Evaluation of turbulent premixed flame properties

J.A.M de Swart[1], R.J.M. Bastiaans[1], J.A. van Oijen[1], L.P.H. de Goey[1]
[1]Eindhoven University of Technology, department of Mechanical Engineering
P.O. Box 513, 5600 MB, Eindhoven, The Netherlands

1 Background and Motivation

Clean and efficient combustion is a hot topic. More stringent environmental legislation forces us to look for clean and efficient types of combustion and fuel mixtures. One road towards clean combustion is adding hydrogen to natural gas used in gas turbines used for electricity production. A key issue in this approach is the flame stability of a hydrogen/natural gas flame. To numerically simulate the processes in a gas-turbine combustion models are required. The models have to be acccurate and the computational cost should be as low as possible. A good candidate is a LES-CFM-FGM-model, where the flow is simulated using Large Eddy Simulation (LES) and the chemical kinetics are captured using Flamelet Generated Manifolds (FGM). Flow and chemistry are coupled using a Coherent Flame Model (CFM). A first step towards this goal is simulating a premixed turbulent flame using DNS-FGM. Here, the flow is solved using Direct Numerical Simulation (DNS), while FGM is used for the chemistry. The strength of Direct Numerical Simulations (DNS) is that no modeling of turbulence is required. This means that the flow is solved numerically up to the smallest scales in the system and no modeling errors are made. The basic idea behind FGM [1–5] is that the structure of the inner reaction layer of a flame in a turbulent environment remains intact. This holds for certain values of scaled turbulence intensity and length scale ratio, as displayed in the combustion diagram by Peters [6]. Because of this property the flame can be precomputed and tabulated. Together with the conservation equations for density, velocity and temperature, we solve an equation for the reaction progress variable and look up other variables in a precomputed datafile. The results of these DNS-FGM simulations will be used to gain insight in the elementary processes that occur locally in the flame brush and it can also be used as a benchmark for future models. In this paper we will discuss two different cases of a premixed, statistically flat, turbulent flame structure. A lean methane/air mixture is used as fuel. Both cases are located in the so-called thin-reaction zones regime, as discussed by Peters [6]. The only difference between the cases is that u' differs a factor of two. We will discuss key parameters in turbulent combustion, such as turbulent mass consumption and flame surface area. Also we will look at flame stretch.

2 Settings and Numerics

2.1 Physical properties

In this study a fully compressible DNS code is used to simulate turbulent combustion statitically flat flames. The position of the two cases in the combustion diagram are characterized by $u'/s_L = 6.9$ and $l/l_F = 2.2$ for case 1 and $u'/s_L = 3.5$ and $l/l_F = 2.2$ for case 2. Preferential diffusion is not taken into account, i.e. $Le_i = 1$ for all species i. We study premixed turbulent flames with an equivalence ratio of $\phi = 0.7$. This equivalence ratio is also found in a lot of industrial applications. An initially laminar flame solution is superimposed on a decaying turbulent field. The laminar flame solutions were

Correspondence to : j.a.m.d.swart@tue.nl

computed using the one-dimensional flame code CHEM1D [7], using detailed chemistry. Precomputed flamelets were computed using the GRI3.0 chemical mechanism [8] and stored in a database. The GRI3.0 methane mechanism has 53 species and 325 fundamental reactions.

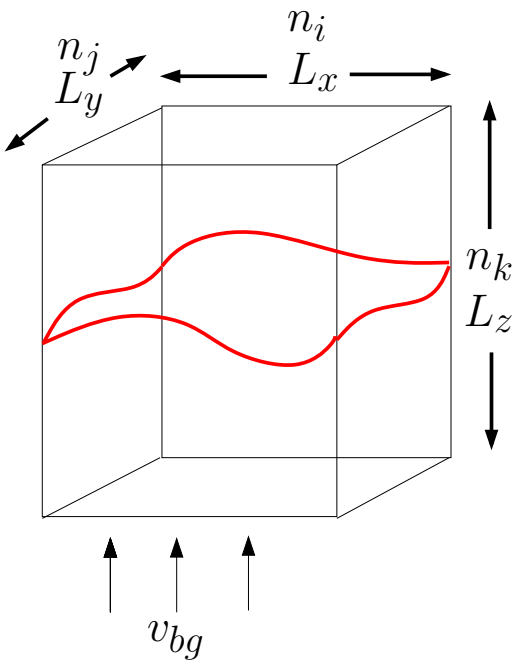


Figure 1: Numerical domain

In the DNS-FGM simulations conservation equations are solved for density (ρ), three velocity components (u,v and w) and temperature (T). The pressure is determined using an equation of state. Also an equation is solved for the progress variable. The governing equations can be found in [4]. One progress variable will be used and this progress variable is used to look up the unclosed (chemical and thermal) source terms and transport properties. In this study the mass fraction of carbon dioxide, which is monotonously increasing, was used as progress variable, $Y_{cv} = Y_{CO_2}/Y_{CO_2}^{burnt}$. The numerical domain is shown in figure 1. We can see a flame structure in the xy-plane and we also see a background velocity from the bottom. The flame propagates in negative z-direction and remains in the domain because of the background velocity.

