Turbulent Premixed Combustion with Flamelet Generated Manifolds in COMSOL Multiphysics®

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Abstract: In this paper a new method for turbulent combustion modeling is introduced in the Comsol environment. The method is called Flamelet Generated Manifolds (FGM). The method is based on the concept of flamelets, elemental reaction layers in combustion. The only hypothesis is that the turbulent combustion takes place in the Thin Reaction Zones regime (TRZ). A regime that normally is the case in gas turbines combustion and that assumes that the Kolmogorov scale of turbulence is able to penetrate the preheat zone of the reaction layers. However they are not able to penetrate the chemical conversion layer. This is because their energy is too small and their size is too large. An experimental case is simulated and an acceptable agreement is found.

Keywords: Turbulent combustion, Flamelets, Flamelet Generated Manifolds (FGM), Thin reaction zones regime (TRZ), Reynolds Averaged Navier-Stokes (RANS).

1. Introduction

In reacting flows, and especially in combustion, the problem is always attached to the representation of the chemistry. In general there are many reactions between lots of species. The current consensus on what is a good kinetic scheme involves 53 species and 325 reactions for simple methane combustion. Besides the fact that transport equations have to be solved for many species, also short time scales are involved making the problem stiff. This requires very many very small timesteps. At Eindhoven University we developed the method of Flamelet Generated Manifolds (FGM) [1]. It can be used for laminar and turbulent combustion and premixed and non-premixed situations.

Up till now FGM has been used in RANS, LES and DNS codes. Often the first two were involved with large commercial finite volume codes and the second two mainly in research codes. Here we present the use of the method in combination with Comsol. We will consider a turbulent case, being a burning backward facing step flow. This was investigated in a physical experiment published by El Banhawy et al. [2].

2. Use of COMSOL Multiphysics

The reactive backward facing step was operated burning methane at an equivalence ratio of 0.9.

The experimental geometry was 4 cm high and there was a restriction at the upper side of 2 cm. The depth of the physical geometry was 15.7 cm but in principle this is not relevant in this 2 dimensional simulation.

For solving the problem we defined 3 studies in a simulation. The first two were dedicated to solve the turbulent stationary cold flow with the k-ε model. The Reynolds number was 10,000 and the mean flow was 9 m/s. We did this in an incompressible mode. The density was set to 1.23 kg/m^3 and the viscosity was taken as 1.79 e-5 Pa s. A good value of the recirculation length was obtained.

In the 3rd step we solve an unsteady transport equation for the time, or ensemble, average progress variable. A flame brush is initialized on top of the steady cold flow result with a hyperbolic tangent profile of 2 cm thickness, centered at the step location.

$$c' = \frac{a\Delta^2}{12}\left(\frac{\partial c}{\partial x_i}\right)^2$$

Turbulence is represented by the variance of the progress variable with a gradient model. With the progress variable and its variance a manifold is approached to look up the source term of the progress variable, necessary to advance this equation in time. The manifold is pre-computed with the dedicated 1D chemistry code CHEM1D. A laminar flamelet at the correct equivalence ratio is taken and convoluted with a β-PDF chance distribution. This is done for all possible progress variable variances ranging from 0 to 0.25 for a scaled progress variable in the range 0 to 1.

3. Construction of the laminar manifold

Basically the construction of the laminar manifold consists of 5 steps and the extension to a turbulent manifold is done in an extra step. In the first step a laminar adiabatic flame is calculated in detail. This is done with our in house code CHEM1D. This code solves the system in physical space and the result is depicted in Figs 1 and 2, for a certain species and its source term respectively. Here CO_2 is taken as an example. It can be observed that the source term has a sharp peak and it can only be resolved by using many grid points.

