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Intrinsic Disturbed Flame Equations and Stretched Premixed Flamelet Model: Two Descriptions of Premixed Flame-Flow Interaction

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Abstract

Over the last few years, two new descriptions of flame-flow interaction have been developed independently, viz. the 'Intrinsic Disturbed Flame Equations' (IDFE) and 'Stretched Premixed Flamelet Model' (SPFM). Both descriptions employ a coordinate system attached to the flame. The conservation equations for a premixed flame are rewritten in this coordinate system, eventually resulting in a quasi one-dimensional system. We present applications in theory, numerics and data analysis. This includes burning velocity relations, stability and predictions of a triple flame. The description seems promising for turbulent combustion modelling.

Keywords: premixed combustion, curvilinear coordinates, flamelets, flame stretch, flame speed, asymptotic methods, integral analysis

1 Introduction

Fossil fuels remain the primary source for our energy demand. In order to reduce toxic combustion by-products such as nitrogen oxides (NO_x), unburned hydrocarbons and soot, improved combustors are being developed. In advanced combustion processes, premixed combustion plays an increasingly important role. For example, in stationary lean-burn gas turbines fuel is first vaporized, next premixed with air, and finally burned in the combustion chamber. Premixed combustion allows to avoid extreme values of temperature and creates fairly uniform conditions along the flame resulting in a significant reduction of NO_x and other combustion by-products.

At present the potential of advanced combustion processes to reduce pollutants cannot yet be exploited to its full extent. Complex phenomena which are not fully understood prohibit operation at favorable conditions. With the exception of very small burners, combustion takes place in a turbulent flow field. Thus the interactions of the combustion process with the flow and vice versa appear to be stochastic and nonlinear.

The actual location of the reaction zone depends on details of the flow-flame interaction. This makes all the well-known difficulties of predicting turbulent flows even more acute for premixed combustion.

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Even if the chemical mechanism of a premixed flame is well-specified and documented so that the emission of pollutants can be accurately calculated and predicted for the case when the flame is laminar, i.e., not disturbed by a turbulent flow, predictions become unreliable when the flame is stretched and curved by the turbulent fluid flow. The rapid increase of available computer resources allows in many fields of science to model at a fundamental level and to compute the problem of technical interest by crude computer power. This may be feasible for nonreacting turbulent flows and the problem of complex chemistry in simple flows, but we will have to wait at least for another decade before the problem of turbulent premixed combustion in applications of technical relevance can be attacked using pure computer power. Hence, our goal is the development of methods and models which allow for the autonomous evaluation of the chemistry and the fluid flow which yet preserve the interaction between them.

Over the last few years, two new descriptions have been developed independently, viz. the 'Intrinsic Disturbed Flame Equations' (IDFE) [11] [3] and 'Stretched Premixed Flamelet Model' (SPFM) [6] [18]. In both descriptions a small element of a flame is considered which is subjected to a general flow field.

The IDFE-method is based on the mathematics of asymptotic series expansions and matched asymptotics. Exploited is the fact that the flame structure is typically thin, so that the ratio of the length scales of the flame thickness to the fluid length scale may be used as a small parameter in asymptotic series expansions. The flame structure represents a thin inner region which is embedded within a nonreactive outer flow. Two terms of the asymptotic series are evaluated, where the leading order corresponds to an undisturbed flame and the next order accounts for the interactions with the flow. The flow fields on either side of the flame structure are related by jump conditions, which include the effect of viscosity and thermal expansion in the flame structure. The propagation of the flame relative to the unburned gases is described by a flame speed equation. This flame speed equation has been derived for global single-step Arrhenius chemistry but also for flames with realistic complex chemistry. The flame speed relation includes the effects of stretch, curvature, unsteadiness, and the nonlinear coupling of neighboring flame elements.

Following the approach of SPFM, the system of 3D unsteady reacting flow equations is decoupled in a) a set of equations for the flow and mixing processes, b) a kinematic equation for the flame structure and c) a set of quasi-1D flamelet equations describing the inner flamelet structure. The flamelet structure is also considered thin, and the detailed behaviour of the flow, stretch and curvature within the flamelet is taken into account. Applying an integral analysis to the flamelet equations yields an algebraic system describing the flame response in terms of the stretch rate, which also holds for higher stretch rates. The model can be considered as an extension of the laminar flamelet concept, which originally was developed for diffusion flames. Recently an extension has been introduced of SPFM in which the kinematic equation is replaced by a transport equation for a progress variable (e.g. temperature). This new model, referred to as 'Flamelet-Generated Manifold' (FGM) model [15] is an ideal mix of 1) SPFM, 2) earlier flamelet models and 3) chemical reduction techniques like ILDM. The FGM model has been used numerically to model 2D and 3D Bunsen-type flames, partially-premixed flames (triple-flames) and flames on a ceramic foam burner in a radiating furnace [16].

In both descriptions the number of parameters responsible for flame / flow interactions may be reduced to a relatively small number. The resulting equations are closely related to those of laminar premixed combustion and may be solved using standard techniques. The main advantage of IDFE and SPFM is that the effect of fluid flow on the flame is considered in a relatively general and simple way.