2.2 Numerics

The governing equations are solved with a higher order finite difference method. Temporal discretization is performed with a compact storage (two memory locations) third order Runge-Kutta method, as reported by Wray [9]. Spatial discretization is done using higher order compact discretization schemes, both central and upwind, typically 6th and 5th order accurate, as proposed by Lele [10] and De Lange [11], respectively. The non-reflecting NSCBC for a subsonic in- and outflow [12] are used for the streamwise (z) direction. In the spanwise directions (x and y), periodic boundary conditions are used. More details about the code can be found in [13]

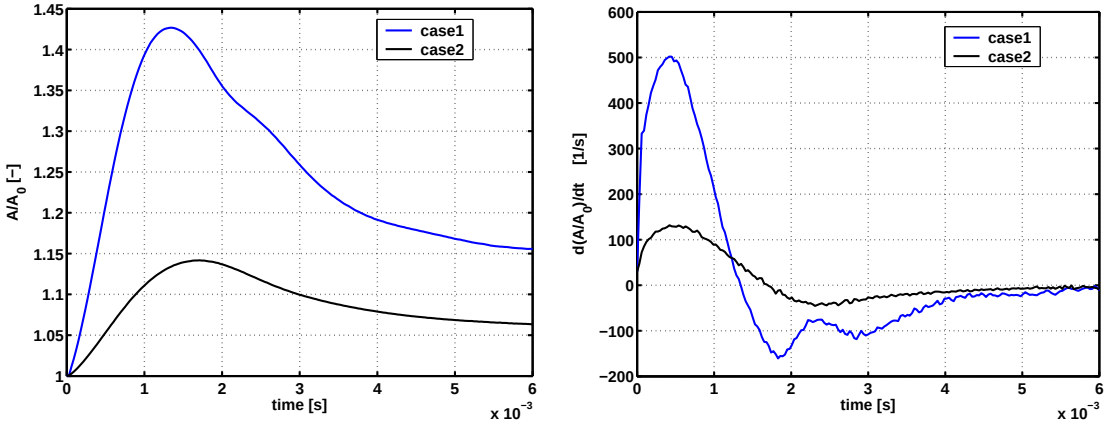
3 Results and Discussion

First we take a look at the actual flame surface area. We can see (figure 2) that the surface area increases from time $t = 0$ until it has a peak value and then starts to decrease. The turbulence is decaying in time. On the concave side of a wrinkled flame there is relatively much flame surface area moving in on a certain pocket of fuel (or products). This means that more fuel is consumed in these pockets and that the wrinkled structure tends to become less wrinkled. As the turbulence becomes weaker, this mechanism becomes more important. This might cause the flame surface area to decrease after some time. From the actual flame surface area we can compute the flame stretch rate, which is defined as:

$$K = \frac{d(A/A_0)}{dt} \tag{1}$$

where A is the actual flame surface area [m^2], A_0 is the flame surface area [m^2] at time $t = 0$ and t is the time [s]. The flame stretch rate is displayed in figure 2. We can see that the overall flame stretch rate is not equal to zero. It is possible that local values are a lot higher than these mean values. Also,

by definition, the flame stretch rate should be positive immediately after time $t = 0$, since A_0 is the smallest flame surface area possible. After the peak in the flame surface area, the flame stretch rate will become negative.



(a) scaled flame surface area (b) flame stretch rate

Figure 2: Flame surface area and flame stretch rate

Another parameter of interest is the turbulent mass consumption. The turbulent mass consumption can be found by integrating the chemical source term over the volume:

$$m_T = \frac{1}{A_{cs}} \int_V \dot{\omega} \mathrm{d}V \tag{2}$$

where $A_{cs} = L_x * L_y$ is the projected cross-sectional area $[m^2]$, $\dot{\omega}$ represents the chemical source term $[kg/m^3 s]$ and V is the volume $[m^3]$. The turbulent mass consumption $[kg/m^2 s]$ is shown in figure 3.

