated is of 6.5%

4.2.2 Temperature

Looking at figure 4 it is possible to see the how the temperature profiles inside the shock tube are printed.

With the results taken from Fluent it was possible to see that there was a considerable difference between the temperatures in region 2 from both approaches. This is due to the fact that turbulent flow is assumed and from figure 5, we know that as the flow develops, the boundary layer gets thicker and reflects the shock creating oblique shocks which lead to more heating applied to the mixture. Because of this, the maximum error for T_2, calculated for the last time step, from both approaches is 20.11% which is quite considerable. However, when looking at T_3, calculated for the last time step, a difference between values practically doesn't exist as the boundary layer ends up not affecting region 3 as the flow moves in the other direction. This leads to a maximum error of just 1.33%.

The same happens for methane, however since the shock is much weaker, the temperature reached in region 2 is smaller than for hydrogen. Comparing both approaches we extract a maximum error of 18.9% for T_2 and 0.93% for T_3.

4.2.3 Density

With equation 6 it is possible to calculate the entire density profile of the mixtures, as the density at regions 1 and 4 are known from the ideal gas law.

If the gas was the same in both regions, the density would rely only on the temperature leading to a density profile very similar to the pressure profile, however since the gases are different the density profile for hydrogen/air mixture is very similar, visually, to the temperature profile due to the fact that the universal gas constant for hydrogen is 14 times greater than the one from air. This lead to a maximum error of just 5.06% between the two approaches, calculated for the last time step, which proves the validity of the assumptions made. For methane/air mixtures the results came out very different printing a $\frac{\rho_2}{\rho_3}$ much smaller than the one for hydrogen/air. However, the calculated error for the last time step, was bigger at 8.57%

4.2.4 Velocity

Through Bernoulli's principle we know that for two fluids at constant height with different pressures, the flow will move in the direction of the low pressured fluid in order to try to find a balance. The bigger the pressure difference, the faster the velocity of the flow which means that, when we increase the pressure of the driver section, the velocity will also increase when comparing to lower pressured driver sections. With this, as the initial pressure is increased, so does the flow velocity increase.

Considering turbulent flow, we know that in the boundary layer the flow is sped up, which means that the maximum velocity reached is at the boundary layer. Using equation 9, values for velocities using both approaches are calculated. Considering that hydrogen/air creates a much stronger shock wave, the flow velocities reached will be much faster. For example at 40 bar of driver pressure the flow reaches a velocity of 1102.2m/s. Comparing the values from both approaches, for the last time step calculated, we get a maximum error of 21.52% for hydrogen and 37.96% for methane. Since methane produces weaker shocks, the flow velocities will be much lower leading to a max velocity at 40 bar of 699.5 m/s. The main reason that leads to the difference in results is the assumption of viscous flow. Since viscosity is not applied to the equations in the analytical approach, the flow velocities calculated are much faster than the ones printed in the numerical work.

Considering that all of these results were taken for the last time step calculated and only for comparison purposes, the originated error from both approaches is flexible. This means that it might be different if other tube dimensions or other time steps are chosen to be compared with the analytical results. However, the main difference relies on the way that both approaches are calculated. In the analytical approach a steady state is studied with simple 1D equations, while for the numerical work a transient state is assumed with complicated Navier-Stokes equations used. This obviously leads to different results.

4.3. Fluent Results for case 2

In case 2 the effects of the length of the tube were tested. For this a geometry, just like the one used in case 1, was designed with the dimensions of 360mm, 420mm and 480mm all with the same diameter of 20mm. As previously, driver and driven sections were designed with the same length meaning that half of the total length of the tube belonged to the driver section and the other half to the driven section. With all the assumptions mentioned before, the driver section was initialized for all 3 lengths with 20 bar, as it was proven that it was enough to reach the spontaneous ignition of hydrogen, and the driven section with atmospheric conditions. For this reason only hydrogen is going to be tested and the results are shown for the last time step calculated.