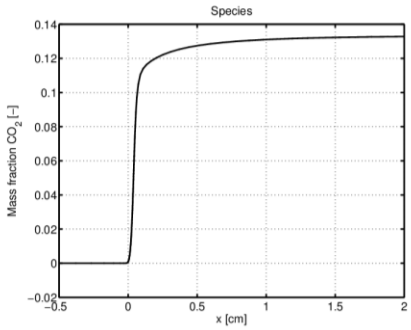

Figure 1. Laminar adiabatic methane flame with ϕ=0,9: species: CO_2

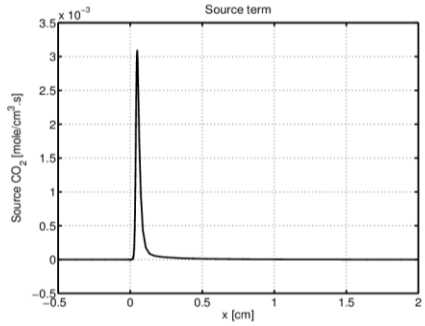

Figure 2. Laminar adiabatic methane flame with ϕ=0,9: source term of CO_2.

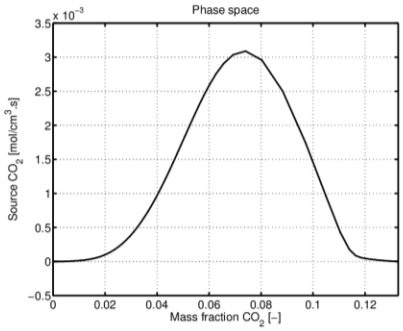

Figure 3. Laminar adiabatic methane flame with ϕ=0,9: phase space; source term as function of species.

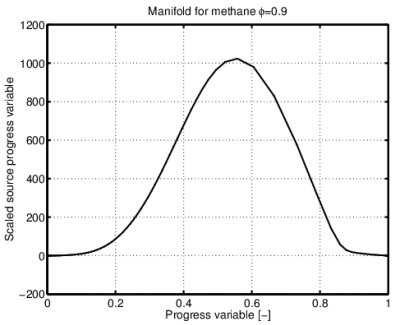

Figure 4. Laminar adiabatic methane flame with ϕ=0,9: phase space and rescaled.

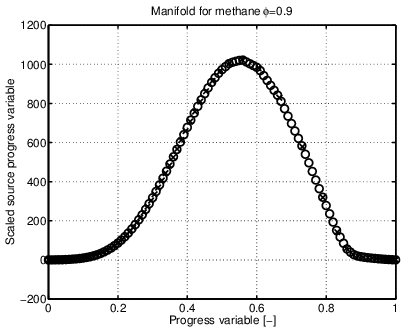

Figure 5. Laminar adiabatic methane flame with ϕ=0,9: phase space and rescaled and reinterpolated. Crosses are form the original physical space simulation, circles denote the new redistribution in phase space.

Now research on this fundamental laminar flame structure learns us that all other species are correlated uniquely with the profile of CO_2, in case of the combustion of methane at ϕ=0,9. This can be seen when plotting all species as function of CO_2. This means that we only have to

track a transport equation for CO_2. Usually we scale this variable from 0 to 1 and then we call it the progress variable, c. The mixture is unburnt if c=0 and burnt when c=1. So if we do a flame calculation we solve a transport equation for the progress variable only (all other species have a perfect correlation and can be retrieved as well). From now on the basic structure, with which the manifold will be filled, is called a flamelet.

However solving a transport equation for the progress variable requires knowledge about its source term ω_c. Therefore we go over to phase space and tabulate the source term from the laminar calculation as function of the carbon-dioxide mass fraction. This is given in Fig. 3. In Fig. 4 a scaling is carried out from mass fraction to progress variable. Furthermore to cover the flame structure properly a redistribution of numerical points is carried out, as can be seen in Fig. 5.

In principle now we have created a laminar manifold. Now we can simulate stationary and unsteady laminar combustion by using fluid dynamics software and incorporate the use of the manifold. Besides looking up the source term of the progress variable we can also add other species to the manifold as well. Examples are minor species, but also e.g. viscosity and density to improve the prediction. In principle we can also use a second progress variable to include for instance heat loss effects. In that case we need to solve a second progress variable in the CFD and in the manifold. In this study this is not yet implemented but instead we want to focus on implementation of turbulent combustion effects in Comsol.

