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A PRIORI TABULATION OF TURBULENT FLAME SPEEDS VIA A COMBINATION OF A STOCHASTIC MIXING MODEL AND FLAMELET GENERATED MANIFOLDS

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Abstract. *In the paper we propose a technique of an a priori turbulent flame speed tabulation (TFST) for a chosen parameter space. In a first step, stationary laminar flamelets are computed and stored over the progress variable following the ideas of flamelet generated manifolds (FGM). In a second step, the incompressible one-dimensional Navier-Stokes equations supplemented by the equation for the progress variable are solved on a grid that resolves all turbulent scales. Additionally, turbulent transport is implemented via the linear eddy model (LEM). The turbulent flame structures are solved until statistically stationarity of the mean of the turbulent flame speed is reached. The results are stored in a table that could be used by large scale premixed combustion models, e.g. front tracking schemes.*

1 INTRODUCTION

Due to the interaction between many different time and length scales, turbulent premixed combustion simulation remains a challenging task. Wheras the largest turbulent

scales and the slow chemical processes are resolvable, the small scale turbulence/chemistry interaction often has to be modelled. Therefore, the reactive Navier Stokes equations are filtered, dividing the original solution into resolved and unresolved parts, where the latter needs closure. This is commonly done using parameterizations that relate the unresolved parts to the resolved field. For example, the unresolved turbulent flame speed, s_t, is an important quantity[1].

This parameter is used in many approaches to premixed combustion modelling, e. g., level set methods, flame surface density models, and progress variable type approaches[2, 3, 4]. There are different possibilities to evaluate this property. The simplest and perhaps least physical is an algebraic expression, where often s_t is a function of the unburnt (indicated by subscript u) thermodynamic state and turbulent fluctuations, say

$$s_t = f(u', \boldsymbol{Y}_u, T_u, p_u), \tag{1}$$

where $u', \boldsymbol{Y}, T, p$ are the velocity fluctuation, species mass fraction, temperature and thermodynamic pressure. Additionally, curvature and stretch effects can be taken into account. More recent methods use so-called superparameterizations to determine s_t. Here a one dimensional microstructure evolution for turbulence chemistry interaction, e.g.[5], is forced by the resolved solution. Suitable integrals over the microstructure yield some of the needed closure terms like the turbulent flame speed. However this procedure is done "online", increasing the costs of such a computation considerably. Even for (stand alone) one dimensional calculations of turbulent premixed flames using detailed chemistry and the Linear Eddy Model[6] for the turbulent transport, the effort is quite high[7, 8].

In this paper, we propose a technique of a priori tabulation of s_t for a given reactive setup, e.g., geometric scales, reaction type, and so on. The different s_t for the table are computed evolving one-dimensional turbulent flame structures to a statistical steady state. The steady state assumption is tested with unit root tests and looking at the convergence of the mean. In the flame structure computation we use the Linear Eddy Model (LEM) for the turbulent transport and the idea of flamelet generated manifolds (FGM)[9] for the chemistry tabulation. Both are linked to an implicit solver for the one-dimensional Navier-Stokes equations[10].

As long as the smallest turbulent eddies do not enter the reaction zone, (laminar) chemistry and turbulence can be treated separately. For the chemistry we apply FGM[9] using the code from[8]. In a first step we compute steady one-dimensional laminar flamelets with detailed chemistry and tabulates all relevant chemical details as a function of suitable progress variables, e. g. CO_2 for a methane air mixture. Additional parameters for tabulation depending on their physical relevance could be stoichiometry, enthalpy, curvature, or flame stretch.

This paper proceeds as follows. In the next section, we outline our model approach using FGM and LEM. Some results of turbulent premixed flames for different equivalence ratios and turbulence intensities are presented in section 3. The paper ends with some conclusions on the approach and an outlook for further investigations.

2 MODEL FORMULATION

In fact, our model approach may be regarded as a combination of different stand alone models, where each of them tries to reduce the complexity of turbulent reactive multi dimensional flow computations. The main steps are (i) constructing a FGM table by computing a sequence of laminar flames to a steady state, (ii) computing a sequence of turbulent flame structures using LEM and a progress variable approach using the FGM results, (iii) extracting the turbulent burning speed for each run when convergence of the mean is reached, and (iv) building the turbulent data base.