4.3.1 Pressure

As mentioned above the pressure was the same for each case so that there would be just one variable, the length of the tube. From the results gathered from Fluent it was possible to conclude that the pressure profile wont change with the current settings. The only possible thing to be observed is the fact that for smaller lengths of tube, region 2 and 3 are more unstable creating some fluctuations of pressure across the diameter of the tube. However, it was possible to clearly identify all for regions of the shock tube as it is possible to see in the following figure 8 for the length of 360mm, at the last time step calculated.

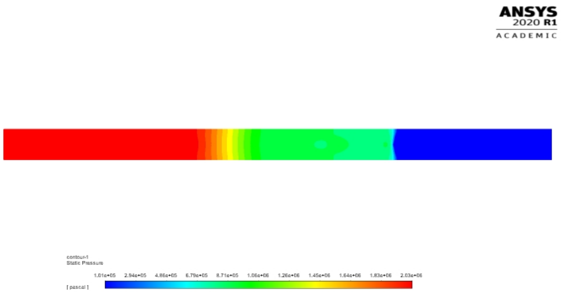

Figure 8: Pressure profile inside the 360mm shock tube

4.3.2 Temperature

Although there was no visible change in the pressure profile with the increase of length, temperature profiles had the opposite reaction. It is known that the turbulent boundary layer thickness grows with the length of the tube and with this increase, the shock wave is more affected by shock reflections of off the boundary layer. With these reflections, oblique shocks are created which lead to a higher temperature of the flow. This being said, it was expected that the temperature would increase with the increase of tube length. This assumption was verified. It was found that at a tube length of 360mm, the shock produced by a downstream pressure of 20 bar was enough to cause a spike of temperature up to 836.6K, at the last time step registered, which means that for this length of tube smaller pressures could lead to spontaneous ignition of the hydrogen/air mixture in the presence of good mixing. On the opposite thought for this downstream pressure, a smaller tube might be able to cause the same effect. Although it was verified that with the increase of length the maximum temperature would rise, the minimum temperature on the other hand, remains constant which is expected since region 3 is not affected by the shock wave. In the following figure 9 we can see how the temperature profile behaves inside the tube with the use of contours, for the 360mm long tube, at the last time step.

As it is possible to see, the four regions are easily identifiable with the highest temperature being recorded at the tube walls due to the boundary layer.

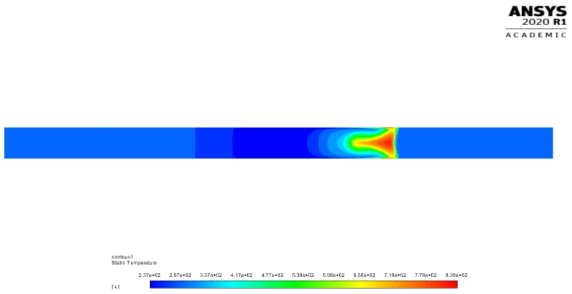

Figure 9: Temperature profile inside the 360mm shock tube

4.3.3 Density

As previously discussed the density profile inside the shock tube is very similar to the temperature profiles. It was possible to observe that due to the increase of temperature in region 2 and the temperature in region 3 maintaining similar values, the density ratio across the shock wave, $\frac{\rho_2}{\rho_3}$, becomes smaller as ρ_2 decreases with the increase of temperature. In the following figure 10 we can see that the density profile at the last time step, once again for the 360mm long tube, is very similar to the one shown in figure 9 as the density varies with the temperature of the region.

