

# Towards a generalized level-set/in-cell-reconstruction approach for accelerating turbulent premixed flames

Heiko Schmidt and Rupert Klein

Freie Universität Berlin

Berlin, Germany

heischmi@math.fu-berlin.de

## 1 Introduction

Due to the feedback between turbulence, gas expansion and flame front dynamics a continuous acceleration of premixed flames can occur. This process occurs, e.g., in large scale gas explosions and astrophysical nova- and supernova explosions. In the context of flame accelerations and DDT one is faced with rapidly changing thermodynamic, mean flow and turbulence conditions. One consequence is that the internal structure of the propagating combustion front will become inherently time dependent. In addition, the turbulence intensities associated with the accelerating flow will increase and grow rapidly beyond the characteristic burning velocity of a laminar flame. While turbulence intensities are still low, quasi laminar combustion takes place in thin “flamelets”. Turbulent combustion modelling will in this case aim at a description of the net flame surface area and of the mean quasi-laminar burning velocity in order to arrive at the net rate of unburnt gas consumption. If, on the other hand, turbulence intensities increase dramatically, then the turbulence-induced strains will locally distort the flamelet structures or even quench them completely and a more stochastic interaction between reaction, turbulent transport and diffusion becomes significant. As a consequence in these regimes, the “thin-reaction-zone regime” and the “well-stirred reactor” regime, very different effective turbulent combustion models must be employed, (*Peters*) [5, 6, 7].

Thus a numerical code that is supposed to cover the full range of combustion phenomena during flame acceleration and DDT must be capable of dynamically accessing the correct combustion model for all the regimes the solution passes through. Here we present a new numerical technique which—given such a set of (turbulent) combustion models—allows us to consistently represent laminar deflagrations, fast turbulent deflagrations as well as detonation waves. Supplemented with suitable DDT criteria, the complete evolution of a DDT process can be implemented in principle.

The original algorithm of *Smiljanovski et al.* [11] we started from, is shortly described in the next section. It implements a version of the flamelet model of turbulent premixed combustion combining level-set techniques with conservative finite volume methods for compressible flows. Our extensions of that method, allowing us to model the completely opposite well stirred reactor regime, are presented in section three. Finally, first results of the method are shown in section four. Sample implementations incorporate one combustion model based on a classical pdf-approach by *Pope* [8, 9] and one based on the linear eddy model (LEM) by *Kerstein* [2].

## 2 Basic Capturing/Tracking Hybrid Scheme

The deflagration capturing/tracking hybrid scheme of *Smiljanovski et al.* [11] allows a robust representation of turbulent high speed combustion. A deflagration is considered as a reactive discontinuity, which is embedded in a compressible surrounding flow. The flame surface is represented as the level set of a dynamically evolving scalar function. Flame flow coupling is realized by explicitly invoking Rankine-Hugoniot type jump conditions at the front. The original scheme uses the standard Rankine-Hugoniot conditions and an explicit burning rate law expressing the net unburnt gas mass consumption as a function of the unburnt gas conditions. This approach is strongly limited to conditions where such burning rate laws are available and where the standard Rankine-Hugoniot conditions are applicable.

The present developments are based on the reactive Euler equations in conservation form. Here the following notation is used:  $\rho$  is the density,  $\vec{v}$  the flow velocity,  $p$  the pressure,  $Q$  the specific heat release of a one-step chemical reaction,  $E$  the sum of internal and kinetic energy and  $\gamma$  the isotropic coefficient. With these conventions the governing equations read

$$\begin{aligned}\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho\vec{v}) &= 0 \\ \frac{\partial}{\partial t}(\rho\vec{v}) + \nabla \cdot (\rho\vec{v} \circ \vec{v} + p\mathbf{I}) &= 0 \\ \frac{\partial}{\partial t}(\rho E) + \nabla \cdot ([\rho E + p]\vec{v}) &= \rho Q\omega_Y\end{aligned}\tag{1}$$

