Some Aspects on Level-set Modelling of Premixed Turbulent Combustion

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Abstract

A level-set flamelet library approach is investigated, especially in terms of the level-set flame position tracking formulation. Different methods for the numerical propagation of a distance function, denoting the distance to the mean flame surface, have been tested. One of them, the Fast Marching Method with extension velocities has shown beneficial thanks to the extension velocity algorithm.

The mean turbulent flame is assumed to be an ensemble of locally laminar flamelets fluctuating around a mean flame position. Each flamelet has its own local structure of temperature and species as a function of the flamelet coordinate. This structure is simulated in a laminar flame calculation and stored in a table, called a flamelet library. The G-equation is employed to trace the mean flame surface, and a presumed Gaussian distribution of position around the surface is employed to average the locally laminar flamelet properties over the turbulent flame.

The turbulent flow modelling frame work is that of standard $k-\epsilon$ and the computational field is discretized using Finite Differences on a staggered Cartesian grid.

Measurements from the VAC Validation Rig 1, in which lean premixed propane/air V-shaped flame is stabilised behind a triangular prismatic flame holder in a rectangular channel, are utilised for some assessment of the simulated data.

1 Level-set Flamelet Library Approach

The turbulent flame is considered to consist of flamelets, assumed to locally have the structure of a laminar flames [1]. Using a detailed chemical mechanism prior to the CFD simulations, the laminar flame is simulated and the results (density, temperature, species molar fractions, etc.) are stored in a table, a flamelet library.

A level-set formulation, the G-equation [2], is employed to trace the position of the mean flame surface. Then a presumed Gaussian distribution of position around the surface is employed to average the locally laminar flamelet properties over the turbulent flame. The width of the distribution, roughly the flame thickness, is estimated from the experiments and set to be a linearly increasing function of position in the domain.

The Favre averaged G-equation, where $\widetilde{G} = 0$ is defined to be the mean flame surface, has the following form:

$$\frac{\partial \widetilde{G}}{\partial t} + \widetilde{u_i}\frac{\partial \widetilde{G}}{\partial x_i} = s_T \left| \frac{\partial \widetilde{G}}{\partial x_k} \right| \tag{1}$$

The turbulent flame speed, s_T is the speed by which the surface where $\widetilde{G}=0$ propagates into the unburned fluid. It includes a modification for curvature (κ) in s_T [3].

$$\frac{\partial \widetilde{G}}{\partial t} + u_i \frac{\partial \widetilde{G}}{\partial x_i} = \left(s_T^0 - D\kappa\left(\widetilde{G}\right)\right) \left|\frac{\partial \widetilde{G}}{\partial x_k}\right| \tag{2}$$

where D is a measure of the influence of the mean flame curvature. Here s_T^0 is computed from the laminar flame speed and characteristic turbulent velocity fluctuation as

$$s_T^0 = s_L + 0.46u' + 0.2\sqrt{s_L u'} \tag{3}$$

The modification in practice means that s_T^0 does not contain effects due to curvature of the mean surface. As can be seen from Figure 1, the curvature modification decreases the turbulent flame speed at curved sections. In this case the effect is self limiting as the decrease of s_T leads to a less curved shape. The present flame is however already rather planar and the effect is therefore hard to assess further here. (For a thorough explanation of the level-set approach for combustion, see [4].)