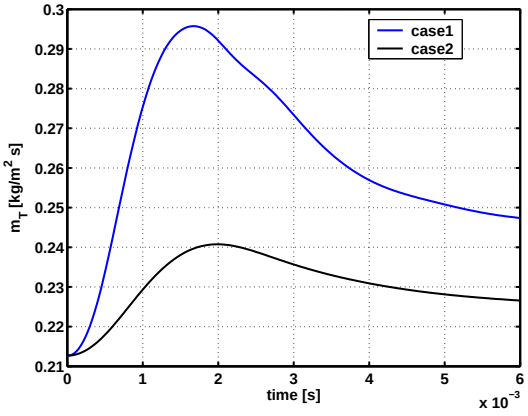


Figure 3: Turbulent mass consumption

It must be recognized that the overall change of the mass consumption is caused by two effects. First the local burning velocity s'_L changes and second the flame surface area increases. We can see that in our case the mass consumption increases from time $t = 0$. For the cases presented in this study, the length scale ratio is relatively small. This means that the turbulent eddies are relatively small and they will enhance mixing in the preheat zone. This will increase local burning velocities. We can say that the increase in turbulent consumption is partly due to enhanced mixing in the preheat zone. On the other hand, the flame surface area increase also influences the turbulent consumption. A third test case that has an equal turbulence intensity and a different length scale ratio could be used to show these separate effects. It can also be seen that the peak values in the flame surface area and the turbulent mass consumption occur at different times. First there is a peak in the area, which is followed by a peak in mass consumption. This shows that the change in mass consumption is not only caused by area increase but that there is another effect, i.e. change in local flame speed.

4 Conclusions and Outlook

It has been shown that DNS-FGM gives promising results and the results have been explained and discussed. It was shown that the flame surface area and the turbulent mass consumption increase from time $t = 0$. After some time, the flame surface area and the turbulent consumption start decreasing after some time. A possible reason for the decrease in flame surface area and turbulent mass consumption has been discussed. The values found for the flame surface area, the flame stretch rate and the turbulent mass consumption can be used to check future models in LES modeling. More analysis will focus on extracting flamelets and more detailed analysis on the local flame/flow interactions.

References

[1] J.A. van Oijen, L.P.H. de Goey. Modeling of premixed laminar flames using flamelet-generated manifolds, *Combust. Sci. Technol.*, 161: 113-137 (2000)

[2] J.A. van Oijen, L.P.H. de Goey. Modeling of premixed counterflow flames using the flamelet-generated manifolds, *Combust. Theory Modeling*, 6: 463-478 (2002)

[3] G.R.A. Groot, L.P.H. de Goey. A computational study of propagating spherical and cylindrical premixed flames. *Proc. Combust. Institute*, 29: 1445-1451 (2002)

[4] R.J.M. Bastiaans, J.A. van Oijen, S.M. Martin, L.P.H. de Goey, H. Pitsch. DNS of lean premixed turbulent spherical flames with a flamelet generated manifold. CTR Annual Research Briefs, pp257-268 (2004)

[5] J.A. van Oijen, R.J.M. Bastiaans, G.R.A. Groot, L.P.H. de Goey. Direct numerical simulations of premixed turbulent flames with reduced chemistry: validation and flamelet analysis. *Flow, Turb. Comb.*, 75: 67-84 (2005)

[6] N. Peters. *Turbulent combustion.* Cambridge University Press (2000)

[7] CHEM1D. A one-dimensional laminar flame code. Eindhoven University of Technology. http://www.combustion.tue.nl/chem1d/

[8] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B. Eiteneer, M. Goldenberg, C.T. Bowman, R.K. Hanson, S. Song, W.C. Gardiner Jr., V.V. Lissianski, Z. Qin. http : //www.me.berkeley.edu/gri_mech/ (1999)

[9] A.A. Wray. Minimal storage time-advancement schemes for spectral methods. Technical report, NASA Ames Research Center, Moffet Field, Ca. 94035 (1990)

[10] S.K. Lele. Compact finite difference schemes with spectral-like resolution. *J. Comp. Phys.*, 103: 16-42 (1992)

[11] H.C. de Lange. Inviscid flow modelling using asymmetric implicit finite difference scheme. *Int. J. Num. Meth. Fluids*, 49: 1033-1051 (2005)

[12] T.J. Poinsot, S.K. Lele. Boundary conditions for direct simulations of compressible viscous flows. *J. Comp. Phys.*, 101: 104-129 (1992)

[13] R.J.M. Bastiaans, L.M.T. Somers, H.C. de Lange. DNS of non-premixed combustion in a compressible mixing layer. *Modern Simulation Startegies for Turbulent Flow*, Editors: B.J. Geurts, R.T. Edwards Publishers, Philadelphia, USA, pp 247-262 (2001). ISBN 1-930217-04-8