

Direct numerical simulation of ignition by hot moving particles

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1 Introduction

Mechanical sparks play an important role in safety-related assessments of the ignition of combustible mixtures in process industry and aviation. They are mechanically generated from solid materials by grinding, abrasive cutting, or mechanical impact. In general, the particle temperature required for ignition sharply increases with decreasing particle size [1–6]. Another important factor is the relative velocity between particle and gas phase. Using electrically heated cylindrical rods, Mullen et al. [7] studied the ignition of different fuel/air mixtures at various fluid velocities between 25 and 150 m/s. Higher ignition temperature was recorded for increasing velocity, lower rod diameters as well as lower initial gas temperature and pressure. High-speed photography showed that ignition begins in the stagnant region near the downstream face of the heated cylinder. The results are consistent with earlier experiments by Paterson [8] who shot hot 2 mm diameter platinum and 3.5 mm diameter quartz spheres at 10–65 m/s into coal gas-air mixtures. Kumagai and Kimura [9] used nichrome cylinders of varying diameter to ignite city gas-air mixtures at much lower stream velocities between 0.2 and 10 m/s. Up to about 1 m/s the surface temperature remains the same as in the quiescent gas. At higher fluid velocities the behavior depends on the cylinder diameter.

Previous numerical studies have been limited to asymptotic analysis using simplified models [1, 2, 8, 10, 11]. Only recently, Melguizo-Gavilanes et al. [12, 13] published 2D simulations of a particle with a diameter of 4 mm falling into a stoichiometric hydrogen/air mixture and studied the formation of the ignition kernel as a function of particle temperature as well as differential diffusion. Until now there is no numerical study available that systematically investigates the whole range of velocities observed in the experiments. Especially the low velocity region is of considerable interest, because it represents the typical range of speeds of frictional sparks [9]. This work presents 2D and 3D direct numerical simulation (DNS) studies of the ignition of hydrogen/air and methane/air mixtures in dependence on the relative velocity between the hot particle and the fluid as well as stoichiometry.

2 Numerical Setups

The governing equations in terms of the conservation equations for total mass, species masses, momentum and energy are solved in their compressible formulation with OpenFOAM [14], employing the finite

volume method. The detailed calculation of chemical reactions and molecular diffusive fluxes has been accomplished by coupling OpenFOAM with the open-source chemical kinetics library Cantera [15, 16]. The reaction mechanisms developed by Konnov et al. [17] (9 species and 38 reactions) and GRI 3.0 [18] (53 species and 325 reactions) are used to describe the reaction system for hydrogen/air and methane/air combustion. A fully implicit second order scheme for the time derivative and a fourth order, unbounded interpolation scheme for convective and diffusive terms are used.

By assuming axial symmetry, the computational domain is built from a 2D slice of a cylindrical domain ($12.5 d$ radius and $25 d$ height with the diameter of the spheric particle $d = 0.8$ mm), which spans over an angle of 3 degrees along its perpendicular direction (see Fig. 1 on the left). The particle is located at the center of the domain. Premixed fuel-air mixtures at $T_0 = 300$ K, $p = 1$ bar enter the domain from the bottom side and leave the domain at the top. The spatial resolution directly at the surface of the particle is $20 \mu\text{m}$, both in radial and circumferential direction. This resolution has been chosen after performing a grid convergence study, which showed that further refinement of the grid does not affect the time of ignition. For higher inflow velocities, the flow around the particle becomes unstable leading to vortex shedding at the spherical particle, so that the axisymmetric assumption is violated. Therefore, a 3D grid consisting of 650 000 finite volumes and with the same mesh topology as the 2D grid has been built for inflow velocities larger than 5 m/s. Figure 1 on the right shows a cut through the 3D grid passing through the center of the sphere, which illustrates the resolution of the particle surface and its surroundings. The 3D DNS have been performed only for the hydrogen case to reduce computational costs.

The surface of the particle is set as no-slip wall and the two lateral faces of the domain are defined as symmetry planes. For hydrogen and methane mixtures the initial temperature of the particle surface is set to 900 K and 1400 K respectively, which increases linearly in time with a rate of 2200 K/s. This heating rate was chosen from a similar experimental setup [6]. The simulation domain is initially filled with combustible fuel/air mixture, which becomes heated by the hot particle, leading to an ignition of the mixture and a spherically expanding flame. The ignition is defined as the time at which the maximum heat release rate detaches from the particle surface [6]. The temperature of the particle surface at that time is denoted as $T_{\text{surf,ign}}$.

