

Lecture 12

The Level Set Approach for Turbulent Premixed Combustion

A model for premixed turbulent combustion, based on the **non-reacting scalar G** rather than on the progress variable, has been developed in recent years.

It avoids complications associated with counter-gradient diffusion and, since G is non-reacting, there is **no need for a source term closure**.

An equation for G can be derived by considering an iso-scalar surface

$$G(\mathbf{x}, t) = G_0$$

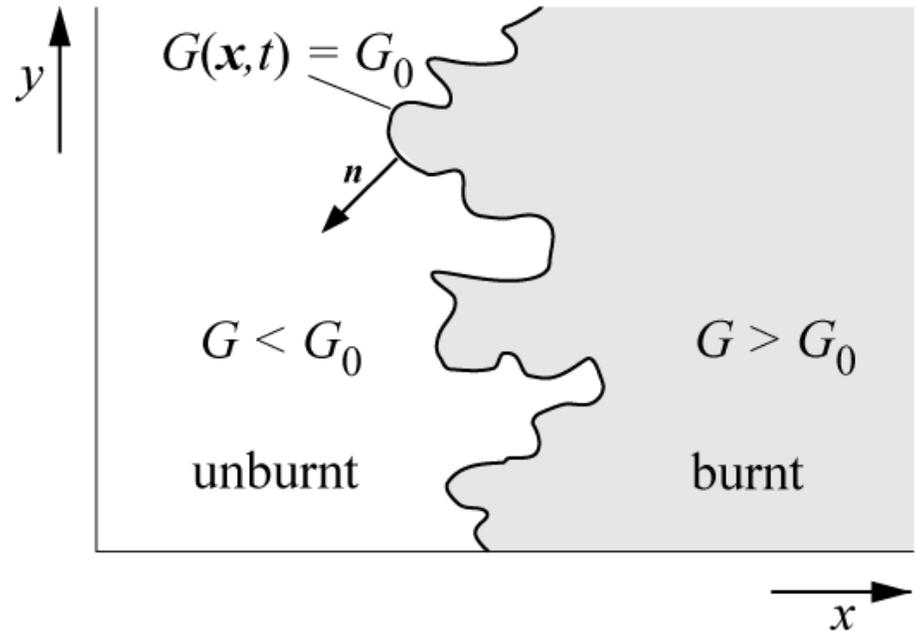
This surface divides the flow field into two regions where

$G > G_0$ is the region of burnt gas

and

$G < G_0$ is that of the unburnt mixture.

The choice of G_0 is arbitrary, but fixed for a particular combustion event.



We introduce the vector normal to the front in direction of the unburnt gas, as by

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|}$$

In a general three-dimensional flow field the propagation velocity dv_f/dt of the front is equal to the sum of the flow velocity and the burning velocity in normal direction

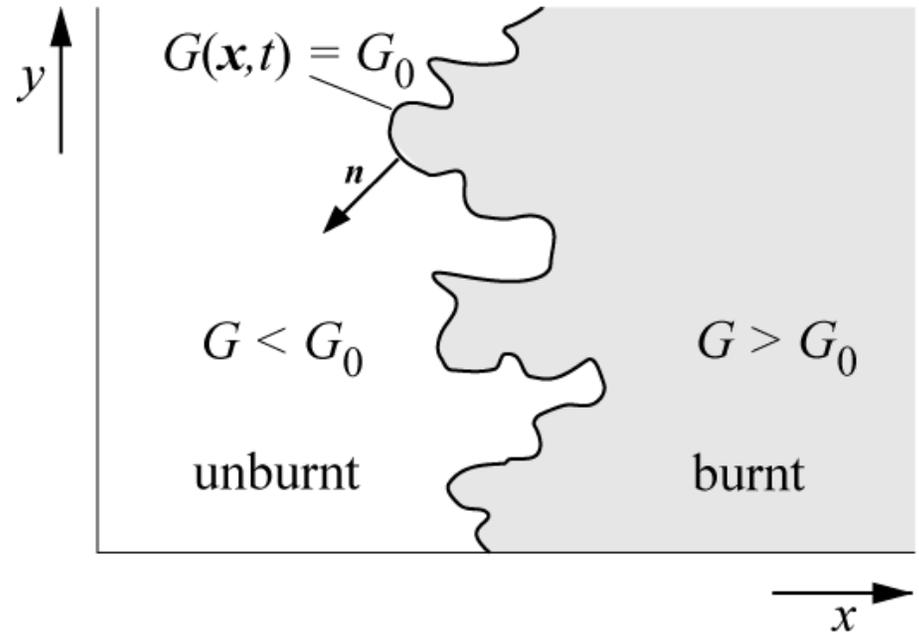
$$\frac{d\mathbf{x}_f}{dt} = \mathbf{v}_f + \mathbf{n} s_L$$

A field equation can now be derived by differentiating

$$G(\mathbf{x}, t) = G_0.$$

with respect to time

$$\frac{\partial G}{\partial t} + \nabla G \cdot \frac{d\mathbf{x}_f}{dt} = 0$$



Introducing

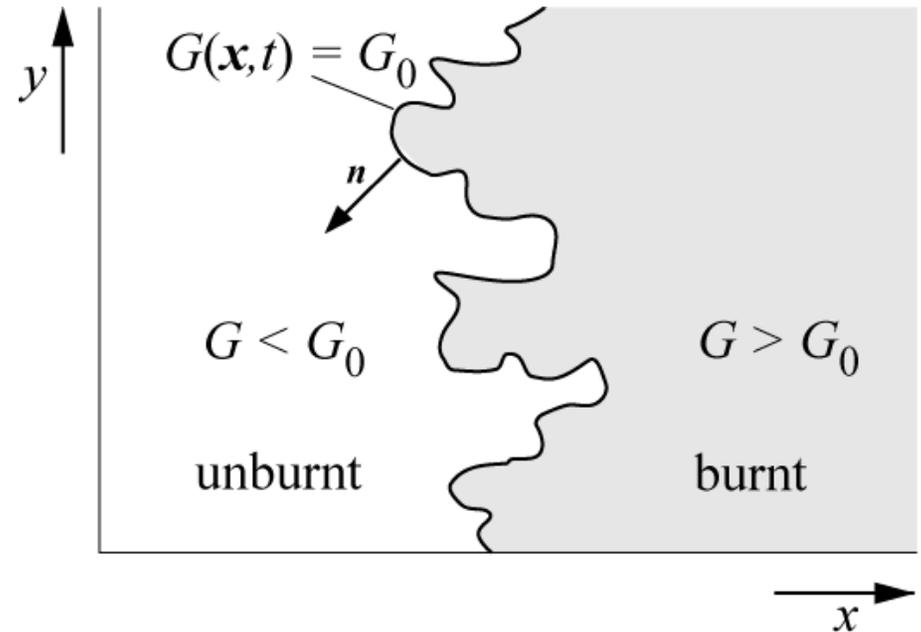
$$\frac{d\mathbf{x}_f}{dt} = \mathbf{v}_f + \mathbf{n} s_L \quad \text{and} \quad \nabla G = -\mathbf{n} |\nabla G|$$

one obtains the field equation

$$\frac{\partial G}{\partial t} + \mathbf{v}_f \cdot \nabla G = s_L |\nabla G|$$

This equation was introduced by Williams (1985).

It is known as the G -equation.



The G -equation is applicable to thin flame structures which propagate with a well-defined burning velocity.

It therefore is well-suited for the description of premixed turbulent combustion in the **corrugated flamelets** regime, where it is assumed that the laminar flame thickness is smaller than the smallest turbulent length scale, the Kolmogorov scale.

Therefore, the entire flame structure is embedded within a locally quasi-laminar flow field and the laminar burning velocity remains well-defined.

The G -equation.

$$\frac{\partial G}{\partial t} + \mathbf{v}_f \cdot \nabla G = s_L |\nabla G|$$

contains a local and a convective term on the l.h.s, a propagation term with the burning velocity s_L on the r.h.s but no diffusion term.