2.1 Flamelet generated manifolds

To make the sequence of turbulent flame structure computations feasible, the flamelet generated manifold (FGM) method[9] is used to describe the reaction kinetics. FGM can be considered as a combination of the flamelet approach and the intrinsic low dimensional manifold (ILDM) method[11] and is similar to the flame prolongation of ILDM, FPI, introduced in[12]. FGM is applied similar to ILDM. However, the thermodynamic data base is not generated by applying the usual steady state relations, but by solving a set of one-dimensional convection-diffusion-reaction equations to a steady state of a laminar flame structure. The main advantage of FGM is that diffusion processes, which are important between the preheat zone and the reaction layer, are taken into account. This leads to an accurate method for premixed flames that uses fewer controlling variables than ILDM. The manifold used in this paper is based on a methane/air kinetic mechanism with 16 species and 36 reactions taken from[13]. Extension of the idea to more complicated mechanisms is straightforward[14].

2.2 Governing equations

To generate the manifolds, we solve the variable-density zero-Mach-number equations in one spatial dimension on a regular grid. The balance equations for species mass fractions, Y_s and temperature, T,t are

$$\rho\frac{\partial Y_s}{\partial t} + \rho u\,\frac{\partial Y_s}{\partial x} = -\frac{\partial j_s}{\partial x} + M_s\,\dot{\omega}_s, \tag{2}$$

$$\rho c_p\frac{\partial T}{\partial t} + \rho u c_p\,\frac{\partial T}{\partial x} = \frac{\mathrm{d}p}{\mathrm{d}t} - \frac{\partial q}{\partial x} - \sum_s j_s\,\frac{\partial h_s}{\partial x} - \sum_s h_s\,M_s\,\dot{\omega}_s, \tag{3}$$

with $s = 1, \ldots, n_s$. Here, ρ is the density, u the velocity, j_s the species diffusive flux, M_s the molecular weight of species s, $\dot{\omega}_s$ the chemical source term of species s, c_p the heat capacity at constant pressure, p the pressure, q the heat flux, and h_s the enthalpy of species s including the heat of formation. In the zero-Mach number limit the pressure is

spatially constant and we have a divergence constraint on the velocity

$$\begin{aligned}\frac{\partial u}{\partial x} &= -\frac{1}{\gamma\, p}\frac{\mathrm{d}p}{\mathrm{d}t} - \frac{1}{\rho c_p T}\left\{\frac{\partial q}{\partial x} + \sum_s j_s \frac{\partial h_s}{\partial x}\right\} \\ &\quad -\frac{1}{\rho}\sum_s \left\{\frac{M}{M_s}\frac{\partial j_s}{\partial x}\right\} + \frac{1}{\rho}\sum_s \left\{\frac{M}{M_s} - \frac{h_s}{c_p T}\right\}\dot{\omega}_s.\end{aligned} \tag{4}$$

Prescribing the inflow velocity and integrating (4) over the whole domain from $x = x_1$ to $x = x_1 + L$ yields the outflow velocity condition. The inflow condition is varied to balance s_t. The density is calculated from the equation of state for an ideal gas $p = \rho\, T \sum_s Y_s\, R_s$. It is important to note that similar to a DNS, in the LEM concept equations (2) and (3) need to resolve all spatial scales of a turbulent reacting flow. The velocity u in eq. (2) and (3) represents the flow velocity induced by dilatational effects due to compression, conduction, and chemical reactions as given by (4).

The zero-Mach-number equations are solved numerically using standard second-order finite-difference discretizations. The time integration of the stiff set of equations is performed using the DAE solver IDA of the SUNDIALS package[10]. Thermodynamic and transport properties as well as reaction rates are calculated using the C++ interface of the CANTERA software package[15]. Diffusion velocities are calculated using a mixture-based formulation with variable Lewis numbers for all species.

2.3 Linear eddy mixing to simulate turbulent transport

Solving equations (3) and (4) together with an equation for the progress variable Y_p,

$$\rho\frac{\partial Y_p}{\partial t} + \rho u\,\frac{\partial Y_p}{\partial x} = -\frac{\partial j_p}{\partial x} + M_p\,\dot{\omega}_p, \tag{5}$$

here CO_2, gives a simplified description for the computation of laminar flamelets. The source terms ω_s appearing in (3) and (4) are taken from the FGM tables, whereas all thermodynamical properties and mixture based transport coefficients are evaluated using the CANTERA package[15].