In addition, the effect of turbulence can be taken into account through a standard  $k-\epsilon$  turbulence model as has been demonstrated by *Smiljanovski et al.*[11]. The chemical source term  $\rho Q\omega_Y$  in the balance equation for thermal and kinetic energy is determined by the net consumption of all energy carrying species. Here we consider a simple two-species system and let  $Y$  denote the mass fraction of the relevant energy carrying fuel species. Then the fuel consumption process is described by the following balance law:

$$\frac{\partial}{\partial t}(\rho Y) + \nabla \cdot (\rho\vec{v}Y) = -\rho\omega_Y\tag{2}$$

The detailed formulation for  $\omega_Y$  depends on the combustion mode considered. For resolved computations we presently use a standard Arrhenius rate law, but our general set-up allows for more sophisticated schemes when needed. The appropriate formulation of a reactive discontinuity is a delta distribution,  $\omega_Y = s \delta(G) |\nabla G|$ , where  $s$  is the flame speed, and  $G(\vec{x}, t)$  is a scalar function whose level set  $G = 0$  coincides with the flame surface. The evolution of the level set function is described by the well-known ‘‘G-equation’’ [13, 5]

$$G_t + (\vec{v} + s\vec{n}) \cdot \nabla G = 0\tag{3}$$

Modern numerical methods for level set equations are described, e.g., by *Sethian* in [10]. In our formulation we use a propagation scheme developed by *Terhoeven* and *Klein* [12], but any of the established methods can be used as well. Tracking the time evolution of a flame surface is only one part of a complete description of gasdynamic discontinuities. The second equally important issue is the description of flame-flow coupling. *Fedkiw et al.* [1] perform this by applying a ghost fluid method. *Smiljanovski et al.* [11] introduce a coupling scheme

that relies on “in-cell reconstruction”. The idea is to construct a finite volume scheme which, between time steps, updates only the averages of all conserved quantities for each grid cell. As described shortly, there is a way to reconstruct the two separate pre- and post-front substates within each “mixed-cell” from the grid cell averages by invoking the Rankine-Hugoniot type jump conditions. Given such a reconstruction, at each intersected cell interface there are two pairs of adjacent cells available: One pair of burnt gas conditions and one pair of unburnt gas conditions. Modern higher order shock capturing schemes use Riemann solvers to derive effective numerical fluxes for mass, momentum and energy from pairs of adjacent states at grid cell interfaces, [3]. An area-weighted superposition of these fluxes then allows an accurate numerical approximation of the net flux across the grid cell interface. A detailed description is given in [11].

### 3 Tracking Flames with Unsteady Internal Flame Structure

In the “well-stirred-reactor regime”, and also in the “thin-reaction-zone regime”, the assumption of a limitingly thin flame sheet is not applicable and, even though flame fronts will still tend to be compact, their internal dynamics must be accounted for. In order to systematically derive the necessary modifications to the existing numerical technique we reconsider the original derivation of the standard Rankine-Hugoniot conditions in a single space dimension first. Conservation of mass, momentum and energy is required for space-time control volume that encloses the discontinuity (see figure 1).

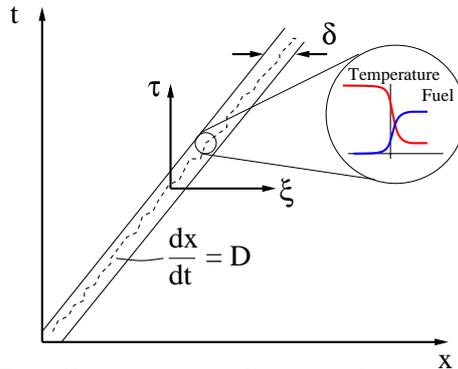


Figure 1: Travelling wave with unsteady internal structure

The general conservation law for the vector of conserved quantities, say  $\underline{U}$ ,

$$\frac{\partial}{\partial t} \underline{U} + \frac{\partial}{\partial x} (\underline{F}(\underline{U})) = 0 \quad (4)$$

is first transformed to a moving coordinate system with  $\xi = x - Dt$  and  $\tau = t$ . The transformed equation then reads

$$\frac{\partial}{\partial \tau} \underline{U} - D \frac{\partial}{\partial \xi} \underline{U} + \frac{\partial}{\partial \xi} (\underline{F}(\underline{U})) = 0 \quad (5)$$