G is a scalar quantity which is defined at the flame surface only, while the surrounding G -field is not uniquely defined.

This originates simply from the fact that the kinematic balance

$$\frac{d\mathbf{x}_f}{dt} = \mathbf{v}_f + \mathbf{n} s_L$$

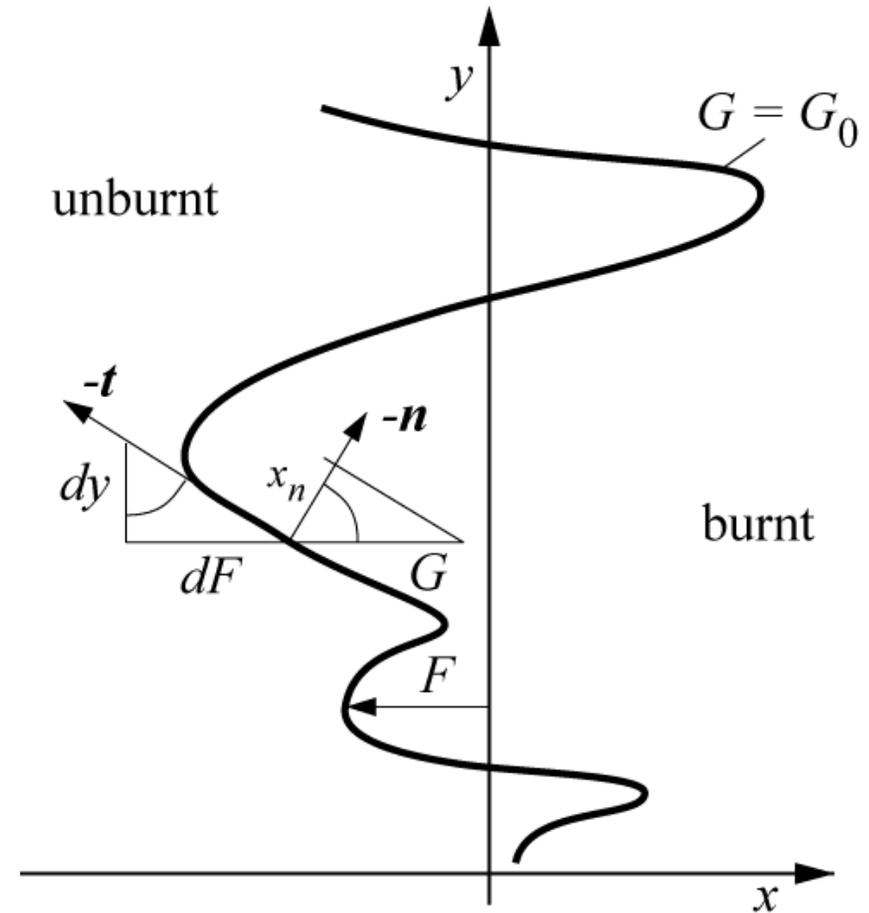
describes the motion of a point on a two-dimensional surface while the G -equation is an equation in three-dimensional space.

The value of σ value depends on the ansatz that is introduced in solving a particular problem using the G -equation.

For illustration purpose we choose as ansatz for the G -field

$$G(x, t) - G_0 = x + F(y, z, t)$$

Thereby the flame front displacement $F(y, z, t)$ is assumed to be a single-valued function of y and z as shown for a two-dimensional case.

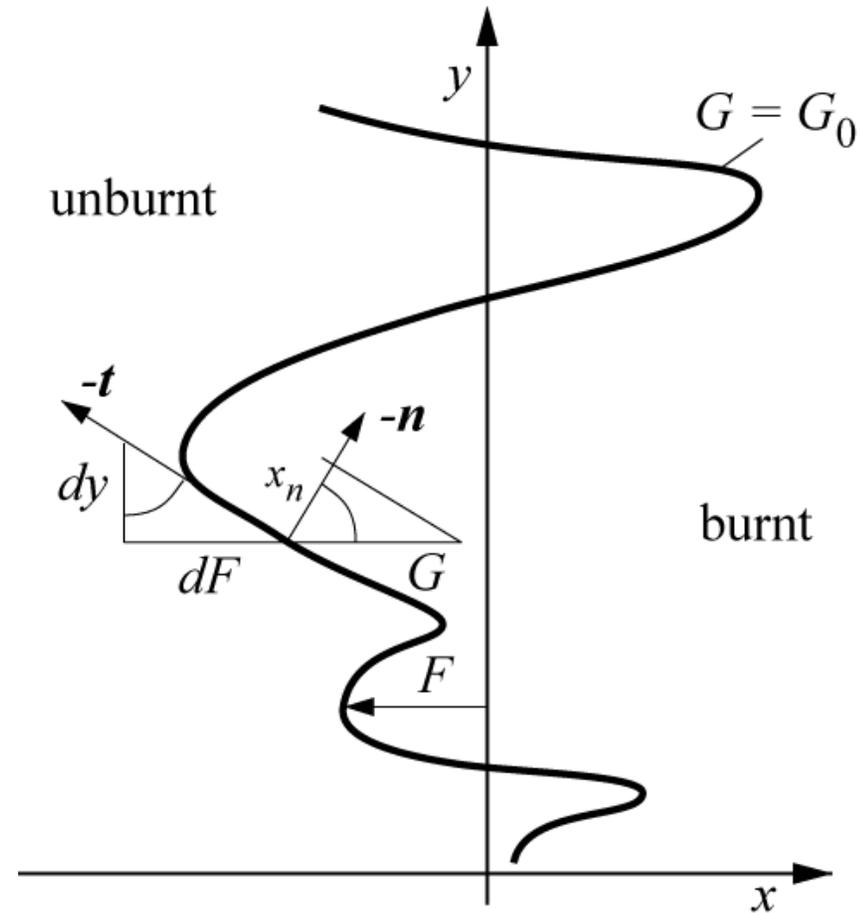


This assumption does not allow for multiple crossings of the flame surface.

Note that x is the co-ordinate normal to the mean flame surface.

G is measured in x -direction.

It is also seen that the angle β between the flame normal direction $-n$ and the x -axis is equal to the angle between the tangential direction t and the y -axis.



In the corrugated **flamelets regime** the reactive-diffusive flame structure is assumed to be thin compared to all length scales of the flow.

Therefore it may be **approximated by jumps** of temperature, reactants and products.

For such a very thin flame structure the iso-scalar surface $G(\mathbf{x},t)=G_0$ is often defined to lie in the unburnt mixture immediately ahead of the flame structure.

Since

$$\frac{\partial G}{\partial t} + \mathbf{v}_f \cdot \nabla G = s_L |\nabla G|$$

was derived from

$$\frac{d\mathbf{x}_f}{dt} = \mathbf{v}_f + \mathbf{n} s_L$$

the velocity \mathbf{v}_f and the burning velocity s_L are values defined at the surface $G(\mathbf{x},t)=G_0$.

In numerical studies values for these quantities must be assigned in the entire flow field.

The flow velocity \mathbf{v}_f can simply be replaced by the local flow velocity \mathbf{v} , a notation which we will adopt in the following.

The burning velocity s_L appearing in

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L |\nabla G|$$

may be modified to account for the effect of flame stretch.

Performing two-scale asymptotic analyses of corrugated premixed flames, Pelce and Clavin (1982), Matalon and Matkowsky (1982) derived **first order correction** terms for **small curvature and strain**.

The expression for the modified burning velocity becomes

$$s_L = s_L^0 - s_L^0 \mathcal{L} \kappa - \mathcal{L} S$$

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$$s_L = s_L^0 - s_L^0 \mathcal{L} \kappa - \mathcal{L} S$$

Here s_L^0 is the burning velocity of the unstretched flame, κ is the **curvature** and S is the **strain rate**.

