

Flame wall interaction of an H₂/O₂ flame

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Abstract-Numerical simulations of the interaction of an H₂-O₂ flame and a wall are performed. Two situations are considered: a premixed flame propagating towards the wall and a diffusion flame staying at a distance from the wall. In both cases the thermal fluxes to the wall are evaluated during the simulation and the maximal value, as well as the interaction duration, are compared. Results show that the premixed flame leads to high fluxes to the wall, during a short time before quenching. The diffusion flame gives lower values for the maximum flux, but for a longer time. Finally the total energy transferred to the wall is comparable for both flames.

1 Introduction

The understanding of the fundamental mechanisms that occur in the near-wall region is essential to predict and improve engine performances. This task usually involves two different aspects: first, the mean fluxes at the wall must be evaluated to design the cooling devices; second, the maximum heat fluxes must also be estimated because they condition the lifetime of the burner. The mean wall fluxes are due to the convection of burnt gases along the chamber wall and can usually be estimated using correlations or CFD codes. The maximum fluxes are more difficult to determine: an important source of large wall fluxes is flame / wall interaction (FWI). This interaction has been studied in premixed flames theoretically (Wichman and Bruneaux, 1995), experimentally (Jarosinski, 1986) and (Ezekoye et al., 1992), and numerically for both laminar (Poinsot et al., 1993), (Poinsot and Veynante, 2001) and turbulent flows (Bruneaux et al., 1992), (Alshaal, 1998). These studies show that two generic FWI cases must be considered for premixed flames: head on quenching (HOQ) occurs when the flame front, parallel to the wall, propagates towards the wall; side-wall quenching (SWQ) occurs when the flame propagates along the wall. FWI studies for turbulent premixed flames suggest that simple estimates may be found for maximum wall fluxes (Poinsot et al., 1993), (Bruneaux et al., 1992): typically, the maximum heat flux that can be observed in a premixed combustion chamber is the flux ϕ_Q^p measured in laminar flames. Although FWI is rather well understood in premixed flames, much less work has been devoted to diffusion flames. For such flames, even identifying the generic FWI configurations is a difficult task. The flames created near the walls in a diffusion burner can have various topologies. One possible situation is similar to the HOQ case observed for premixed flames: the diffusion flame front is parallel to the wall, located at a distance d with oxidizer (or fuel) trapped between the flame and the wall. An important difference between HOQ for premixed and diffusion flames is that the diffusion flame has no propagation velocity. Therefore, it will remain at a fixed distance d from the wall while the temperature diffuses towards the wall.

We present here a study of one-dimensional flame-wall interaction for an H₂/O₂ flame, in the two configurations of premixed flame and diffusion flame (HOQ) including complex chemistry. Wall heat flux histories and the associated chemical mechanisms are studied in detail.

2 Numerical Method

The whole set of the compressible one-dimensional multi-species reacting flows equations is solved using a sixth-order finite difference scheme in space combined with a third-order Runge-Kutta scheme in time. Cross-diffusional effects (Soret and Dufour effects) are taken into account. Chemistry is described using a detailed kinetic scheme, taken from (Miller et al., 1982). Catalytic reactions at the wall are not included in the kinetic model. Fluid properties, molecular transport coefficients and reaction source terms are computed using CHEMKIN (Kee et al., 1989) and TRANSPORT (Kee et al., 1983).

A steady one-dimensional laminar flame is first calculated using PREMIX (Kee et al., 1985) for premixed flames or OPPDIFF (Kee et al., 1989) for diffusion flames. Calculations are initialized with this flame, placed at a distance from the wall. A boundary condition of inert isothermal wall at $T_w = 750K$ is imposed at the left-hand side of the computational domain using the NSCBC method (Poinsot and Lele, 1992). On the right-hand side of the domain, a non-reflecting boundary condition is used.

3 Results

Flame-wall interaction for a premixed flame For an inert wall, and neglecting the radiative heat transfer, the wall heat flux is given by $q_w = \lambda_w(\partial T/\partial x)_w$ where λ_w is the thermal conductivity of the mixture at the wall. Using the laminar flame power of the unstrained flame, $q_l^0 = \rho_u Y_{F,u} S_l^0 \Delta H$, where Y_F is the fuel mass fraction, S_l^0 is the unstretched laminar flame speed and ΔH is the heat produced by the flame, q_w is normalized to obtain the non-dimensional wall heat flux $\phi = q_w/q_l^0$ (here a subscript u denotes unburnt gas and b burnt gas). We are mostly interested by the maximum non-dimensional wall heat flux during the flame-wall interaction, denoted ϕ_Q .

