

## IMPACT OF TURBULENCE ON THE INITIATION OF AN EXPLOSION IN A FUEL/AIR MIXTURE BY HOT JETS

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### ABSTRACT

In this paper we investigate the impact of shear generated turbulence on the initiation of an explosion in a pre-mixed fuel/air mixture which is caused by hot exhaust gas jets. A stand-alone PDF method is used to investigate initiation of such explosion. In order to reduce the computational cost concerning the calculation of fuel/air combustion we use a reaction-diffusion manifold (REDIM) technique to obtain an appropriate reduced kinetic scheme. The simulations are performed for hydrogen/air and propane/air cases in configurations relevant to safety applications. The ignition in the hydrogen case and the propane case, respectively, are investigated using different boundary conditions in order to examine the impact of boundary conditions on the ignition event. It is observed that the ignition delay time is shorter in case where the hot jet enters into the ambient gas right away in comparison to the case where the hot jet enters into an already developed jet of the cold gas.

### INTRODUCTION

Ignition by hot turbulent jets is found in many areas including pulsed engines, pulsed detonation engines and safety relevant applications. The primary motivation of this study is the prevention of an accidental explosion of a combustible mixture in the field of explosion protection. In many industrial plants combustible gases exist in the ambient atmosphere. Due to safety requirements (Hattwig & Steen, 2004) the components that could ignite the combustible ambient can e.g. be enclosed by "flameproof enclosures" (IEC 60079-1, 2014). In such enclosures there exist gaps that cannot be eliminated completely due to practical reasons, such as a joint clearance or other gaps. An internal explosion may lead to jetting of hot exhaust gases into the surrounding which may result in an accidental explosion. In this sense, the explosive gases are usually classified into groups and sub-groups according to their maximum experimental safe gaps (MESG). Typical representative gases for the gas group with lowest MESG is hydrogen and for the gas group with highest MESG is propane. The ignition initiation for various boundary conditions have been investigated for hydrogen/air mixture in our previous work (Ghorbani *et al.*, 2014). One of the contributions of this work is to investigate the impact of flow conditions such as turbulence on the initiation of an ignition for a stoichiometric propane/air mixture and compare the results with that of stoichiometric hydrogen/air mixture.

This investigation is carried out by a numerical simulation. In order to perform the simulation we use a Lagrangian PDF (probability density function) method. In this approach a transport equation is solved for a joint velocity-turbulent frequency-scalar PDF. The transport equation for the joint PDF is solved by a Monte Carlo/particle method, the computational domain is initialized by a large number of notional particles. The notional particles are evolved in time by a set of stochastic differential equations (SDEs). In order to reduce the computational cost concerning the calculation of propane/air combustion we use a reaction-diffusion manifold (REDIM) technique (Bykov & Maas, 2007) to obtain an appropriate reduced kinetic scheme.

### Modelling Approach

In order to model transient turbulent flow, we use the probability density function-projection method (PDF-PM) algorithm which has been developed based on the joint velocity-turbulence frequency-composition PDF model (Ghorbani *et al.*, 2015b). The modeled PDF equation is solved by using a Monte Carlo particle-cell technique. In this method, the flow is modeled by an ensemble of notional particles. The evolution of notional particles is governed by a set of stochastic differential equations. We use the simplified Langevin model (SLM) (Pope, 1985) for the velocity evolution. Here we use same model equations and constants as explained in (Ghorbani *et al.*, 2014). Molecular mixing is modeled by the modified Curl model (Janicka *et al.*, 1979). To reduce the number of dependent variables in the simulation, a reduced description of the thermochemical state is applied using the REDIM method (Bykov & Maas, 2007). It is sufficient to describe the state with a two-dimensional manifold (Ghorbani *et al.*, 2014). The manifold is parametrized with a chemical progress variable and a variable that represent the state of mixing of the two streams, i.e. exhaust gas and fresh unburnt gas. For propane/air case the specific mole number of CO<sub>2</sub>,  $\phi_{CO_2}$ , is used to represent the progress variable.  $\phi_{CO_2}$  is defined as  $w_{CO_2}/M_{CO_2}$ , where  $M_{CO_2}$  is the molar mass and  $w_{CO_2}$  is the mass fraction of CO<sub>2</sub>. The state of mixing is represented by enthalpy, which also accounts for the heat losses due to nozzle walls (Ghorbani *et al.*, 2014). Thus,  $\phi_{CO_2}$  and enthalpy are the only additional variables that has to be solved in the reactive simulations. In case of hydrogen simulations  $\phi_{H_2O}$  is used to represent the chemical progress variable. For REDIM calculations the hydrogen mechanism