The **flame curvature** is defined in terms of the G -field as

$$\kappa = \nabla \cdot \mathbf{n} = \nabla \cdot \left(-\frac{\nabla G}{|\nabla G|} \right) = -\frac{\nabla^2 G - \mathbf{n} \cdot \nabla(\mathbf{n} \cdot \nabla G)}{|\nabla G|}$$

where

$$\nabla(|\nabla G|) = -\nabla(\mathbf{n} \cdot \nabla G)$$

has been used. The flame curvature is positive if the flame is convex with respect to the unburnt mixture.

The **strain rate** imposed on the flame by velocity gradients is defined as

$$S = -\mathbf{n} \cdot \nabla \mathbf{v} \cdot \mathbf{n}.$$

The Markstein length \mathcal{L} is of the same order of magnitude and proportional to the laminar flame thickness.

The ratio \mathcal{L}/ℓ_F is called the **Markstein number**.

For the case of a **one-step reaction with a large activation energy**, constant transport properties and a constant heat capacity, the Markstein length with respect to the unburnt mixture reads, for example

$$\frac{\mathcal{L}_u}{\ell_F} = \frac{1}{\gamma} \ln \frac{1}{1-\gamma} + \frac{Ze(Le-1)(1-\gamma)}{2\gamma} \int_0^{\gamma/(1-\gamma)} \frac{\ln(1+x)}{x} dx$$

This expression was derived by Clavin and Williams (1982) and Matalon and Matkowsky (1982).

Here

$$Ze = E(T_b - T_u) / \mathcal{R}T_b^2$$

is the Zeldovich number, where E is the activation energy, and Le is the Lewis number of the **deficient reactant**.

The Lewis number is approximately unity for methane flames and larger than unity for fuel-rich hydrogen and all fuel-lean hydrocarbon flames other than methane.

Therefore, since the first term on the r.h.s. of

$$\frac{\mathcal{L}_u}{l_F} = \frac{1}{\gamma} \ln \frac{1}{1-\gamma} + \frac{Ze(Le-1)(1-\gamma)}{2\gamma} \int_0^{\gamma/(1-\gamma)} \frac{\ln(1+x)}{x} dx$$

is always positive, the **Markstein length is positive** for most practical applications of premixed hydrocarbon combustion, occurring typically under stoichiometric or fuel-lean conditions.

Whenever the **Markstein length is negative**, as in lean hydrogen-air mixtures, diffusional-thermal instabilities tend to increase the flame surface area.

This is believed to be an important factor in gas cloud explosions of hydrogen-air mixtures.

Although turbulence tends to dominate such local effects the combustion of diffusional-thermal instabilities and instabilities induced by gas expansion could lead to strong flame accelerations.

Introducing

$$s_L = s_L^0 - s_L^0 \mathcal{L} \kappa - \mathcal{L} S$$

into the G -equation it may be written as

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G| - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

Here

$$\mathcal{D}_{\mathcal{L}} = s_L^0 \mathcal{L}$$

is defined as the [Markstein diffusivity](#).

The curvature term adds a second order derivative to the G -equation.

This avoids the formation of **cusps** that would result from

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G|$$

for a constant value of s_L^0 .

For positive Markstein length the mathematical nature of is that of a **Hamilton-Jacobi equation** with a **parabolic** second order differential operator coming from the curvature term.

While the solution of the G -equation with a constant s_L^0 is solely determined by specifying the initial conditions, the parabolic character of

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G| - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

requires that the boundary conditions for each iso-surface G must be specified.

The Level Set Approach for the Thin Reaction Zones Regime

The Eq.

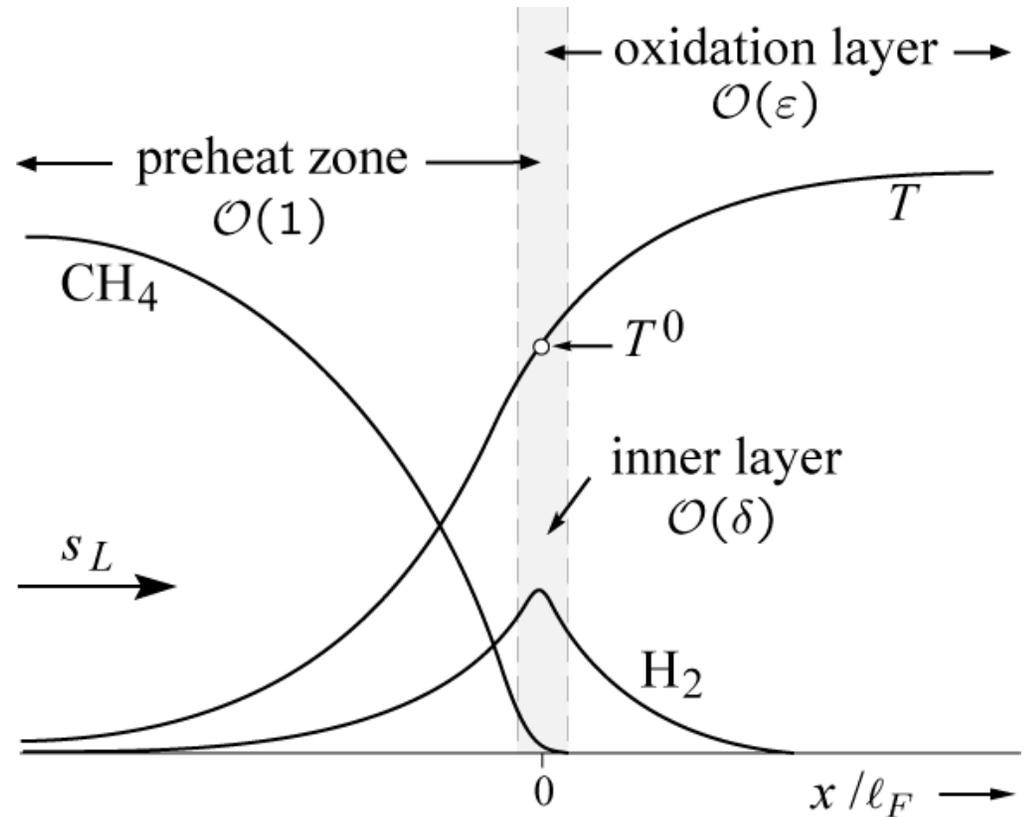
$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G| - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

is suitable for thin flame structures in the corrugated flamelets regime, where the entire flame structure is quasi-steady and the laminar burning velocity is well defined, but not for the thin reaction zones regime.

We now want to derive a level set formulation for the case, where the flame structure cannot be assumed quasi-steady because Kolmogorov eddies enter into the preheat zone and cause unsteady perturbations. The resulting equation will be valid in the thin reaction zones regime.

Since the inner layer shown previously is responsible for maintaining the reaction process alive, we define the thin reaction zone as the inner layer.

The location of the inner layer will be determined by the iso-scalar surface of the temperature setting $T(\mathbf{x}, t) = T^0$, where T^0 is the inner layer temperature.



The temperature equation reads

$$\rho \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \nabla T = \nabla \cdot (\rho D \nabla T) + \omega_T$$

where D is the thermal diffusivity ω_T the chemical source term.

Similar to Eq.

$$\frac{\partial G}{\partial t} + \nabla G \cdot \frac{d\mathbf{x}_f}{dt} = 0$$

for the scalar G the iso-temperature surface $T(\mathbf{x}, t) = T^0$ satisfies the condition

$$\left. \frac{\partial T}{\partial t} + \nabla T \cdot \frac{d\mathbf{x}}{dt} \right|_{T=T^0} = 0$$

Gibson (1968) has derived an expression for the displacement speed s_d for an iso-surface of non-reacting diffusive scalars.

Extending this result to the reactive scalar T this leads to

$$\left. \frac{d\mathbf{x}}{dt} \right|_{T=T^0} = \mathbf{v}_0 + \mathbf{n} s_d$$

where the displacement speed s_d is given by

$$s_d = \left[\frac{\nabla \cdot (\rho D \nabla T) + \omega_T}{\rho |\nabla T|} \right]_0$$

Here the index 0 defines conditions immediately ahead of the thin reaction zone.