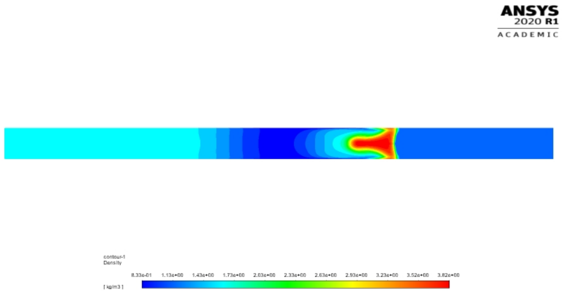

Figure 10: Density profile inside the 360mm shock tube

4.3.4 Velocity

Through Bernoulli, it is known that with the increase of pressure on the driver side, the flow velocity will be faster. However, with the increase of length and the pressure remaining constant, the velocity profile is much harder to predict. With the increase of tube length it is known that the turbulent boundary layer will have more influence on the flow. Also it is also known that the turbulent boundary layer increases the speed of the fluid near the walls. So with these two arguments it could be expected that the velocity would increase with the increase of length. However, with more surface for the fluid to run through, viscous forces will have more influence and therefore the flow velocity will actually decrease through adhesion and friction.

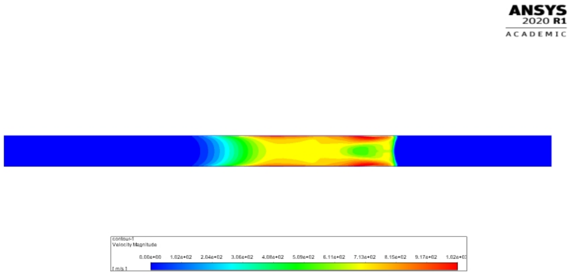

Figure 11: Velocity profile inside the 360mm shock tube[10]

In the previous figure 11 we see just that. For the 360mm long tube we have the fastest flow near the walls of the tube, with the boundary layer being quite visible.

Although the results shown are only for the 360mm long tube the following table presents all the results for the four lengths tested which allow for better conclusions.

Properties	Length of the tube	360mm	420mm	480mm	1000mm
Hydrogen/air:					
Max. Flow velocity (m/s)		1018.8	997.1	976.9	877
P_2(Bar)		9	9	9	9
$T_3(k)$		236.7	236.7	237.3	238.2
$T_2(k)$		836.6	848.4	860.4	918.2
Density ratio (ρ_2/ρ_3)		4.66	4.56	4.53	4.08

Table 2: Temperature profile inside the 360mm shock tube

By looking at table 2, as the length of the tube increases, only two properties are affected directly, the temperature behind the shock wave and the velocity of the flow. With the increase of tube length not only does the maximum temperature increase but the velocity of the flow decreases. Therefore, a longer tube might have a higher probability of causing spontaneous ignition of the mixture fuel/air. Since the numerical work was presented for the last time step, different results for different time steps can be expected. This being said, the next section is dedicated to the study of the shock through time inside the tube.

4.4. Shock Through time

In this section an evaluation of what happens inside the shock-tube throughout the flow time, in terms of temperature is going to be made.

Several studies were made in terms of ignition times and the delay it takes for the spontaneous ignition to happen. One of those studies was done by Mogi et al.[10] in 2007 where jet fire ignition was achieved with an experimental set consisting of a tube with 185mm with 5mm in diameter with a driver pressure of 145 bar with hydrogen/air mixture. With this setting, spontaneous ignition of hydrogen was achieved. With the careful observation of this paper, it was possible to conclude that ignition might start inside the tube and not outside, meaning that at the burst of the contact surface, mixing might start right away leading to the ignition. With this information, this section is dedicated to studying what happens inside the shock-tube through time.

In previous sections the properties of the mixtures are addressed and what happens to them in case of shock inside of a tube. However, one of the most important things to study when considering combustion is the quality of the mixture. When quality of a mixture is addressed the main aspect to be addressed is the equivalence ratio (Φ). The equivalence ratio studies if a mixture is rich (> 1), lean (< 1) or stoichiometric ($=1$) by dividing the Fuel-air ratio of the mixture by the stoichiometric Fuel-air ratio.