To extend the concept to turbulence we use a stochastic mixing model. In the LEM concept, turbulent advection is implemented explicitly by stochastic eddy events. Each eddy event involves a rearrangement of all scalar quantities using so-called 'triplet maps'. The effect of a triplet map is a three-fold compression of the scalar fields in a selected spatial interval whose size is denoted l. This map increases the scalar gradients within the selected interval, analogous to the effect of compressive strain in turbulent flow, without creating discontinuities. Three parameters are needed to implement the eddy events: eddy size l, eddy location within the domain, and the eddy event frequency. The eddy location is randomly sampled from a uniform distribution, and the eddy size is usually randomly sampled from a given size distribution (e. g., a distribution based on the Kolmogorov

inertial-range scaling). The integral length scale l_t and the turbulent diffusivity D_t are the required inputs to the LEM formulation used here. D_t is determined from $D_t = C_D\, l_t u'$ with $C_D = 1/15$ taken from[7, 8, 16, 17].

2.4 The turbulent burning speed

Each coupled LEM/hydrodynamic simulation yields a time series of turbulent premixed methane flame structures. The net mass burning rate is evaluated as an integral over the source terms of the progress variable

$$\rho_u s_t = \frac{1}{Y_{p,\zeta_1} - Y_{p,\zeta_0}} \int_{\zeta_0}^{\zeta_1} \rho \omega_p d\zeta, \tag{6}$$

where ρ_u is the density of the unburnt mixture, ζ the one-dimensional coordinate and ω_p the source term of the progress variable Y_p. Hence, the outcome of each LEM run is a time series $s_t(t)$. From this series one could construct the pdf of s_t for the given turbulence level and composition. Therefore one has to check for strong convergence, whereas for a steady mean value and variation, only weak convergence is required. Here, we focus on the latter. Wether one has fast or slow convergence depends strongly on the studied process. If the pdf is near gaussian, it is reached much faster than for, e.g. burning speeds of flames in the thin reaction zone regime, where a typical pdf(s_t) is far from Gaussian. Here, the runs are stopped when the mean converges.

3 RESULTS AND DISCUSSION

In this section we give an example of how to build a data base for the turbulent flame speed that later might be used by, e.g., a level set front tracking scheme or any other numerical method for premixed turbulent combustion using s_t. The main steps are (i) constructing a FGM table by computing a sequence of laminar flames to a steady state, (ii) computing a sequence of turbulent flame structures using LEM and a progress variable approach using the FGM results, (iii) extracting the turbulent burning speed for each run when (at least) weak statistical convergence is reached, and (iv) building the turbulent data base.

3.1 The FGM tabulation

In Figure 1 the tabulated chemical source term of the progress variable using the chemical reaction mechanism from[13] is plotted as a function of the progress variable CO_2 and stoichiometry ranging from lean to stoichiometric conditions. The source terms of all other variables are stored as well. Results of some laminar flame properties are summarized in Table 1.