The normal vector on the iso-temperature surface is defined as

$$\mathbf{n} = -\frac{\nabla T}{|\nabla T|} \Big|_{T=T^0}$$

We want to formulate a G -equation that describes the location of the thin reaction zones such that the iso-surface $\mathbf{T}(\mathbf{x},t)=T^0$ coincides with the iso-surface defined by $G(\mathbf{x},t)=G^0$.

Then the normal vector defined by

$$\mathbf{n} = -\frac{\nabla T}{|\nabla T|} \Big|_{T=T^0}$$

is equal to that defined by

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|}$$

and also points towards the unburnt mixture.

Using $n = -\frac{\nabla G}{|\nabla G|}$ and $\frac{\partial G}{\partial t} + \nabla G \cdot \frac{d\mathbf{x}_f}{dt} = 0$

together with

$$s_d = \left[\frac{\nabla \cdot (\rho D \nabla T) + \omega_T}{\rho |\nabla T|} \right]_0$$

leads the G -equation

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = \left[\frac{\nabla \cdot (\rho D \nabla T) + \omega_T}{\rho |\nabla T|} \right]_0 |\nabla G|$$

Peters et al. (1998) show that the diffusive term appearing in the brackets in this equation may be split into one term accounting for curvature and another for diffusion normal to the iso-surface

$$\nabla \cdot (\rho D \nabla T) = -\rho D |\nabla T| \nabla \cdot \mathbf{n} + \mathbf{n} \cdot \nabla (\rho D \mathbf{n} \cdot \nabla T)$$

This is consistent with the definition of the curvature

$$\kappa = \nabla \cdot \mathbf{n} = -\frac{\nabla^2 G - \mathbf{n} \cdot \nabla (\mathbf{n} \cdot \nabla G)}{|\nabla G|}$$

if the iso-surface $G(\mathbf{x}, t) = G^0$ is replaced by the iso-surface $T(\mathbf{x}, t) = T^0$ and if ρD is assumed constant.

Introducing

$$\nabla \cdot (\rho D \nabla T) = -\rho D |\nabla T| \nabla \cdot \mathbf{n} + \mathbf{n} \cdot \nabla (\rho D \mathbf{n} \cdot \nabla T)$$

into

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = \left[\frac{\nabla \cdot (\rho D \nabla T) + \omega_T}{\rho |\nabla T|} \right]_0 |\nabla G|$$

one obtains

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = (s_n + s_r) |\nabla G| - D \kappa |\nabla G|$$

Here

$$\kappa = \nabla \cdot \mathbf{n} = -\frac{\nabla^2 G - \mathbf{n} \cdot \nabla (\mathbf{n} \cdot \nabla G)}{|\nabla G|}$$

is to be expressed by in terms of the G -field.

The quantities s_n and s_r are contributions due to normal diffusion and reaction to the displacement speed of the thin reaction zone and are defined as

$$s_n = \frac{\mathbf{n} \cdot \nabla (\rho D \mathbf{n} \cdot \nabla T)}{\rho |\nabla T|},$$

$$s_r = \frac{\omega_T}{\rho |\nabla T|}$$

In a steady unstretched planar laminar flame we would have

$$s_n + s_r = s_L^0$$

In the thin reaction zones regime, however, the unsteady mixing and diffusion of chemical species and the temperature in the regions ahead of the thin reaction zone will influence the local displacement speed.

Then the sum of

$$s_n + s_r = s_{L,s} \neq s_L^0$$

is a fluctuating quantity that couples the G -equation to the solution of the balance equations of the reactive scalars.

There is reason to expect, however, that $s_{L,s}$ is of the same order of magnitude as the laminar burning velocity.

The evaluation of DNS-data by Peters et al. (1998) confirms this estimate.

In that paper it was also found that the mean values of s_n and s_r slightly depend on curvature.

This leads to a modification of the diffusion coefficient which partly takes Markstein effects into account.

We will ignore these modifications here and consider the following level set equation for flame structures of finite thickness

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - D\kappa |\nabla G|$$

This equation is defined at the thin reaction zone.

\mathbf{v} , $s_{L,s}$, and D are values at that position.

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - D \kappa |\nabla G|$$

is very similar to

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G| - \mathcal{D}_L \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

which was derived for thin flame structures in the corrugated flamelets regime.

An important difference is the difference between \mathcal{D}_L and D and the disappearance of the strain term.

The latter is implicitly contained in the burning velocity $s_{L,s}$.

In an analytical study of the response of one-dimensional constant density flames to time-dependent strain and curvature, Joulin (1994) has shown that in the limit of high frequency perturbations the effect of strain disappears entirely and Lewis-number effects also disappear in the curvature term such that

$$\mathcal{D}_{\mathcal{L}} \approx D$$

This analysis was based on one-step large activation energy asymptotics with the assumption of a single thin reaction zone.

It suggests that

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - D\kappa |\nabla G|$$

could also have been derived from

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G| - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

for the limit of high frequency perturbations of the flame structure.

This strongly supports it as level set equation for flame structures of finite thickness and shows that unsteadiness of that structure is an important feature in the thin reaction zones regime.

The important difference between the level set formulation

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - D\kappa |\nabla G|$$

and the equation for the reactive scalar

$$\rho \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \nabla T = \nabla \cdot (\rho D \nabla T) + \omega_T$$

is the appearance of a burning velocity which replaces normal diffusion and reaction at the flame surface.

It should be noted the level set equations

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G| - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

and

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - D \kappa |\nabla G|$$

are only defined at the flame surface,

while

$$\rho \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \nabla T = \nabla \cdot (\rho D \nabla T) + \omega_T$$

is valid in the entire field.

A Common Level Set Equation for Both Regimes

The G -equation applies to different regimes in premixed turbulent combustion:

corrugated flamelets regime $\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - D\kappa |\nabla G|$

thin reaction zones regime $\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 |\nabla G| - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L}S |\nabla G|$

In order to show this we will analyze the order of magnitude of the different terms in the first equation.

This can be done by normalizing the independent variables and the curvature in this equation with respect to Kolmogorov length, time and velocity scales

$$t^* = t/t_\eta, \quad \mathbf{x}^* = \mathbf{x}/\eta, \quad \mathbf{v}^* = \mathbf{v}/v_\eta,$$

$$\kappa^* = \eta\kappa, \quad \nabla^* = \eta\nabla.$$

Using $\eta^2/t_\eta = \nu$ one obtains

$$\frac{\partial G}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* G = \frac{s_{L,s}}{v_\eta} |\nabla^* G| - \frac{D}{\nu} \kappa^* |\nabla^* G|,$$

Since Kolmogorov eddies can perturb the flow field as well as the G -field, all derivatives, the curvature and the velocity \mathbf{v}^* are typically of order unity.

In flames D/v is also of order unity.

However, since $s_{L,s}$ is of the same order of magnitude as s_L ,

The definition

$$\text{Ka} = \frac{t_F}{t_\eta} = \frac{\ell_F^2}{\eta^2} = \frac{v_\eta^2}{s_L^2}$$

shows that the ratio $s_{L,s}/v_\eta$ is proportional to $\text{Ka}^{-1/2}$.

Since $\text{Ka} > 1$ in the thin reaction zones regime it follows that

$$s_{L,s} < v_\eta$$

in that regime.

The propagation term therefore is small and the curvature term will be dominant.

We want to base the following analysis on an equation which contains only the leading order terms in both regimes.

Therefore we take the propagation term with a constant laminar burning velocity s_L^0 from the corrugated flamelets regime and the curvature term multiplied with the diffusivity D from the thin reaction zones regime.

The strain term $\mathcal{L} S$ will be neglected in both regimes.

The leading order equation valid in both regimes then reads

$$\rho \frac{\partial G}{\partial t} + \rho \mathbf{v} \cdot \nabla G = (\rho s_L^0) \sigma - (\rho D) \kappa \sigma$$

For consistency with other field equations that will be used as a starting point for turbulence modeling, we have multiplied all terms in this equation with ρ . This will allow to apply Favre averaging to all equations.

