# Numerical investigation and comparison of hydrogen/air and propane/air explosion by hot jets

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## 1 Introduction

In this paper we investigate numerically the initiation of an explosion in a premixed propane/air mixture which is caused by hot exhaust gas jets (of its own combustion products). 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 [1, 2] the components that could ignite the combustible ambient can e.g. be enclosed by "flameproof enclosures" [1]. 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. The ignition initiation for various boundary conditions have been investigate the impact of flow conditions such as turbulence on ignition event for propane/air mixture.

In order to perform the simulation we use the PDF-PM algorithm [4] which has been developed based on a Lagrangian PDF (probability density function) method [5], in conjunction with a projection method to calculate mean pressure for transient flows. In this approach a transport equation is solved for a joint velocity-turbulent frequency-scalar PDF [6]. 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 chemical reactions we use a reaction-diffusion manifold (REDIM) technique [7] to obtain an appropriate reduced kinetic scheme.

Calculations of propane/air case shows that the ignition (as in hydrogen case) first appears at the jet head. However, in contrast to hydrogen case, it is observed that for propane the initiation of an ignition (when occurs) appears with considerable larger delay times. This will be explained by comparison of time scales relevant for chemical reactions and mixing processes. The aim of the current study is to investigate qualitatively the conditions and processes that lead to ignition. The results of these investigations will be used as a basis in our following work in order to understand and prevent accidental explosions.

## 2 PDF Approach

In order to model transient turbulent flow, we use PDF-PM algorithm which has been developed based on the joint velocity-turbulence frequency-composition PDF model [4]. The modeled PDF equation

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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) [5] for the velocity evolution. Here we use same model equations and constants as explained in [3]. Molecular mixing is modeled by the modified Curl model [8]. To reduce the number of dependent variables in the simulation, a reduced description of the thermochemical state is applied using the REDIM method [7]. For the reactive case in the current work it is sufficient to describe the state with a two-dimensional manifold [3]. The manifold is parametrized with a chemical progress variable and a variable that represent 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 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 [3]. 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 from [9] and the propane mechanism from [10] was applied.

## 3 Simulation setup

Here, we consider a round jet of hot exhaust gas which enters the ambient with a statistically stationary flow rate at the nozzle exit. For nozzle diameter D values in a range of 0.6 mm to 3 mm are considered. The simulations are performed using a 2D axisymmetric cylindrical coordinate system. The computational domain is rectangular and extends about 10D-20D along the radial direction and 60D for hydrogen case and up to 200D for propane case along the axial direction. A non-uniform grid with  $100 \times 100$  points and a nominal number of 320 particles per cell are used to discretize the computational domain. 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 condition. At the inlet the turbulent frequency is described by a gamma distribution [6]. 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 with an equilibrium composition where the inlet temperature  $T_j$  is varied in the range of 1400–1550 K.

## 4 Results and discussion

In this section first we present simulation results for hydrogen and propane cases. The aim is to have an overall perception concerning the qualitative behaviour in both cases of hydrogen and propane. As with any comparison, to compare both hydrogen and propane simulations, an optimal approach would be to use same parameters. However, for simulations with a meaningful result for practical applications it is not easy to have exact same initial conditions (regarding burnt gas temperature at the jet inlet, mean velocity and nozzle diameter). For example if a typical configuration which results in an ignition with a *delay time* in hydrogen/air case is used for propane case, it might not lead to an ignition. This is due to different behaviour regarding re-ignition, ignition delay times and location, in hydrogen and

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propane gases (which of course is a result of different chemical time scales). Yet, it is very useful to see the different behaviour of the two combustible, even with slightly different setups. Afterwards in the subsequent of this section these different behaviour shall be explained with the help of chemical and turbulent mixing time scales.

Figure 1 shows contour plots for mean temperature shortly after initiating of explosion in the ambient. Also contour levels of mean mixture fraction are shown to approximate the boundaries of the jet. Figure 1a shows the simulation results for hydrogen and Fig. 1b for propane case. In the hydrogen case the nozzle diameter D is 1 mm, mean temperature of exhaust gas  $T_j$  is 1500 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. Despite favourable condition in propane case, i.e. larger nozzle diameter, higher temperature and lower velocity (which means lower shear stress) it can be easily observed that the ignition delay time is of order of magnitude higher in the case of propane.

Figures 2a and 2b show ignition delay times for hydrogen and propane case, respectively. The ignition delay times in Fig. 2a for hydrogen case are shown for simulations with  $T_j = 1400$  K,  $U_j = 300$  m/s and nozzle diameter from 0.6 mm up to 1 mm. It can be seen that, as expected, by decreasing the nozzle diameter the ignition delay time increases and, eventually, at 0.6 mm no ignition is observed (regarding given boundary condition). Figure 2b shows the ignition delay time for propane case with boundary conditions of  $T_j = 1450$  K,  $U_j = 50$  m/s and nozzle diameter from 1 mm up to 3 mm. For the propane case, despite relatively lower temperature in hydrogen case, the ignition delay times are much higher. Also it can be seen that a temperature of 1450 K at nozzle exit does not lead to an ignition for diameters less than 1 mm.

The reason for the increase in the ignition delay time with decrease in nozzle diameter, as discussed in [3], is due the fact that the shear generated turbulence impacts the core of the jet more in small nozzles than large cases. As a result the diameter of the hot core region and the mass flow rate are reduced. Subsequently, the turbulent mixing has more impact on the center of the hot jet region. Whether the hot jet leads to ignition depends on the chemical time scales and scalar mixing time scales [11] during the penetration of the jet into the combustible ambient.