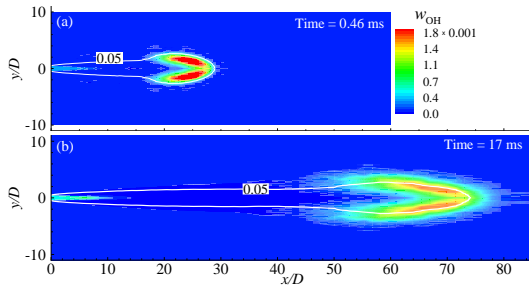


Figure 1: Contour plot of the mean mass fraction of the OH radicals shortly after ignition. The contour line of mixture fraction  $\xi$  of with value of 0.05 (white line) is also shows approximate boundary of the jet. (a) Simulation results for hydrogen case;  $T_j = 1400$  K,  $U_j = 300$  m/s and  $D_j = 1$  mm. (b) Simulation results for propane case;  $T_j = 1550$  K,  $U_j = 50$  m/s and  $D_j = 1.5$  mm.

from (Warnatz *et al.*, 2006) and the propane mechanism from (Kathrotia, 2011) was applied.

### Simulation setup

Here, we consider a round jet of hot exhaust gas which enters the ambient. For nozzle diameter  $D$  values in a range of 1.0 mm to 1.5 mm are considered. The simulations are performed using a 2D axisymmetric cylindrical coordinate system. Due to symmetry only half of the domain is resolved.

At the inlet the PDF of the joint velocity is assumed to have a normal distribution. The mean values and fluctuations are defined based on fully developed turbulent pipe flow conditions. At the inlet the turbulent frequency is described by a gamma distribution as explained in (Van Slooten & Pope, 1998). Symmetry conditions are applied at the centreline ( $r = 0D$ ), and a slip boundary condition is assumed at the side wall. At the outlet the mean pressure is assumed to be uniform. The composition and the density at the inlet are set to be uniform. The co-flow is a fresh stoichiometric fuel/air mixture at a temperature of  $T_e = 300$  K. In the experimental measurements a strong cooling down of exhaust gas due to the nozzle wall is observed. Consequently, the emitted hot exhaust gas has a lower temperature than an adiabatic flame of the considered fuel. To be close to such conditions the composition of the jet inlet is set to the exhaust gas of a stoichiometric mixture where the inlet temperature  $T_j$  is varied in the range of 1400–1550 K.

## RESULTS AND DISCUSSIONS

Figure 1 shows contour plots for mean mass fraction of OH radicals  $w_{OH}$  shortly after initiating of explosion in the ambient. Also contour level of mean mixture fraction for  $\xi = 0.05$  is shown to point out the boundaries of the jet. Figure 1a shows the simulation results for the hydrogen case and Fig. 1b for the propane case. In the hydrogen case the nozzle diameter  $D$  is 1 mm, mean temperature of exhaust gas  $T_j$  is 1400 K and the mean velocity at the nozzle exit  $U_j$  is 300 m/s. On the other hand in the propane case the boundary conditions are  $D = 1.5$  mm,  $T_j = 1550$  K and  $U_j = 50$  m/s. In this plot both cases have the same max-

imum of  $w_{OH}$ . Despite favourable conditions in propane case, i.e. larger nozzle diameter, higher temperature and lower velocity (which means lower shear stress) it can be observed that the ignition delay time is much higher in the case of propane. The ignition process is governed by an interaction of mixing and reaction. Thus, in order to determine whether an ignition is possible, it is necessary to investigate the competing time scales of reaction and mixing (Ghorbani *et al.*, 2015c). In (Ghorbani *et al.*, 2015a) it was shown that the relevant time scales of chemistry and turbulent mixing have major impact on the ignition event.