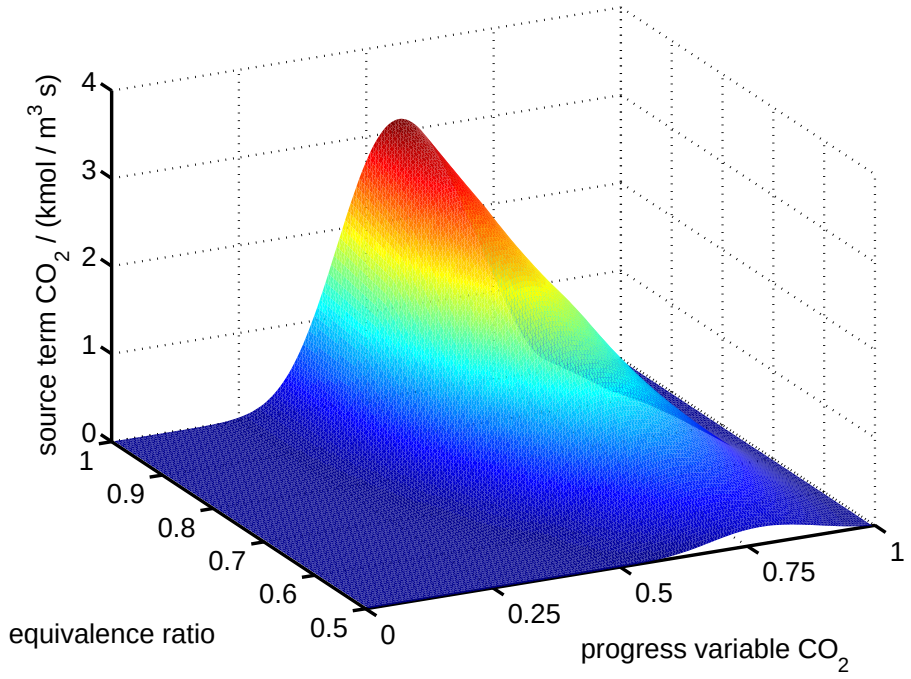

Figure 1: Tabulated source term of the progress variable, CO_2, over stoichiometry mixture using methane/air chemistry.

$\phi[-]$	0.5	0.6	0.7	0.8	0.9	1.0
l_F[mm]	1.348	0.746	0.556	0.478	0.449	0.442
s_l[cm/s]	6.57	14.11	21.60	27.81	31.97	33.63

Table 1: Laminar flame thickness (l_F) and the laminar burning speed (s_l) for different equivalence ratios ϕ.

3.2 Turbulent flame structures

In a second step we use the FGM generated source terms as an input for the LEM computations of the turbulent flame structures. This approach reduces the number of species within the LEM module to the number of progress variables of the FGM and allows a fast computation over a large parameter space.

Some snapshots of a calculated turbulent methane/air flame structure for $\phi = 0.7$, $l_t = 5$mm, and $u' = 0.6$m/s are plotted in Figure 2 (main species) and Figure 3 (minor species). Most of the lean structures can be seen as perturbed laminar flames, whereas the for the near stoichiometric a transitional behavior towards flamelet regime structures is observed.

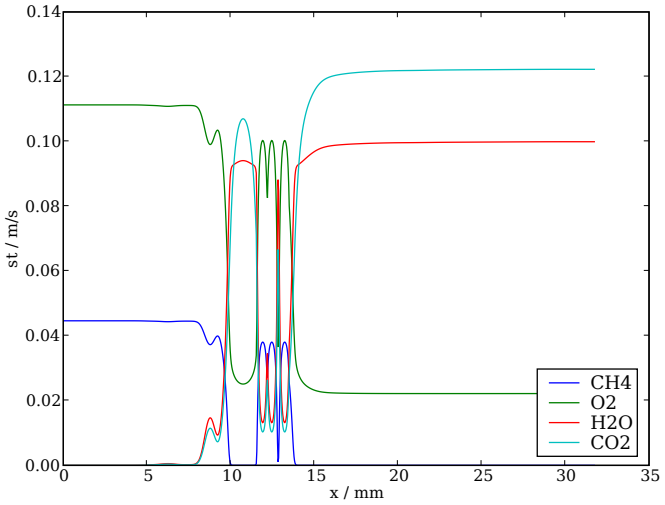

Figure 2: Snapshot of the major species of the turbulent methane flame for $\phi = 0.8$, $l_t = 5$mm, and $u' = 0.6$m/s

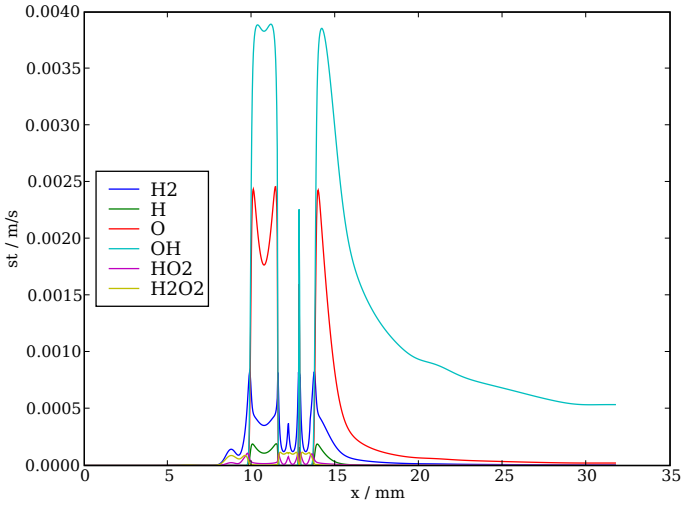

Figure 3: Snapshot of the minor species of the turbulent methane flame for $\phi = 0.8$, $l_t = 5$mm, and $u' = 0.6$m/s