When the structure is a stationary travelling wave, then for a suitable choice of  $D$  the time derivative  $\underline{U}_\tau$  vanishes identically and straight forward integration w.r.t.  $\xi$  yields the standard Rankine-Hugoniot conditions, with  $[\Phi] = (\Phi_b - \Phi_u)$  denoting a jump of a quantity  $\Phi$ ,

$$-D[\underline{U}] + [\underline{F}] = 0 \quad (6)$$

This, however, is a special situation and the general result of such an integration is

$$-D[U] + [F] = \int_0^L \frac{\partial}{\partial \tau} U d\xi \quad (7)$$

Our extension of the flame front algorithm may be summarized shortly as follows:

- In the in-cell reconstruction step, the homogeneous jump conditions are replaced by a discrete analogue of the inhomogeneous Rankine-Hugoniot conditions described above.
- The source term as well as the net unburnt gas mass consumption rate  $\rho_u s$  are computed by suitable integrations over the time dependent internal flame structure.
- A separate quasi-onedimensional computation module is running parallel to the overall flow solver and provides the needed flame structure information.
- The flame structure module receives its input from the “outer flow computation”. The coupling is done by forcing suitable integral expressions from the inner and outer computation to match.

## 4 First Results

To describe premixed combustion in a highly turbulent environment, we have adopted a turbulent premixed combustion model based on the pdf approach. The joint-pdf of enthalpy and species is solved using a Monte-Carlo method as described by *Pope* [8]. The flame structure model uses a reduced chemical model for Hydrogen combustion derived from a detailed chemical kinetic mechanism by *Maas* and *Warnatz* [4]. The description of turbulent flame propagation is decomposed into one operation (flame tracking) that locates the reaction zone and another (pdf-module) that determines its internal structure. Figure 2 displays an illustrative snapshot of the “inner” (pdf) and “outer” (tracked) solution.

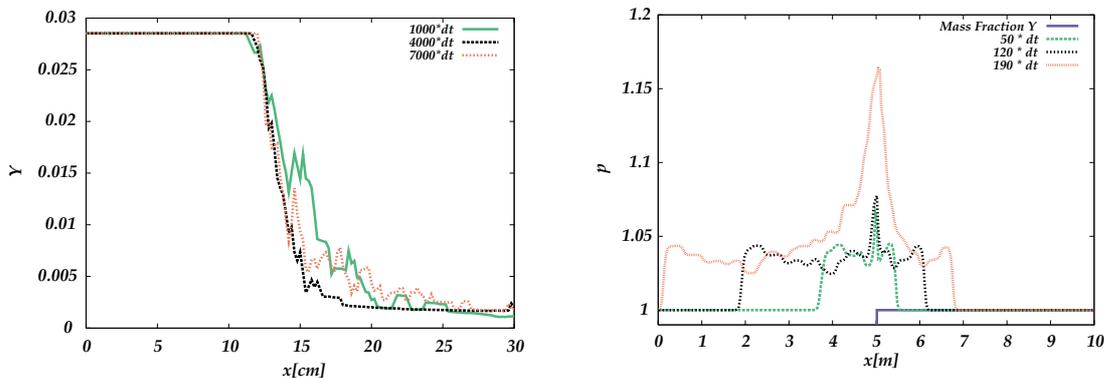


Figure 2: left: Fluctuating hydrogen mass fraction distribution with pdf-module; right: Pressure waves in the “outer” flow solution generated by sudden, highly turbulent combustion

To study the transition of a flame in the flamelet regime to burning in the distributed reaction zone regime we applied the LEM-method to an incompressible onedimensional subgrid flow solver. The advantage of the LEM method is that the small turbulent scales which might be crucial for turbulent combustion are fully resolved in one space dimension. Qualitative results for flame structures at different turbulent Reynolds numbers  $Re_t$  are plotted in figure 3.