Furthermore, we have set $\rho s_L^0 = \rho_u s_{L,u}$ constant and denoted this by paranthesis.

This takes into account that the mass flow rate ρs_L^0 through a planar steady flame is constant as shown by

$$\rho u v_u = \rho u s_L$$

The paranthesis of ρD also denote that this product was assumed constant in deriving

$$\nabla \cdot (\rho D \nabla T) = -\rho D |\nabla T| \nabla \cdot \mathbf{n} + \mathbf{n} \cdot \nabla (\rho D \mathbf{n} \cdot \nabla T)$$

There it was defined at T^0 , and since

$$\rho D = \lambda / c_p$$

it is equal to λ / c_{p0} used in the definition of the flame thickness

$$\ell_F = \frac{(\lambda / c_p)_{T^0}}{(\rho s_L)_u}$$

Modeling Premixed Turbulent Combustion Based on the Level Set Approach

If the G -equation is to be used as a basis for turbulence modeling, it is convenient to ignore at first its non-uniqueness outside the surface $G(\mathbf{x}, t) = G_0$.

Then the G -equation would have similar properties as other field equations used in fluid dynamics and scalar mixing.

This would allow to define, at point \mathbf{x} and time t in the flow field, a probability density function $P(G; \mathbf{x}, t)$ for the scalar G .

This is the probability density of finding the flame surface $G(\mathbf{x},t)=G_0$ at \mathbf{x} and t given by

$$P(G_0, \mathbf{x}, t) = \int_{-\infty}^{+\infty} \delta(G-G_0)P(G; \mathbf{x}, t)dG = P(\mathbf{x}, t).$$

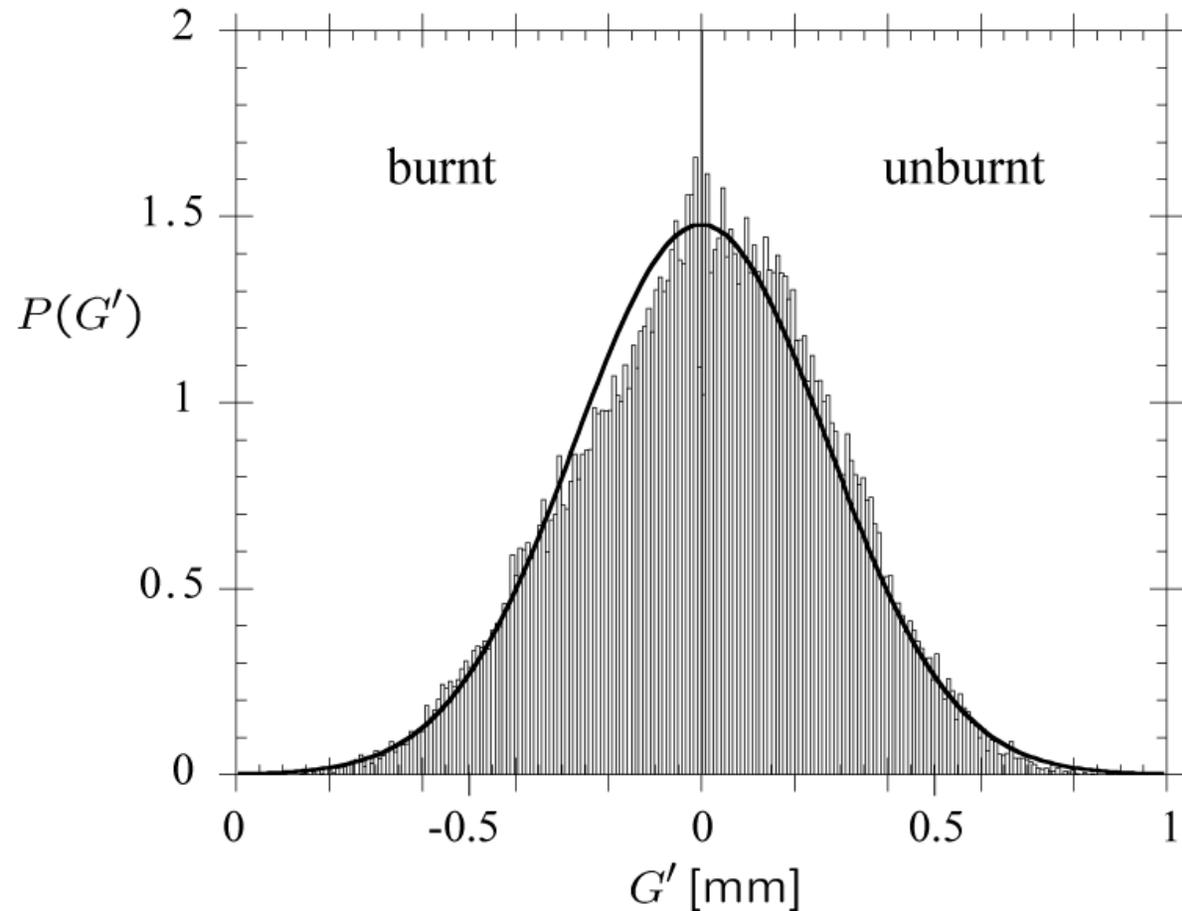
This quantity can be measured, for instance, by counting the number of flame crossings in a small volume ΔV located at \mathbf{x} over a small time difference Δt .

Experimental data for the pdf (Wirth et al., 1992, 1993) from a transparent spark-ignition engine.

Smoke particles, which burnt out immediately in the flame front, were added to the unburnt mixture.

Thereby the front could be visualized by a laser sheet as the borderline of the region where Mie scattering of particles could be detected.

The pdf represents the pdf of fluctuations around the mean flame contour of several instantaneous images.



By comparing the measured pdf with a Gaussian distribution it is seen to be slightly skewed to the unburnt gas side.

This is due to the non-symmetric influence of the laminar burning velocity on the shape of the flame front:

there are rounded leading edges towards the unburnt mixture, but sharp and narrow troughs towards the burnt gas.

This non-symmetry is also found in other experimental pdfs.

Without loss of generality, we now want to consider a one-dimensional steady turbulent flame propagating in x -direction.

We will analyze its structure by introducing the flame-normal coordinate x , such that all turbulent quantities are a function of this coordinate only.

Then the pdf of finding the flame surface at a particular location x within the flame brush simplifies to $P(G_0; x)$ which we write as $P(x)$.

We normalize $P(x)$ by

$$\int_{-\infty}^{+\infty} P(x) dx = 1$$

and define the mean flame position x_f as

$$x_f = \int_{-\infty}^{+\infty} x P(x) dx$$

The turbulent flame brush thickness $\ell_{F,t}$ can also be defined using $P(x)$.

With the definition of the variance

$$\overline{(x - x_f)^2} = \int_{-\infty}^{+\infty} (x - x_f)^2 P(x) dx$$

a plausible definition is

$$\ell_{F,t} = \left(\overline{(x - x_f)^2} \right)^{1/2}$$

We note that from $P(x)$ two important properties of a premixed turbulent flame, namely the **mean flame position** and the **flame brush thickness** can be calculated.

Peters (1992) considered turbulent modeling of the G -equation in the corrugated flamelets regime and derived Reynolds-averaged equations for the mean and the variance of G .

The main sink term in the variance equation was defined as

$$\bar{\omega} = -2 s_L^0 \overline{G' \sigma'}$$

This quantity was called kinematic restoration in order to emphasize the effect of local laminar flame propagation in restoring the G -field and thereby the flame surface.

Corrugations produced by turbulence, which would exponentially increase the flame surface area with time of a non-diffusive iso-scalar surface are restored by this kinematic effect.

From that analysis resulted a closure assumption which relates the main sink term to the variance of G and the integral time scale

$$\bar{\omega} = c_{\omega} \frac{\varepsilon}{k} \overline{G'^2}$$

where $c_{\omega}=1.62$ is a constant of order unity.