Due to complex chemistry, there is no single and univoque definition of the flame position. Indeed, the position of the flame may be located either at the maximum heat release $\dot{\omega}_{max}$ or at the maximum fuel reaction rate $\dot{\omega}_{F,max}$, which are generally different. The corresponding flame-wall distances will be noted $\delta_{\dot{\omega}_{max}}$ and $\delta_{\dot{\omega}_{F,max}}$ respectively. The quenching distances will be denoted by the subscript "Q". Most authors normalize these distances by a characteristic flame thickness $\delta_l^0 = \lambda_u/(\rho_u C_p S_l^0)$, that yields to the Peclet numbers, $Pe = \delta_{\dot{\omega}_{max}}/\delta_l^0$ and $Pe_F = \delta_{\dot{\omega}_{F,max}}/\delta_l^0$ respectively. The flame thickness is defined as $\delta_f = \Delta T/(\partial T/\partial x)_{max}$, where $\Delta T = T_b - T_u$. One can also define a characteristic time of the interaction: t_Q , which represents the time needed to have the heat flux increase from $\phi_Q/2$ to ϕ_Q . The corresponding non-dimensional time is given by $\tau_Q = t_Q/t_l^0$ where $t_l^0 = \delta_l^0/S_l^0$ is a characteristic flame time.

The unburnt gas mixture H2/O2 placed at the wall is in stoichiometric proportions at 750K and 1 bar. The main characteristics of the laminar premixed flame are the burnt gas temperature $T_b = 3130K$, the flame speed $S_l^0 = 3197cm/s$ and the flame thickness $\delta_f = 3,075.10^{-2}cm$.

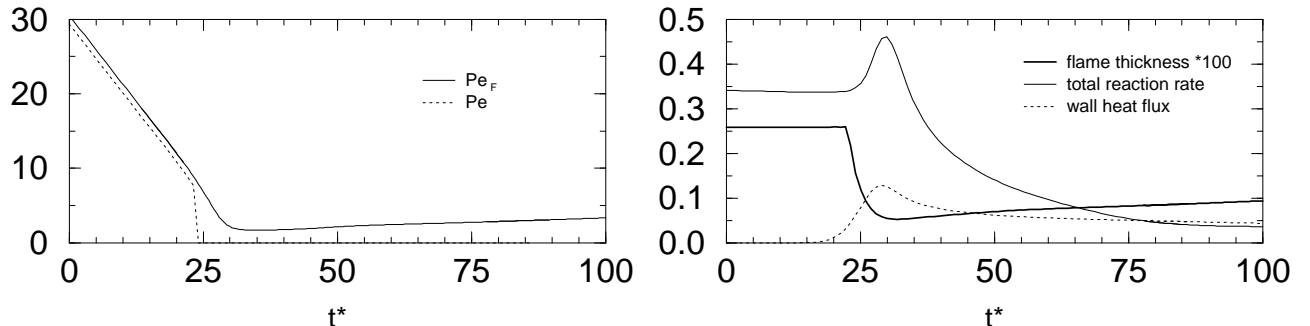


Figure 1: non-dimensional characteristic parameters of the flame-wall interaction.

In figure 1, non-dimensional characteristic parameters of the flame-wall interaction are plotted versus the non-dimensional time $t^* = t/t_l^0$. This head-on-quenching process may be split up into three distinct stages. In the first stage, the flame propagates at a constant speed equal to the laminar flame speed. All the species, temperature and heat release profiles are identical with those of the equivalent undisturbed flame. The mechanism of the flame propagation is the classical mechanism of a premixed flame. Just in front of the flame, in the induction zone, the stable species H_2 reacts with radical species to produce H atoms as: $H_2 + OH \rightarrow H_2O + H$ (R1) and $O + H_2 \rightarrow OH + H$ (R2). Then, these H atoms are oxidized in the reaction zone to produce other radical species, and the main part of the heat of reaction is released. Far from the wall, these radical species diffuse from the reaction zone to the induction zone to feed the

