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Two quasi-one-dimensional descriptions of premixed flames
based on flame coordinates

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Abstract. Two different curvilinear, flame coordinate systems are introduced. These form the basis for either the Intrinsic Disturbed Flame Equations (IDFE) or the Strongly Stretched Flamelets Equations (SSFE), which are quasi-one-dimensional systems of differential equations describing the inner structure and propagation velocity of stretched, premixed flames. Integral analysis is applied to derive relations for the mass burning rate, and for the IDFE, to derive jump conditions. The feasibility of both descriptions has been demonstrated. Finally, an efficient solution strategy for premixed flames is proposed, that combines both formalisms.

Keywords. Premixed flames, flame surface(s), flame coordinates, tensor formulation of conservation laws, stretch rate, instrinsic disturbed flame equations (IDFE), strongly stretched flamelets equations (SSFE), jump conditions, burning speed, mass burning rate.

1 Introduction

A premixed flame can be considered as the thin layer where all chemical reactions and heat production take place, separating the burned and unburned gas mixtures. It can be either stationary, as in most domestic heating equipment, or time dependent, occurring, when a flame is acoustically perturbed or in turbulent flames. Numerical simulation of premixed flames is still a demanding task since it requires the solution of a large number of nonlinear, three-dimensional conservation laws characterised by many different space and time scales. However, the very small thickness of a flame allows us to reformulate the conservation laws as a system of quasi-one-dimensional differential equations describing the propagation and/or inner structure of the flame in the direction normal to itself. This can be easily accomplished for some flames, like stagnation flames, using Cartesian coordinates, or spherically expanding flames, using spherical coordinates. In general, this is not so easy, since premixed flames are usually not aligned with a standard coordinate system. It is therefore convenient to construct curvilinear coordinate systems attached to a flame that do have this property.
Recently, two such coordinate systems have been developed independently [6, 11, 37]. In this paper we will present these two coordinate systems and refer to these as flame coordinates. Both systems allow a reformulation of the conservation laws in terms of a quasi-one-dimensional system of differential equations. From these quasi-one-dimensional systems we can derive analytical models describing the propagation and inner structure of a flame, using asymptotics and/or integral analysis. Moreover, numerical simulation of these quasi-one-dimensional systems is much cheaper than the numerical simulation of the complete system of three-dimensional conservation equations, yet giving accurate results. The combination of a particular flame coordinate system and an analytical/numerical solution strategy is referred to as a quasi-one-dimensional description. We will compare and assess two different quasi-one-dimensional descriptions. Our final goal is to combine these two descriptions in order to have a very efficient and accurate solution method for premixed flames.

We define two curvilinear flame coordinate systems $\xi = (\xi^1, \xi^2, \xi^3)$ such that the $\xi^1$-lines are perpendicular to the coordinate surfaces $\xi^i = \text{const}$. In the first system (uniform flame coordinates) we choose the coordinate surface $\xi^1 = 0$ inside the flame, referred to as the flame surface, and take all other surfaces $\xi^1 = \text{const} \neq 0$ equidistant to the flame surface. Any smooth surface within the flame can be used as the flame surface, however, in the following we will make a specific choice that turns out to be advantageous. On the other hand, in the second system (iso-scalar flame coordinates) we take iso-surfaces $Y(x,t) = \text{const}$ of a suitable progress variable $Y$ as coordinate surfaces $\xi^i = \text{const}$. This is possible, provided $\nabla Y \neq 0$ everywhere in the flame. In this case, the surfaces $\xi^i = \text{const}$ are not equidistant. Both coordinate systems can be time dependent and moving with the flame.

Next, we reformulate the conservation laws of premixed flames in terms of the flame coordinates $\xi$ using tensor notation. The resulting equations are quite complicated, containing the metric tensor describing the (local) geometry of the flame. However, significant simplifications are possible, observing that variations along the flame surfaces are small compared to variations across the flame. Consequently, as a first approximation, we can neglect all diffusive fluxes in the flame surfaces, resulting in a quasi-one-dimensional system of differential equations only containing derivatives in $\xi^1$-direction. For the uniform flame coordinates we assume that the $\xi^\alpha$-surfaces ($\alpha = 2, 3$) are moving with the flow tangential to the flame surface, so that transverse convection terms disappear to first order approximation, yet accounted for at higher order in an asymptotic series expansion. Thus, at higher order, variations of all variables along the flame are accounted for. For the iso-scalar flame coordinates, the quasi-one-dimensional equations contain terms describing convective transport along the flame surfaces, which arise since flow usually is not normal to the flame surfaces. These convective terms are described as stretch terms. The resulting quasi-one-dimensional system is referred to as Intrinsic Disturbed Flame Equations (IDFE) for the uniform flame coordinates and Strongly Stretched Flamelets Equations (SSFE) for the iso-scalar flame coordinates. Both coordinate systems have been used in previous work [11, 12, 13, 6] to describe the influence of flame stretch, curvature and unsteady effects on the mass burning rate.

There are a number of previous theories which are closely related to either IDFE or SSFE. Darrieus [9] and Landau [19] independently considered a model of a flame as a gasdynamic discontinuity, based on the observation that flames are often very thin. They assumed that mass and momentum are conserved across the flame and that the mass burning rate is constant. In fact, their theory is identical to the IDFE leading order result for near-equidiffusional flames, i.e., flames for which the ratio of mass and heat diffusivities is close to 1 for all species. Applying a stability analysis, they showed that such a simple model is not sufficient to describe real flames, as their theory yields unconditional instability of the flame with respect to perturbations of any wave length. Later theories tried to resolve this issue by deriving mass burning rate relations that account for the flow and the shape of the flame, even though not being rigorous asymptotic approaches. In fact, Markstein [21, 22], Eckhaus [10] and Karlovitz [16] proposed
mass burning rate relations that account for flame curvature, strain and stretch. In order to derive these
relations they focused on specific aspects of the combustion problem and excluded other effects, which
they considered less important, based on a profound physical understanding of the problem. Even though
they captured the essential features of flame dynamics, they could not yet provide quantitative relations
based on physico-chemical parameters. The SSFE approach is based on first principles, i.e., all chemical
reactions and transport processes in the flame are taken into account, but instead of employing heuristic
arguments only, we verified the validity of our assumptions by analysing detailed numerical simulations
of premixed flames [12, 36]. In the current paper we support this further by presenting estimates for the
terms neglected. For the IDFE we follow a more formal approach to determine which terms in the com-
bustion problem must be considered and which terms may be excluded. Asymptotic series expansions
have proven to be a very effective tool to construct models of a desired order of accuracy.