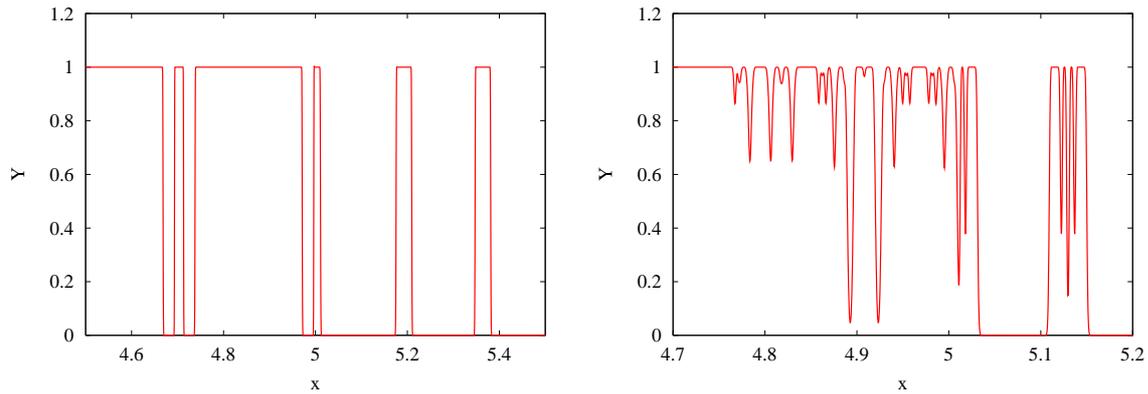


Figure 3: left: Fuel mass fraction distribution with linear eddy model for different turbulent Reynoldsnumbers. left:  $Re_t = 3$ ; right:  $Re_t = 10$

In our presentation we will summarize the numerical technique, explain some relevant details of the implementation of different turbulent combustion models, and discuss further applications including comparisons between combustion models and some recent results on flame – acoustic interactions.

## References

- [1] FEDKIW, R., ASLAM, T. AND XU, S.: *The Ghost Fluid Method for Deflagration and Detonation Discontinuities*, Journal of Computational Physics, **154**, 393-427, 1999
- [2] KERSTEIN, A. R.: *Linear-eddy model of turbulent transport ii*, Combustion and Flame, **75**, 397-413, 1989
- [3] LEVEQUE, R.: *Numerical Methods for Conservation Laws*, Birkhäuser, Basel, 1992
- [4] MAAS, U., WARNATZ, J.: *Ignition processes in hydrogen-oxygen mixtures*, Combustion and Flame, **74**, 53-69, 1988
- [5] PETERS, N.: *Laminar flamelet concepts in turbulent combustion*. The Combustion Institute, Pittsburgh, PA, USA, Volume **21**, 1291-1301, 1986
- [6] PETERS, N.: *The turbulent burning velocity for large scale and small scale turbulence*. Journal of Fluid Mechanics, 384:107-132, 1999
- [7] PETERS, N.: *Turbulent Combustion*. Cambridge University Press, 2000
- [8] POPE, S. B.: *A Monte Carlo method for the PDF equations of turbulent reactive flow*. Combustion Science and Technology 25:159-174, 1981
- [9] POPE, S. B.: *PDF methods for turbulent reactive flows*. Prog. Energy Combustion Science 11:119-192, 1985
- [10] SETHIAN, J. A.: *Level Set Methods and Fast Marching Methods*, Cambridge Univ. Press, 1999
- [11] SMILJANOVSKI, V., MOSER, V. AND KLEIN, R.: *A Capturing-Tracking Hybrid Scheme for Deflagration Discontinuities*, Journal of Combustion Theory and Modelling, 2(1):183-215, 1997
- [12] TERHOEVEN, P.: *Ein numerisches Verfahren zur Berechnung von Flammenfronten bei kleiner Machzahl*, Dissertation, RWTH-Aachen, Deutschland, 1998
- [13] WILLIAMS, F. A.: *Turbulent Combustion*, in J. Buckmaster, editor, The Mathematics of Combustion, 97-131, 1985