This expression shows that kinematic restoration plays a similar role in reducing fluctuations of the flame front as scalar dissipation does in reducing fluctuations of diffusive scalars.

It was also shown by Peters (1992) that kinematic restoration is active at the Gibson scale, since the cut-off of the inertial range in the scalar spectrum function occurs at that scale.

Equations for the Mean and the Variance of G

In order to obtain a formulation that is consistent with the well-established use of Favre averages in turbulent combustion, we split G and the velocity vector v into Favre means and fluctuations

$$G = \tilde{G} + G'' , \quad v = \tilde{v} + v''$$

Here the Favre means are at first viewed as unconditional averages.

At the end, however, only the respective **conditional averages** are of interest.

The turbulent burning velocity s_T^0 is obtained by averaging over

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 \sigma - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

By setting $\bar{v} = s_T^0$ one finds for the stationary unstretched flame front

$$s_T^0 |\nabla G| = \overline{s_L^0 \sigma}$$

Using a number of additional closure assumptions described in Peters (2000), one finally obtains the following equations for the Favre mean and variance of G :

$$\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{G} = (\bar{\rho} s_T^0) |\nabla \tilde{G}| - \bar{\rho} D_t \tilde{\kappa} |\nabla \tilde{G}|$$

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \widetilde{G''^2} = \nabla_{||} (\bar{\rho} D_t \nabla_{||} \widetilde{G''^2}) + 2 \bar{\rho} D_t (\nabla \tilde{G})^2 - c_s \bar{\rho} \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{G''^2}$$

It is easily seen that

$$\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{G} = (\bar{\rho} s_T^0) |\nabla \tilde{G}| - \bar{\rho} D_t \tilde{\kappa} |\nabla \tilde{G}|$$

has the same form as

$$\rho \frac{\partial G}{\partial t} + \rho \mathbf{v} \cdot \nabla G = (\rho s_L^0) \sigma - (\rho D) \kappa \sigma$$

and therefore shares its mathematical properties.

It also is valid at $\tilde{G}(\mathbf{x}, t) = G_0$ only.

The solution outside of that surface depends on the ansatz for the Favre mean of G that is introduced.

In order to solve

$$\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{G} = (\bar{\rho} s_T^0) |\nabla \tilde{G}| - \bar{\rho} D_t \tilde{\kappa} |\nabla \tilde{G}|$$

a model for the turbulent burning velocity s_T^0 must be provided.

A first step would be to use empirical correlations from the literature.

Alternatively, a modeled balance equation for the mean gradient $\bar{\sigma}$ will be derived.

According to Kerstein (1988) this quantity represents the [flame surface area ratio](#), which is proportional to the turbulent burning velocity.

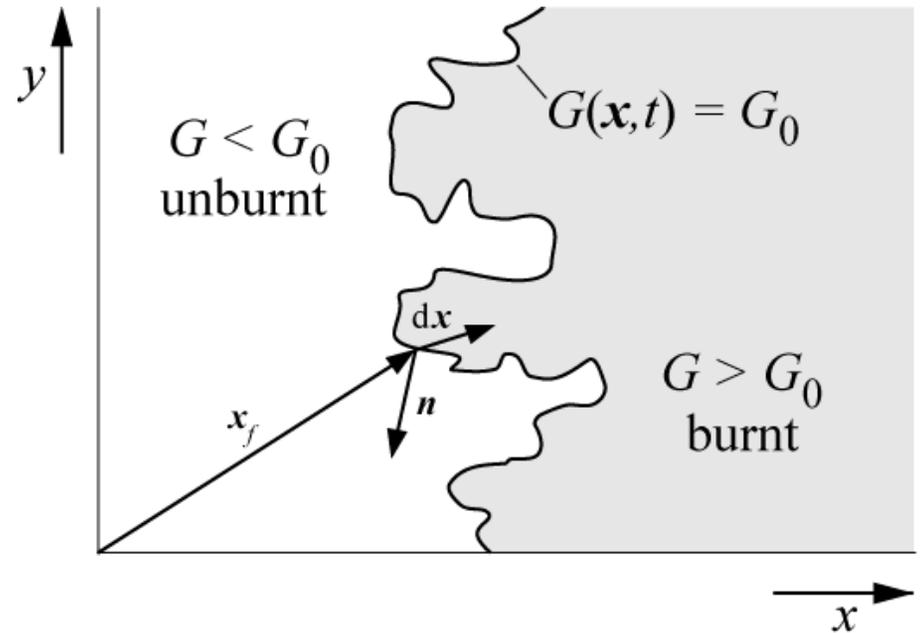
Appendix

In this respect $G(\mathbf{x},t)$ differs fundamentally from the mixture fraction $Z(\mathbf{x},t)$ used in nonpremixed combustion, which is a conserved scalar that is well defined in the entire flow field.

The distance x_n from the flame surface in normal direction, however, can be uniquely defined by introducing its differential increase towards the burnt gas side by

$$dx_n = -\mathbf{n} \cdot d\mathbf{x} = \frac{\nabla G}{|\nabla G|} \cdot d\mathbf{x}$$

Here $d\mathbf{x}$ is a differential vector pointing from the front to its surroundings.



If we consider a frozen G -field, a differential increase of the G -level is given by

$$dG = \nabla G \cdot dx$$

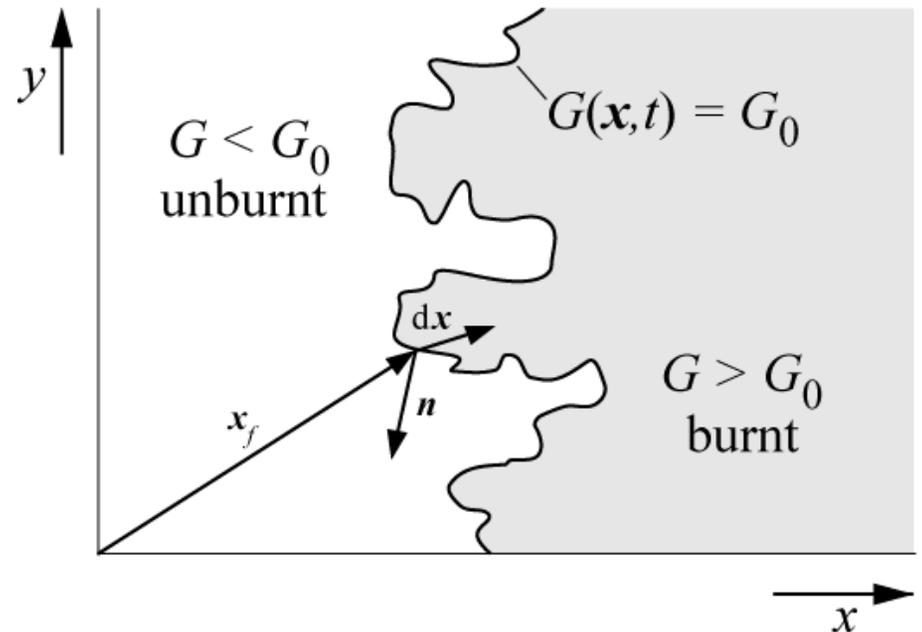
Introducing this into $dx_n = -n \cdot dx = \frac{\nabla G}{|\nabla G|} \cdot dx$

it is seen that the differential increase dx_n is related to dG by

$$dx_n = \frac{dG}{|\nabla G|}$$

In the following the absolute value of the gradient of G at $G(\mathbf{x},t)=G_0$ will be denoted by

$$\sigma = |\nabla G|$$



The Eq.

$$\frac{\mathcal{L}_u}{\ell_F} = \frac{1}{\gamma} \ln \frac{1}{1-\gamma} + \frac{Ze(Le-1)(1-\gamma)}{2\gamma} \int_0^{\gamma/(1-\gamma)} \frac{\ln(1+x)}{x} dx$$

is valid if s_L is defined with respect to the unburnt mixture.

A different expression can be derived, if both, s_L and \mathcal{L} are defined with respect to the burnt gas (cf. Clavin (1985)).