Alcock et al. [3], demonstrated that hydrogen/air stoichiometric mixture requires a minimum ignition energy of just 0.02 mJ, however the flammability limits present a very wide range of % of hydrogen in air. With this, it is possible to conclude that the easiest way for hydrogen to ignite when mixed with air, is to have a concentration mixture at stoichiometric conditions which is 29.5% of hydrogen in air. Since this is a numerical study, it is impossible to say for sure that combustion happens, however, through temperature and quality of the mixture it is possible to say if the conditions necessary for the mixture to ignite are gathered. In order to study this, two tube lengths, 1m and 0.36m, were used to test two initial pressures, 5 and 40 bar, to a total of four different analysis. Since Fluent does not produce the equivalence ratio as a result property, a user defined function was developed where the mass fraction of H_2 was divided by stoichiometric hydrogen% in air

4.4.1 360mm Long tube

As mentioned before, two different pressure ratios are going to be tested, 5 and 40 bar. As seen from case 1, it is known that for 5 bar of initial pressure, the temperature achieved by the mixture is not going to be enough to cause spontaneous ignition as the maximum temperature recorded was 471.6K. However, analysing the equivalence ratio hydrogen/air mixtures, it was possible to conclude that the location of the highest temperature achieved was also where the mixture was stoichiometric. This being said it is possible to say that if there is a bigger input of pressure that leads to a bigger spike of temperature, it might lead to spontaneous ignition.

From the figure 12 we prove the assumption made in the previous paragraph where, for 40 bar of pressure, the temperature achieved by the stoichiometric mixture is higher than the recorded spontaneous ignition for hydrogen at 737k. As it is possible to see from the figure, in the temperature profiles, right from $5e^{-5}s$, the temperatures recorded behind the shock wave are already enough to cause spontaneous ignition of the mixture. Moreover, from the equivalence ratio profiles, it is possible to say that the mixture stays stoichiometric throughout the length of the tube, meaning that at the interface separation of the mixture with air, the conditions are stoichiometric. Combining these two factors it is possible to say that for a driven section of 180mm and an initial pressure input of 40 bar, the conditions necessary to ignite and produce flame from a hydrogen/air mixture are gathered.

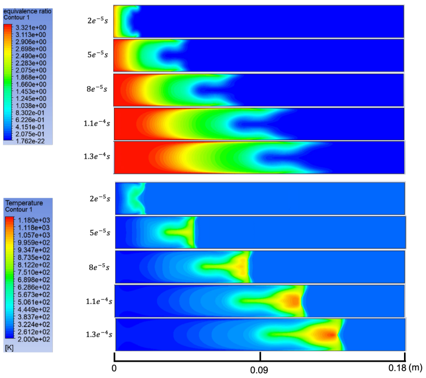

Figure 12: Hydrogen/air equivalence ratio profile (top), and temperature profile (bottom) for the 360mm long tube at 40 bar of initial pressure.

4.4.2 1m Long tube

As said before, from case 1, with an input pressure of 5 bar for a 1m long tube, the temperatures produced are not high enough to lead the mixture to spontaneous ignition as the maximum temperature achieved is of 533.5K with a lean mixture. However, when analyzing the 40 bar profiles for 1 meter long tube with figure 13, the profiles observed are very different than for 5 bar. In the temperature profile observed it is possible to see that the maximum temperature achieved by the shock wave is 1233K which is well above the spontaneous ignition temperature but is located at the boundary layer. However, most of the temperature profile exhibits temperatures in the range of 1000K (in yellow) which is still well above the temperature required. When looking at the equivalence ratio profile, a very interesting conclusion can be taken from its observation. Although in the beginning of the tube, at $7.9e^{-5}s$, the mixture creates a shape that resembles a horse shoe where near the edges, the mixture in light blue, is stoichiometric. However with the flow development, at the time stamp of $4e^{-4}s$ the mixture starts to face and becomes lean with $\Phi < 1$. So, although the conditions at $7.9e^{-5}s$ are gathered for a possible spontaneous ignition of the mixture, with the flow development, the mixture becomes lean which leads to bad conditions for ignition. So although a longer tube might produce higher temperatures, with the flow development mixture fades over time, where Φ decreases below the stoichiometric value and ignition is no longer possible. So in the early stages there might be combustion but at the end of the tube the combustion will be extinct producing no flame to the outside.