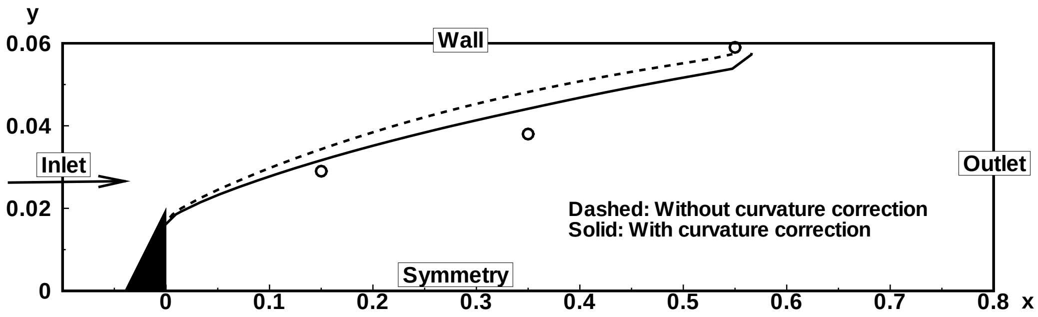

Figure 1: Mean flame position with and without modification for curvature in s_T

The propagation of $\widetilde{G}=0$ can be achieved in different ways. In one approach, $\widetilde{G}$ is computed in points close to $\widetilde{G}=0$, solving Equation 1, then the rest of the field is re-normalised, see next section. In the Fast Marching Method [8], the points are updated in the order of proximity to the $\widetilde{G}=0$ surface. The ordering is based on a preliminary calculation of the distance to the $\widetilde{G}=0$ surface.

2 $\widetilde{G}$ as a Distance Function

In a level-set formulation, the level used for tracing the surface can be arbitrarily chosen. It is convenient to chose the $\widetilde{G}=0$ level and then define $\widetilde{G}$ to denote the normal distance to the traced surface. This means that $\widetilde{G}$ becomes a distance function. As the turbulent flame speed is only defined at the mean flame surface, the $\widetilde{G}$ field outside this surface is a function of this surface. The solution of this can be obtained in some different ways.

In the present work, the re-normalisation based method [10] and the Fast Marching Extension velocity methods (FME) [8] have been tested. Both have their own benefits and deficits. The re-normalisation approach has, in its simplest form, a very easy implementation. The FME is somewhat more complicated to implement algorithmically, especially in three dimensions. In its simplest form, the re-normalisation may distort the surface, under some circumstances even more than the usual order of accuracy - the grid size. This problem can be remedied by more or less complicated fixes to the algorithm [9] [11]. The FME has a built in protection for the $\widetilde{G} = 0$ level. There is also the difference between the FME and the re-normalisation based methods with the computational effort. When the initial field is almost accurate, the re-normalisation procedure converges fast and is more effective than the FME. If, however, the initial field is poor, the FME will give faster results.

An important aspect of the difference between the two methods was noticed. As the FME propagation is based on the previous $\widetilde{G}$-field, not only on the present $\widetilde{G} = 0$ surface, it may cause an updated field which does not fully comply with what is wanted, i.e. the distance to the $\widetilde{G} = 0$ surface. Assume that the present flame (which is however stationary) would be propagating upstream, e.g. due to a decrease in the inlet mass flow. As can be seen from Figure 2, if the $\widetilde{G} = 0.01$ iso-contour is propagated normal to itself in

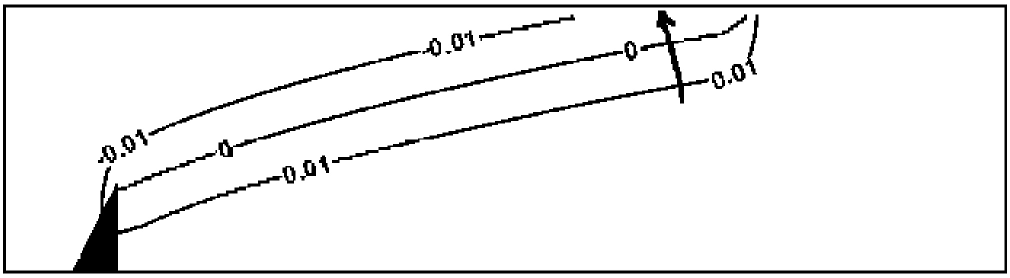

Figure 2: Sketch of some $\widetilde{G}$ iso-contours

the direction of the arrow, the curved shape around the end of the $\widetilde{G} = 0$ contour would disappear. The $\widetilde{G} = 0.01$ iso-contour would look as if the $\widetilde{G} = 0$ had propagated out through the wall and *still exists there.* This means that G would yield a to low distance to the mean flame surface, and hence place the studied point too early in the flame, close to the wall. A simple remedy for this is to make a re-normalisation, which would recreate the curved shape around the end of the $\widetilde{G} = 0$ contour.