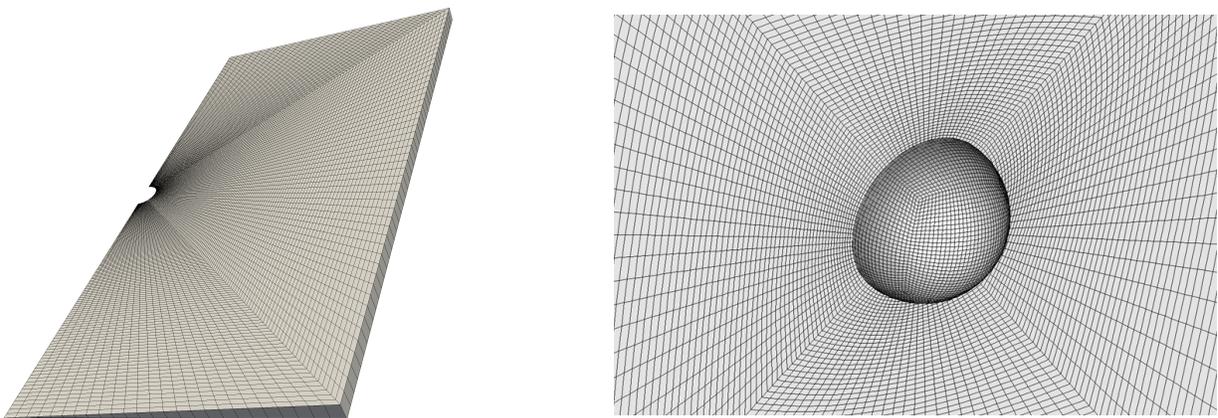


Figure 1: Computational mesh of the 2D simulation (left) and cut through the 3D mesh including the surface mesh on the spherical particle of the 3D setup (right).

3 Simulation Results

3.1 Flow and Temperature Fields

Figure 2 depicts the temperature field and the streamlines of the flow on a cutting plane from the 3D simulation for H_2/air at $\phi = 1.02$ shortly before ignition. The flow around the hot spherical particle is axisymmetric for $v = 1 \text{ m/s}$ and 2 m/s . At $v \geq 5 \text{ m/s}$, the flow develops a vortex street. Flow and temperature field vary periodically in time, so that the ignition process may be additionally influenced by the time history of the flow. The region with the highest temperature indicating the location of the ignition kernel is located at the far side of the particle for all cases, where the flow velocity is lowest and the thermal boundary layer is thickest. In this region, a thermal reservoir with homogeneously high temperature is built up, which supports an early ignition due to less heat losses.

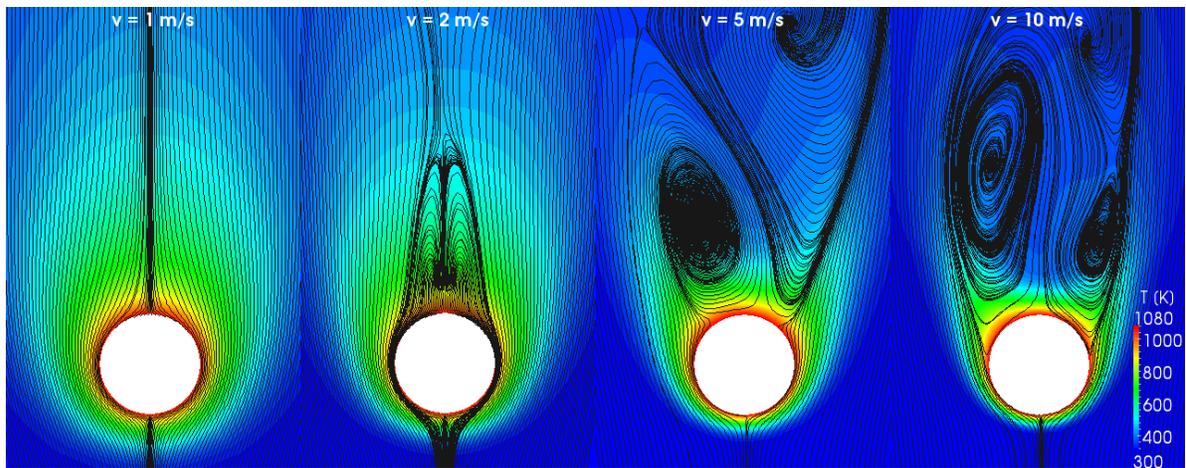


Figure 2: Temperature field and streamlines on a cutting plane through the centerline axis of the 3D simulation for a time shortly before ignition and inflow velocities of $v = 1 \text{ m/s}$ to $v = 10 \text{ m/s}$.

3.2 Correlation of Ignition Temperature with Fluid Velocity

Figure 3 presents $T_{\text{surf,ign}}$ calculated from DNS in dependence on the incoming flow velocities v . The black and white symbols represent results from the 2D and 3D DNS. For both the methane/air (left) and hydrogen/air (right) mixtures, $T_{\text{ign,surf}}$ increases monotonously with v at fixed equivalence ratios ϕ , because higher stream velocities lead to a thinner thermal boundary layer around the particle and therewith higher heat losses (Fig. 2). At fixed velocities, $T_{\text{surf,ign}}$ is larger for mixtures with higher ϕ , which is in agreement with the quiescent case with $v = 0 \text{ m/s}$ [4, 5]. Moreover, $T_{\text{surf,ign}}$ increases similarly with v for different ϕ values, and faster at lower flow velocities than at higher velocities.