In the presentation we will review a number of problems, which we have solved using the Intrinsic Disturbed Flame Equations or Stretched Premixed Flamelet Model. We will compare both methods and we will give a perspective view of the class of combustion applications that can be solved using the approach of IDFE or SPFM.

2 Equations in flame coordinates

Before we discuss results which have been derived from either description, we briefly resort to the mathematics and in particular to tensor calculus. We do our best to present it in a form which is understandable for a reader without a profound background in tensor analysis. Both methods, IDFE and SPFM, have independently been proposed to analyse the behaviour of premixed flames in arbitrary flow fields. In both methods the equations are first transformed to a moving system of coordinates which is attached to the flame. The coordinate systems are selected, in a way which simplifies the equations substantially. Yet, the actual choice of the coordinate systems is quite different, resulting in a number of differences between IDFE and SPFM.

Consider the conservation equation for a scalar quantity ϕ in a suitable nondimensional notation

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla \cdot (\rho\mathbf{v}\phi) = \frac{1}{\text{PeLe}_\phi} \nabla \cdot (\lambda \nabla \phi) + \omega_\phi, \quad (2.1)$$

where t is time, ρ is density, \mathbf{v} is the velocity field, λ is ratio of the thermal conductivity to its unburned value and ω_ϕ is the chemical source term of ϕ . The Peclet number Pe is the ratio of the hydrodynamic length scale to the flame thickness, which is often large. The Lewis number Le_ϕ is the ratio of the thermal diffusivity to the diffusivity of the scalar quantity ϕ and is assumed to be constant. The scalar quantity may be the temperature or the concentration of any species.

Employing tensor calculus we rewrite equation (2.1) as

$$\frac{\partial}{\partial t}(\sqrt{g}\rho\phi) + \frac{\partial}{\partial x^i}(\sqrt{g}m^i\phi) = \frac{1}{\text{PeLe}_\phi} \frac{\partial}{\partial x^i} \left(\lambda \sqrt{g} g^{ij} \frac{\partial \phi}{\partial x^j} \right) + \sqrt{g} \omega_\phi, \quad (2.2)$$

where x^i are the moving coordinates. In this equation, the Einstein summation convention is employed with $i, j = 1, 2, 3$. The quantity m^i is the contravariant mass flux relative to the moving coordinate system, defined as $m^i = \rho(v^i - u^i)$, where v^i is the contravariant flow velocity and u^i is the velocity of the coordinate system relative to a fixed frame of reference. Obviously, if the coordinate system is convected with the flow, then the mass flux m^i vanishes. The contravariant metric tensor is g^{ij} and \sqrt{g} is the control volume defined by the coordinate system which is related to the metric tensor through the relation $g = 1/\det(g^{ij})$. Note that the relation between physical quantities and covariant tensors is given by: $m^i = \sqrt{g^{ii}}m(i)$, $v^i = \sqrt{g^{ii}}v(i)$ and $u^i = \sqrt{g^{ii}}u(i)$, where no summation applies and $m(i)$, $v(i)$ and $u(i)$ denote the physical mass flux, flow velocity and velocity of the coordinate system, respectively.

The continuity equation is obtained if we set $\phi = 1$ and $\omega_\phi = 0$, i.e.

$$\frac{\partial}{\partial t}(\sqrt{g}\rho) + \frac{\partial}{\partial x^i}(\sqrt{g}m^i) = 0. \quad (2.3)$$

A kinematic relation for \sqrt{g} is obtained if we transform the trivial equation $\partial(1)/\partial t = 0$, to moving coordinates, i.e.

$$\frac{\partial}{\partial t}(\sqrt{g}) - \frac{\partial}{\partial x^i}(\sqrt{g}u^i) = 0. \quad (2.4)$$

As a flame represents a layer of finite, but small thickness, in which the variables change from their unburned to their burned values, the changes in normal direction are much larger than they are in tangential direction. Therefore, the normal direction plays a distinct role in the analysis. In both IDFE and SPFM the normal direction x^1 is orthogonal to the transverse directions x^2, x^3 . This property results

in $g^{12} = g^{21} = g^{13} = g^{31} = 0$, so that mixed derivatives involving one of the transverse directions and the normal direction simultaneously do not occur. The quantity g becomes $g = a/g^1$ where $a = 1/\det(g^{\alpha\beta})$, with $\alpha, \beta = 2, 3$, so that \sqrt{a} represents a surface element on the surfaces $x^1 = \text{const}$.

This is as far as the coordinate systems are identical for IDFE and SPFM. In order to derive the IDFE we assume that within the flame structure there is a distinguished surface, so that all the properties of the coordinate system should be expressed in terms of the intrinsic properties of this distinguished surface. Eventually our goal is to derive equations, which describe the propagation of the distinguished surface normal to itself. In SPFM a simplification of the equations is obtained by selecting iso-surfaces of a specific scalar ϕ as the coordinate surfaces $x^1 = \phi = \text{const}$. Note that ϕ must be a monotonous function, e.g., the fuel concentration. Each of these surfaces propagates at its own speed, so that as the surfaces propagate their distance may change both in space and time. The propagation speed of each individual surface $\phi = \text{const}$ has a physical meaning, while for IDFE only the propagation of the distinguished surface has a physical meaning.