Barenblatt et al. [2] introduced high activation energy asymptotics and derived a first mass burning
rate relation based on physico-chemical parameters, but they ignored thermal expansion; see also [40].
Sivashinsky [35] accounted for thermal expansion and derived a mass burning rate relation by strict
asymptotics. Even though his theory accounts for flame stretch it does not resolve the problem of the
flame being unconditionally unstable. On the other hand, the theories of Clavin and Williams [5] and
Matalon and Matkowsky [23] both consider near-equidiffusional flames to derive a mass burning rate
which now yields acceptable results as long as the fuel diffusivity is not larger than a critical value. In
the unified IDFE theory of Class et al. [6] the theories of Sivashinsky [35] and of Matalon and Matkowsky
[23] are unified and extended to account for short wave flame corrugations. This eventually resolves the
problem of flame instability for any fuel diffusivity.

Both from the IDFE and SSFE we will derive a mathematical model describing the inner structure
and the propagation speed of the flame. For the IDFE we apply an integral analysis to derive a model
of the flame as a gasdynamic discontinuity. We then use asymptotic expansions to derive expressions
for the laminar burning speed and jump conditions for mass, momentum, specific enthalpy, species mass
fractions and element mass fractions across the flame. Our asymptotic theory exploits the fact that flame
perturbations like stretch and curvature are often weak and thus may be employed for an asymptotic
series expansion. At leading order, we obtain one-dimensional equations. These determine the flame
structure as a function of the local mass burning rate. Moreover, for near-equidiffusional flames, the
mass burning rate can be determined as well and turns out to be identical to the mass burning rate of
unstretched stationary flames. For near-equidiffusional flames, corrections of the mass burning rate are
computed at higher orders of the asymptotic expansion, while for other flames the leading order mass
burning rate is computed at higher orders.

For the SSFE we do not use asymptotic expansions, but we also use integral analysis [8] in order to
derive a relation for the mass burning rate. Carrying out this analysis for both a stretchless and a stretched
flame, we can derive a relation between the mass burning rates of both flames. It turns out that the mass
burning rate depends on the detailed structure of the flame. The SSFE theory has proven to be able to
describe the behaviour of flames with complex chemistry [36] and flames characterised by strong stretch
and curvature, as occurring in turbulent flames [24]. There are also a number of other theories which
account for complex chemistry which rely on high activation energy; see e.g. Class and Klimenko [17],
and Seshadri and Peters [33]. The asymptotic approach followed in these last studies inherently restricts
the analysis to small perturbations while the SSFE model is applicable for strong stretch. In the latter
case, the detailed behaviour of stretch and curvature have to be integrated through the flame to determine
the local flame response.

In the current paper we present the main features of the IDFE and SSFE theories. For the first
time, we present a rigorous derivation of the SSFE using tensor notation. Moreover, we show that
the transverse transport terms in the SSFE are small compared to transport terms normal to the flame surfaces, and can be neglected indeed. The IDFE are formulated in terms of the primitive variables, rather than the coefficient functions in an asymptotic series, and likewise for the corresponding jump conditions. For the IDFE we present for the first time the equations and jump conditions for element mass fractions. The description of both theories is uniform, which makes comparison very easy. We discuss the applicability of both methods and indicate their advantages and disadvantages. Finally, we propose a combination of both descriptions, in order to construct an efficient yet accurate solution strategy for premixed flames.

We have organised this paper as follows. In Section 2 we briefly review the governing equations of premixed flames and reformulate these in general curvilinear coordinates, using tensor notation. Furthermore, we derive the IDFE and the SSFE. Next, in Section 3, we apply integral analysis to both IDFE and SSFE in order to derive jump conditions and a model for the mass burning rate, respectively. A comparison of both theories is given is Section 4. Application of the IDFE and SSFE are presented in Section 5. In the final discussion section, we propose new solution strategies for premixed flames by combining both theories.

2 Governing equations in flame coordinates

In this section we present a mathematical model for laminar, premixed flames under atmospheric conditions. Typically, we consider the combustion of hydrocarbons in air. The species in the flame are numbered 1 through \( N_s \). Species \( N_s \) is nitrogen (\( N_2 \)) and is present in abundance, while the other species are considered trace species. The governing equations for such flames are the conservation equations of mass, momentum and energy of the gas mixture, the balance equations of mass for the trace species and the thermal and caloric equations of state [39, 31]. These can be written in the following form [37]:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0,
\]

\[
\frac{\partial}{\partial t}(\rho v) + \nabla \cdot (\rho vv) = -\nabla p + \nabla \cdot \mathbf{T},
\]

\[
\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho vh) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) = \nabla \cdot \mathbf{J}_h,
\]

\[
\frac{\partial}{\partial t}(\rho Y_n) + \nabla \cdot (\rho v Y_n) - \nabla \cdot \left( \frac{\lambda}{Le_n c_p} \nabla Y_n \right) = \omega_n, \quad n = 1, 2, \ldots, N_s - 1,
\]

\[
p_{\text{amb}} = \frac{\rho RT}{M}, \quad \frac{1}{M} = \sum_{n=1}^{N_s} Y_n \frac{M_s,n}{M_{s,n}},
\]

\[
h = \int_{T_{\text{ref}}}^{T} c_p(T', Y_1, Y_2, \ldots, Y_{N_s}) \, dT' + \sum_{n=1}^{N_s-1} h_{n,\text{ref}} Y_n.
\]

