Effect of orientation on the ignition of stoichiometric ethylene mixtures by stationary hot surfaces

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1 Introduction

The risk of accidental ignition of flammable mixtures by a hot surface is of particular importance for industry. Accurate measurements and modeling of the minimum surface temperature for ignition to occur are needed to estimate the risk of hot surface ignition. Previous work for stationary hot surfaces have determined critical conditions for ignition in terms of surface size [1–3], material [3] and heating rate [4, 5]. However, less attention has been paid to studying the effect that the orientation of the hot surface has on the reported ignition thresholds. The present study examines this question by numerically determining the minimum surface temperature required to ignite a stoichiometric ethylene-air mixture using a stationary vertical and horizontal hot cylinder.

2 Computational methodology

2.1 Governing equations, transport and chemical models

The motion, transport and chemical reaction in the gas surrounding the heated surface were modeled using the low Mach number, variable-density reactive Navier-Stokes equations with temperature-dependent transport properties [6]. Differential diffusion effects were taken into account using a constant but non-unity Lewis number for each species, Le_i, as proposed by [6]. The form that the heat and mass diffusion fluxes take when written as a function of Le_i can be found in [7] along with all the spatial and temporal discretization details, and models used to account for the functional temperature dependence of mixture viscosity, thermal conductivity and specific heat. Thermodiffusion (Soret effect) and radiation were neglected. The governing equations were solved using the Open source Field Operation And Manipulation (OpenFOAM) toolbox [8]. Our implementation of the code is well validated as it has been used succesfully in various ignition studies comprising different geometries, modes of heat transfer (e.g. forced and natural convection), and ignition timescales [7, 9–12]. The chemistry was modeled using a reduced version of Mével's mechanism [13] targeting ethylene oxidation which includes 29 species and 93 reactions. This mechanism has been validated, and reproduces flame speeds and ignition delay times to a reasonable degree of accuracy over a wide range of concentrations ($0.5 < \Phi < 4$) [14].

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2.2 Domain, initial and boundary conditions

The geometries simulated corresponded to: (i) a vertical cylinder or radius $r = 5$ mm, and length 70 mm with a heated section of 10 mm placed between 30 mm $< y <$ 40mm; (ii) a horizontal cylinder of radius $r =$ 3.1831 mm so that the arc length, $s = r\theta$, between the front and the back stagnation point of the cylinder (θ = 180°) equaled 10 mm. This choice of geometries ensured heated sections of identical length for both setups. For the vertical configuration, a 2D-axisymmetric mesh was used with approximately 80,000 cells. For the horizontal configuration, a 2D mesh using vertical half-symmetry with 60,000 cells in the computational domain was employed. For both cases, the cells were compressed near the wall of the heated surface, using a minimum cell size of $40\,\mu$m to properly resolve the thermal and hydrodynamic boundary layers. The initial conditions were $\mathrm{p}_o = 101\,\mathrm{kPa}$, $\mathrm{T}_o = 300\,\mathrm{K}$, $\mathrm{U}_o = (0, 0)$ m/s, and mass fractions $\mathrm{Y}_{\mathrm{C_2H_4}}$ = 0.06372, $\mathrm{Y}_{\mathrm{O_2}}$ = 0.21808, $\mathrm{Y}_{\mathrm{N_2}}$ = 0.7182, corresponding to a stoichiometric C_2H_4-air mixture. On the heated surface, a time dependent boundary condition given by $\mathrm{T}_{\mathrm{surf}}$ (t) = 300 + α t was imposed with a heating rate of $\alpha = 220$ K/s.

3 Results

Numerical fields of temperature, magnitude of velocity and velocity vectors, product mass fraction (CO_2), and mass fraction of OH (important intermediate species) during ignition and early stages of flame propagation are shown in this section for both configurations considered. The ignition criteria used was to monitor the gas temperature, T, until its maximum in the computational domain reached 50 K beyond the heated surface temperature, $\mathrm{T}_{\mathrm{surf}}$ (t). Using this definition, the time to ignition, τ_{ign}, can be accurately determined from the temperature maxima history during the simulation and the heating ramp imposed on the heated surface.

