

Only recently, three-dimensional direct numerical simulations (DNS) with detailed chemistry have become possible. These types of simulations will have an important impact on combustion science because of the data they provide. Obtaining similar data sets through experimental characterization is very challenging and requires joint measurements of a multitude of chemical species concentrations in addition to temperature and velocity fields. Gruber *et al. (J. Fluid Mech.*, vol. 658, 2010, pp. 5–32) have performed a detailed chemistry DNS to understand the physics of flame/wall interactions. They found that flames interact with streamwise vortical structures close to the wall, and that these structures can push the flame towards or away from the wall. The flames get extinguish when they are too close to the wall. Interestingly, the extinction process actually causes an order-of-magnitude increase in heat release, and therefore, strongly amplifies wall heat transfer.

Key words: boundary layers, flames, turbulent reacting flows

## 1. Introduction

Combustion has been called the oldest science of mankind. While preserving a burning flame was essential for the survival of early humans, today's questions are related to the joint optimization of efficiency, stability and emissions. Because of combustion's complexity, its multi-scale and multi-physics nature, and the strong inherent non-linearities, answering these questions presents a tremendous challenge to modern science. Although there is an urge to move to alternative energy sources, the 2009 International Energy Outlook projects that under current law and policies, carbon dioxide emissions will increase by almost 40 % between 2006 and 2030, and that in the year 2030, fossil fuels will still provide over 80 % of marketed energy (Energy Information Administration 2009).

A game-changing achievement towards mitigating the harmful consequences of burning fossil fuels would be the ability to perform reliable multi-objective optimization of combustion systems, which could improve present processes through enhanced efficiency and reduced emissions or even lead to radically new combustor designs. However, a necessary requirement for this is the availability of predictive models at sufficiently low computational cost. Combustion systems often involve complex turbulent flows, liquid fuels, spray dynamics, atomization, evaporation, interactions with walls, radiation, and of course chemistry. Each of these physical



processes interacts with one another, influences the combustion process, and is in turn influenced by heat release.

In particular, the interaction of flames with walls is an important process in many technical applications. Flame extinction at walls of internal combustion engines can lead to emissions of smoke and unburned hydrocarbons. In aircraft engines, efforts to increase efficiency have led to higher temperatures and smaller combustors. Similarly, efforts to reduce total fuel cost and reduce emissions of greenhouse gases have led to increased interest in small-scale micro-turbines for co-generation of heat and power. This makes flame/wall interactions more important, yet present computational models do not adequately consider the effect of walls on the flame, and they cannot predict the unsteady wall heat transfer caused by near-wall turbulence.

Direct numerical simulations (DNS) have become an essential tool in turbulence research for illuminating and understanding complex physical processes. While for non-reactive flows the computational cost is essentially governed by the Reynolds number, the chemistry/fluid interaction creates its own length and time scales, which considerably increase the stiffness of the governing systems of equations. Because of these difficulties, DNS of reactive flows has in the past mostly been performed either in only two dimensions, which is known to misrepresent small-scale turbulence, or using only single-step chemistry, which is fundamentally different from realistic chemistry, especially for wall-bounded flows. Only in the past few years three-dimensional DNS with realistic chemical schemes have been performed for laboratory-type configurations, and now the paper by Gruber *et al.* (2010) describes a carefully executed very large-scale DNS that uses detailed chemistry to compute a premixed flame in a channel.

## 2. Overview

The aim of this paper is to study the interaction of a flame with walls, which are at the temperature of the unburnt gases. The flame itself is stabilized by a lateral flame anchor located at the channel centreline. While several similar studies have been performed in the past, three-dimensional DNS have so far used only one-step chemistry. However, it is shown here that in order to capture the leading order physics, the consideration of realistic multi-step chemistry is essential.