The ignition process is governed by an interaction of mixing and reaction. Thus, in order to determine whether an ignition is possible, it is necessary to investigate the competing time scales of reaction and mixing. The reaction time scales are estimated by means of the REDIM reduced system dynamics.

Figure 2a shows chemical source term of the progress variable  $S(c)$  on the (reduced) scalar state space for propane. By definition mixture fraction  $\xi$  is 1 for pure jet and 0 for ambient gas. The progress variable  $c$  is 1 for completely burnt gas and 0 for unburnt gas. In the state space which is defined by  $(\xi, c)$  the point  $(\xi = 0, c = 0)$  is attributed to the pure unburnt ambient and  $(\xi = 1, c = 1)$  to the pure burnt exhaust jet. In Fig. 2a the two initial points also are shown, namely, pure jet  $T = 1550$  K and pure fresh unburnt ambient ( $T = 300$  K). The line that connects these two initial points is called mixing line, since, by pure mixing (no chemical reactions) only this line would be accessible in the state space. Figure 2b shows the chemical source term of the progress variable for the hydrogen/air case (where the temperature of burnt mixture is 1400 K). Chemical reactions lead to an upward advancement of composition. After a small fluid element is advanced along the progress variable direction (which is called *local ignition*), it can also push other fluid elements off the mixing line by mixing. Indeed, sequences of these processes are that lead to initiation of global ignition (i.e. rise of *mean* temperature). The details of these processes and their impact on location of global ignition have been investigated in (Ghorbani *et al.*, 2015c).

In Fig. 2 it can be seen that the highest rates of the progress variable are close to  $(\xi = 0, c = 0.6)$  (6000/s for propane and 40000/s for hydrogen). This region is not accessible as explained above (by pure mixing) at initial times. Hence, one relevant time scale that is interesting to look into is the time that it takes to ignite for a fluid element that resides along the mixing line. If a fluid element progress along the progress variable to a 80% of maximum possible value ( $c_{80\%}(\xi)$ ) for a given mixture fraction then it is assumed as burnt. In Fig. 2a a line that represents  $c_{80\%}(\xi)$  is also illustrated. The chemical rates of progress variable in Fig. 2 show that the highest rates are around  $c_{60\%}(\xi)$ . Taking any other values in the range 0.6–0.8 for the criteria shall not change the reasoning which will be followed.

Figure 3 shows the inverse of the time that just discussed above (i.e. the time that takes for a fluid element at the mixing line to ignite i.e. reach  $c_{80\%}(\xi)$ ). In this plot the inverse of the time is shown (instead of the time itself) in order to obtain a chemical rate which will be compared with the turbulent mixing rate. In Fig. 3 the time scales (or rates) are shown for both hydrogen (red line) and propane (blue line). Not surprisingly, it can be seen that propane has much lower rates in comparison to hydrogen.

Figure 4 compares the time scales regarding turbulent mixing and chemical reactions as mentioned above at sta-

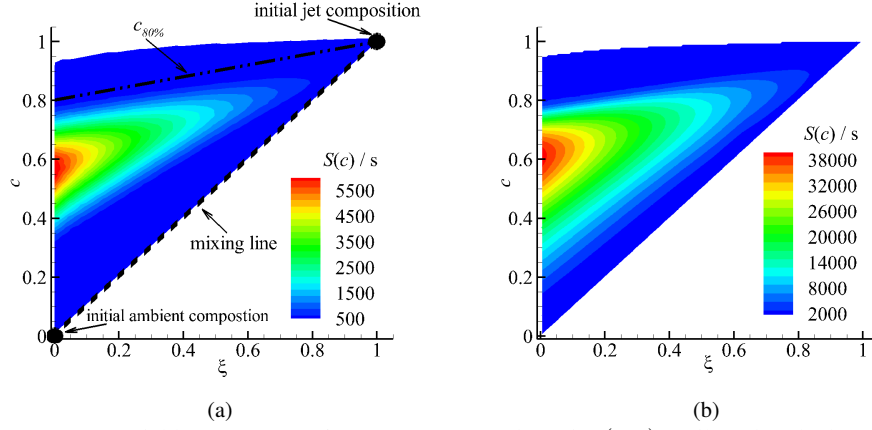


Figure 2: (a) Progress variable source term for propane case. The point (1,1) attributed to the hot exhaust gas with a temperature of 1550 K. (b) Progress variable source term for hydrogen case. The point (1,1) attributed to the hot exhaust gas with a temperature of 1400 K.