3.1 Flow field

Vertical cylinder As explained in subsection 2.2, we simulated a vertical cylinder of 70 mm in length and of radius 5 mm with a heated section of 10 mm placed between 30 mm $< y <$ 40 mm (see T field on Fig.1 top row). The heating of the surface induces a buoyancy flow that results in a thermal boundary layer as can be observed in this figure. This thermal boundary layer grows in the direction of the flow as expected. Parcels of cold gas enter the thermal boundary layer from the bottom (see U field on Fig.1 top row), and heat up as they travel upward in close proximity to the heated surface. Significant chemical activity starts after these parcels have traveled 5 mm along the thermal boundary layer (see mass fraction fields on Fig.1 top row). Near this region (35 mm $< y <$ 40 mm), after 3.847 s of heating, the gas temperature reached T = $\mathrm{T}_{\mathrm{surf}}$ (τ_{ign}) + 50 K, yielding a surface temperature at ignition of $\mathrm{T}_{\mathrm{surf}}$ (τ_{ign}) = 1146 K. Two milliseconds later, a flame kernel forms that will subsequently develop into a radially expanding flame that consumes the rest of the combustible mixture.

Horizontal cylinder The flow field for this configuration is shown in Fig. 2 top left. The thermal boundary layer appears to have a constant thickness up until $\theta = \pi/2$. Beyond that location, it merges with the thermal plume resulting in a thicker thermal boundary layer (shallower temperature gradient) at the back stagnation point of the cylinder. This configuration allows for higher gas temperatures at a longer distance from the