Strain due to flow divergence can be interpreted as stream line curvature.

Since strain and curvature have similar effects on the burning velocity they may be summarized as **flame stretch** (cf. Matalon (1983)).

The concept of stretch was generalized to account for finite flame thickness (cf. de Goey and Ten Thijs Boonkhamp 1997, de Goey et al. 1997 and Echehki ,1997).

In these papers a [quasi-one-dimensional analysis](#) of the governing equations was performed to identify different contributions to flame stretch.

Experimental studies of stretched flames were performed by Egolfopoulos et al. 1990, Erard et al. 1996, Deshaies and Cambay 1990 and many others.

For the iso-surface $G(\mathbf{x},t) = G_0$ in particular, the flame front position at the boundaries is that where the flame is anchored.

As an illustration of the level set approach, in Lecture 4 Section 4.3 we already presented an examples of laminar flames to determine the flame front position by solving the G -equation.

$$\frac{\mathcal{L}_u}{\ell_F} = \frac{1}{\gamma} \ln \frac{1}{1-\gamma} + \frac{Ze(Le-1)(1-\gamma)}{2\gamma} \int_0^{\gamma/(1-\gamma)} \frac{\ln(1+x)}{x} dx$$

Since the derivation of

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - D\kappa |\nabla G|$$

was based on the balance equation

$$\rho \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \nabla T = \nabla \cdot (\rho D \nabla T) + \omega_T$$

for the temperature, the diffusion coefficient is the thermal diffusivity.

However, a similar derivation could have been based on any other reactive scalar defining the position of the inner layer.

Then the diffusivity of that particular scalar would appear.

In order to obtain the same result we therefore must assume equal diffusivities for all reactive scalars.

It can be shown that the equal diffusivities are a good choice for the flamelet equations in the thin reaction zones regime.

Since the temperature plays a particular role in combustion due to the strong temperature sensitivity of chemistry, the use of the thermal diffusivity D is the appropriate.

Relative small mean values of $s_{L,s}$ may, for instance, result from instantaneously negative values of the burning velocity.

Even though wrinkling of the reaction zone by small eddies leading to large local curvatures is an important feature, it is the enhanced mixing within the preheat zone that is responsible for the advancement of the front.

On the contrary, as can be shown by a similar analysis of

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L^0 \sigma - \mathcal{D}_{\mathcal{L}} \kappa |\nabla G| - \mathcal{L} S |\nabla G|$$

in the corrugated flamelets regime where $Ka < 1$ and therefore

$$s_L^0 > v_\eta$$

the propagation term $s_L^0 \sigma$ is dominant.

Since the Markstein length is of the order of the flame thickness, this term is unimportant in the corrugated flamelets regime, where

$$\mathcal{L} < \eta$$

A term called scalar-strain co-variance resulting from this term is effective in the diffusive subrange of the scalar spectrum only (cf. Peters, 1992).

It therefore does not interact with the turbulent part of the spectrum and is unimportant for leading order scaling arguments required for turbulent closure.

With that definition the last term in

$$\rho \frac{\partial G}{\partial t} + \rho \mathbf{v} \cdot \nabla G = (\rho s_L^0) \sigma - (\rho D) \kappa \sigma$$

can also be expressed as

$$(\rho s_L^0) \ell_F \kappa \sigma$$

Again the Eq. above is defined at the flame surface $G(\mathbf{x}, t) = G^0$ only.

From this pdf the first two moments of G , the mean and the variance, can be calculated as

$$\bar{G}(\mathbf{x}, t) = \int_{-\infty}^{+\infty} GP(G; \mathbf{x}, t)dG ,$$

$$\overline{G'^2}(\mathbf{x}, t) = \int_{-\infty}^{+\infty} (G - \bar{G})^2 P(G; \mathbf{x}, t)dG$$

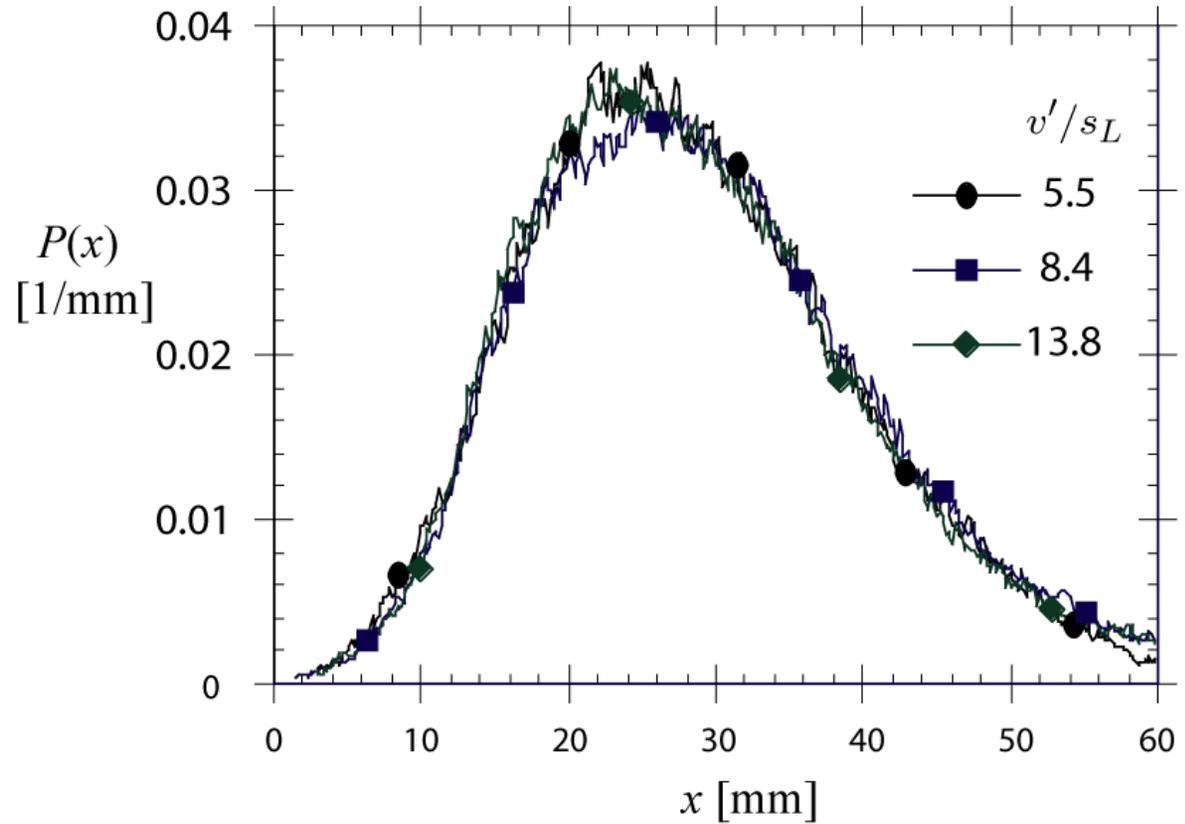
If modeled equations for these two moments are formulated and solved, one could use the presumed shape pdf approach to calculate pdf by presuming a two-parameter shape function.

However, since G is only defined at the flame front, the pdf and its moments carry the non-uniqueness of its definition outside $G(\mathbf{x}, t)=G^0$.

Plessing et al. (1999) have measured the probability density of finding the flame surface in steady turbulent premixed flames on a weak swirl burner.

The flames were stabilized nearly horizontally on the burner thus representing one-dimensional steady turbulent flames.

Temperature data obtained from Rayleigh scattering are averaged. The three profiles of $P(x)$, for three velocity ratios v'/s_L , nearly coincide and are slightly skewed towards the unburnt gas side.



The G -equation has been used in a number of papers to investigate quantities relevant to premixed turbulent combustion.

An early review was given by Ashurst (1994).

Kerstein et al. (1988) have performed direct numerical simulations of Eq.

$$\frac{\partial G}{\partial t} + \mathbf{v}_f \cdot \nabla G = s_L |\nabla G|$$

in a cubic box assigning a stationary turbulent flow field and constant density.