3.3 The extracted turbulent burning speed and statistical convergence

From each flame structure we extract the turbulent burning speed via equation (6). A typical time history of s_t is plotted in Figure 4. The mean value of s_t in Figure 5 indicates that we have not reached a statistically steady state yet. To obtain strong

statistical convergence, one has to wait until the whole pdf of s_t is converged. Here, we stop the computations when the first moment is converged to a steady state. This constraint is even less than is normally meant by weak statistical convergence that requires convergence of mean and variance. But, it can be concluded from Figure 4. that, even to get convergence of the mean of s_t, it is necessary to calculate over a time interval that is quite large compared to the integral eddy turn over time. For the different set-ups, the factor ranges from about 20 to 200. Generally, this is a much longer time than standard DNS cases are run for, but DNS runs may be less intermittent. A run over a longer time interval is shown for a different case in Figure 6.

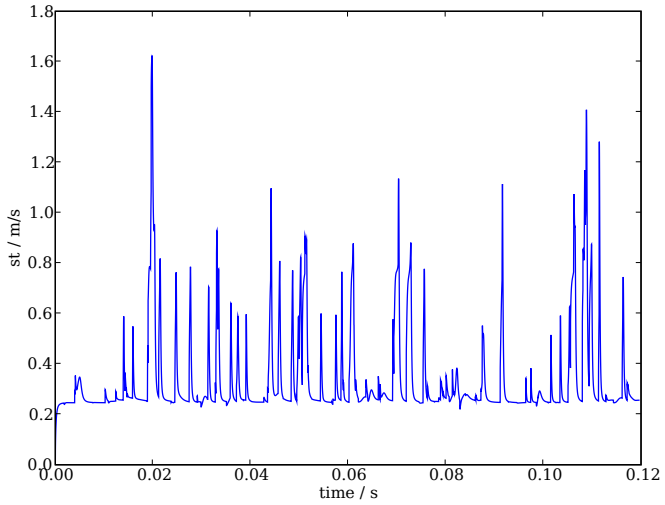

Figure 4: Time history of the turbulent burning velocity for the case $\phi = 0.7$, $l_t = 5$mm, and $u' = 0.6$m/s

3.4 A data base for the turbulent burning velocity

To construct a data base of s_t values, we repeat the turbulent flame structure computations for different turbulent fluctuations and stoichiometry values. The tabulated region is shown in the well known Borghi diagram, see Figure 7.

The exact coordinates of the computations which depend in our example on stoichiometry and turbulence conditions are summarized in Table 2.

The results for the mean turbulent burning speed are shown in Table 3 and the interpolated manifold is plotted in Figure 8.

The interpolated s_t shows a monotone behaviour. Highest values are reached for the stoichiometric flame at the highest turbulence intensity. For lean mixtures changes in turbulence levels have a smaller effect than for fuel richer flames. This could be explained by the different laminar flame thicknesses.

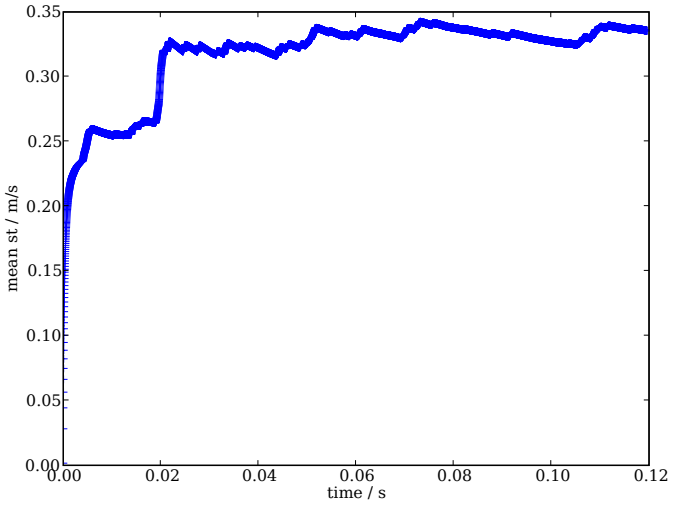

Figure 5: Time history of the mean turbulent burning velocity for the case $\phi = 0.7$, $l_t = 5$mm, and $u' = 0.6$m/s