4. Introducing turbulence

In the case of turbulent combustion we have to take into account turbulent events that can not be resolved. In the case of velocity fluctuations in RANS these phenomena are taken into account by the kinetic energy and kinetic energy dissipation of the unresolved temporal scales.

Usually the unresolved fluctuations of scalars are taken into account by their variances. So in this case we have the mean and variance of the progress variable, c and $'$. It is known that the extended probability of finding a certain value of c at a certain time is governed by a β-PDF. This kind of PDF exhibits a very rich behavior, comprising bimodal as well as uni-modal distributions for either burnt and unburnt but also constant probability and Gaussian like behavior for small variances. This especially considering the fact that it is supported by only 2 variables. The β-PDF can be calculated by c and c'. So we need an equation for both of them in the CFD. Furthermore we can derive the effective turbulent source term by convolution of the laminar source term with the PDF on the basis of all possible variances of the progress variable. This is done in Fig. 6. One can observe that at zero variance you have a laminar flame as depicted in Fig. 5. When the variance increases the source term decreases, as should be.

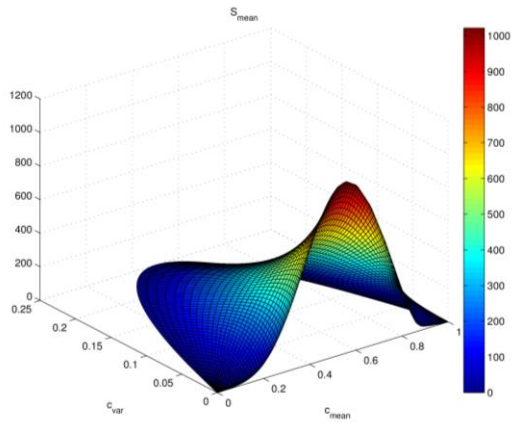

Figure 6. Turbulent manifold, Step 5 convoluted with a β-PDF.

By having a transport equation for the progress variable and the algebraic model for the variance we can now lookup the turbulent source term in the turbulent manifold, Fig.6.

5. Results

5.1 Cold flow results

The cold flow for this case is calculated and displayed in Fig. 7. This result is for the coarsest grid (on a physics controlled mesh). First a grid convergence study is performed to see what mesh would be required to obtain an accurate solution. The accuracy is measured by the length of the recirculation zone in terms of *h*. This is defined by the location where the (dividing) streamline is perpendicular to the wall and hits it. The value of *h* is both the height of the channel as well as the step-size. The mesh density was varied in 7 steps starting at "Extremely coarse" up to the "Finer" level, and the associated computation time varied between 1 minute and 1.5 hours.

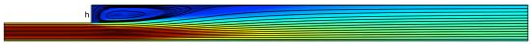

Figure 7. Backward facing step flow with Re=10,000, the recirculation length is l=6.65*h*

Table 1. Recirculation length of backward facing step flow with Re=10,000, as function of the numerical resolution.

Grid	Recirculation length
Extremely coarse	6.65 h
Extra coarse	7.75 h
Coarser	7.79 h
Coarse	7.78 h
Normal	7.50 h
Fine	7.30 h
Finer	7.25 h

The results of the grid study are given in Table 1. It must be noted that all the calculation are started from scratch. It seems that there is some convergence in the coarser grids approaching the Coarser and Coarse grids (starting from Extremely Coarse), but then going to higher resolution a new convergence takes place. A study on a fundamental change of the recirculation structure must be conducted to find the reason for this convergence behavior.

5.2 Reacting flow results

The reacting flow is defined by starting with the cold flow result. Then at the expansion position an initial progress variable profile is generated with a thickness of 2 cm. It is defined as

$$c(x,y,t) = c(x,y,o) = \left(\tanh\left(\frac{x}{0.02}\right) + 1\right)/2.$$

With this initial profile of progress and the cold flow profile on top we start a time-integration considering the evolution of the progress variable. Clearly the initial thickness is much too big because initially this thickness starts to contract and convect away from the flow expansion position. Anyway within some time the convection is balanced by the turbulent burning rate and a stationary state appears. This typically takes place in 0.05 secs.

Table 2. Burning length of burning backward facing step flow with Re=10,000, as function of the numerical resolution.