The constant density assumption has the advantage that the flow field is not altered by gas expansion effects.

The gradient $\partial \bar{G} / \partial x$ in direction of mean flame propagation was fixed equal to unity and cyclic boundary conditions in the two other directions were imposed.

In this formulation all instantaneous G -levels can be interpreted as representing different flame fronts.

Therefore G_0 was considered as a variable and averages over all G -levels were taken in order to show that for large times the mean gradient $\bar{\sigma}$ can be interpreted as the [flame surface area ratio](#).

A dissipation term involving a positive Markstein diffusivity was shown to be effective at the Obukhov-Corrsin scale and a term called scalar-strain co-variance was shown to be most effective at the Markstein length.

In the corrugated flamelets regime the Gibson scale is larger than the Corrsin scale and the Markstein Length.

Therefore these additional terms are higher order corrections, which, in view of the order of magnitude assumptions used in turbulence modeling, will be neglected.

A similar analysis was performed by Peters (1999) for the thin reaction zones regime.

In that regime the diffusion term in

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_{L,s} |\nabla G| - \mathcal{D} \kappa |\nabla G|$$

is dominant as shown by the order of magnitude analysis of

$$\frac{\partial G}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* G = \frac{s_{L,s}}{v_\eta} |\nabla^* G| - \frac{D}{\nu} \kappa^* |\nabla^* G|,$$

This leads to a dissipation term replacing kinematic restoration as the leading order sink term in the variance equation. It is defined as

$$\bar{\chi} = 2D\overline{(\nabla G')^2}$$

Closure of that term is obtained in a similar way as for non-reacting scalars and leads to

$$\bar{\chi} = c_\chi \frac{\varepsilon}{k} \overline{G'^2}$$

Below we will use the two closure relations

$$\bar{\omega} = c_\omega \frac{\varepsilon}{k} \overline{G'^2} \quad \text{and} \quad \bar{\chi} = 2D\overline{(\nabla G')^2}$$

as the basis for the [modeling of the turbulent burning velocity](#) in the two different regimes.

Since in a turbulent flame G was interpreted as the scalar distance between the instantaneous and the mean flame front, evaluated at $G(\mathbf{x},t)=G_0$, the Favre mean

$$\tilde{G} = \overline{\rho G} / \bar{\rho}$$

represents the Favre average of that distance.

If $G(\mathbf{x},t)=G_0$ is defined to lie in the unburnt mixture immediately ahead of the thin flame structure, as often assumed for the corrugated flamelets regime, the density at $G(\mathbf{x},t)=G_0$ is constant equal to ρ_u .

Similarly, if it is an iso-temperature surface, as assumed for the thin reaction zones regime, changes of the density along that surface are expected to be small.

The same argument holds for

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \widetilde{G''^2} = \nabla_{||} (\bar{\rho} D_t \nabla_{||} \widetilde{G''^2}) + 2\bar{\rho} D_t (\nabla \tilde{G})^2 - c_s \bar{\rho} \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{G''^2}$$

since the variance is a property of the flame front.

The solution of that equation will provide the conditional value $(\widetilde{G''^2})_0$ at the mean flame surface.

Following

$$\ell_{F,t} = \left(\overline{(x - x_f)^2} \right)^{1/2}$$

its square root is a measure of the flame brush thickness, which for an arbitrary value of $|\nabla \tilde{G}|$ at the front, will be defined as

$$\ell_{F,t} = \left. \frac{(\widetilde{G''^2}(\mathbf{x}, t))^{1/2}}{|\nabla \tilde{G}|} \right|_{\tilde{G}=G_0}$$

An Example Solution for the Turbulent Flame Brush Thickness

For illustration purpose we want to solve the variance equation

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{v} \nabla \widetilde{G''^2} = \nabla_{||} (\bar{\rho} D_t \nabla_{||} \widetilde{G''^2}) + 2 \bar{\rho} D_t (\nabla \tilde{G})^2 - c_s \bar{\rho} \frac{\tilde{\varepsilon}}{\bar{k}} \widetilde{G''^2}$$

for a one-dimensional unsteady planar flame using $|\nabla \tilde{G}| = 1$

We pose the problem such that at time $t = 0$ a one-dimensional steady laminar flame with flame thickness ℓ_F is already present and that the laminar flow is suddenly replaced by a fully developed turbulent flow field.

We assume that the turbulence diffusivity D_t , the Favre mean turbulent kinetic energy and its dissipation are constant, independent of time.

Since the flame is planar and, furthermore, since the variance must not depend on the coordinate normal to the mean flame, if it is supposed to represent the conditional variance, **all gradients of G -variance must vanish.**

$$\widetilde{G''^2} = 0$$

Therefore, the convective and diffusive terms in

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \widetilde{G''^2} = \nabla_{||} (\bar{\rho} D_t \nabla_{||} \widetilde{G''^2}) + 2 \bar{\rho} D_t (\nabla \tilde{G})^2 - c_s \bar{\rho} \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{G''^2}$$

disappear entirely.

For modeling purposes we will use a turbulent Schmidt number $Sc_t = \nu_t / D_t = 0.7$ and the empirical relations given in Tab. of Lecture 13.

constant	equation	suggested value	origin
a_1	$\bar{\varepsilon} = a_1 v'^3 / \ell$	0.37	Bray (1990)
a_2	$k = a_2 v'^2$	1.5	definition
a_3	$\tau = a_3 \ell / v'$	4.05	$\tau = k / \bar{\varepsilon}$
a_4	$D_t = a_4 v' \ell$	0.78	$D_t = \nu_t / 0.7$
b_1	$s_T = b_1 v'$	2.0	experimental data
b_2	$\ell_{F,t} = b_2 \ell$	1.78	$(2a_3 a_4 / c_s)^{1/2}$
b_3	$s_T^0 / s_L^0 = b_3 (D_t / D)^{1/2}$	1.0	Damköhler (1940)
c_0	$c_0 = c_{\varepsilon 1} - 1$	0.44	standard value
c_1	Eq. (13.18)	4.63	DNS
c_2	Eq. (13.18)	1.01	$a_4 c_1 / (b_1 b_2)$
c_3	Eq. (13.18)	4.63	$c_1 = c_3$
c_s	Eq. (12.47)	2.0	spectral closure

The empirical values follow from Eqs.

$$\nu_t = c_\mu \frac{\tilde{k}^2}{\tilde{\varepsilon}}, \quad c_\mu = 0.09, \quad \tau = \frac{k}{\varepsilon}$$

and relate the turbulent quantities to the velocity fluctuations, the flame thickness and the turbulent time scale.

Non-dimensionalizing the time in

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{v} \cdot \nabla \widetilde{G''^2} = \nabla_{||} (\bar{\rho} D_t \nabla_{||} \widetilde{G''^2}) + 2 \bar{\rho} D_t (\nabla \tilde{G})^2 - c_s \bar{\rho} \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{G''^2}$$

by the integral time scale, the variance equation becomes an equation for the turbulent flame brush thickness

$$\frac{\partial l_{F,t}^2}{\partial (t/\tau)} = 2 a_3 a_4 l^2 - c_s l_{F,t}^2$$

The equation for the turbulent flame brush thickness has the solution

$$\ell_{F,t}^2 = b_2^2 \ell^2 [1 - \exp(-c_s t / \tau)] + \ell_F^2 \exp(-c_s t / \tau)$$

where $b_2 = (2a_3 a_4 / c_s)^{1/2} = 1.7$ for $c_s = 2.0$

Here the laminar flame thickness was used as initial value.

In the limit $\ell_F / \ell \rightarrow 0$ one obtains

$$\ell_{F,t} = b_2 \ell [1 - \exp(-c_s t / \tau)]^{1/2}$$

The unsteady development of the flame brush thickness in the limit $\ell_F/\ell \rightarrow 0$

For large times it becomes proportional to the integral length scale ℓ .