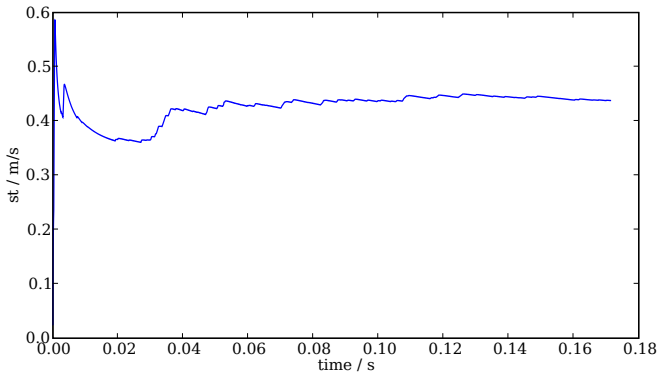

Figure 6: Time history of the mean turbulent burning velocity for the case $\phi = 0.9$, $l_t = 5$mm, and $u' = 0.6$m/s

u'[m/s]\ϕ	0.5	0.6	0.7	0.8	0.9	1.0
0.33	5.02; 3.71	2.34; 6.70	1.53; 8.99	1.19; 10.46	1.03; 11.14	0.98; 11.31
0.66	10.04; 3.71	4.68; 6.70	3.06; 8.99	2.37; 10.46	2.06; 11.14	1.96; 11.31
0.99	15.07; 3.71	7.02; 6.70	4.58; 8.99	3.56; 10.46	3.10; 11.14	2.94; 11.31
1.30	19.79; 3.71	9.21; 6.70	6.02; 8.99	4.67; 10.46	4.07; 11.14	3.87; 11.31

Table 2: Coordinates (y; x) = $s_t/u'; l_t/l_F$ in the Borghi diagram for the cases considered

4 Summary and Outlook

A technique of an a priori turbulent flame speed tabulation (TFST) for a chosen parameter space is presented. In a first step, stationary laminar flamelets are computed and

