

Application of a stand-alone PDF method to investigate the ignition of propane/air and hydrogen/air mixture by unsteady turbulent jets

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Abstract

A stand-alone particle method which has been developed for transient reacting flows (PDF-PM) is used to investigate ignition events of a combustible environment by hot jets. The initiation of an explosion in a premixed fuel/air mixture which is caused by hot exhaust gas jets (of its own combustion products) is investigated using this method. 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 hydrogen case and propane case are investigated by comparison of time scales relevant for chemical reactions and mixing processes. Calculations of propane/air case shows that the ignition (as in hydrogen case) first appears at the jet head.

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 investigated for hydrogen/air mixture in our previous work [3]. One of the contributions of this work is to 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 (if it occurs) appears with considerable larger delay times. This will be explained by a 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.

Modelling Approach

In order to model transient turbulent flow, we use the PDF-PM algorithm which has been developed based on the joint velocity-turbulence frequency-composition PDF model [4]. 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) [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]. 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 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 CO₂, ϕ_{CO_2} , is used to represent the

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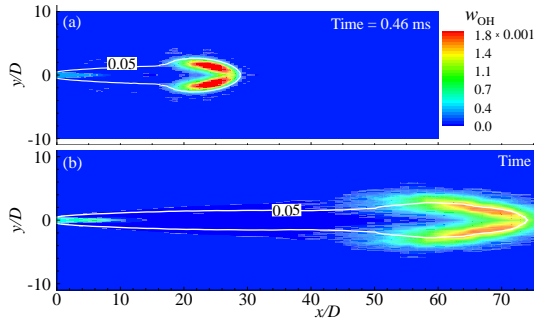


Figure 1: Contour plot of the mean mass fraction of the OH radicals shortly after ignition. (a) Simulation results for hydrogen case; $T_j = 1400$ K, $U_j = 300$ m/s and $D_j = 1$ mm. (b) Simulation results for propane case; $T_j = 1550$ K, $U_j = 50$ m/s and $D_j = 1.5$ mm.

progress variable. ϕ_{CO_2} is defined as $w_{\text{CO}_2}/M_{\text{CO}_2}$, where M_{CO_2} is the molar mass and w_{CO_2} is the mass fraction of CO_2 . The state of mixing is represented by enthalpy, which also accounts for the heat losses due to nozzle walls [3]. Thus, ϕ_{CO_2} and enthalpy are the only additional variables that has to be solved in the reactive simulations. In case of hydrogen simulations $\phi_{\text{H}_2\text{O}}$ is used to represent the chemical progress variable. For REDIM calculations the hydrogen mechanism from [9] and the propane mechanism from [10] was applied.

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 100×100 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 as explained in [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 where the inlet temperature T_j is varied in the range of 1400–1550 K.

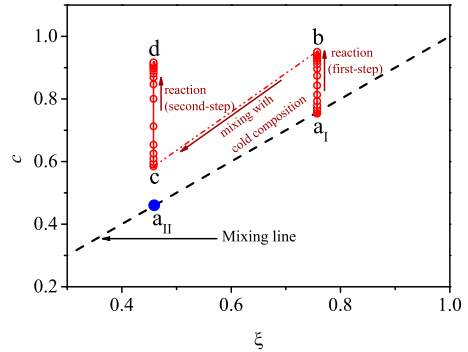


Figure 3: An example of pathway of a fluid element due to reaction and mixing in the reduced scalar state space starting from mixing line.

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 the 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 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. This different behaviour shall afterwards be explained with the help of chemical and turbulent mixing time scales.

