Direct numerical simulation of non-premixed flame–wall interactions

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Abstract. The overall objective of this poster presentation is to illustrate how detailed numerical modelling may be used to bring basic information on fundamental problems in combustion science. We consider in the following the interaction of non-premixed flames with cold solid wall surfaces. Flame-wall interactions are an important feature in many combustion systems, that result in significant changes in the flame and wall dynamics: the flame strength is reduced near cold wall surfaces, leading possibly to (partial or total) quenching, while the gas-solid heat flux takes peak values at flame contact. The questions of turbulent fuel-air-temperature mixing, flame extinction and wall surface heat transfer are here studied using direct numerical simulation (DNS). The DNS configuration corresponds to an ethylene-air diffusion flame stabilized in the near-wall region of a chemically-inert solid surface. Simulations are performed with adiabatic or isothermal wall boundary conditions, and with different turbulence intensities. The simulations feature flame extinction events resulting from excessive wall cooling, and convective heat transfer up to 90 kW/m². The structure of the simulated wall flames is studied in terms of a classical mass mixing variable, i.e. the fuel-air-based mixture fraction, and a less familiar heat loss variable, i.e. the excess enthalpy variable, introduced to provide a measure of non-adiabatic behavior due to wall cooling.

1. Introduction
Flame-wall interactions (FWI) play an important role in many combustion systems. For instance in Internal Combustion (IC) engines, cooled walls combined with occurrences of short flame-wall distances result in flame quenching and FWI has a negative impact on engine performance, both in terms of thermal efficiency and pollution propensity. Similar effects are observed in aeronautical propulsion and power-generation applications. Enclosure fires are another combustion topic in which FWI plays an important (albeit different) role. For instance, the burning of a vertical flammable wall is a generic configuration where the fuel is released and consumed within the buoyancy-driven wall boundary layer, and the entire combustion process may be considered as FWI.

The subject of flame-wall interactions in IC engines has received significant interest in the past fifteen years. Previous studies have focused primarily on the quenching problem of laminar or turbulent premixed flames near cold wall boundaries [1-14]. Results from these studies indicate that: (1) quenching events occur near cold wall surfaces; (2) these quenching events also correspond to maximum values of the gas-solid heat flux; (3) depending on wall temperature and fuel type, premixed flames may loose a significant fraction of their reference power when driven to quenching. The maximum heat flux may be as high as 0.5-1 MW/m² for atmospheric hydrocarbon flames.
References [13-14] also consider the case of a laminar diffusion flame impinging on a cold wall in a stagnation point flow configuration. It is found that at high strain rates, the diffusion flame comes remarkably close to the wall surface (prior to quenching) and the gas-solid heat flux takes very large values. For the hydrocarbon-air flames studied in Ref. [13], the peak value of the gas-solid heat flux may be higher than that obtained in the corresponding premixed stoichiometric configuration.

We now turn to enclosure fire applications and consider three different configurations featuring substantial flame-wall interactions [15-16]: a first configuration corresponding to a flammable vertical wall, in which the flame is fueled by the thermal decomposition of the wall material; a second configuration in which the flame is fueled by a separate burner and where it develops adjacent to an inert vertical wall; and a third configuration in which the flame is again fueled by a separate burner and impinges on an inert horizontal (ceiling) wall. These configurations are representative of the large variety of flame spread and heat transfer mechanisms found in fire problems and correspond to different flame-wall arrangements. Typical values for the wall heat flux are: up to 50 kW/m² in the case of vertical wall fires [15-18]; up to 120 kW/m² in the case of vertical walls exposed to a separate adjacent flame [15-16,19-20]; and up to 150 kW/m² in the case of horizontal walls exposed to an impinging, buoyancy-driven flame [15-16,21-22]. It is worth emphasizing that those estimates correspond to time-averaged values and cannot be compared directly to the time-resolved, instantaneous peak values discussed above in the context of IC engine applications. In fire configurations, the magnitude of the wall heat flux will also depend on the optical thickness of the flame gases: previous studies indicate for instance that while the gas-solid heat flux in small non-sooty flames is controlled by convective heat transfer, the contribution of radiation heat transfer becomes dominant in large flames with significant smoke production [15-16].

The present study is a continuation of the laminar FWI study in Ref. [13] and an extension to the case of turbulent flame-wall interactions. Because of space limitations, we focus our discussion in the following on a presentation of the numerical study and an analysis of the observed wall-induced modifications of the flame structure. Additional information may be found in Ref. [23].