To write the equations in their final form we introduce flame stretch. The definition of flame stretch is different in SPFM and IDFE. In IDFE the flame behaviour is described in terms of intrinsic properties of the distinguished surface. Therefore, the original definition of flame stretch may be used, i.e.

$$\chi = \frac{1}{\sqrt{a^*}} \frac{d\sqrt{a^*}}{dt}, \quad (2.5)$$

where $\sqrt{a^*}$ represents a surface element on the distinguished surface, and the total derivative includes transport along the surface only. Throughout this manuscript the asterisk "*" denotes quantities evaluated at the distinguished surface. Without loss of generality we may assume that the coordinate system is normalized, i.e., the surfaces $x^1 = \text{const}$ are parallel surfaces and x^1 is identical to the signed distance function so that $g^{11} = 1$, $\sqrt{g} = \sqrt{a}$, and the normal contravariant tensor components are identical with their physical components, i.e., $m^1 = m(1)$, $v^1 = v(1)$, and $u^1 = u(1)$. The points of this surface element are convected along the surface with the local tangential flow field, so that if these points increase their distance as the flame evolves the flame element is growing in size and thus the flame experiences a positive stretch. In the analysis the tangential velocity components u^2 and u^3 are not specified yet. We select them requiring that the term $\partial(\sqrt{g} m^\alpha \phi) / \partial x^\alpha$ vanishes. Since the flame has a finite width this cannot be done pointwise. We only have the freedom to select the x^2 and x^3 -lines and thus the coordinate velocities u^2 and u^3 on the distinguished surface. Orthogonality of the coordinate system uniquely defines the x^2 and x^3 -lines and thus u^2 and u^3 on other surfaces $x^1 = \text{const}$. We require that the integral contribution of the term $\partial(\sqrt{g} m^\alpha \phi) / \partial x^\alpha$ vanishes. This requires $m^\alpha \approx 0$, i.e., $u^\alpha \approx v^\alpha$. Therefore, the flame stretch simply becomes

$$\chi = \frac{1}{\sqrt{g^*}} \frac{\partial \sqrt{g^*}}{\partial t} \quad (2.6)$$

and has to be evaluated at the distinguished surface.

In SPFM a different definition of flame stretch is used. Since the coordinate surfaces are iso-surfaces of a scalar, the mass in a volume element, which is convected along the flame is changing due to strain and also due to flame thickening. Both these effects are assumed to be equally important and included in the mass based stretch rate K , which is the fractional rate of change of mass in the volume element [8], i.e.

$$K = \frac{1}{\rho \sqrt{g}} \frac{d}{dt} (\sqrt{g} \rho) = \frac{1}{\rho \sqrt{g}} \left(\frac{\partial}{\partial t} (\sqrt{g} \rho) + \frac{\partial}{\partial x^\alpha} (\sqrt{g} m^\alpha) \right). \quad (2.7)$$

Note that $K = K(x^1)$. Employing the mass based stretch rate we rewrite the conservation equation for a general scalar field ψ (one of the concentrations or temperature) as

$$\frac{1}{\sqrt{g}} \frac{\partial}{\partial x^1} (\sqrt{g} F_\psi^1) - \omega_\psi = -\rho K \psi + Q_\psi, \quad (2.8)$$

where F_ψ^1 is the contravariant normal flux of ψ given by

$$F_\psi^1 = m^1 \psi - \frac{\lambda g^{11}}{\text{PeLe}_\psi} \frac{\partial \psi}{\partial x^1}, \quad (2.9)$$

and where Q_ψ describes transverse transport of ψ , i.e.

$$Q_\psi = - \left(\rho \frac{\partial \psi}{\partial t} + m^\alpha \frac{\partial \psi}{\partial x^\alpha} \right) + \frac{1}{\text{PeLe}_\psi} \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^\alpha} \left(\lambda \sqrt{g} g^{\alpha\beta} \frac{\partial \psi}{\partial x^\beta} \right). \quad (2.10)$$

In general the $Q_\psi \neq 0$, but for the special case that $\psi = \phi$, the scalar field used to define the flame adapted coordinate system, we have $Q_\phi = 0$, simply because the kinematic condition

$$\rho \frac{\partial \phi}{\partial t} + m^\alpha \frac{\partial \phi}{\partial x^\alpha} = 0 \quad (2.11)$$

holds and due to the fact that the gradient of ϕ is in x^1 -direction implying that $\partial \phi / \partial x^\beta = 0$ ($\beta = 2, 3$). Furthermore, if scalars ψ and ϕ (such as temperature and concentrations) are correlated to each other, we have that both $\partial \phi / \partial t + m^\alpha \partial \phi / \partial x^\alpha$ and $\partial \phi / \partial x^\beta$ are small leading to $|Q_\phi| \ll 1$ and these contributions are neglected. This is typical for flames with thin reaction zones and was verified from full numerical simulations of various flames [7].