pre-oxidization of H_2 . After $t^* = 20$ ($Pe = 10.7$ and $Pe_F = 12.1$), in a second stage, the flame starts to feel the influence of the wall. The flame-wall interaction begins with a slight increase in the total reaction rate, followed by a sharp drop in the flame thickness around $t^* = 23$. At that time, the wall heat flux has reached a value of about 25% of its maximum value. At $t^* = 24$, the peak value of heat release reaches the wall ($Pe = 0$), but the increase in total reaction rate is still very low. The maximum wall heat flux $\phi_Q = 0.129$ is obtained at $t^* = 29$, while the total heat release keeps on increasing until $t^* = 30$ to reach a value equal to 1.33 time the reference value of the free propagating flame. Then as the induction zone temperature decreases (due to wall thermal losses), recombination reactions occur and the pre-oxidation of H_2 slows down. The consumption speed of the flame then reduces up to the quenching at $t^* = 32$ and at a distance $Pe_{F,Q} = 1,7$ from the wall. These second stage mechanisms are well known and identical whatever the fuel is (see (Westbrook et al., 1981)) for example).

In the third stage of the flame-wall interaction that follows, the total reaction rate and the wall heat flux decrease slowly to zero but the combustion is not completed yet. Indeed, H_2 molecules which have not been consumed diffuse now towards the hot burned gas where radical species concentrations are high to allow its post-oxidization. This is the reason why Pe_F increases after $t^* = 32$. Of particular interest is the fact that all these mechanisms seem to remain unchanged in a large range of pressure and equivalence ratio.

The interaction characteristic parameters ($\phi_Q = 0.129$, $Pe_{F,Q} = 1.7$ and $\tau_Q = 4,69$), appear to be notably different from the ones of a hydrocarbon-air flame (see (Huang et al., 1986) and (Vosen et al., 1984) for example). The main difference concerns the non-dimensional wall heat flux ϕ_Q : many studies present values equal to one-third approximately whereas we obtain only 0.129. The high wall heat flux and the short interaction time show a very intense and very fast flame-wall interaction compared to the hydrocarbon-air flames. This is due first to the components nature (H_2/O_2 flames are very exothermic, rapid and hot flames) and second to the a high wall temperature (the wall heat flux is known to increase with increasing wall temperature (Ezekoye et al., 1992)). Another reason is the fact that a H_2/O_2 flame, being fast and therefore thin, can go much closer to the wall before quenching compared to a methane- or propane-air flame.

Looking at the chemical species profiles, the main feature is an accumulation of species HO_2 and H_2O_2 directly at the wall. This phenomenon is particularly striking for the stable intermediate species H_2O_2 since its peak value is multiplied by 7 compared to the free propagating flame. This is due to the three low-activation reactions: $H + O_2 + M \rightarrow HO_2 + M$ (R4), $H + 2O_2 \rightarrow HO_2 + O_2$ (R5), and $HO_2 \rightarrow H_2O_2 + O_2$ (R6), that occur in the near-wall region due to the natural presence of HO_2 ahead of the induction zone and to the low temperature in this zone. This also explains the low decrease of O_2 concentration compared to the H_2 one, although the mixture is in stoichiometric proportions. Reaction (R6) is exothermic and results in a high heat release directly at the wall.

This process is all the more remarkable as HO_2 and H_2O_2 have very low concentrations in the free flame (about 10^{-3} for HO_2 and 10^{-4} for H_2O_2) and do not seem to play a crucial role there. The presence of the wall completely changes the kinetic mechanism and it appears necessary to have a good description of these two species, though it strongly raises computing times. To confirm this, calculations without HO_2 and H_2O_2 have been run, showing that the maximum wall heat flux is reduced by about 30%, whatever the pressure or the equivalence ratio.

After $t^* \approx 29$, all the species profiles become flat because of diffusion from the near-wall cold region to the burned gas hot region. H_2 and H , having the lowest molecular weight are the fastest to diffuse and are finally post-oxidized in the hot gas. The flame thickness decrease, by approximately 80%, leads to an important stiffening of the temperature profile, with a corresponding increase of the temperature gradient by a factor of 5 approximately.

Flame-wall interaction for a diffusion flame One can distinguish two different situations for HOQ of a diffusion flame, depending on whether the dihydrogen or the dioxygen is trapped between the flame

and the wall. In this study, the species on the wall side is the dioxygen as it is known to lead to higher wall heat flux (dihydrogen is generally used to protect chamber walls). Temperatures are 750K for O_2 and 300K for H_2 .