2. DNS solver and numerical configuration
The present study is performed using an advanced DNS solver called S3D [24]. S3D is a fully compressible Navier-Stokes solver coupled with an integrator for combustion chemistry, and is based on 8th-order finite differencing, 4th-order explicit Runge-Kutta time integration, characteristic-based boundary conditions treatment, a CHEMKIN-compatible description of chemical kinetics, and a rectangular Cartesian mesh capability. In addition, S3D is a massively parallel solver based on Message Passage Interface (MPI) libraries, and is currently re-designed and enhanced for increased performance and capability by a consortium of research institutions [24].

The selected FWI configuration corresponds to a momentum-driven, chemically reacting, ethylene-air, mixing layer developing parallel to an inert solid wall surface (Figure 1). While S3D features a detailed chemical kinetics capability as well as new soot formation and thermal radiation capabilities [24], the present study takes an intermediate step and treats the FWI configuration in a two-dimensional domain, with global chemistry, and without soot and radiation. Future work will be aimed at removing these limitations with the goal of achieving more quantitative simulations.

As seen in figure 1, the combustion region is well-ventilated with plenty of air supplied from the free stream while ethylene flow is confined to the near-wall region. The wall boundary conditions correspond to zero velocity, zero mass flux, and either zero heat flux (adiabatic wall case) or prescribed temperature (non-adiabatic wall case). The free stream inflow boundary at \( x = 0 \) corresponds to a uniform flow of air seeded with turbulent-like perturbations. The mean velocity is \( u_\infty = 5 \text{ m/s} \); the perturbations use a variant of the random fluctuation method of Ref. [25]. In the present study, the turbulent inflow perturbations are characterized by a moderate-to-high forcing intensity, \( 1 \leq u' \leq 2.5 \text{ m/s} \), and a small integral length scale, \( l_i = 0.17 \text{ cm} \); the corresponding turbulent flow Reynolds number, \( Re_t = \frac{u' \times l_i}{\nu} \), where \( \nu \) is the free stream kinematic viscosity, ranges from 108 to 270. The near-wall region of the inflow boundary corresponds to a prescribed velocity profile that satisfies the
the no-slip wall condition, and prescribed profiles of species mass fractions and fluid temperature that are specified according to a moderately-strained counter-flow laminar flame solution.

The initial fields correspond to a one-dimensional laminar flame solution and are constructed from the inflow boundary profiles. The computational grid size is $1216 \times 244$. The grid spacing is uniform in the $x$-direction, $\Delta x \approx 66 \, \mu m$, while variable in the $y$-direction: the $y$-grid is uniform in the near wall/flame region, $\Delta y \approx 50 \, \mu m$ for $0 \leq y \leq 0.8$ cm, and is stretched in the free-stream region. Computations are performed for a total duration corresponding typically to 4 free stream transit times, or 64 ms. S3D is run in a parallel mode, using MPI and more than 200 processors on an IBM SP Power 3 super-computer, called Seaborg and located at the National Energy Research Scientific Computing Center at Lawrence Berkeley Laboratory. On the Seaborg platform, the cost of performing a single simulation of total duration 64 ms is approximately 32,000 processor hours.

![Numerical configuration corresponding to a non-premixed turbulent wall-flame](image)

### Figure 1.
Numerical configuration corresponding to a non-premixed turbulent wall-flame. The domain is two-dimensional and features a turbulent inflow boundary at $x = 0$ (flow is from left to right); a solid wall boundary at $y = 0$; and non-reflecting boundaries at $x = 8$ cm and $y = 4$ cm. The inflow boundary is used both for air and fuel injection. The plot shows a typical snapshot of temperature iso-contours (adiabatic wall case).

| Case | 1    | 2    | 3    | 4    |
|------|------|------|------|------|
| Inflow turbulence | $u' = 1$ m/s | $u' = 2.5$ m/s | $u' = 1$ m/s | $u' = 2.5$ m/s |
| Wall condition | adiabatic | adiabatic | $T_w = 300$ K$^{(a)}$ | $T_w = 300$ K$^{(a)}$ |

$^{(a)}$ $T_w$ is the gas-solid wall temperature

### 3. Results
We consider in the following a series of four simulations: the simulations differ by the choice of inflow turbulence intensity and/or thermal boundary condition applied at the solid wall surface (table 1). The flame structures observed in cases 1-4 are found to correspond to different topologies and belong to one of the following three categories: a continuous flame sheet without extinction; multiple flame sheets without extinction; or multiple flame sheets with extinction. Figure 2 provides examples of the first and third categories.