In order to present equation (2.8) in its final form the contravariant normal flux F_ψ^1 is rewritten in terms of the corresponding physical flux $F_\psi(1) = F_\psi^1 / \sqrt{g^{11}}$, and the coordinate x^1 is normalized employing $\partial / \partial s = \sqrt{g^{11}} \partial / \partial x^1$, yielding a quasi-one-dimensional equation for any scalar combustion variable ψ (including ϕ) of the form:

$$\frac{\partial}{\partial s} (F_\psi) - \omega_\psi = -\rho K \psi + 2c F_\psi, \quad (2.12)$$

where c is the mean Gaussian curvature, given by

$$2c = -\frac{1}{\sqrt{a}} \frac{\partial}{\partial s} (\sqrt{a}). \quad (2.13)$$

Note that in previous publication the minus sign and the factor 2 did not appear, but are employed here in agreement with the definition of Gaussian curvature in differential geometry. In (2.12), $F_\psi = F_\psi(1)$ is the physical normal flux of the scalar ψ , given by

$$F_\psi = m \psi - \frac{\lambda}{\text{PeLe}_\psi} \frac{\partial \psi}{\partial s}, \quad (2.14)$$

with the physical normal mass flux $m = m(1)$.

The terms K and c in (2.12) contain perturbations from one-dimensional behaviour. For a given $K = K(s)$ and $c = c(s)$ equation (2.12) may be solved. This is done in most applications numerically,

but for special situations this may also be done analytically. It should be noted that the quasi-stationary one-dimensional equation (2.12) can be solved much more effectively than the original multidimensional equations.

In IDFE the goal of the analysis are analytical expressions for the jump conditions across the flame and flame speed relations. These are obtained employing asymptotic series expansions for the scalar ϕ , the fluxes, and source terms in the form

$$\phi \sim \sum_n \text{Pe}^{-n} \phi_{(n)}. \quad (2.15)$$

The small parameter is Pe^{-1} which is the ratio of the flame thickness to the hydrodynamic length scale. In the x^1 -variable the flame structure has a small thickness. To study the flame structure it is necessary to introduce a stretched normal coordinate $X = \text{Pe} x^1$, so that derivatives with respect to X become $O(1)$ inside the flame structure. The volume element \sqrt{g} is Taylor expanded as $\sqrt{g} = \sqrt{g^*} + \text{Pe}^{-1} (\partial \sqrt{g} / \partial x^1)^* X$, so that \sqrt{g} is constant at leading order. Writing two terms of the series expansion we obtain the intrinsic disturbed flame equations

$$\frac{\partial}{\partial X} F_{(0)}^1 = \omega_{(0)}, \quad (2.16)$$

$$\left(\frac{\partial}{\partial t} + \chi \right) \phi_{(0)} + \frac{1}{\sqrt{g^*}} \frac{\partial}{\partial x^\alpha} \left(\sqrt{g^*} F_{(0)}^\alpha \right) + \frac{\partial}{\partial X} \left(F_{(1)}^1 - 2cX F_{(0)}^1 \right) = \omega_{(1)} - 2cX \omega_{(0)}, \quad (2.17)$$

where

$$F_\phi^i = m^i \phi - \frac{\lambda g^{ij}}{\text{Pe} \text{Le}_\phi} \frac{\partial \phi}{\partial x^j}, \quad (2.18)$$

is the flux vector. Note that the continuity equation is obtained if we set $\phi = 1$ and $\omega_\phi = 0$, so that $F_\phi^i = m^i$. At leading order the normal changes of the fluxes balance the source terms. Due to the absence of a source term in the continuity equation the leading order normal mass flux $m_{(0)} = \text{const}$. The $O(\text{Pe}^{-1})$ terms contain the perturbative effects of stretch and curvature. In SPFM the term containing the transverse flux $F_{(0)}^\alpha$ is generally neglected. In IDFE, the term is shown to be a corrective perturbation, but it is retained in the $O(\text{Pe}^{-1})$ equations. The term is the origin for the transverse coupling of neighbouring flame elements. It is also non-negligible in the momentum equations which are not considered in the SPFM so far.

Both SPFM and IDFE represent a simple frame work to derive explicit flame models, or effective numerical algorithms for premixed flame propagation.

3 Applications

3.1 The unified model of premixed flames as gasdynamic discontinuities

In [3] a model of a premixed flame is derived, in which the flame is viewed as a gasdynamic discontinuity surface separating the unburned from the burned gases, i.e., the philosophy of the original model of [5] and [13] is employed. In contrast to the original model, which includes leading order terms only, in [3] perturbative corrections are considered which account for the effects of stretch, unsteadiness and curvature. The model consists of incompressible fluid equations on either side of the flame, jump conditions

for fluid variables across the flame and a flame speed relation, describing the propagation of the flame surface normal to itself. The derivation of the jump conditions requires the following steps. In addition to the reactive model which describes the details within the flame structure, a hydrodynamic model is formulated which holds on either side of the flame. In the hydrodynamic model density is piecewise constant on both sides of the flame, while in the reactive model density is continuous. The equations of both the reactive and the hydrodynamic model are transformed to moving flame-attached coordinates. The equations in the flame region are analyzed using asymptotic series expansions, i.e., the IDFE are employed. Only the $O(1)$ solution of the IDFE must be determined, both for the reactive and the hydrodynamic model. The IDFE of the hydrodynamic model are subtracted from those of the reactive model. Outside the flame region both models and their solutions are identical. Differences occur in the flame region only. Integrating these differences across the flame region yields the jump conditions of the hydrodynamic model. These jump conditions are called the intrinsic disturbed flame jump conditions. The jump conditions are calculated up to $O(\text{Pe}^{-1})$.