Figure 1 shows contour plots for mean mass fraction of OH radicals w_{OH} shortly after initiating of explosion in the ambient. Also contour levels of mean mixture fraction are 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 maximum 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 [11]. The reaction time scales are estimated by means of

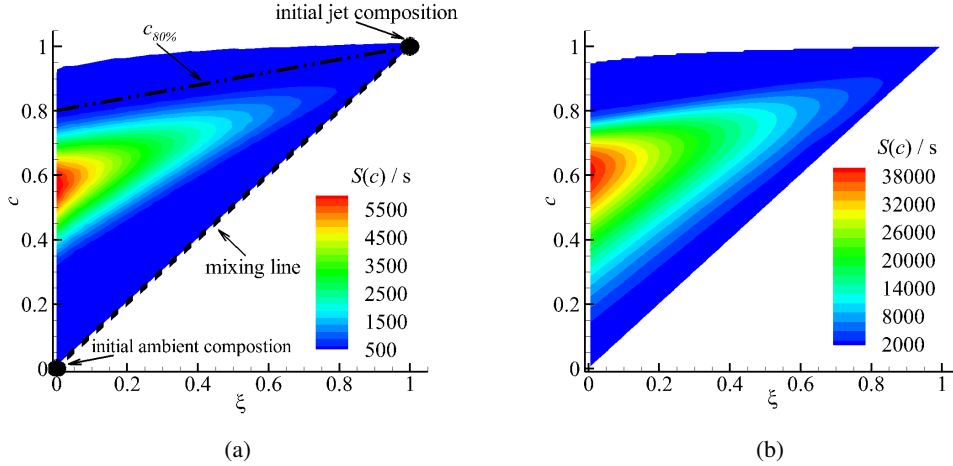


Figure 2: (a) Progress variable source term for propane case. The point (1, 1) attributed to the hot exhaust gas with a temperature of 1550 K. (b) Progress variable source term for hydrogen case. The point (1, 1) attributed to the hot exhaust gas with a temperature of 1400 K.

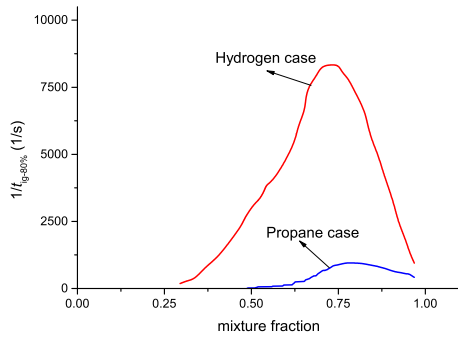


Figure 4: A chemical rate for hydrogen and propane which is obtained from $1/t_{c,80\%}$. $t_{c,80\%}$ is the time necessary (using REDIM reduced system dynamics) for a fuel/air mixture at a given mixture fraction along the mixing line to reach $c_{80\%}$ as defined by Eq. (1).

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 ξ 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 ξ 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 (ξ, 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 2a shows chemical source term of the progress variable $S(c)$ on the (reduced) scalar state space for propane. In this plot 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 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 [11].

This mixing and reaction process just discussed above is well represented by an example in Fig. 3. The red symbols in Fig. 3 show the pathway of a small packet of fluid in scalar state space by means of reaction and mixing. For example the fluid element with a composition $(\xi = 0.76, c = 0.76)$ on mixing line first, due to chemical reaction, advances in the direction of progress variable axis, i.e. a_1 to b. Then the fluid element mixes with an unburnt composition which obtains a value of $(\xi = 0.48, c = 0.58)$ in scalar state space (b to c). Because of mixing with a fresh gas now combustible gas is available, hence, the fluid element advances again in c direction and burns (c to d). The time that takes for this pathway (including only chemical times¹), i.e. from a_1 to d is about 2 ms. On the other hand if we look at a system dynamic which ends up to the point d in which only chemical source terms are involved (i.e. from a_{II} to d) this time is about 90 ms. This clearly shows that the compositions with smaller mixture fractions in the state space will only be available (at the relevant time scales of explosion, e.g. ignition delay times etc) if flow elements with higher temperatures mixes with fresh gas only in a small amount and afterwards burns due to chemical reactions, and so on and so forth. This, indeed, is very similar to that of reaction-diffusion processes in laminar combustion, however, here it is shown for its turbulent counterpart.

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

¹At this stage only time scales of chemistry are considered.