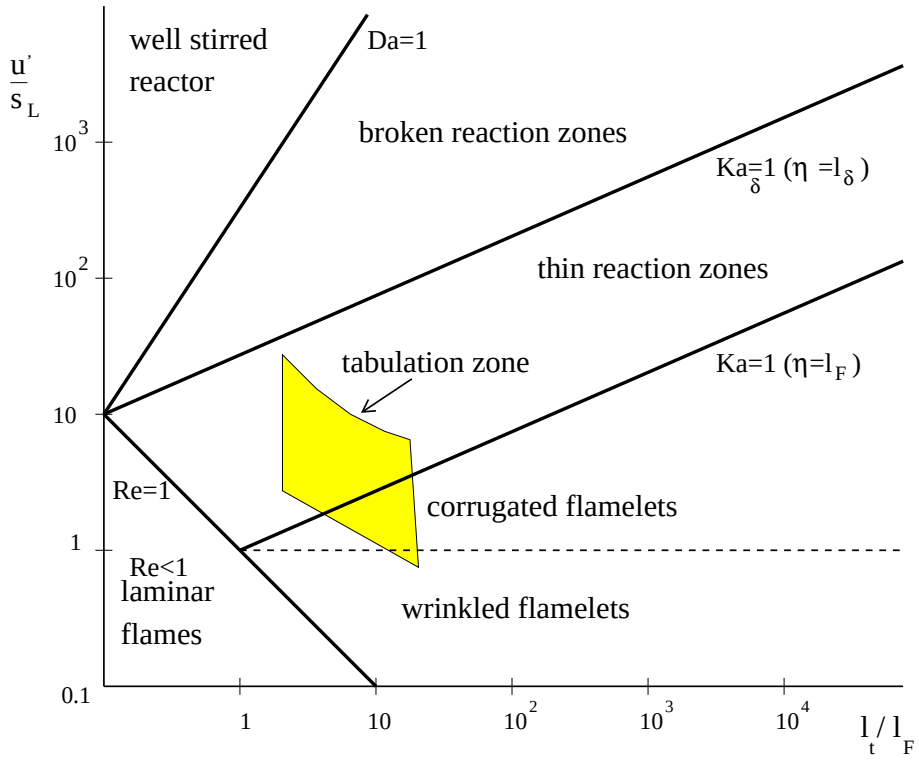

Figure 7: Diagram of turbulence/chemistry regimes

u'[cm/s] \ ϕ	0.5	0.6	0.7	0.8	0.9	1.0
0.33	8.62	17.28	29.02	33.50	38,59	38,65
0.66	9.28	20.95	27.23	38.34	42.53	43,52
0.99	9.70	22.45	37.29	45,32	48.01	50,82
1.30	10.94	23.72	40.32	45.94	53.72	56.75

Table 3: The mean turbulent burning speed, s_t, as a function of stoichiometry and velocity fluctuations for the different calculations

stored over a chosen progress variable following the ideas of flamelet generated manifolds (FGM). In a second step, the incompressible one-dimensional Navier-Stokes equations supplemented by the equation for the progress variable are solved on a grid that resolves all turbulent and chemical scales. In addition, turbulent transport is implemented via the linear eddy model (LEM). The turbulent flame structures are solved until a statistically stationary state for the mean flame speed is reached. The time for convergence is quite high compared with eddy turnover times. This is due to fact that statistically rare events, like the big turbulent eddies, have a major impact on the flame structure and the burning speed. Only after a higher number of these events does the mean value converge. The results are stored in a table that could be used by large scale premixed combustion models, e.g. front tracking schemes.

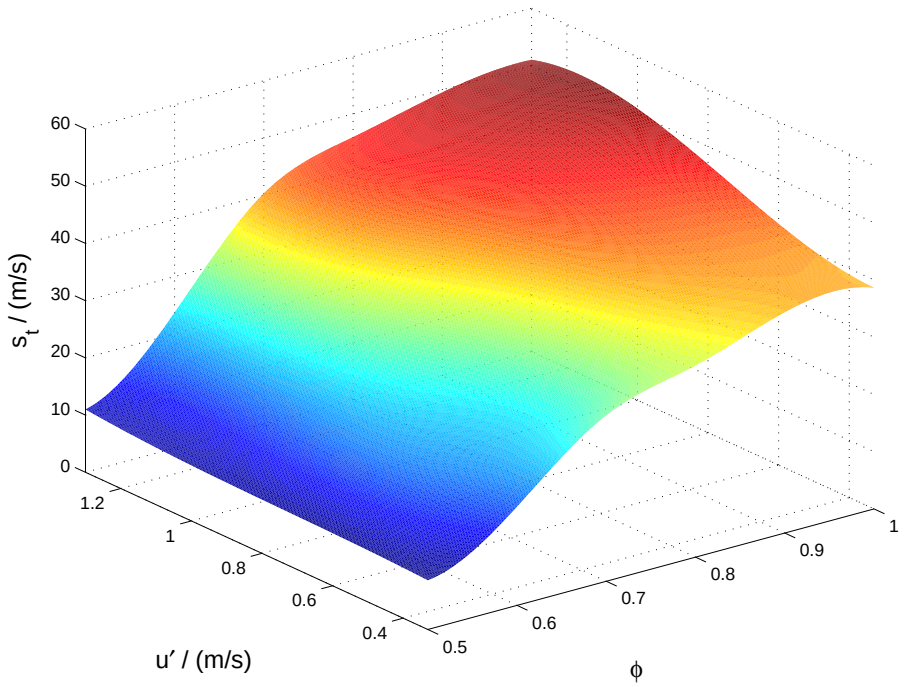

Figure 8: Tabulated turbulent burning speed as a function of stoichiometry and velocity fluctuations

In the future, the idea can easily be extended to other parametric dependencies of the turbulent burning speed. This could be, e.g, stretch, curvature, and integral length scale effects. Our strategy could also be applied for building a pdf of subgrid scale (SGS) s_t values which could then be used in large eddy simulations (LES). The pdf can be build by averaging the LEM solutions over time intervals corresponding to LES time steps. Finally, the LES samples the s_t values from the constructed pdf.

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