The fluid fields on the two sides of the flame surface are related by the jump conditions for the normal mass flux (3.1), normal momentum flux (3.2), and tangential momentum flux (3.3)

$$[m] = 0, \quad (3.1)$$

$$[m v_n + p - \sigma_{nn}] = -\frac{2}{\text{Pe}} c m I_\sigma, \quad (3.2)$$

$$[m \mathbf{v}_\perp - \sigma_{n\perp}] = -\frac{1}{\text{Pe}} \nabla_\perp (m I_\sigma). \quad (3.3)$$

Here the square bracket $[*]$ denotes the jump of the quantity $*$ across the flame surface, i.e., the burned minus the unburned value, $v_n = \mathbf{v} \cdot \mathbf{n}$ is the normal velocity component with respect to the flame surface. The normal vector on the flame surface \mathbf{n} is pointing into the burned products. The tangential velocity vector on the flame surface is $\mathbf{v}_\perp = \mathbf{n} \times \mathbf{v} \times \mathbf{n}$, and similarly the tangential derivative is $\nabla_\perp(*) = \mathbf{n} \times \nabla(*) \times \mathbf{n}$. The normal and tangential viscous stresses σ_{nn} and $\sigma_{n\perp}$ at the discontinuity surface are $\sigma_{nn} = \mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n}$ and $\sigma_{n\perp} = \mathbf{n} \times (\boldsymbol{\sigma} \cdot \mathbf{n}) \times \mathbf{n}$, respectively. The jump condition (3.1) states that normal mass flux is continuous across the flame. According to the jump condition (3.2) the normal component of momentum exhibits an $O(\text{Pe}^{-1})$ jump which is proportional to the curvature c of the flame surface. The term $-\text{Pe}^{-1} m I_\sigma$ plays a role similar to surface tension but is here referred to as surface compression since it has the opposite sign. Gradients of surface compression result in a jump of tangential momentum (3.3), which is the analog of Marangoni forces. The quantity $I_\sigma > 0$, in the reaction sheet approximation, is given by

$$I_\sigma = \frac{4}{3}(\text{Pr} + 1)(T_b^{3/2} - 1) - 2(T_b - 1), \quad (3.4)$$

where T_b is the ratio of the burned to the unburned temperature.

The propagation of the flame normal to itself is governed by

$$C I_H \left(\overbrace{\partial/\partial t}^{\text{inertia}} + \overbrace{\chi}^{\text{stretch}} \right) (1/m) - \overbrace{C \text{Pe}^{-1} I_\Delta \nabla_\perp^2 (1/m)}^{\text{transverse coupling}} + \overbrace{C \text{Pe}^{-1} I_{\nabla^2} m (\nabla_\perp (1/m))^2}^{\text{nonlinear coupling}} + \underbrace{m \ln \left(m + \text{Pe}^{-1} \left(\underbrace{(I_Y - I_X) \chi/m}_{\text{stretch}} + \underbrace{2c I_X}_{\text{curvature}} \right) \right)}_{\text{nonlinearity}} = 0, \quad (3.5)$$

a nonlinear partial differential equation which we refer to as the unified flame speed relation.

Here, $C = \text{Pe}^{-1} \text{Ze} (1 - \text{Le}^{-1})$ is a nondimensional number which measures the combined effect of preferential diffusion, i.e., the Lewis number Le of the deficient component of the mixture, and the temperature sensitivity of the flame speed, i.e., the Zeldovich number Ze . The positive constants I_H , I_Δ , I_{∇^2} , I_Y , and I_X are integrals of the leading order solutions, i.e., integrals which may be evaluated from planar unperturbed flames.

The time derivative indicates that the mass flux m needs a definite amount of time to adjust to new conditions. The operator $\nabla_\perp^2(*) = \nabla \cdot (\mathbf{n} \times \nabla(*) \times \mathbf{n})$ is the surface Laplacian. Thus, neighbouring points on the flame cannot propagate at uncorrelated speeds. A second mechanism coupling neighbouring flame elements is provided by the nonlinear term $(\nabla_\perp(1/m))^2 = (\nabla_\perp(1/m)) \cdot (\nabla_\perp(1/m))$.

If we ignore the transverse coupling terms the unified flame speed relation reduces to the flame speed relations previously derived in [17] and [14].

The unified model describes the flame propagation by nonreactive incompressible fluid equations, jump conditions for the flow variables and a flame speed relation. The effects of the reactive flow enter the constants of the model and may be evaluated from stationary planar flames. The unified model is attractive for numerical computations, as it replaces the reactive equations, involving small length scales and stiff reaction terms, by nonreactive equations. The thin flame structure is replaced by a surface of discontinuity. This eliminates the necessity to resolve thin internal layers. The propagation of the surface of discontinuity may be computed using the levelset method, which is also referred to as the G -equation.