Figures 2(a)-(b) present instantaneous snapshots of temperature and fuel mass reaction rate, as obtained in case 1 (adiabatic wall). The figures illustrate the flame response to incoming flow perturbations and confirm that significant turbulent mixing and flame wrinkling take place in the vicinity of the wall. Figure 2(c) presents the location of the stoichiometric fuel-air interface and a comparison between figures 2(b) and 2(c) indicates that the flame is active along the entire stoichiometric interface: the flame displays the classical downstream weakening of combustion intensity as the reactants get depleted and replaced by combustion products, but it remains free of any aerodynamic flame extinction event. In the absence of extinction, the temperature levels are particularly high in the near-wall region (Figure 2(a)): the wall boundary is almost everywhere in contact with hot gases at temperatures in excess of 2000 K.

Figures 2(d)-(f) presents the results obtained in case 3 (cold wall temperature). A comparison between figures 2(e) and 2(f) indicates that case 3 features several flame extinction events. As seen in figure 2(d), the structure of the thermal boundary layer is quite different from that observed in figure 2(a): a thin cold sub-region develops near the wall and the flame is now exposed to wall-induced heat
losses. These heat losses occasionally become super-critical and lead to the extinction events seen in figure 2(e).

Figure 2. Instantaneous spatial variations of: (a)(d) fluid temperature; (b)(e) fuel mass reaction rate. Figures (c)(f) present the location of the corresponding stoichiometric iso-contour of mixture fraction $Z$. Case 1 (left) and case 3 (right) solutions. Two wall-induced flame extinction events are observed in figure 2(e). Figure 2(f) also presents the spatial variations of excess enthalpy $H$.

In Ref. [23], the flame response to wall cooling is studied in terms of the classical fuel-air-based mixture fraction $Z$ and a less familiar quantity called the excess enthalpy variable $H$ [26-27]:

$$Z = \frac{Y_F - \left(\frac{Y_{O_2}}{r_s}\right) + \left(\frac{Y_{O_2}^{\infty}}{r_s}\right)}{Y_F^{\infty} + \left(\frac{Y_{O_2}^{\infty}}{r_s}\right)}; \quad H = \frac{c_p(T - T^{\infty})}{\Delta H_c} \left(\frac{1}{Y_F^{\infty}} + \frac{1}{Y_{O_2}^{\infty}}\right) + \frac{Y_F}{Y_F^{\infty}} \frac{Y_{O_2}}{Y_{O_2}^{\infty}} - 1$$

where $Y_k$ is the species $k$ mass fraction and $Y_k^{\infty}$ its value in the $k$-supply stream; $r_s$ the stoichiometric oxygen-to-fuel mass ratio; $T$ the fluid temperature and $T^{\infty}$ its free-stream value; $c_p$ the specific heat at constant pressure (assumed constant); and $\Delta H_c$ the heat of combustion per unit mass of fuel. $H$ is a non-dimensional quantity that varies between (-1) and 0. Under adiabatic conditions, $H = 0$. Under non-adiabatic conditions, $H \neq 0$ and the deviations of $H$ from 0 give a local measure of the amount of heat loss resulting from the wall cooling process. Figure 2(f) compares the location of the wall-cooled region (i.e. the region that exhibits negative values of $H$) to that of the flame (i.e. the stoichiometric fuel-air interface); occurrences of wall-induced extinction events are possible when the wall-cooled region extends to the flame zone (see Ref. [23] for a discussion of the critical flame extinction conditions).
4. Conclusion
This poster presentation demonstrates that the S3D direct numerical simulation (DNS) capability developed with SciDAC support is well-suited to our objectives of bringing basic information on flame-wall interactions (FWI). The simulations correspond to ethylene-air turbulent wall-flames, and feature sub-critical flame dynamics, in the case of an adiabatic wall, and super-critical flame dynamics, in the case of a cold wall. DNS simulations allow for fundamental and unique observations of the micro-physics of FWI, including the location of the wall-cooled region, the dynamics of flame extinction events, and the quantification of the statistical variations of the wall heat flux.

In Ref. [23], the DNS results are also analyzed and compared to classical results from turbulent diffusion flame theory. This leads to an extension of the classical flamelet description of diffusion burning and extinction events to the case of non-adiabatic combustion, using mixture fraction, scalar dissipation rate and excess enthalpy as controlling variables. A modified flame extinction criterion is also proposed that provides a correction factor to the criterion obtained in the adiabatic flame theory. Overall, we feel that this study illustrates how DNS combined with large-scale parallel computing resources does contribute to combustion science, as a tool for exploration, analysis and modeling.

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