For the hydrogen/air case on the right of Fig. 3, 3D and 2D results agree well in the low velocity range with $v \leq 3 \text{ m/s}$. At $v = 5 \text{ m/s}$, $T_{\text{surf,ign}}$ is approximately 10 K higher in the 3D simulations than in the 2D simulations. The reason for this can be seen in Fig. 2. The flow is axisymmetric for $v = 1 \text{ m/s}$ and 2 m/s , but at higher velocities ($v > 5 \text{ m/s}$), the flow develops a vortex street which is not axisymmetric anymore and can therefore not be considered by the 2D simulations. A steeper increase of $T_{\text{surf,ign}}$ from $v = 5 \text{ m/s}$ to $v = 10 \text{ m/s}$ on the right of Fig. 3 compared to the low velocity range is observed, because the heat loss in

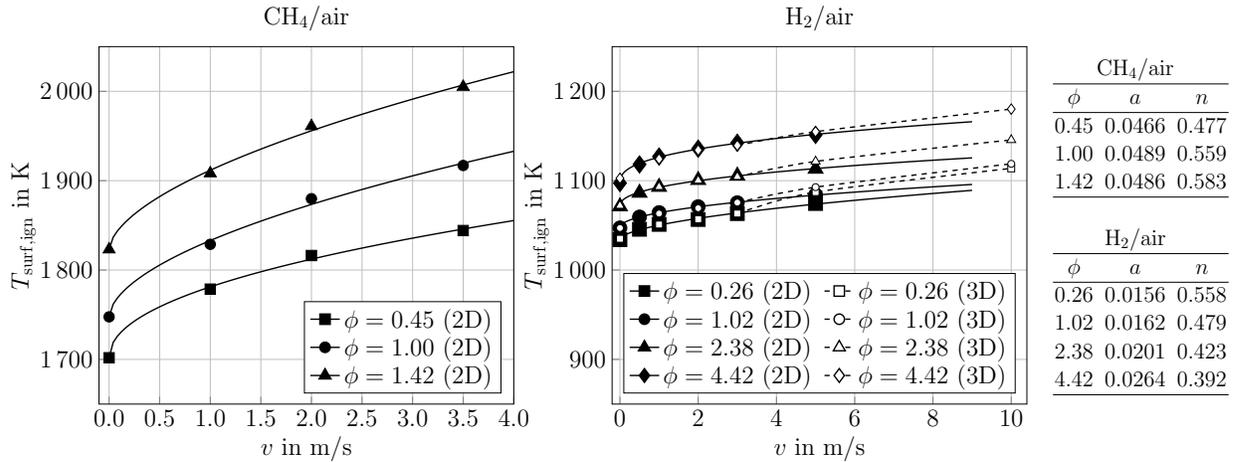


Figure 3: Ignition temperature of methane/air (left) and hydrogen/air (right) mixtures at a hot particle for different flow velocities calculated from 2D and 3D direct numerical simulation with OpenFOAM. Additionally, parameters of the fit to Eq. (1) are included.

the unsteady flow regime increases even stronger with higher Reynolds numbers Re , in accordance with a thinner boundary layer and therewith higher heat losses at the far side of the particle.

To find a general dependence of ignition temperature on flow velocity, the 2D simulation results for $v \leq 5$ m/s have been fitted to

$$\frac{T_{\text{surf,ign}}}{T_{\text{surf,ign},0}} = 1 + a v^n \quad (1)$$

where $T_{\text{surf,ign},0}$ is the temperature at ignition in the quiescent fluid and a and n are the fitting parameters. The solid lines in Fig. 3 show the results of this fit. As shown in the tables on the right of Fig. 3, the exponent n is approximately 0.5 for all cases, so that the ignition temperature depends on the square root of the flow velocity or Reynolds number, respectively. This is the same dependency as for the general transfer of heat in laminar flows, which is also used in the Nusselt number in Eq. (3).