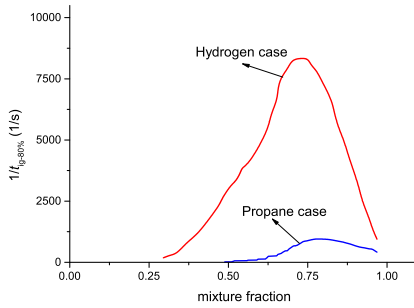


Figure 3: Chemical rates for hydrogen and propane which is obtain from  $1/t_{c,80\%}$ .  $t_{c,80\%}$  is the time necessary (using REDIM reduced system dynamics) for a fuel/air mixture at a given mixture fraction along the mixing line to ignite (i.e. reach  $c_{80\%}$ ).

tionary state. Indeed, initiation of an ignition as discussed in (Ghorbani *et al.*, 2015c) is more complicated than that can be accurately described by stationary state flow condition. The stationary state, by simplifications, allows to observe some of the important aspects of the ignition event under study. Hence, in Fig. 4 the profiles are shown for steady state condition. The results for the hydrogen case are shown in Fig. 4a. In this plot the mean mixing frequency (blue symbol line) and root mean squared of mixture fraction  $\xi_{rms}$  (green solid line) and progress variable  $c_{rms}$  (red dashed line) along the centreline axis are shown. The importance of the comparison between  $\xi_{rms}$  and  $c_{rms}$  is that  $\xi$  appears as an inert scalar, therefore, its fluctuation is only due to fluid dynamics (e.g. turbulent mixing), while, fluctuations in  $c$  are due to both fluid dynamics and chemical reactions.

Due to the mixing of the jet and ambient gas close to the nozzle the scalar fluctuations increase (Mi *et al.*, 2001). As shown in Fig. 4a both  $c_{rms}$  and  $\xi_{rms}$  increase at locations very close to the nozzle exit until the end of core region of the jet is reached which in this case is around  $5/D$ . After this point due to molecular diffusion the fluctuations reduce. It can be seen that  $c_{rms}$  and  $\xi_{rms}$  are very similar at upstream locations. At downstream (i.e.  $25 - 35D$ ), however, they

depart from each other.

The black dashed line specifies the maximum chemical rate for hydrogen in Fig. 3, which is about 8000/s. It can be seen that the departure of  $c_{rms}$  and  $\xi_{rms}$  (i.e. an increase in  $c_{rms}$  at downstream which is due to chemical reactions) occurs at a point where the mixing frequency becomes less than (or close to) these chemical rates.  $c_{rms}$  and  $\xi_{rms}$  are close to each other at upstream, which reveals that the mixing is dominant and the fluctuations are governed by mixing processes. On the other hand, as the turbulence reduces downstream, the chemistry becomes dominant which in turn increases  $c_{rms}$ .

Figure 4b shows the same data for propane case. It is interesting to see that for propane case also the same behaviour can be observed. This result, indeed, supports the assumption that in order a global ignition to occur one of the requirements are that mixing time scales should be in order of the initial chemical time scale of the compositions along the mixing line.

On the other hand in (Sadanandan, 2007) it was observed that the ignition appears first at the jet head vortex. A numerical investigation in (Ghorbani *et al.*, 2015c) has shown that the conditions at the jet head is the most suitable location to initiate the ignition. In order to further investigate the impact of the jet head vortex on e.g. ignition delay time two cases are considered. In one case the hot jet impinges into a (quasi<sup>1</sup>) quiescent ambient right away. In the second case at first the same gas mixture as in the surrounding enters the ambient and develops a statistically stationary jet. Afterwards the hot jet is issued into the already developed jet. In the second scenario at the time the hot jet enters the surrounding, due to the fact that the jet is already developed, there is no head vortex at the tip of the hot jet.

Figure 5 shows the jet shortly after ignition for both scenarios (which hydrogen is used as fuel). The first scenario is shown in the upper half of the plot and the lower half shows the second scenario. It can be seen that the ignition delay time (the time at which a global ignition occur after the hot jet enter the surrounding) is increased significantly (almost 65%) in the second scenario in comparison to the first scenario. This, obviously, emphasises again the importance of the turbulent field on the ignition of hot jet.