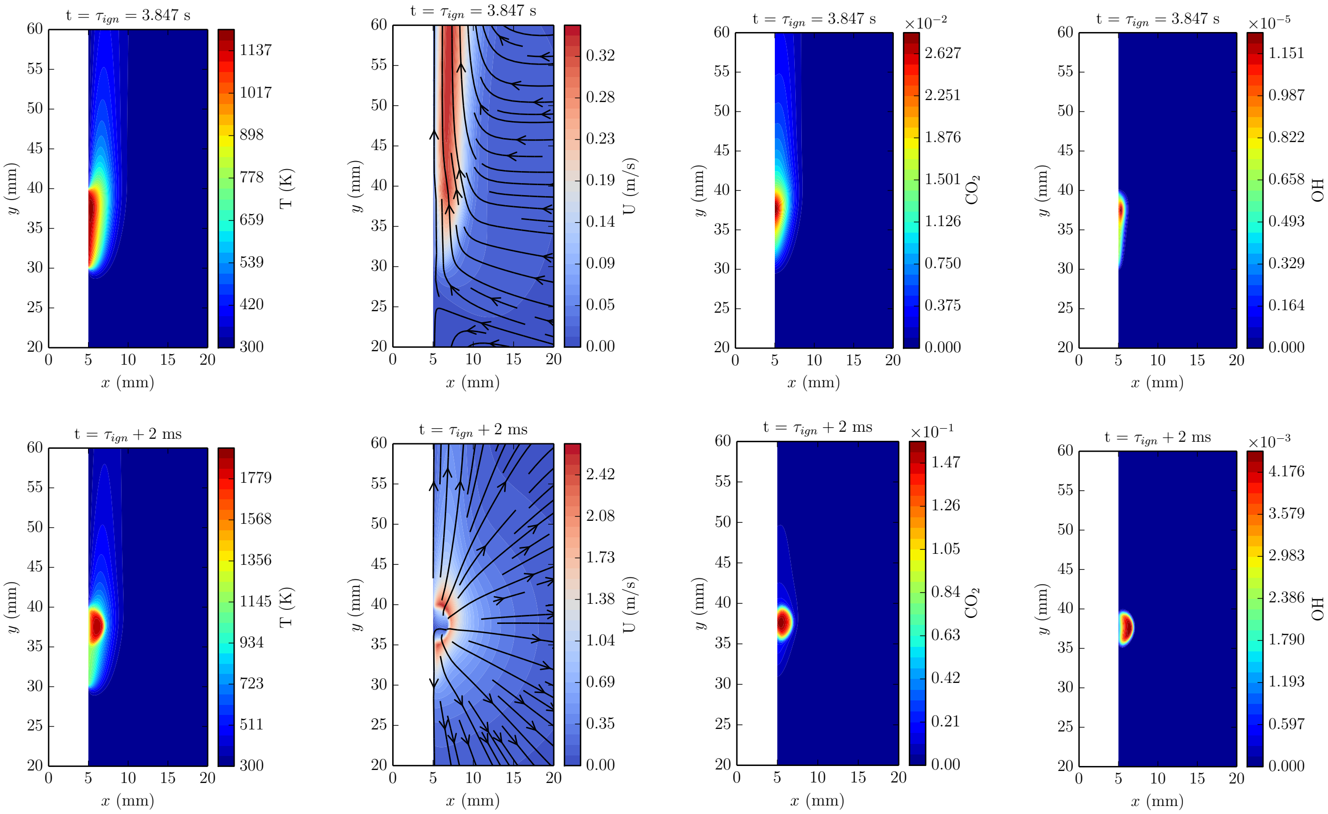

Figure 1: vertical cylinder – temperature, magnitude of velocity and mass fraction (CO_2 and OH) fields during ignition (t = τ_{ign} = 3.847 s), and early stages of flame propagation (t = τ_{ign} + 2 ms).

heated surface. The velocity vectors show how the cold gas gets entrained in the thermal boundary layer, and travels along the circumference of the cylinder to then continue its upward journey within the thermal plume. In contrast with the previous case, strong chemical activity is confined to a small region (of roughly $s = 2$ mm) on the back of the cylinder (see Fig.2 top right). Although this evolution seems to be consistent with previous observations [7,15] where flow/boundary layer separation was found to play an important role in creating the ideal conditions for ignition to take place, in this configuration, the boundary layer does not separate. However, as mentioned above, the merging of the thermal boundary layer with the thermal plume results in a thicker boundary layer at the back of the cylinder. This is precisely the same outcome observed, namely a thicker thermal boundary layer near the ignition location, in cases where flow separation occurs. Shortly after ignition takes place (2.5 ms later), a flame kernel forms that propagates preferentially upward within the thermal plume. The surface temperature at ignition for this configuration was found to be T_{surf} (τ_{ign}) = 1018 K.

3.2 Predicted ignition thresholds

Figure 3 summarizes the ignition results described above. Heated cylinders placed vertically and horizontally in an initially stagnant reactive gas resulted in ignition thresholds of 1146 K and 1018 K, respectively.