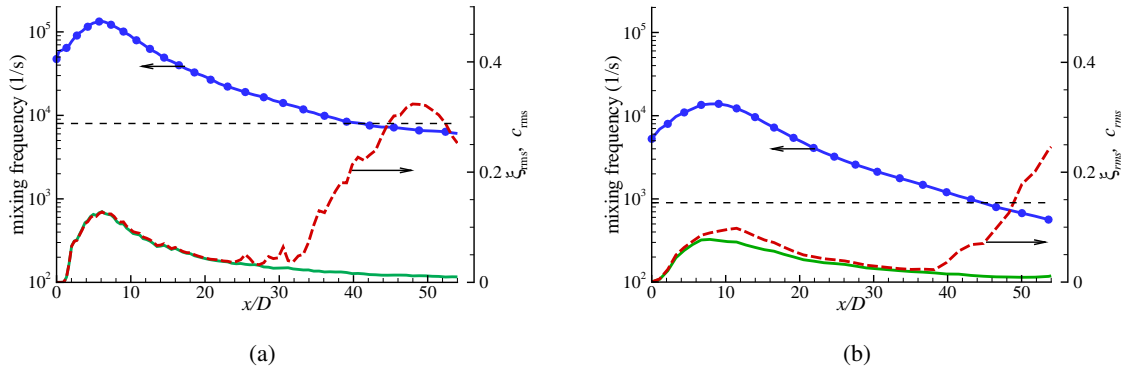


Figure 5: Scalar mixing frequency (symbols), fluctuations of mixture fraction ξ_{rms} (green solid line) and fluctuations of progress variable c_{rms} (red dashed line) along the centreline at stationary state. (a) Simulation results for the hydrogen case. $T_j = 1400$ K, $D = 1$ mm and $U_j = 300$ m/s. (b) Simulation results for propane case. $T_j = 1550$ K, $D = 1.5$ mm and $U_j = 50$ m/s.

times. Regarding the discussion for Fig. 3 one relevant time scale is a time that takes for a fluid element with a composition along the mixing line to ignite (first step of the pathway). A fluid element is regarded burnt if it advances in c direction in amount of 80% of its path from the mixing line to the maximum value of c , which is defined by

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

where $c(\xi)$ is the progress variable of a composition along the mixing line with a mixture fraction of ξ .² The time that takes for a fluid element at mixing line to reach a progress variable of $c_{80\%}(\xi)$ gives a time scale that one can compare with turbulent time scales. 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 Eq. (1) in the range 0.6–0.8 for the criteria shall not change the reasoning which will be followed.

Figure 4 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 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. 4 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 5 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. The stationary state, by simplifications, allows to observe some of the important aspects of the ignition event under study. Hence, in Fig. 5 the profiles are shown for steady state condition. The results for the hydrogen case

are shown in Fig. 5a. In this plot the mean mixing frequency (blue symbol line) and root mean squared of mixture fraction ξ_{rms} (green solid line) and progress variable c_{rms} (red dashed line) along the centreline axis are shown. The importance of the comparison between ξ_{rms} and c_{rms} is that ξ 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 [12]. As shown in Fig. 5a both c_{rms} and ξ_{rms} increase at locations very close to the nozzle exit until the 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 ξ_{rms} are very similar at upstream locations. At downstream (i.e. $25 - 35 D$), however, they depart from each other.

The black dashed line specifies the maximum chemical rate for hydrogen in Fig. 4, which is about 8000/s. It can be seen that the departure of c_{rms} and ξ_{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 ξ_{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 5b 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 initial burning time scale of the compositions at the mixing line.

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.

²Since along the mixing line the progress variable c is a monotonic function of ξ , therefore c can be represented by $c(\xi)$ along this line. But that is not true in the whole state space.

Using this method ignition events in hydrogen/air and propane/air cases are compared, in configurations relevant to safety applications. It was observed that the initiation of an ignition in both cases of hydrogen and propane appears first at the jet head. However, in contrast to the hydrogen case, for propane the initiation of an ignition (if it occurs) happens with a considerable larger delay time. It was shown that the competition between time scales of turbulent mixing and chemical time scales at the mixing line (in scalar state space) governs ignition. We have seen that the global ignition occurs where the mixing time scales reduce to values in order of the chemical time scales along the mixing line. This has been observed both for propane and hydrogen case, with different setups, which further supports this hypothesis.

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