3.3 Correlation of Ignition Temperature using Van't Hoff's criterion

The van't Hoff criterion can be used to predict ignition at hot surfaces [1, 19]. If the heat release rate from chemical reactions balances the heat losses to the surroundings, there is no net heat transfer between the surface and the gas phase and ignition can occur. Using a one-step kinetic, Laurendeau [19] developed a model that correlates the surface temperature at ignition with the Nusselt number and an apparent activation energy of the combustion reaction:

$$\log \left[\frac{\theta}{(\theta - 1)^2 Nu^2} \right] = \log \left[\frac{E^*}{D} \right] + \frac{E^*}{\theta} \quad (2)$$

Here, θ is the surface temperature at ignition divided by the temperature of the incoming flow $\theta = T_{\text{surf,ign}}/T_0$, the Arrhenius number $E^* = E/(RT_0)$ is the apparent activation energy E divided by the universal gas constant R times the fluid temperature T_0 . The parameter $D = 2Da_1Da_2$ is the product of two Damköhler numbers Da_1 and Da_2 , which represent the ratio of convective-diffusive time scale to the chemistry time

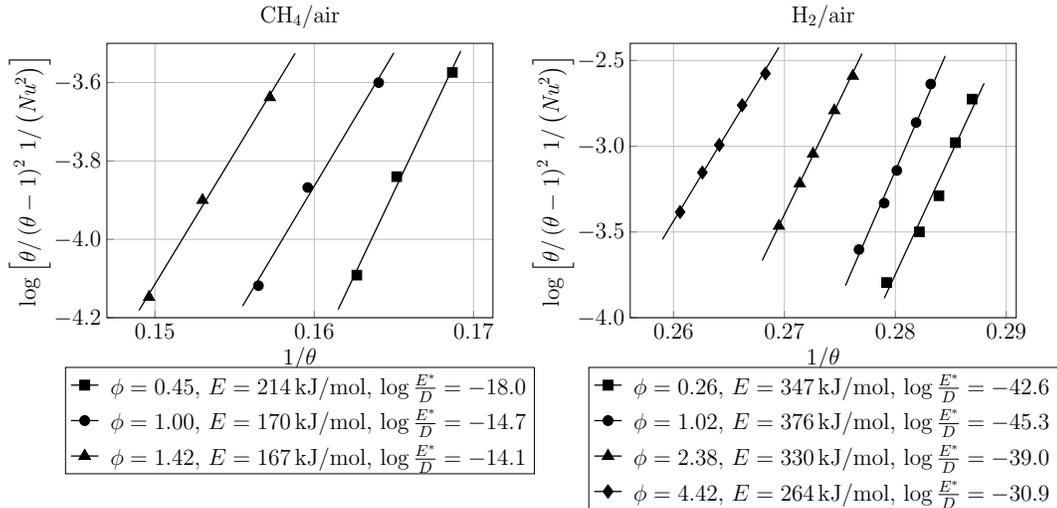


Figure 4: Correlation of simulation results using Eq. (2).

scale and the ratio of heat generated by the chemical reactions to the heat losses to the fluid [19]. The Nusselt number Nu is calculated from [20]

$$Nu = 2 + 0.664 Re^{\frac{1}{2}} Pr^{\frac{1}{3}} \quad (3)$$

where $Re = vd/\nu$ is the Reynolds number with regard to the particle diameter d , and $Pr = \nu/a$ is the Prandtl number. Thermal diffusivity a and kinematic viscosity ν have been calculated from kinetic gas theory [15] for the unburnt mixture at the temperature of ignition.

Figure 4 shows the results of fitting the simulation data from Fig. 3 to Eq. (2) for the velocity range with $v < 5$ m/s, where the flow mostly retains its laminar, steady-state nature. E^* and the first term on the r.h.s. are the parameters used in the fit. The apparent activation energy E lies between 160 kJ/mol and 210 kJ/mol for methane and between 260 kJ/mol and 380 kJ/mol for hydrogen. For methane/air they are similar to those reported by Laurendeau ($E/R \approx 20\,000$ – $25\,000$ K) [19]. The apparent activation energies E for hydrogen are larger than those for methane. This is attributed to the fact that E appears not only in the linear term on the r.h.s. of Eq. 2 but also in the logarithm. The activation energies from the Laurendeau model are therefore not directly comparable to those obtained from other models [1, 6, 8].

4 Conclusion

Direct numerical simulations of the ignition of premixed hydrogen/air and methane/air mixtures by heated moving particles with a diameter of 0.8 mm are performed. The objective is to study the influence of particle velocities on the ignition process. 2D and 3D simulations yield the same surface temperature at ignition for small velocities, but deviate at larger velocities due to the formation asymmetric flow structures caused by more complex flow patterns. For the same stoichiometry, the ignition temperature increases with flow velocity or movement speed of the particle. This is attributed to the fact that the thermal boundary layer is reduced and the surroundings of the particle are heated up slower due to greater heat losses. The ignition kernel is shown to be located on the opposite side of the stagnation point, where the flow velocity is approximately

zero and the temperature boundary layer is at its thickest. Two correlations are provided which can be used to predict the temperature at ignition. The first correlation shows that the ignition temperature depends on the square root of the flow velocity or Reynolds number, respectively. A model by Laurendeau has been applied which yields the apparent activation energies of the ignition depending on the Nusselt number.

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