<sup>1</sup>Ambient has a small velocity

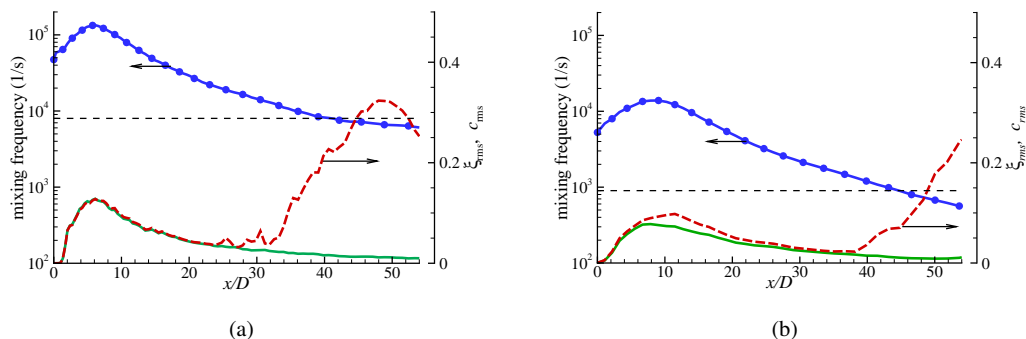


Figure 4: Scalar mixing frequency (blue line with symbols), fluctuations of mixture fraction  $\xi_{rms}$  (green solid line) and fluctuations of progress variable  $c_{rms}$  (red dashed line) along the centreline at stationary state. (a) Simulation results for the hydrogen case.  $T_j = 1400\text{ K}$ ,  $D = 1\text{ mm}$  and  $U_j = 300\text{ m/s}$ . (b) Simulation results for propane case.  $T_j = 1550\text{ K}$ ,  $D = 1.5\text{ mm}$  and  $U_j = 50\text{ m/s}$ .

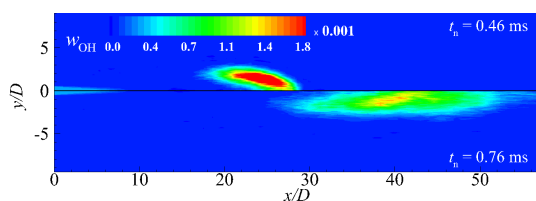


Figure 5: Contour plot of the mean mass fraction of the OH radicals shortly after ignition. Upper half: The hot burnt gas impinges into quiescent ambient. Lower half: Initially the jet is cold unburnt gas (i.e. the same as the surrounding gas), which the hot burnt gas enters the ambient after the initial jet obtains a statistically steady state.

## Conclusion

In this work a PDF approach was used to investigate the initiation of an explosion in a premixed fuel/air mixture which is caused by hot exhaust gas jets. Using this method ignition events in hydrogen/air and propane/air cases are compared, in configurations relevant to safety applications. In contrast to the hydrogen case, for propane the initiation of an ignition occurs with a considerable larger delay time, which is expected as the chemical rates are slower in propane. The relevant chemical time scales are compared with the turbulent mixing time scales in order to explain the ignition delay time.

Here, also the impact of shear turbulence as well as the head jet vortex on initiation of an ignition were investigated. It was observed that the initiation of an ignition in both cases of hydrogen and propane appears first at the jet head, if the hot jet impinges into the quiescent ambient. However, if the hot gas impinges into an already developed jet, the ignition is initiated in a broader locations. This suggests that, in case of ignition by hot jet, one needs to take into account the fact that whether the hot jet enters into a quiescent ambient or into an already developed jet. The importance of this issue reveals itself when one observe that in a practical condition due to existence of cold gas in the nozzle the hot jet first pushes out the cold gas and leads to development of a turbulent jet. In such a condition, therefore, it is important this effect to be accounted for.

## Acknowledgements

This work was supported in part by the Deutsche Forschungsgemeinschaft within the Research Group FOR 1447. The authors gratefully acknowledge the support of DLR–Institute of Combustion Technology, Stuttgart, Germany for providing access to the detailed propane mechanism.

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