Computational Methods for Turbulent Premixed Combustion

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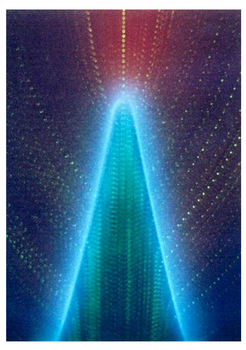
Turbulent premixed combustion

Turbulent flames occur in car engines, industrial burners and gas turbines among other applications. Turbulence, in contrast to laminar combustion, enhances mixing and thus enables higher rates of combustion. In premixed flames no diffusion of different species to form a combustible mixture has to be considered; a homogeneous air-fuel gas is already injected into the combustion chamber. Reaction complexity, involving numerous intermediates, requires reliable simulation models which reduce chemistry to a computationally processable extend.

Premixed Bunsen flame



Tip of a methane flame

Figure 1: *Premixed flame of a Bunsen burner*

The laminar burning velocity s_L incorporates all chemical aspects of a specific reaction in a laminar combustion process. When stretch, strain and curvature of the flame start to play a role at higher Reynolds numbers, s_L has to be modified to account for turbulent effects (Markstein length $\mathcal{L}$). The flame front is assumed to burn always in the normal direction of its current shape.
Large gradients of velocity, pressure, temperature, concentrations and material properties (e.g. density) are found within the reaction zone and their correct numerical reproduction is a challenging task. If the chemical length scales are small compared to the turbulent length scales (wrinkled and corrugated flame regimes), the reaction zone can be considered infinitely thin. Hence, burnt and unburnt gases are separated by the flame front which is modelled as a sharp interface. As a result, velocity and pressure can be described as discontinuous fields at the interface.

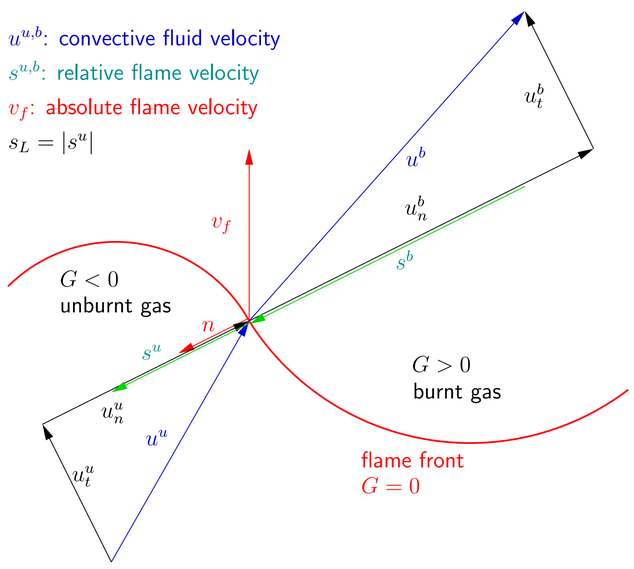


Figure 2: *Velocities at the flame front and G-function*

Both convection velocity and burning velocity determine the movement and propagation of the flame front (see Figure 2).

$$\mathbf{v}_f = \mathbf{u}^{u,b} + \mathbf{s}^{u,b} \quad \text{with} \quad \mathbf{s}^u = s_L \cdot \mathbf{n}.$$

Predicting turbulent flame fronts accurately with advanced Finite Element Methods is the objective of this project.

Level set function / G-function formulation

A variety of models and approaches to premixed combustion exist in the literature. The promising, so-called *G-equation* formulation is pursued in this project. It involves a level set function for the scalar G which is given by

$$\frac{\partial G}{\partial t} + \mathbf{v}_f \cdot \nabla G = 0, \qquad \text{with the normal vector } \mathbf{n} = -\frac{\nabla G}{|\nabla G|}$$

pointing into the unburnt domain.
A fixed constant *level* G_0 of this continuous function (usually $G_0 = 0$) defines the shape and position of the flame front. Off the respective iso-line (2D problem) or iso-surface (3D problem) the G-function has no physical meaning. It is defined as a *signed distance function*, being negative in the unburnt domain and positive in the burnt domain (see Figure 2).

$G < 0$	in the unburnt domain
$G = 0$	on the flame front
$G > 0$	in the burnt domain

If turbulent effects such as stretch, strain or curvature are taken into account, the G-equation becomes non-linear. Then it can be classified as a non-linear convection-diffusion equation.
The level set function G is convected by the fluid field ($G(\mathbf{u})$). Simultaneously, the location of the flame front affects the fluid field ($\mathbf{u}(G)$). Since velocity and pressure fields exhibit jumps at the flame interface, the FEM integration procedure over the fluid elements has to account for these discontinuities. Thus the computational combustion problem becomes a coupled two-field problem with the fluid field (Navier-Stokes equations) interacting with the level set field (G-equation). The fluid velocity and the position of the interface are the two quantities transferred between the two fields in an iterative procedure.