A special benefit of the FME is that it takes almost no extra effort to distribute the information about the $\widetilde{G}$-variance, $\widetilde{G''^2}$, to all points along a line normal to the mean flame surface. $\widetilde{G''^2}$ is closely related to the turbulent flame thickness. Due to the presumption of a one-dimensional distribution (in this case Gaussian) of flame position around the mean flame surface, the variance $\widetilde{G''^2}$ should be constant along a normal to the mean flame surface. A deviation from this could lead to strange species distributions due to the way the ensemble averaging over the distribution is performed [5],

$$\overline{Y} = \int_{-\infty}^{\infty} Y(G)\wp(\overline{G} - G)dG \tag{4}$$

The unphysical sharp fall off of the profile (in the circle) in Figure 3 is due to the variance not being constant in the preheat zone along the mean flame normal. It is effective to compute the extension $\widetilde{G''^2}$ at the same time the extension velocity is computed. Therefore,

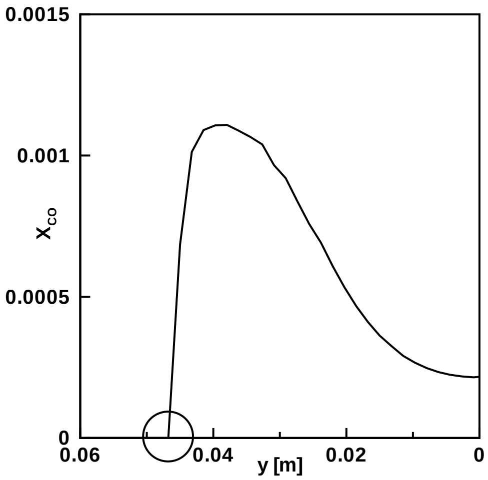

Figure 3: CO molar fraction at x=0.35m

even if the extension velocity method is not beneficial for a stationary flame compared to using frequent re-normalisation, it may be worth while in combination with the extension $\widetilde{G''^2}$.

3 Simulated Species Fractions

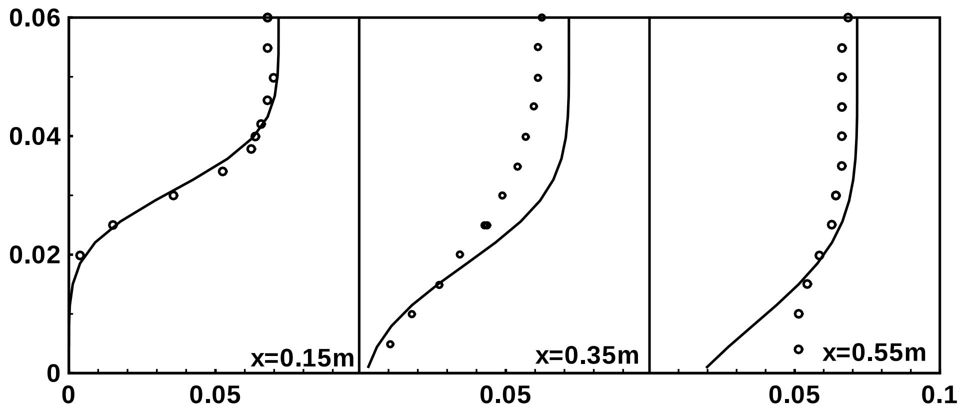

Figure 4: CO_2 molar fraction at three stations downstream of the flame holder.

The benefits of the level-set flamelet library approach in terms of accurate simulations of species is shown elsewhere. The effect of stretch rate on intermediate species, such as CO, has been investigated [7]. A transport modelling based on rates from the flamelet library has also been developed and shown beneficial for the simulation of species with slow formation paths, such as NO [6].

Here only an example, the CO_2 molar fraction, is compared to experimental data. The simulation shows a good match, with the exception of the region close to the wall at the

$x = 0.55m$ section. This discrepancy is probably due to a slight misplacement of the mean flame surface, which in turn is probably due to a misprediction of the turbulent flame speed here.

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