The independent variables in (2.1) are the density \( \rho \), the flow velocity \( v \), the hydrodynamic pressure \( p \), the specific enthalpy \( h \), the species mass fractions \( Y_n \) and the temperature \( T \). Other variables/consts in (2.1) are the stress tensor \( \mathbf{T} \), the thermal conductivity \( \lambda \), the specific heat at constant pressure \( c_p \), the enthalpy diffusion flux \( \mathbf{J}_h \), the Lewis numbers \( Le_n \), the reaction rates \( \omega_n \), the ambient pressure \( p_{\text{amb}} \), the universal gas constant \( R \), the species molar masses \( M_s,n \), the average molar mass \( M \) and the specific enthalpies of formation \( h_{n,\text{ref}} \) at a reference temperature \( T_{\text{ref}} \).
In Section 3 we need the element mass fractions \( Z_q \). Assume that the elements are numbered 1 through \( N_e \) and that nitrogen \((N)\) is the \( N_{e,0} \)th element. The element mass fractions of the other elements are defined by

\[
Z_q := \sum_{n=1}^{N_e-1} \alpha_{q,n} Y_n, \quad q = 1, 2, \ldots, N_e - 1,
\]

where \( \alpha_{q,n} \) is the mass fraction of element \( q \) in species \( n \), i.e., \( \alpha_{q,n} = M_{e,q} a_{q,n}/M_{s,n} \) with \( M_{e,q} \) the molar mass of element \( q \) and \( a_{q,n} \) the number of atoms of element \( q \) in a molecule of species \( n \). Taking the proper linear combination of the species equations (2.1d), we get the following conservation equations for \( Z_q \):

\[
\frac{\partial}{\partial \tau}(\rho Z_q) + \nabla \cdot (\rho \mathbf{v} Z_q) - \nabla \cdot \left( \frac{\lambda}{\rho C_p} \nabla Z_q \right) = \nabla \cdot \mathbf{J}_{Z_q}, \quad q = 1, 2, \ldots, N_e - 1,
\]

where \( \mathbf{J}_{Z_q} \) is the mass diffusion flux of element \( q \); for more details see [11, 37]. These conservation equations are, of course, not independent of the set (2.1d).

Next, we like to reformulate the conservation equations (2.1a)-(2.1d) and (2.3) in terms of a curvilinear coordinate system moving with the flame. To that purpose, we describe the flame in terms of so-called flame surfaces. Two specific choices for the flame surfaces will be made in Section 2.1 and Section 2.2, respectively, but for the time being we consider the flame as a set of these surfaces. We choose the curvilinear coordinate system \( \xi = (\xi^1, \xi^2, \xi^3) \), such that \( \xi^1 \) is the coordinate normal to the flame surfaces, whereas the coordinates \( \xi^\alpha (\alpha = 2, 3) \) are (orthogonal) coordinates in each flame surface. Moreover, we introduce the variable \( \tau \) as the time corresponding to the curvilinear coordinate system. Obviously, \( \tau = t \). Referring to Appendix A for the exact form of the relevant differential operators, the conservation equations in (2.1) and (2.3) read:

\[
\frac{\partial}{\partial \tau}(\sqrt{g} \rho) + \frac{\partial}{\partial \xi^2}(\sqrt{g} m^i) = 0, \tag{2.4a}
\]

\[
\frac{\partial}{\partial \tau}(\sqrt{g} \rho u^i) + \frac{\partial}{\partial \xi^2}(\sqrt{g} m^i v^j) = -\frac{\partial}{\partial \xi^2}(\sqrt{g} p \ell^i) + \sqrt{g} g^j g^k - v^k \partial_j \partial_k u^i - \frac{2}{3} \sqrt{g} g^{ji} \partial_k \left( \frac{\lambda}{\rho C_p} \right) \ell_j \left( \sqrt{g} v^k \right) \ell_j, \tag{2.4b}
\]

\[
\frac{\partial}{\partial \tau}(\sqrt{g} \rho h) + \frac{\partial}{\partial \xi^2}(\sqrt{g} m^i h) - \frac{\partial}{\partial \xi^2}(\sqrt{g} \frac{1}{\rho C_p} \partial_i u^j \partial_j \ell^i) = \sqrt{g} J^i_k, \tag{2.4c}
\]

\[
\frac{\partial}{\partial \tau}(\sqrt{g} \rho Y_n) + \frac{\partial}{\partial \xi^2}(\sqrt{g} m^i Y_n) - \frac{\partial}{\partial \xi^2}(\sqrt{g} \frac{1}{\rho C_p} \partial_i \partial_j \partial_i Y_n) \ell_j \left( \sqrt{g} \omega_n \right), \tag{2.4d}
\]

\[
\frac{\partial}{\partial \tau}(\sqrt{g} \rho Z_q) + \frac{\partial}{\partial \xi^2}(\sqrt{g} m^i Z_q) - \frac{\partial}{\partial \xi^2}(\sqrt{g} \frac{1}{\rho C_p} \partial_i \partial_j \partial_i Z_q) \ell_j \left( \sqrt{g} \omega_q \right), \tag{2.4e}
\]

where \( \sqrt{g} \) is the Jacobian of the coordinate transformation \( x \mapsto \xi \), \( g^j \) are the components of the contravariant metric tensor, \( m^i := \rho a^i \cdot (v - \dot{x}) \) is the contravariant component of the mass flux vector relative to the coordinate system moving with velocity \( \dot{x} = \frac{\partial x}{\partial \tau} \) and \( u^i := a^i \cdot u \) is the contravariant component of a vector \( u (u = v, J_h, J_Z) \). Moreover, in equation (2.4b), \( \ell_i \) and \( \ell^i \) are the covariant and contravariant components of a vector \( \ell \), respectively, which is an arbitrary constant vector in Cartesian coordinates, i.e., the vector \( \ell \) has constant length and direction. Thus, equation (2.4b) is a conservation law for the velocity component \( v \cdot \ell = v^i \ell_j \) and represents the scalar momentum balance in the direction of the vector \( \ell \). Note that we have to apply (2.4b) to three linearly independent vectors \( \ell \).
2 GOVERNING EQUATIONS IN FLAME COORDINATES