The almost steady position of the diffusion flame makes the initial flame wall distance a key point of the resulting wall heat flux. Considering that the wall heat flux is directly linked to the ratio $\Delta T/d$ with $\Delta T = T_{max} - T_w$, it is reasonable to say that a minimal distance d (defined as the distance between the wall and the maximum temperature location) corresponds to a maximal wall heat flux. This minimum distance is directly linked to the flame thickness, itself related to the strain rate of the flame Λ . If we suppose that a variation of the strain rate does not imply a significant variation of the flame maximum temperature T_{max} , one can estimate that the maximum wall heat flux during head-on-quenching of a H_2/O_2 diffusion flame occurs for a strain rate close to the extinction strain rate as it corresponds to the minimum possible flame-wall distance d .

Non-dimensional heat release profiles are displayed in Fig.2 at five distinct times t^* , for an initial distance $d^* = 1.045$ and an initial strain rate of $3400s^{-1}$ (low compared to the extinction strain rate). Here t^* is an acoustic time defined as $t^* = ct/L_{ref}$ where c is the sound velocity on the H_2 side, x^* is given by $x^* = x/L_{ref}$. Little by little, intermediate species accumulate directly at the wall. Like in the

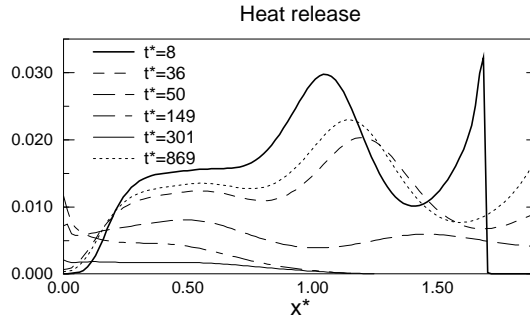


Figure 2: Non-dimensional heat release profiles for $d^* = 1.045$.

premixed case, HO_2 and H_2O_2 , which peak farthest on the oxidizer side, are the first species to reach the wall. However, for the diffusion flame, these concentrations remain relatively low. This is due to two effects. First HO_2 and H_2O_2 concentrations are initially lower in the diffusion flame than in the premixed flame. Second, the H atoms necessary to the formation of HO_2 via low activation recombination reactions (R4) and (R5) are mainly concentrated on the fuel side and not close to the wall. Consequently, peak values of heat release remain in the high temperature region, i.e. at a finite distance to the wall, and not directly at the wall as in the premixed case.

Although the mechanisms including HO_2 and H_2O_2 species seemed to be less important in the interaction process in the case of a diffusion flame, calculations have shown that the contribution of HO_2 and H_2O_2 species to the wall heat flux is still about 30%, i.e. of the same order of magnitude as in a premixed flame. This would be probably wrong if the reactant trapped between the wall and the flame was H_2 , since HO_2 and H_2O_2 are almost non-existent on the fuel side.

The peak value of heat release reaches the wall only at $t^* = 160$, i.e. right in the middle of the interaction whereas, for the premixed flame, it happened at the beginning of the interaction (i.e. at the beginning of what we have called "second stage"). The time $t^* = 301$ corresponds approximatively to the time of maximum wall heat flux. At this time, the heat release is almost equal to zero in the whole domain except in the near-wall region.

The next step is to vary the initial flame-wall thickness, and use the minimal flame-wall distance, in order to reach the maximum wall heat flux that can be obtained with this flame. As we already mentioned, the diffusion flame thickness is imposed by the strain rate Λ . Initial values for the non-dimensional strain

rate Λ^* (using the extinction strain rate as the reference value) have been taken from 0.03 to 0.5.

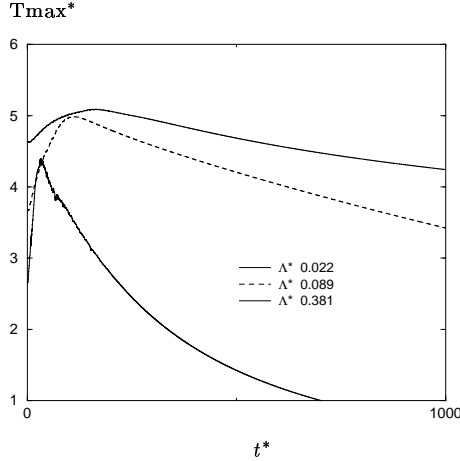


Figure 3: Time evolution of maximum temperature during interaction for different strain rates.