The unified model is also attractive with respect to analytical studies of flame behavior. The incompressible nonreactive flow equations are substantially simplified compared to the original compressible reactive equations and may often be treated analytically. An example of an analytical study is presented in the next subsection.

Even though the unified model was derived for a single step global chemistry, it is shown in [12] that the model may be extended to complex reaction mechanisms.

3.2 Stability of planar flames

The stability of steadily propagating planar premixed flames has been the subject of numerous studies since Darrieus and Landau showed that in their model flames are unstable to perturbations of any wave length. Moreover, the instability was shown to persist even for very small wave lengths, i.e., there was no high wave number cutoff of the instability. In addition to the Darrieus-Landau instability, which results from thermal expansion, analysis of the diffusional thermal model indicates that premixed flames may exhibit cellular and pulsating instabilities as a consequence of preferential diffusion. However, previous theories did not capture all of the instabilities including a high wave number cutoff for each. In [2] the stability of a uniformly propagating planar flame is considered employing the unified model of premixed flames as gasdynamic discontinuities [3]. It is shown that the unified model is the only model to capture the Darrieus-Landau, cellular and pulsating instabilities including a high wave number cutoff for each. Figure 1 shows two typical stability diagrams. Plotted is the amplification rate ω of perturbations versus the wave number k of the perturbations. Positive amplification rates correspond to unstable flames. Oscillatory behaviour is indicated if a curve is shown together with a shaded region, where the width of the shaded region is a measure of the frequency of the oscillations. Figure 1a) corresponds to the typical situation of intermediate Lewis numbers. For small wave numbers, i.e., long wave perturbations we observe the Darrieus Landau instability including its cutoff, i.e., a positive Markstein number. For shorter wave length perturbations the flame shows stable behaviour. Within the stable region we observe both oscillatory and aperiodic behaviour. Figure 1b) corresponds to the case of negative Markstein numbers. We observe a destabilizing trend of the Darrieus-Landau instability for small wave numbers.

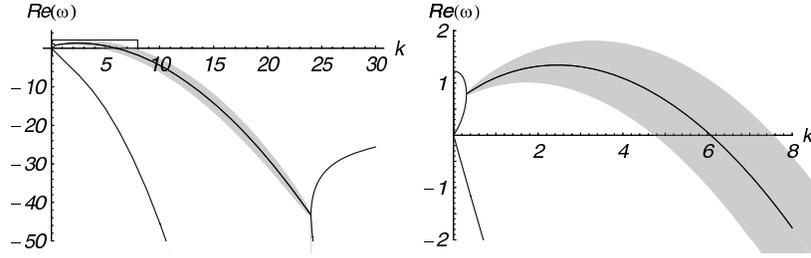


Figure 1: Stability diagrams for a) intermediate and b) small Lewis numbers.

For shorter wavelength perturbations (higher k) the instability becomes oscillatory and for yet higher wavelength the high-wave number cutoff of the oscillatory instability is found.

3.3 Algebraic Stretched Flamelet Model

While in the unified model a large Peclet number is used to allow for an asymptotic series expansion, i.e., weak curvature is assumed, in the stretched premixed flamelet model, the term Q_b in (2.12) is neglected, due to physical arguments. This assumption has been verified for typical test cases. Therefore no explicit assumption on curvature or stretch must be employed.

Integrating the set of quasi 1D flamelet equations (2.12) across the flame front, we obtain integral balances for the enthalpy H and the element mass fractions Z_j and a relation for the mass burning rate $m_b = (\rho s_L)_b$ in the burnt gas mixture. These equations read

$$\begin{aligned} \Delta H_b &:= H_b - H_u = -\sum_{i=1}^N H_i^0 \left(\frac{\text{Ka}_i}{\text{Le}_i} - \text{Ka}_T \right) (Y_{i,b} - Y_{i,u}), \\ \Delta Z_{j,b} &:= Z_{j,b} - Z_{u,j} = -\sum_{i=1}^N w_{ji} \left(\frac{\text{Ka}_i}{\text{Le}_i} - \text{Ka}_T \right) (Y_{i,b} - Y_{i,u}), \\ m_b(H_{T,u}, H_b, Z_{j,b}) &\approx (1 - \text{Ka}_T) m_b^0(H_{T,u}, H_b^0 + \Delta H_b, Z_b^0 + \Delta Z_b), \end{aligned} \quad (3.6)$$

where the Karlovitz integrals Ka_i are defined by

$$\frac{\text{Ka}_i}{\text{Le}_i} = \int_{s_u}^{s_b} \sqrt{g} \rho K \tilde{Y}_i ds / (\sqrt{g_b} m_b^0), \quad (3.7)$$

i.e. Ka_i/Le_i is the mass flow rate $\sqrt{g} \rho K$ along the flame surfaces weighted with the normalized species mass fraction \tilde{Y}_i , integrated across the flame and scaled with the stretchless mass burning rate $\sqrt{g_b} m_b^0$. A similar interpretation holds for Ka_T . This set of algebraic equations is referred to as the Algebraic Stretched Flamelet Model (ASF) and completely describes the detailed influence of stretch and curvature on the flame speed. For more details the reader should consult [6].