2.1 Intrinsic disturbed flame equations

Observations of premixed flames typically show that the burned products are separated from the unburned mixture by a thin layer. Variations across this layer are typically much larger than along the layer. Viewed on the larger hydrodynamic scale, the flame layer shrinks to a surface that propagates normal to itself with the laminar burning speed $s_L$. It is the propagation speed of this surface relative to the unburned mixture. We will give a more precise definition below. Note that within the layer, thermal expansion results in a strong variation of the flow velocity. On the other hand, the mass burning rate $m$ shows small variations across the flame layer, so that it is more appropriate to describe the propagation of the flame surface.

We choose a flame coordinate system $\xi = (\xi^1, \xi^2, \xi^3)$ attached to the flame as follows. First, we select a suitable surface inside the flame layer and identify it with the coordinate surface $\xi^1 = 0$. We call it the flame surface. Even if the flame is a layer of finite extend we may choose such a surface, where we have some freedom in choosing it. Once we have selected the flame surface, we may choose arbitrary $\xi^\alpha$ ($\alpha = 2, 3$)-coordinate lines on the surface at time $\tau = 0$. The coordinate system $(\xi^1, \xi^2, \xi^3)$ outside the flame surface is constructed in such a way that the resulting equations become as simple as possible, and such that intrinsic properties of the surface, in particular the mean curvature and stretch, appear as explicit coefficients in the equations. More precisely, we assume that the $\xi^1$-lines are orthorgonal to the $\xi^1$-surfaces and that the $\xi^1$-surfaces are uniformly spaced, i.e.,

$$\frac{\partial x}{\partial \xi^1} \cdot \frac{\partial x}{\partial \xi^\alpha} = 0 \quad (\alpha = 2, 3) \quad \text{and} \quad |\nabla \xi^1| = \text{const} := 1. \quad (2.5)$$

With these two requirements the coordinate system on the flame surface uniquely defines the coordinate system in the entire flame layer. The (symmetric) covariant and contravariant metric tensors now take the form

$$(g_{ij}) = \begin{pmatrix} g^{11} & 0 & 0 \\ 0 & g^{22} & g^{23} \\ 0 & g^{23} & g^{33} \end{pmatrix}, \quad (g^{ij}) = \begin{pmatrix} g^{11} & 0 & 0 \\ 0 & g^{22} & g^{23} \\ 0 & g^{23} & g^{33} \end{pmatrix}, \quad (2.6)$$

with $g^{11} = g_{11} = 1$. It is interesting to note, that with our specific choice $|\nabla \xi^1| = 1$ the normal component of any covariant or contravariant vector is identical to the corresponding physical component, i.e., $u_1 = u^1 = u \cdot n$ where $n$ is the unit normal vector on the $\xi^1$-surfaces directed towards the burned gas mixture. Moreover, note that the volume element $dV := \sqrt{g} d\xi^1 d\xi^2 d\xi^3$ and the surface element of $\xi^1$-surfaces $dS := \sigma d\xi^2 d\xi^3$ are essentially the same since

$$g = \det(g_{ij}) = g_{11} \det(g_{\alpha\beta}) = \sigma^2, \quad \sigma := \left| \frac{\partial x}{\partial \xi^2} \times \frac{\partial x}{\partial \xi^3} \right|. \quad (2.7)$$

Next, we will give the expressions for the mean curvature and stretch. Locally, the flame surface can be characterized by its two principle curvatures. In each principle direction line elements on the surface can be approximated by arcs. The principle radius of curvature of these arcs can be calculated by taking the derivative of the arc length with respect to normal distance. The sum of the two principle curvatures is called the mean curvature $c$ and can be computed using the normal derivative of $\sigma = \sqrt{g}$ as follows:

$$2c = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^1} (\sqrt{g}). \quad (2.8)$$
In addition, we introduce the auxiliary variables \( q_i \) defined as in (2.8), where the index 1 should be replaced by \( i (i = 1, 2, 3) \). Note that \( c_1 = c \). The flame stretch \( \chi \) is defined as the relative temporal rate of change of a surface element on \( \xi^1 = 0 \) due to the movement of the surface with the tangential fluid velocity. Note, that the tangential velocity is weakly varying within the flame layer. Therefore, depending on the specific choice of the flame surface we get weakly varying flame stretch. Employing a weighted mean value of the tangential velocity component within the flame layer, rather than the local value of the tangential velocity on the flame surface, results in a flame stretch that becomes independent of the choice of the flame surface. We will specify the procedure below. We refer to the weighted mean value of the tangential velocity as the projected tangential velocity. Furthermore, we let the two-dimensional coordinate system in \( \xi^1 = 0 \) move with the same tangential velocity. The surface element \( dS = \sqrt{g} d\xi^2 d\xi^3 \) on \( \xi^1 = 0 \) is the same as in the flame stretch definition, and consequently

\[
\chi = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \tau} (\sqrt{g}), \tag{2.9}
\]

Strictly speaking, the stretch is defined for the flame surface only, but we will apply (2.9) formally to other coordinate surfaces \( \xi^1 = \text{const} \neq 0 \) as well.