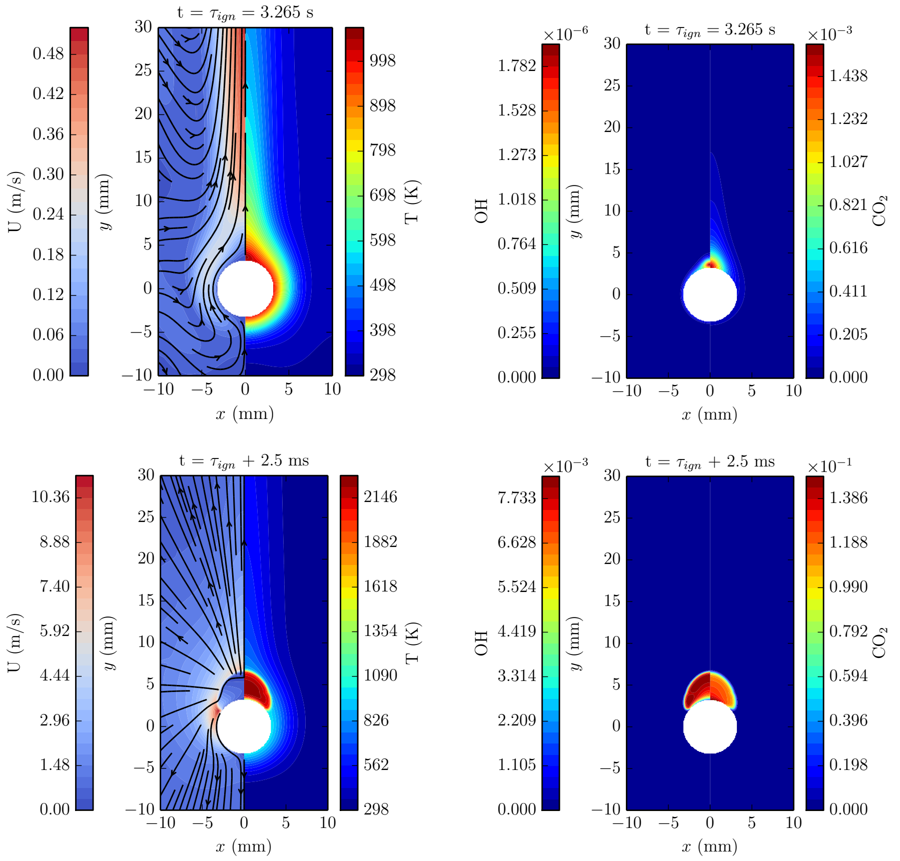

Figure 2: horizontal cylinder – temperature, magnitude of velocity and mass fraction (CO_2 and OH) fields during ignition (t = τ_{ign} = 3.265 s), and early stages of flame propagation (t = τ_{ign} + 2.5 ms).

Keeping all the variables of the problem fixed (mixture composition, extent of heated section on surface and surface heating rate), and varying the orientation only, yielded a threshold 128 K lower for the horizontal cylinder than for the vertical cylinder. This result supports our previous investigations where we concluded that the interaction of the hot surface with the induced buoyancy flow, creates regions where ignition is more likely to occur (thermal boundary layer separation). Although in this particular case the thermal boundary layer does not separate, we can make a more general statement: regions where the temperature gradients are shallower (thicker thermal boundary layers) result in an increased likelihood of ignition because higher gas temperatures are reached further away from the surface (i.e. minimizing heat losses) which in turn result in higher reaction rates, and more heat deposition in the gas. This result also provides further evidence that determining ignition thresholds by using, for example, standardized auto ignition temperature (AIT) tests and extrapolating these values to heated surfaces may result in poor estimates. Hot surface ignition thresholds are not a definite number or a mixture property but vary significantly depending upon a variety of factors such as the state of the hot surface with respect to the combustible gas (i.e. moving or stationary), mode of heat transfer (i.e. forced vs. natural convection), surface material properties, and, as shown in this study, orientation. It is also important to note that depending on the activation energy of the mixture around the temperature at which ignition is expected to occur, based for instance on constant pressure ignition delay time calculations, the predicted hot surface ignition threshold as a function of orientation will be affected to a lesser or greater degree.

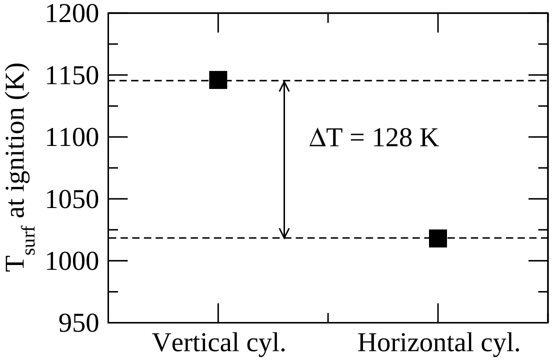

Figure 3: predicted surface temperature at ignition for vertical and horizontal cylinder.

4 Conclusion

The ignition of a stoichiometric ethylene-air mixture by stationary vertical and horizontal cylinders with heated sections of equal length was numerically studied. Temperature, velocity and mass fraction fields were used to explain the ignition evolution, and temperature maxima histories allowed to determine the minimum surface temperature that resulted in the ignition of the mixture for both configurations. Results showed that for the mixture considered, simply changing the orientation of the heated surface, while keeping the remaining parameters of the problem fixed, yielded an ignition threshold that is 128 K lower for the horizontal cylinder than the threshold obtained when the vertical cylinder was used. This outcome provided further evidence that numerical determination of hot surface ignition thresholds requires a detailed simulation that includes appropriate initial and boundary conditions, and that is capable of capturing the interaction of the hot surface with the buoyancy flow induced by the heating of the gas. It is precisely this interaction that results in regions where the thermal boundary layer is thicker favoring the establishment of the critical conditions for ignition to occur. Future work will include comparison with experimentally determined thresholds, a detailed analysis of the temperature, velocity and species profiles, as well as analysis of the competition of convective, diffusion and chemical reaction terms within the thermal boundary layer. Additionally, the effect of orientation on the chemical pathways under near-critical conditions will be studied.

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