The ASF has the following properties:

1. the detailed behaviour of stretch and curvature fields inside the flame structure is taken into account
2. the model is applicable for strong stretch, curvature and detailed reaction mechanisms

3. for weak stretch and a single step reaction, previous results from Matalon et al. [14], Clavin [4] and others are recovered
4. a comparison with a series of numerical results has shown that a quantitative prediction of m_b is possible.

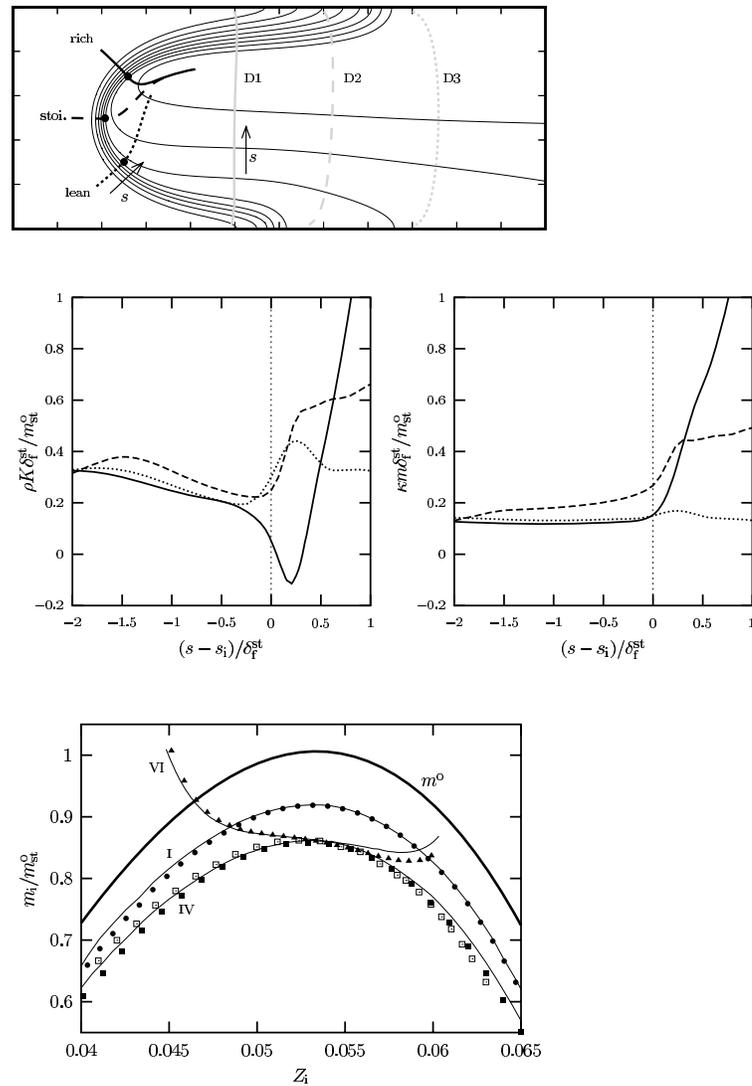
These properties open the way to use the model in a number of ways, which will be summarised below.

3.4 Analytical Application of ASFM

First of all, as ASFM is valid for general (detailed) chemistry and strong stretch and curvature, the ASFM gives the possibility to investigate the predictive power of asymptotic theories like the IDFE approach. In particular the maximum stretch rate and the minimum radius of curvature, up to which these theories yield quantitative results may be evaluated. This will be one of the main goals of our collaboration in the future. On the other hand, as the unified model offers jump conditions for all variables, the flame stability theory evolving from the unified model can be improved employing the detailed chemical kinetics of ASFM. The power of ASFM to predict the influence of stretch and curvature on the flame speed in even very complicated cases has recently been shown. Consider the example presented in Figure 2, in which the local mass burning rate of a triple flame, computed numerically is compared to the results from ASFM by integrating the numerically computed stretch (Figure 2b) and curvature (Figure 2c) fields along the flamelet contours (Figure 2a) as predicted by the model. This is very convincing since the flame speed depends on the local stoichiometry Z_i which changes rapidly along the premixed triple flame front. The upper thick line in Figure 2d) is the unstretched flame speed as function of Z_i , the thin lines denote the local flame speed in three different flames computed numerically and the symbols indicate the results of ASFM, which are very close to the numerical results. We noted, that this result has been obtained for unit Lewis numbers so that the effects of preferential diffusion are absent. At the moment it is not yet possible to reach a similar accuracy with ASFM if Lewis numbers are non-unit. ASFM will be improved in the near future to account for these effects.