Substituting the expressions for \( \chi \) and \( q_i \) into the the conservation equations (2.4a)-(2.4e) we obtain the following set of equations:

\[
\begin{align*}
\left( \frac{\partial}{\partial \tau} + \chi \right) \rho + \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) m^i &= 0, \tag{2.10a} \\
\left( \frac{\partial}{\partial \tau} + \chi \right) \left( \rho v^j \ell_j \right) + \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( m^i v^j \ell_j \right) &= - \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( p \ell^i \right) + \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left[ \mu \left( g^{ik} \frac{\partial v^i}{\partial \xi^k} + g^{ik} \frac{\partial v^i}{\partial \xi^k} - v^k g^{ji} + 2c_k v^k \right) \ell_j \right], \tag{2.10b} \\
\left( \frac{\partial}{\partial \tau} + \chi \right) \left( \rho h \right) + \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( m^i h \right) - \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( \frac{\lambda}{c_p} g^{ij} \frac{\partial h}{\partial \xi^j} \right) &= \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) J^i_h, \tag{2.10c} \\
\left( \frac{\partial}{\partial \tau} + \chi \right) \left( \rho Y_n \right) + \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( m^i Y_n \right) - \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( \frac{1}{\rho_0} \frac{\lambda}{c_p} g^{ij} \frac{\partial Y_n}{\partial \xi^j} \right) &= \omega_n, \tag{2.10d} \\
\left( \frac{\partial}{\partial \tau} + \chi \right) \left( \rho Z_q \right) + \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( m^i Z_q \right) - \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) \left( \frac{\lambda}{c_p} g^{ij} \frac{\partial Z_q}{\partial \xi^j} \right) &= \left( \frac{\partial}{\partial \xi^i} + 2c_i \right) J^i_{Z_q}. \tag{2.10e}
\end{align*}
\]

The equations in (2.10) are exact and no assumptions are made. However, for thin flames we may introduce the following simplifications. The tangential velocity components \( v^i (\alpha = 2, 3) \) are constant across the flame to leading order in an asymptotic series expansion in powers of the reciprocal Peclet number \( \text{Pe} \), which is defined as \( \text{Pe} := \ell / \delta_f \) with \( \ell \) the hydrodynamic length scale and \( \delta_f \) the (thermal) flame thickness. The Peclet number is large in general, thus the projected tangential velocity field is to leading order identical to the local tangential velocity component and \( m^i = \rho a^p \cdot (v - \dot{x}) = o(1) (\alpha = 2, 3) \). Therefore, \( m^\alpha \) may be neglected since variations along the flame are much smaller than variations normal to the flame, so that transverse variations of the small quantity \( m^\alpha \) are yet smaller. In the convection terms only the term \( \frac{\partial}{\partial \xi^i} + 2c \) remains and the corresponding contravariant index 1 in \( m^1 \) is skipped, i.e., \( m := m^1 \). Moreover, transverse derivatives of all quantities are small so that diffusion fluxes along the flame may be neglected. Finally, for thin flames the stretch \( \chi \) and the curvature \( c \) are constant to leading
order in the asymptotic series expansion in powers of $\text{Pe}^{-1}$. Details of the asymptotics can be found in [6]. Introducing these simplifications into system (2.10) yields

\[
\left(\frac{\partial}{\partial \tau} + \chi\right)\rho + \left(\frac{\partial}{\partial \xi^1} + 2c\right)m = 0, \quad (2.11a)
\]

\[
\left(\frac{\partial}{\partial \tau} + \chi\right)(\rho u^j \ell_j) + \left(\frac{\partial}{\partial \xi^1} + 2c\right)(mv^i \ell_j) = -\left(\frac{\partial}{\partial \xi^1} + 2c_i\right)\left(p e^j\right) + \left(\frac{\partial}{\partial \xi^1} + 2c_i\right)\left[\mu \left(g^{jk} \frac{\partial v^k}{\partial \xi^1} + g^{ik} \frac{\partial v^j}{\partial \xi^1}\right) - v^k \frac{\partial g^{ji}}{\partial \xi^1} - 2g^{ji} \left(\frac{\partial}{\partial \xi^1} + 2c_i\right) v^k \right] \ell_j, \quad (2.11b)
\]

\[
\left(\frac{\partial}{\partial \tau} + \chi\right)(\rho h) + \left(\frac{\partial}{\partial \xi^1} + 2c\right)(m h) - \left(\frac{\partial}{\partial \xi^1} + 2c\right)\left(\frac{\lambda}{c_p} \frac{\partial h}{\partial \xi^1}\right) = \left(\frac{\partial}{\partial \xi^1} + 2c\right)J_{h1}, \quad (2.11c)
\]

\[
\left(\frac{\partial}{\partial \tau} + \chi\right)(\rho Y_n) + \left(\frac{\partial}{\partial \xi^1} + 2c\right)(m Y_n) - \left(\frac{\partial}{\partial \xi^1} + 2c\right)\left(\frac{\lambda}{c_p} \frac{\partial Y_n}{\partial \xi^1}\right) = \omega_n. \quad (2.11d)
\]

\[
\left(\frac{\partial}{\partial \tau} + \chi\right)(\rho Z_q) + \left(\frac{\partial}{\partial \xi^1} + 2c\right)(m Z_q) - \left(\frac{\partial}{\partial \xi^1} + 2c\right)\left(\frac{\lambda}{c_p} \frac{\partial Z_q}{\partial \xi^1}\right) = \left(\frac{\partial}{\partial \xi^1} + 2c\right)\frac{1}{2}J_{Z_q}. \quad (2.11e)
\]

These equations contain the parameters $c$ and $\chi$, which are the intrinsic properties of the flame surface and for this reason we refer to system (2.11) as the Intrinsic Disturbed Flame Equations (IDFE). The IDFE (2.11) can formally be solved in an asymptotic series expansion in powers of $\text{Pe}^{-1}$, where variations in normal direction are assumed to be large, more precisely of $\mathcal{O}(\text{Pe})$ while all other terms are assumed to be $\mathcal{O}(1)$. At each order we thus find a system of equations which is one-dimensional in space. Time dependency and transverse variations are accounted for by the contributions of leading order terms to lower order equations.