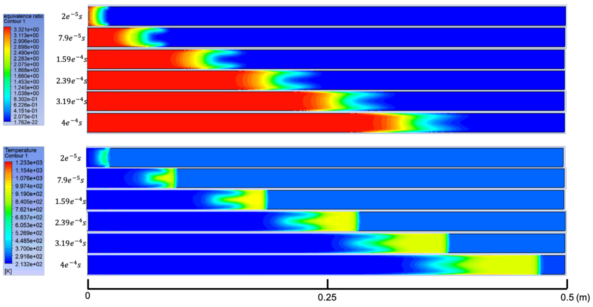

Figure 13: Hydrogen/air equivalence ratio profile (top), and temperature profile (bottom) for the 360mm long tube at 40 bar of initial pressure.

With all the analysis made with fluent, it is possible to conclude at what lengths and pressure there might be an ignition considering that the conditions are gathered for such phenomena to take place. With the studied analysis, it is concluded that for 5 bar of initial pressure, much like for 10 bar, the shock wave produced is not strong enough to cause enough increase of temperature to lead the mixture to spontaneous ignition. However, for 20 bar and up, it is possible to see that for some tube lengths the conditions are gathered for spontaneous ignition to take place. With the results from case 1 and 2 it is possible to conclude that the higher the pressure input, the longer the mixture quality is sustained. With the results from the analysis made it is possible to plot the following graph where ignition is expected to occur under such conditions of initial pressure and tube length.

With all the analysis made it is possible to conclude whether it is possible or not to have ignition. In figure 14 we see just that, where above the black line it is concluded that the conditions to have spontaneous ignition are gathered and such phenomena is possible to occur.

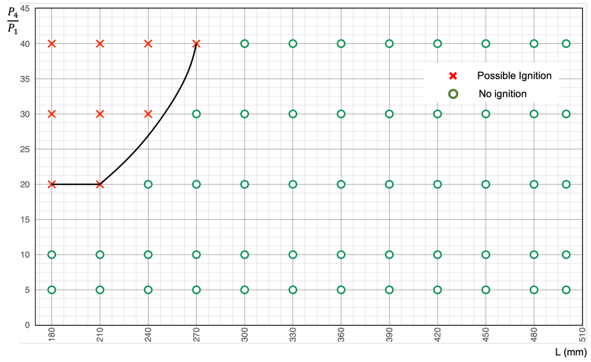

Figure 14: Initial pressure as a function of the length of the tube where the conditions are or not gathered for spontaneous ignition to occur.

5. Conclusions

This dissertation had two objectives. For the first objective analytical calculations were compared to the CFD work. For this the governing equations were used for the analytical part and fluent was used for the CFD part. The same setting was implied to both approaches where certain assumptions were made in fluent. Comparing the results it was possible to conclude that the assumptions made were correct where the error printed between the two approaches, even though sometimes considerable, was minimal in most cases. The biggest difference in results was seen for the temperature and velocity profiles as both are affected by viscous flow. However, considering that only the last time step was used to compare values, it is possible to say that for a different time step, the error might be different.

For the second objective, various lengths of tube were tested. This allowed the study of the properties with the increase of length and the study of exactly what happens inside the shock tube. It is possible to say that a longer tube allows for a bigger build of temperature behind the shock wave. However, in order to have combustion, good mixture is also necessary and for a longer tube, the mixture might fade with time, whereas for a smaller tube the mixture maintains better quality for longer time. This leads to the conclusion that for a smaller tube, if the input pressure leads to a temperature above the spontaneous ignition line, ignition is more likely to happen than for a longer tube. This being said, for certain tube lengths, there is a minimum critical pressure that might lead the mixture to ignite, as seen in figure 14.

6. Future Work

In order to complement the work done in this dissertation, further work on what happens when the mixture spouts into the atmosphere is needed. Work such as what conditions lead to stabilized jet fire of hydrogen spontaneous ignited leaks could be very useful.

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