3.5 Numerical Application of SPFM

Secondly, the theory of SPFM offers the possibility to develop new fast, efficient and accurate numerical (flamelet) models for premixed flames. Groot et al. [9] for instance used SPFM recently to simulate and investigate propagating spherical and cylindrical flames. The kinematic equation for ϕ has been solved for the motion of a series of iso-surfaces of ϕ in the flame area (between ϕ_u and ϕ_b). The 1D stretched and curved flamelet system was solved during each time step to predict the change in the inner structure and the local flame speed. This decoupling of the stiff reacting system for the inner structure and the flame motion (without chemistry) shows that a reduction in computing time compared to a direct solution of the full system of a factor of 10 is easily possible. Also, the theory of ASFM and the numerical model were used to compute the Markstein numbers for spherical and cylindrical flames and again a very good quantitative agreement was found. Furthermore, it was shown that it makes no sense to decouple the Markstein number for flame stretch in separate contributions due to strain and curvature, because the value for the Markstein number of strain proved to depend on the combustion situation and is not unique [10].



1

Figure 2: Verification of ASFM in a triple flame.

3.6 Flamelet Generated Manifold Model

A disadvantage of the numerical model based on the kinematic equation and ASFM is that it is very difficult to use the model directly in numerical simulations. Solving the kinematic equation (similar to the G-equation) for one iso-surface is often used in literature, but the solution of the kinematic equation of a series of isoplanes in an area was not done before. In the above-mentioned study, Groot and de Goeij [9] showed that it is possible to do this for 1D spherical or cylindrical flames, but it seems to be very difficult

to extend this numerical procedure to arbitrary flame geometries. The reason for this is that different iso-surfaces are not connected and a diffusive term coupling the iso-planes is missing in the kinematic equations for the separate iso-surfaces. To get around this problem, the so-called Flamelet-Generated Manifold (FGM) method has been developed recently [15]. The starting point of this approach is that the kinematic equation for ϕ is combined with the flamelet-equation for ϕ , leading again to the 3D transport equation for ϕ . The model remains equivalent to SPFM: we now have 1) a set of flow- and mixing equations, 2) a set of quasi-1D flamelet equations for the internal structure and 3) a 3D instationary transport equation for ϕ (instead of a kinematic equation) for the flame motion. The FGM method has proved to be very efficient and very accurate [15] [16]. A reduction in computing time of a factor of 100 compared to direct numerical solution is possible. In a number of papers it has been shown that FGM is also very accurate. Bunsen flames are computed and even in the highly curved tip and near the flame base close to the burner very accurate results are found. In Figure 2, results of FGM are compared to direct numerical solutions, showing the power of the method. FGM is used similarly as ILDM or other manifold methods, in the sense that species mass fractions and source terms are stored as function of the progress variables (like ϕ). In spite of the accuracy of FGM the disadvantage of the model is that it cannot be used for non-premixed flames like ILDM because the database is constructed from premixed flamelets. For this reason, we recently introduced the so-called Phase-Space ILDM method [1], in which the system SPFM is treated in a similar way as in ILDM. This method has not been applied so far, but theory predicts that it might be used to all kinds of flames in the near future.

4 Future applications

In the previous section we have shown that IDFE and SPFM represent a general framework to investigate dynamic flame behaviour in theory, numerics and data analysis. Examples include stability analysis, effective implementations of flame codes and the study of stretch effects in premixed flames using field data. These are only a few examples of problems to which our method is applicable.

Let us consider some future applications for our theory. In the reaction zone of a premixed flame a radical pool is created, which in the burned mixture yields toxic combustion by products. A great deal of research has been focused reducing these toxics for a clean environment. Our approach enables us to provide a quantitative prediction of the radical pool as a function of flame stretch and geometry in an efficient manner. As an example consider thermal nitrogen oxide, which is very sensitive to temperature variations. Due to the interaction with the flow, the burned temperature may exhibit local peaks, where the production of nitrogen oxide is much larger, than anywhere else in the flame. Other toxics are generated by fairly slow reactions in the burned products but still depend on the precise value of the radical pool, which we provide.

Another field of interest to the combustion community is turbulent premixed or partially premixed combustion. A typical approach is to first simulate a turbulent flame by direct numerical simulation, next to seek correlations, and finally to employ these correlations in turbulence modelling. Unfortunately the numerical effort for this is prohibitively large if detailed combustion models are employed. Our approach gives the possibility to greatly reduce the numerical effort. There are basically two approaches which seem promising.

If a calculation is needed which resolves a large number of turbulent length scales, which are larger than the flame thickness, it is not possible to employ a detailed combustion model. We propose to use a flame speed relation and the corresponding jump conditions for the flow, which increases the total computational cost only slightly compared to those of a nonreactive DNS.

If on the other hand detailed chemistry is required, we propose to employ the Flamelet Generated Manifold method, which reduces the numerical effort significantly, since it replaces the multidimensional reactive equations, by a much smaller number of multidimensional combustion equation and a set of quasi-stationary one-dimensional equations for the remaining species. The reduced multidimensional system does not suffer from the severe time step restrictions as the original system.

In the far future we intend to develop turbulence models for premixed and partially premixed combustion similar to the conditional moment closure method. In these models the closure of turbulent correlations is conditioned on a suitable progress variable. Our theory provides the framework to determine which variables may be employed as progress variables.

The problems which we already have solved and those which we intend to solve show the potential of our framework in getting a better understanding of flames and eventually will suit to better control combustion processes.

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