### 2.2 Strongly stretched flamelet equations

In this section we present a second choice for the flame coordinate system and reformulate the conservation equations in terms of these coordinates. The derivation in this section is a reformulation of the theory in [11, 37].

We define a premixed flame as the region in space where $\mathcal{Y}_u \leq \mathcal{Y} \leq \mathcal{Y}_b$, for some suitable progress variable $\mathcal{Y}$, taking the values $\mathcal{Y}_u$ and $\mathcal{Y}_b$ in the unburned and burned gases, respectively. The variable $\mathcal{Y}$ can be, say, one of the species mass fractions or the temperature. We assume that $\nabla \mathcal{Y} \neq 0$ everywhere in the flame. Consequently, we can identify iso-surfaces of $\mathcal{Y}$, i.e., surfaces where $\mathcal{Y}(x, t) = \mathcal{Y}_0$ for some constant $\mathcal{Y}_0 (\mathcal{Y}_u \leq \mathcal{Y}_0 \leq \mathcal{Y}_b)$. We refer to these iso-surfaces as flame surfaces. We now define a curvilinear coordinate system $\xi = (\xi^1, \xi^2, \xi^3)$ by the relations

\[
\mathcal{Y}(x_1, x_2, x_3, t) = \mathcal{Y}(\xi^1), \quad \frac{\partial x^\alpha}{\partial \xi^1} \frac{\partial x^\alpha}{\partial \xi^1} = 0 \quad (\alpha = 2, 3), \quad \text{for} \quad \mathcal{Y}_u \leq \mathcal{Y} \leq \mathcal{Y}_b, \quad (2.12)
\]

i.e., coordinate surfaces $\xi^1 = \text{const}$ coincide with flame surfaces and the $\xi^1$-coordinate lines are orthogonal to the $\xi^\alpha$-coordinate lines ($\alpha = 2, 3$). In each flame surface, $(\xi^2, \xi^3)$ is a curvilinear coordinate system, not necessarily orthogonal, and will not be specified further. Consequently, the (symmetric) covariant and contravariant metric tensors are the same as in (2.6) with $g^{11} = 1/g_{11} = (|\nabla \mathcal{Y}|/\mathcal{Y})^2$, where $\mathcal{Y}''$ denotes the derivative of $\mathcal{Y}$ with respect to $\xi^1$. In the following we assume that $\mathcal{Y}'' > 0$. Note that the scaling of the $\xi^1$-coordinate is not determined by the relations in (2.12).
For time-dependent flames the iso-surfaces will move in the spatial domain, resulting in a time-dependent coordinate system, i.e., \( \xi = \xi(x, t) \). The motion of these surfaces is described by the kinematic condition

\[
\frac{dY}{dt} := \frac{\partial Y}{\partial t} + v_I \cdot \nabla Y = 0, \quad v_I := v - s_L n,
\] (2.13)

with \( v_I \) the velocity of the flames surfaces, \( s_L \) the laminar burning speed and \( n = \nabla Y/|\nabla Y| \) the unit normal vector to the flame surfaces, directed towards the burned gas mixture. Alternatively, differentiating with respect to \( \tau \), we find

\[
\frac{\partial Y}{\partial \tau} = \frac{\partial Y}{\partial t} + \dot{x} \cdot \nabla Y = 0,
\] (2.14)

with \( \dot{x} = \frac{\partial}{\partial \tau}(x) \) the velocity of the moving coordinate system. Combining the conditions in (2.13) and (2.14), we conclude that \((v_I - \dot{x}) \cdot \nabla Y = 0\), i.e., the flame velocity \( v_I \) and the velocity \( \dot{x} \) of the moving coordinate system have the same component normal to the flame surfaces. On the other hand, the tangential component of the velocity \( \dot{x} \) of the moving coordinate system is not determined by (2.12), and for this we simply choose \( \alpha = 2, 3 \). This choice implies that \( \dot{x} = v_I \) and \( \frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} \).

In [14] we introduced the mass-based stretch rate \( K \), defined as the fractional rate of change of the mass contained in an infinitesimal small control volume \( \Omega(t) \) moving in the flame with velocity \( \upsilon \). We derived the following expression

\[
\rho K = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v_I).
\] (2.15a)

Substituting \( q = \rho \) and \( u = v_I = \dot{x} \) in relation (A.5e), we can derive the following expression for the stretch rate

\[
K = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \tau} \left( \sqrt{g} \right) + \frac{1}{\rho} \frac{\partial \rho}{\partial \tau}.
\] (2.15b)

Compared to the stretch rate \( \chi \) defined in (2.9), the stretch rate \( K \) contains the additional term \( \frac{1}{\rho} \frac{\partial \rho}{\partial t} \), which is the fractional rate of change of the density. Moreover, the first term in (2.15b) represents the fractional rate of change of the volume of \( \Omega(t) \) whereas the same term in (2.9) represents the fractional rate of change of the area of a surface element on the flame surface. Once more applying relation (A.5e), this time with \( q = 1 \) and \( u = v_I \), we recover the familiar expression for \( K \) derived in [14], i.e.,

\[
K = \nabla \cdot v_I + \frac{1}{\rho} \frac{d \rho}{dt}.
\] (2.15c)

In the derivation of (2.15c) we also used the relation \( Y_I = \dot{x} \).