Since 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 [11]. The reaction time scales are estimated by means of the REDIM reduced system dynamics. Starting from an initial condition, a chemical source term, obtained from the REDIM table, is integrated. We define a mixture fraction  $\xi$  and a progress variable c, that serve as reduced variables. The initial conditions are calculated by mixing the chemical states of the hot exhaust and the fresh gas. 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. Figure 3a shows source term for progress variable on the whole state space. In this plot the two initial points also are shown, namely, pure jet and pure fresh unburnt ambient. The line that connects these two points is called mixing line, since, by pure mixing (no chemical reactions) only this line would be accessible in the state space. Chemical reactions lead to 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 [11].

In Fig. 3a it can be seen that highest rates of progress variable are close to ( $\xi = 0, c = 0.6$ ). This region is not accessible (by pure mixing) at initial times. Therefore, it is important to look into the chemical time scales along the mixing line. One time scale that we have looked into is a time that takes for a fluid

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Figure 1: Contour plot of mean temperature shortly after ignition. (a) Simulation results for hydrogen case.  $T_j = 1500 \text{ K}, U_j = 300 \text{ m/s}$  and  $D_j = 1 \text{ mm}$ . (b) Simulation results for propane case.  $T_j = 1550 \text{ K}, U_j = 50 \text{ m/s}$  and  $D_j = 1.5 \text{ mm}$ .



Figure 2: Sensitivity of the ignition delay time to the nozzle diameter. (a) Simulation results for hydrogen case.  $T_j = 1400 \text{ K}$  and  $U_j = 300 \text{ m/s}$ . (b) Simulation results for propane case.  $T_j = 1450 \text{ K}$  and  $U_j = 50 \text{ m/s}$ .

element (with composition along the mixing line) to ignite and reach 80% progress, i.e.

$$c_{80\%}(\xi) = c(\xi) + 0.80(1 - c(\xi)),\tag{1}$$

where  $c(\xi)$  is the progress variable of a composition along the mixing line with a mixture fraction of  $\xi$ .<sup>1</sup>  $c_{80\%}(\xi)$  is also shown in Fig. 3a. Other values than 80% also can be used, but values higher than 80% is not advisable since chemistry becomes again very slow. The chemical rates of progress variable in Fig. 3a show that the highest rates are around 60%. Taking any value in the range 60%–80% for the criteria shall not change the reasoning which will be followed.

Figure 3b shows the time scale that just discussed above, i.e. inverse of the time that is needed for a fluid element on the mixing line to reach  $c_{80\%}(\xi)$  of the progress variable. Indeed, this plot shows the inverse of the time to obtain a chemical rate which will be compared with the mixing rate. This time scale is important because the fluid elements that are burnt along the mixing line makes other scalar state space accessible at later times (e.g. global ignition or explosion to occur). In this plot  $c_{80\%}(\xi)$  time scales (or

<sup>&</sup>lt;sup>1</sup>Since along the mixing line progress variable c is a monotonic function of  $\xi$ , therefore c can be represented by  $c(\xi)$  along this line. But that is not true in the whole state space.



Figure 3: (a) Progress variable rates in the scalar state space for propane case. The point (1, 1) attributed to the hot exhaust gas with a temperature of 1550 K. (b) A chemical rate 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 reach  $c_{80\%}$  as defined by Eq. (1).

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 stationary state. Indeed, initiation of an ignition as discussed in [11] is more complicated than that can be accurately described by stationary state flow condition. However, the stationary state allows by simplifications, 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 hydrogen case are shown in Fig. 4a. In this plot the mean mixing frequency (blue symbol line) and the mean temperature (red solid line) along the centreline axis are shown. The black dashed line specifies the maximum chemical rate for hydrogen in Fig. 3b, which is about 8000/s. It can be seen that the increase in the mean temperature occurs at a point where the mixing frequency becomes less than (or close to) these chemical rates. 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 results, indeed, supports the assumption that in order to a global ignition to occur one of the requirements are that mixing time scales should be in order of initial burning time scale of the compositions at the mixing line.

## 5 Conclusion

In this work the PDF-PM algorithm [4] was used to investigate the initiation of an explosion in a premixed fuel/air mixture which is caused by hot exhaust gas jets. The simulations were performed for hydrogen/air and propane/air cases, in configurations relevant to safety applications. As for the hydrogen case which have been discussed in [11], for the propane case the ignition appears first at the jet head. However, in contrast to hydrogen case, for propane initiation of an ignition (if it occurs) happens with a considerable larger delay time. This can be explained by a comparison of time scales relevant for chemical reactions and mixing processes. We have seen that the global ignition occurs where mixing time scales reduce to values in order of the chemical time scales along the mixing line in composition state space. This have been observed both for propane and hydrogen case, with different setups, which further supports this hypothesis.



Figure 4: Scalar mixing frequency (symbols) and mean temperature (soled red line) along the centreline for (a) hydrogen/air and (b) propane/air simulation at stationary state. (a) Simulation results for hydrogen case.  $T_j = 1400 \text{ K}$ , D = 1 mm and  $U_j = 300 \text{ m/s}$ . (b) Simulation results for propane case.  $T_j = 1550 \text{ K}$ , D = 1.5 mm and  $U_j = 50 \text{ m/s}$ .

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