The eXtended Finite Element Method (XFEM)

Originating from crack growth problems in fracture mechanics, an extended version of the standard finite element method was developed. To handle the discontinuous velocity and pressure fields, the finite element solution spaces are enriched by discontinuous shape functions close to the interface. This means that all nodes k located next to the interface ($k \in N^{enr}$) are enriched by additional degrees of freedom $\mathbf{u}_k^{enr}$ and discontinuous functions $\phi_i(\mathbf{x}, t)$ (e.g. the Heaviside function):

$$\mathbf{u}^h(\mathbf{x}) = \sum_{k \in N^0} N_i(\mathbf{x}) \mathbf{u}_k^0 + \sum_{k \in N^{enr}} N_i(\mathbf{x}) \phi(\mathbf{x}, t) \mathbf{u}_k^{enr}.$$

Thus the jump of the variable (here: velocity $\mathbf{u}$) at the interface can be correctly represented as a sharp step from the unburnt to the burnt domain. Mass and momentum conservation across the flame front prescribe the magnitude of the velocity and pressure jumps according to the density decrease due to thermal expansion. These jumps represent constraints for the primary variables at the embedded interface and appear as boundary conditions in the system of equations:

$$\begin{aligned} [\mathbf{u}_n] &= -M \left[\rho^{-1}\right], \\ [\mathbf{u}_t] &= 0, \\ [p] &= M^2 \left[\rho^{-1}\right], \end{aligned}$$

where the brackets denote the jump (e.g. $[\mathbf{u}_n] = \mathbf{u}_n^b - \mathbf{u}_n^u$) and M denotes the mass flux across the flame front: $M = \rho^b(v_n^f - u_n^b) = \rho^u(v_n^f - u_n^u)$.
Lagrange Multipliers can be used to enforce these constraints across the interface in the system of equations. Additional terms are added to the weak form, so that the Lagrange Multipliers are brought as new unknowns into the system of equations. They have to be discretized with care. One option to do so is based on the *Distributed Lagrange Multiplier* technique.

Interface capturing

Integrating over a discontinous domain requires accurate capturing of the moving interface in every time step. Since fluid elements are bisected by the flame front, they have to be decomposed into integration cells to be integrated both over their unburnt and burnt domain. No new elements are added, but according to the value of the G-function within the element (signed distance property), the position of the flame front is determined and matching cells are found in a refinement procedure. Triangular integration cells around the interface are shown in Figure 3.

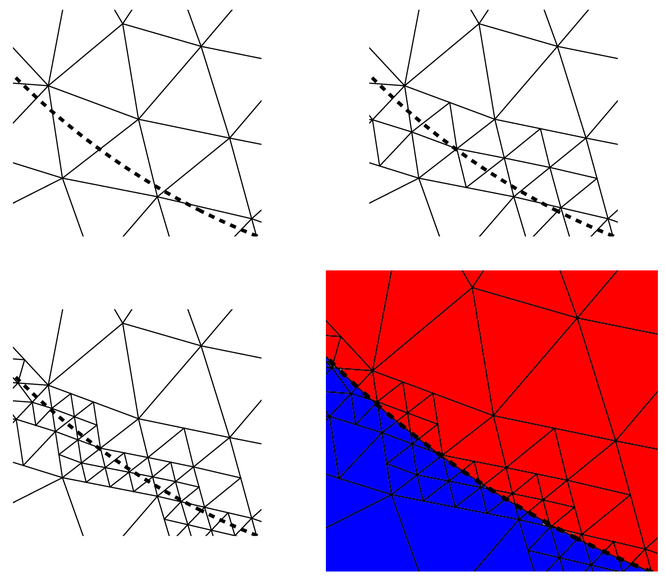
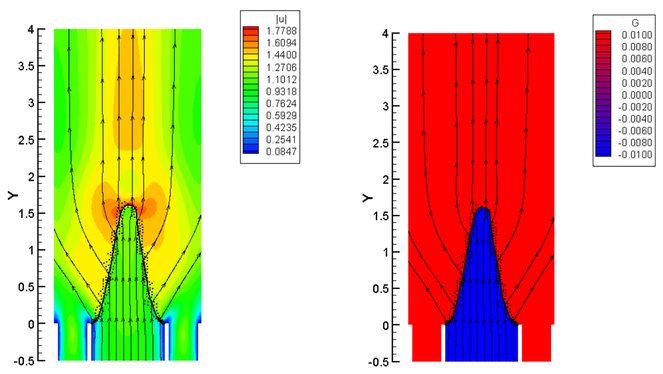


Figure 3: *Refinement of integration cells around the interface in 2D (blue: unburnt gas, red: burnt gas).*

Results

As initial numerical test cases, the Darrieus-Landau instability and a Bunsen burner flame have been simulated successfully in two dimensions. The growth rate of the perturbation of the instable planar flame front in the former example could be accurately reproduced. Exemplarily, the flow fields of the strongly curved Bunsen burner flame are depicted in Figure 4.



magnitude velocity field — G-function field

Figure 4: *Simulation results for a 2D bunsen burner flame. The streamlines show the acceleration of the flow across the flame front (compare to Figure 1).*

Current research projects

- Extension to three dimensions
- Development of a low-Mach-number solver
- Multiscale methods for large eddy simulation of turbulent premixed combustion

Literature

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- **XFEM for combustion**

  Van der Bos, Fedderik and Gravemeier, Volker. Numerical suimulation of premixed combustion using an enriched finite element method. *preprint submitted*, 2008.

Acknowledgement

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