Next, we like to reformulate the conservation equation

\[
\frac{\partial}{\partial t}(\rho Y) + \nabla \cdot (\rho v Y) - \nabla \cdot \left( \frac{1}{1 + \lambda c_p V^2} \nabla Y \right) = \omega Y,
\] (2.16)

for the progress variable \( Y \). Combining this equation with the expression for \( \rho K \) in (2.15a) and the kinematic condition (2.13) and writing all differential operators in \( \xi \)-coordinates, we obtain the quasi-one-dimensional equation

\[
\frac{\partial}{\partial \xi^1} \left( \sqrt{g} m^1 Y \right) - \frac{\partial}{\partial \xi^1} \left( \sqrt{g} \frac{1}{1 + \lambda c_p V^2} \frac{\lambda}{1 + \lambda c_p V^2} \frac{\partial Y}{\partial \xi^1} \right) = \sqrt{g} \left( \omega Y - \rho K Y \right),
\] (2.17)
where $m^1 := \mathbf{a}^1 \cdot \mathbf{m}$ is the first contravariant component of the vector $\mathbf{m} := mn$ and where $m = \rho s$, is the mass burning rate. In the derivation of (2.17) we additionally used the relations $n^\alpha = 0$, $g^1 = 0$ and $\frac{\partial}{\partial \xi^\alpha}(\mathbf{g}) = 0$ for $\alpha = 2, 3$. Because of the specific block structure of the covariant metric tensor in (2.6), we have $\sqrt{\mathbf{g}} = \sqrt{g_{11}} \sigma$; see (2.7). Moreover, since $\mathbf{n} = \mathbf{a}^1 / \sqrt{g^1}$ we have $m^1 = ma^1 \cdot \mathbf{n} = m \sqrt{g^1}$. Substituting the expressions for $m^1$ and $\sqrt{g}$ in (2.17) and applying the relation $g_{11}g^{11} = 1$, this equation can be rewritten as

\[
\frac{1}{h_1} \frac{\partial}{\partial \xi^1} (\sigma m \mathbf{y}) - \frac{1}{h_1} \frac{\partial}{\partial \xi^1} \left( \sigma \frac{1}{\text{Le}_y} \frac{\lambda}{c_p} \frac{1}{h_1} \frac{\partial \mathbf{y}}{\partial \xi^1} \right) = \sigma (\mathbf{w} - \rho K \mathbf{y}), \tag{2.18}
\]

where $h_1 := \sqrt{g_{11}} \sqrt{\mathbf{g}}$ is the scale factor corresponding to the $\xi^1$-coordinate. Finally, introducing the arclength $s$ along a $\xi^1$-coordinate line by the relation $ds = h_1 d\xi^1$, we recover the flamelet equation for $\mathbf{y}$, see [11, 37],

\[
\frac{\partial}{\partial s} (\sigma m \mathbf{y}) - \frac{\partial}{\partial s} \left( \sigma \frac{1}{\text{Le}_y} \frac{\lambda}{c_p} \frac{\partial \mathbf{y}}{\partial s} \right) = \sigma (\mathbf{w} - \rho K \mathbf{y}), \tag{2.19}
\]

Apparently, equation (2.19) is a stationary, one-dimensional conservation equation depending only on the coordinate $s$ perpendicular to the flame surfaces, however, transient terms and convective transport in the flame surfaces is gathered in the term $-\sigma \rho K \mathbf{y}$.

The same procedure can be applied to the scalar conservation equations in (2.1) and (2.3). The result is the following set of quasi-one-dimensional differential equations, referred to as the Strongly Stretched Flamelets Equations (SSFE),

\[
\frac{\partial}{\partial s} (\sigma m) = -\sigma \rho K, \quad \tag{2.20a}
\]

\[
\sigma \rho \frac{\partial h}{\partial \tau} + \frac{\partial}{\partial s} (\sigma mh) - \frac{\partial}{\partial s} \left( \sigma \frac{\lambda}{c_p} \frac{\partial h}{\partial s} \right) - \frac{\partial}{\partial s} (\sigma \mathbf{J}_h \cdot \mathbf{n}) = \sigma (-\rho K h + Q_h), \tag{2.20b}
\]

\[
\sigma \rho \frac{\partial Y_n}{\partial \tau} + \frac{\partial}{\partial s} (\sigma m Y_n) - \frac{\partial}{\partial s} \left( \sigma \frac{1}{\text{Le}_n} \frac{\lambda}{c_p} \frac{\partial Y_n}{\partial s} \right) = \sigma (\mathbf{w}_n - \rho K Y_n + Q_{Y_n}), \tag{2.20c}
\]

\[
\sigma \rho \frac{\partial Z_q}{\partial \tau} + \frac{\partial}{\partial s} (\sigma m Z_q) - \frac{\partial}{\partial s} \left( \sigma \frac{1}{\text{Le}_q} \frac{\lambda}{c_p} \frac{\partial Z_q}{\partial s} \right) - \frac{\partial}{\partial s} (\sigma \mathbf{J}_{Z_q} \cdot \mathbf{n}) = \sigma (-\rho K Z_q + Q_{Z_q}), \tag{2.20d}
\]

where the terms $Q_h, Q_{Y_n}$ and $Q_{Z_q}$, which describe transport in the flame surfaces, arise because the local iso-surfaces of $h, Y_n$ and $Z_q$ generally do not coincide with the iso-surfaces of $\mathbf{y}$. These terms read

\[
Q_h := \nabla_t \cdot \left( \frac{\lambda}{c_p} \nabla_t h \right) + \nabla_t \cdot \mathbf{J}_h, \quad \tag{2.21a}
\]

\[
Q_{Y_n} := \nabla_t \cdot \left( \frac{1}{\text{Le}_n} \frac{\lambda}{c_p} \nabla_t Y_n \right), \quad \tag{2.21b}
\]

\[
Q_{Z_q} := \nabla_t \cdot \left( \frac{\lambda}{c_p} \nabla_t Z_q \right) + \nabla_t \cdot \mathbf{J}_{Z_q}, \quad \tag{2.21c}
\]

where $\nabla_t$ and $\nabla_t$ denote the internal divergence and gradient operator, respectively, restricted to the flame surfaces; see Appendix A.