The simulation results and analysis of Gruber et al. (2010) lead to a clear picture of the structure of the flame as it approaches the wall. As long as the flame is far enough away from the wall, it is hardly influenced. This distance is found to be roughly 10 flame thicknesses, which in the present DNS is equivalent to  $y^+ \approx 120$ . When the flame gets closer to the wall, however, heat losses to the wall start to become significant. Below a distance of about three flame thicknesses, the gradients steepen, heat losses to the wall become very strong, and ultimately the flame extinguishes at a wall distance of approximately one to two flame thicknesses, which is the so-called quenching distance. This quenching process can be understood in the context of the radical balance. While the flame approaches the wall, the heat transfer to the wall leads to larger gradients, and therefore, to a cooling of the flame. When the flame temperature is sufficiently low, radical recombination reactions become dominant, and because of a lack of radicals, the flame extinguishes. The analysis of Gruber et al. (2010) further shows that the recombination reactions are associated with a relatively strong heat release. Because of the high gradients close to the wall, the high local mixing rates of species and thermal energy caused by this, and the resulting



FIGURE 1. Normalized heat flux on the bottom wall (colour) and streaks in the near-wall region (white lines).

amplification of the radical recombination reactions, the extinction process leads to a roughly 10-fold increase in the local heat release, and therefore, to a local amplification of the wall heat transfer. The fact that flame extinction leads to this strong increase in wall heat transfer makes analytic sense, but could not be less intuitive. It is important also to note that one-step global chemistry can obviously not describe this process adequately, because of the lack of the important recombination reactions and the competition with radical-producing reactions, which leads to a distinct cross-over temperature above which combustion becomes fast (Peters & Williams, 1987).

The investigation of the wall heat flux shows strong fluctuations in the region where the flame touches the wall with high peak values, and a decay to substantially smaller levels in the post-flame region (figure 1). This has important consequences, since local peaks can lead to hot spots, and the induced local temperature gradients can lead to strong local straining of the material. The analysis further shows that the root cause for the strong variations along the region where the flame touches the wall is the interaction of the flame with the coherent streamwise vortical structures of the turbulence in the near-wall region. These vortices alternately move the flame away from the wall, or push it towards the wall, causing quenching and hence regions of large heat release. Evidence for this is provided in a temporal and spatial spectral analysis of the wall heat-transfer signature. Characteristic time and length scales observed correlate strongly with those typically observed for streamwise vortices. In this sense, local wall heat transfer in a flame/wall interaction behaves similar to wall skin friction, for which Kravchenko, Choi & Moin (1993) have found that local peaks arise by increased shear rates in the downwash region of the streamwise vortices.

Also, in the outer layer of the channel, the chemistry is found to be fast enough to result in a flame sufficiently thin that it is only wrinkled by the turbulence, but its structure is not disturbed. Close to the wall, however, the flame temperature decreases, as a result the chemical time scale increases, and the flame becomes thicker. When the flame thickness becomes larger than the small scales of the turbulence, turbulent mixing will impact the flame structure, which leads to a fundamentally different local turbulence/chemistry interaction, posing a challenge for the modelling community.



The DNS of Gruber *et al.* (2010) illuminates many interesting features of flame/wall interactions. It should be expected that the physics of these interactions are quite sensitive to some of the chosen simulation parameters. For instance, the simulation highlighted here was performed for hydrogen/air combustion. Hydrogen as a fuel behaves quite differently from hydrocarbon fuels. It was found in laminar flames, for example, that the quenching distance for methane/air flames is approximately twice as large as that for hydrogen/air flames.

Further, as for all DNS, one of the important questions is the effect of the Reynolds number *Re*. For the present DNS, this question is of particular importance, since high Reynolds numbers might lead to a different interaction of the flame with the near-wall turbulence. It was discussed here that the dynamics of wall heat transfer are governed by the interaction of the flame with the streamwise vortical structures close to the wall. These structures are typically found in the near-wall region of  $y^+ < 60$  or so. For the present case, the quenching distance was found to be roughly at  $y^+ = 20$ , corresponding to 1.5 flame thicknesses. Assuming that the ratio of quenching distance to flame thickness is independent of *Re*, increasing the Reynolds number will ultimately lead to a quenching distance that is outside the region where the streamwise vortices are found. It could be speculated, therefore, that the interaction of the flame with these structures vanishes at high Reynolds number. Keeping the flame parameters and channel height the same, for  $Re_{\tau} > 450$  a quenching distance of 1.5 flame thicknesses would lie in a region  $y^+ > 50$ , and the flame dynamics would be unaffected by the streamwise vortices. Here, however, hairpin-type structures could lead to similar down-wash of the flame.

Thinking beyond flame/wall interactions, there are many potential interesting application for three-dimensional, detailed chemistry DNS of reactive flows. Particularly interesting cases are where physical complexity in addition to turbulence/ chemistry interactions makes the analysis and understanding difficult. Examples are spray combustion, soot formation in turbulent combustion, flame stabilization in complex flow fields, and combustion dynamics and instabilities.

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