Figure 3 displays the non-dimensional maximum temperature ($T_{max}^* = (T_{max} - T_{wall}) / (T_{H_2} - T_{wall})$) during the interaction for different strain rates. The flame first experiences a decrease of the strain rate as no straining velocity field is imposed, leading to an increase of flame temperature. Once the flame starts to significantly interact with the wall, the temperature decreases until extinction. However the maximum temperature reached during the simulation still remains a decreasing function of the strain rate. As the flame-wall distance is also lower for higher strain rates, the resulting wall heat flux may be higher or lower, depending on the relative decrease of T_{max} and d .

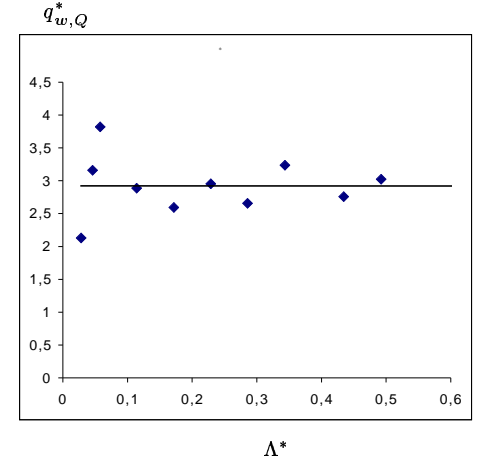


Figure 4: Non-dimensional maximum wall heat flux $q_{w,Q}^*$ for various strain rates.

Theoretically, one can try to estimate the maximum wall heat flux for a fixed distance d . Assuming that the wall heat flux $q_{w,Q}$ is only due to heat conduction in the gas layer of thickness d , one can estimate the flux with the mean temperature gradient: $q_{w,Q} \approx \lambda(T_{max} - T_w)/d$ (Poinsot et al., 1998). Computational results show that this rough approximation proves correct relatively well, with a correction coefficient $\alpha \approx 3$ that relates the local- (at the wall) to the mean temperature gradient. One can then assume the relation: $q_{w,Q}^* = q_{w,Q} / (\lambda_w(T_{max} - T_w)/d) \approx \alpha$, a correlation of great interest for simple heat flux evaluation in such a configuration (See figure 4, where $q_{w,Q}^*$ is plotted for various strain rates). The general trend is an increase of ϕ_Q with the strain rate. However, when going to still higher strain rate, one can expect a decrease due to an abrupt or stronger decrease of T_{max} , corresponding to flame extinction. The H2/O2 flame considered here quenches abruptly at $\Lambda_q = 215000s^{-1}$, and the wall heat flux, estimated just before extinction by the above correlation, is $\phi_Q = 0.0558$. This is the highest possible value for this H2/O2 flame, as the flame can not exist closer to the wall.

Compared to the premixed case, the maximum wall heat fluxes obtained for the diffusion flame are lower but, in the same time, the interaction lasts much longer. The maximum wall heat flux obtained for the diffusion flame rises to approximately one half of the maximal value obtained for the premixed flame at 1 bar.

4 Conclusions

Results of a laminar one-dimensional H2/O2 flame interacting with an inert constant temperature wall ($T_w = 750K$) have been reported for both the premixed and the diffusion flame. Calculations have been performed with detailed reaction mechanisms for a stoichiometric mixture at nearly atmospheric pressure. The flame quenching mechanisms for the premixed flame are approximately the same as for a hydrocarbon-air flame though the characteristic parameters of the interaction (ϕ_Q , $Pe_{F,Q}$, τ_Q) differ

notably. Results have shown the necessity of a good description of minor species HO_2 and H_2O_2 . The low activation energy recombination reactions including these two species are responsible for about 30% of the wall heat flux. Two important assumptions which have been used in this study would merit to be confirmed in the future since their pertinence is not verified at high wall temperature: (i) the lack of catalytic reactions at the wall, (ii) the lack of a thermal boundary layer at the wall.

Concerning the diffusion flame, one interesting result is that the maximum wall heat flux ϕ_Q appears to be one half of the flux obtained for a premixed flame. The maximal wall heat flux ϕ_Q obtained for a given initial strain rate appears to be roughly proportional to $\Delta T/d$ as was also shown in simple chemistry calculations. The maximal wall heat flux that can be obtained with this diffusion flame is reached just before flame quenching at the critical strain rate. For higher strain rates, the flame is quenched and the wall heat flux goes abruptly to zero.

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