Grid	Burning length
Extremely coarse	+/- 10 h
Extra coarse	11.3 h
Coarser	11.0 h
Coarse	10.5 h
Normal	10.3 h
Fine	10.0 h
Finer	10.2 h

In Fig. 8 a result is given of the reacting backward facing step flow. The domain length is 0.5m. This is at the coarsest mesh. At the given time the simulation shows a more or less stationary flame front. At the top small fluctuations take place at the end tip of the flame brush. The burning length is defined as the position where the progress variable is 0.5 where the profile of it hits the wall. For different resolutions these values are given in Table 2 and a similar behavior as in the recirculation of the cold flow is observed for the convergence of the burning length. Typically the burning length extends a bit further then the recirculation at the other side of the channel.

With respect to numerical resources, the time integration of 0.1 sec of the progress variable took almost the same amount as the turbulent flow only, so also ranging from a minute to 1.5

hours. Furthermore it can be observed that a certain grid resolution is required to keep the progress variable that ranges from 0 to 1 within these physical bounds. In the Extremely coarse grid case you easily find overshoots of 20 % at both sides of the limits. At finer grids the overshoot near 1 lowers easily. Near zero it is harder to suppress the overshoot. Even at the finest grid there are still values of the order of 1%.

A direct comparison with the El Banhawy experiment is given by Fig. 9, where iso-contours of the amount of carbon-dioxide are given. These are directly comparable with the profiles of the progress variable in the calculations.

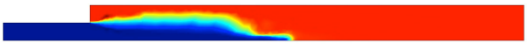

Figure 8. Spatial distribution at t=0.1 sec., of the progress variable, which is the scaled amount of CO_2, blue: fresh mixture, red: burnt

Figure 9. Mean value of CO_2 as reported by Al Banhawi et al.

Fig. 10 shows the coarsest grid to give an idea about grid-sizes used in this study. This grid is chosen because some particularities of the meshing can still be observed; the other meshes are too fine so that they all make up a black plane.

Figure 10. The most coarse mesh that is used in the calculations ('Extremely coarse').

Figure 11. Spatial distribution at t=0.1 sec., of the progress variable, which is the scaled amount of CO_2, blue: finest grid resolution case

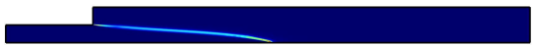

Figure 12. Spatial distribution at t=0.1 sec., of the source term of progress variable: finest grid resolution case

In order to have an overview of high the transient behaves from extremely coarse to finer also the extra coarse solution is given in Fig. 13.

Besides an experimental validation, additional numerical research is performed using OpenFOAM as well as CFX, to arrive at a numerical validation as well. It is observed that similar results are achieved with these numerical tools as well.

6. Improvements

The results of the present study are not bad. However some aspects of the physical phenomena have been excluded deliberately. We would like to introduce the omissions in a stepwise approach. The first step would be to include the expansion effect by using the gas law and introduce density or temperature in the manifold. Furthermore we like to introduce the heat loss at the walls, although we know from another study that the results for progress variable profile will not differ. Furthermore progress towards real 3D geometries and applying LES would be very nice.

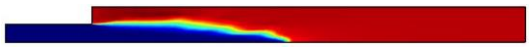

Figure 13. Spatial distribution at t=0.1 sec., of the source term of progress variable: Extra coarse grid resolution case

7. Conclusions

From the present approach and the resulting solutions it can be concluded that the combination of the Comsol flow solver with the FGM method for describing combustion is a good method to calculate reacting flows, presently for laminar and turbulent premixed flames. There seems to be no limitation to also do simulations for non-premixed cases where an equation of the so called mixture fraction has to be solved. Sufficient resolution or grid refinement needs to be used to keep the progress variable within its physical bounds.

8. References

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generated manifolds. Comb. Sci. Technol. 161, 113--137, (2000).
2. Y. El Banhawy, S. Sivasegaram & J.H. Whitelaw, Premixed, Turbulent Combustion of a Sudden Expansion Flow. Comb. & Flame, 50, 153-165,(1983).

9. Acknowledgements

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