The $Q$-terms in (2.20) describe conduction/diffusion along the flame surfaces and are presumably small. In order to investigate this issue more precisely we have to make the flamelet equations (2.20)
and the relations (2.21) dimensionless. As an example consider equation (2.20c) together with relation (2.21b). We consider combustion in the laminar flamelet regime and assume that the surrounding flow, which distorts the flame layer, is characterized by a velocity scale \( U \), length scale \( \ell \) and time scale \( \tau_{\text{ref}} := \ell/U \). The velocity, length and time scales of the flame are the laminar burning speed \( s_0^L \), thermal thickness \( \delta_f \) and \( \tau_f := \delta_f/s_0^L \), respectively. The superscript \(^0\) indicates the stretchless value of the corresponding variable. Note that \( \delta_f \ll \ell \). Other relevant scaling parameters are

\[
m_{\text{ref}} = m_0^b, \quad \rho_{\text{ref}} = \rho_0^b, \quad \omega_{n,\text{ref}} = \rho_0^b Y_{n,\text{ref}} \tau_f, \quad K_{\text{ref}} = \frac{1}{\tau_{\text{ref}}}.
\]

The subscript \( \text{ref} \) on a variable denotes a reference value for the corresponding scaling parameter. We now introduce the following dimensionless variables (indicated by an asterisk \(^*\)):

\[
\begin{align*}
x &= : \ell x^*, \quad s =: \delta_f s^*, \quad \xi^\alpha =: L \xi^{\alpha^*} (\alpha = 2, 3), \quad \tau = \tau_{\text{ref}} \tau^*, \quad q = q_{\text{ref}} q^*,
\end{align*}
\]

where \( q \) is arbitrary variable/parameter in (2.20c) or (2.21b). The resulting dimensionless equation reads (omitting all asterisks):

\[
\sigma K a \rho \frac{\partial Y_n}{\partial \tau} + \frac{\partial}{\partial s} \left( \sigma m Y_n \right) - \frac{\partial}{\partial s} \left( \sigma \frac{1}{\Le c_p} \frac{\lambda}{\partial s} Y_n \right) = \sigma (\omega_n - K a \rho K Y_n + Q Y_n),
\]

where \( K a := \rho_0^b K_{\text{ref}} \delta_f/m_0^b = \tau_f/\tau_{\text{ref}} \) is the Karlovitz number, which is much smaller than 1 in the laminar flamelet regime [30]. The relation for \( Q Y_n \) becomes

\[
Q Y_n = \varepsilon^2 \nabla \cdot \left( \frac{1}{\Le c_p} \frac{\lambda}{\partial} \nabla Y_n \right),
\]

where \( \varepsilon := \delta_f/\ell = K a s_L/U \ll 1 \). Clearly, the diffusion term is much smaller than the stretch term and is negligible, but the time derivative is of the same order of magnitude.

## 3 Integral analysis

In section 2 we derived two different quasi-one-dimensional systems of differential equations, i.e., the IDFE and SSFE. Both systems describe the inner structure and the propagation speed of premixed flames. In this section we will integrate these equations across the flame to derive a model for the mass burning rate, and in case of the IDFE, jump conditions as well.

### 3.1 Flames as gasdynamic discontinuities

The uniform flame coordinate system, introduced in section 2.1, is attached to a specific flame surface. In principle any surface within the flame layer could serve as such a reference surface. Possible choices are an isotherm, an iso-surface for one of the species mass fractions or the surface where the reaction rate reaches its maximum value. The latter choice has been used in most previous work [35, 23, 5]. We will exploit the fact, that any surface can serve as a reference surface, to simplify our equations. At this stage, we just choose some surface.

We follow the philosophy of Darrieus [9] and Landau [19] and construct a model of a flame as a gasdynamic discontinuity. The flame surface separates the unburned mixture from the burned products. In this model the flow on either side of the discontinuity surface is governed by the incompressible
Navier-Stokes equations, and therefore we refer to it as the *hydrodynamic model*. Reaction terms are neglected, and moreover, density, temperature, species mass fractions and other fluid properties are taken constant but distinct on either side of the discontinuity surface. Obviously this hydrodynamic model compromises reality, since a flame is a layer of small but finite thickness. Therefore, a discontinuous model does not reproduce the internal structure of the flame layer. We merely can claim, that the discontinuous model should reproduce the flow outside the flame layer.

We introduce the discontinuous hydrodynamic variables like \( \hat{\rho} \), \( \hat{v} \), \( \hat{m} \) etc., which are the same variables as used in the *reactive model*. The conservation equations in the hydrodynamic model are readily available from the reactive model, which is given in uniform flame coordinates in (2.10) or (2.11). We merely replace the variables \( \rho \), \( v \), \( m \) etc. by the corresponding hydrodynamic variables and delete the reaction terms. Since there is no reaction outside the flame layer anyway, the hydrodynamic model accurately describes the physics outside the flame layer. However, to close the discontinuous model, we have to provide jump conditions for the discontinuous variables. Note that the jumps arise since we neglected the reaction terms in the hydrodynamic model, so that the internal behaviour in the flame layer is no longer reproduced. The jump conditions account for the integral effect of any difference which exists between the hydrodynamic and the reactive models. We subtract the hydrodynamic equations from the corresponding reactive equations. Thus for each term in the equations we find a corresponding difference involving hydrodynamic and reactive variables, respectively. These differences are integrated along a \( \xi \)-coordinate line. Integration is performed separately in the region ahead of the discontinuity surface and behind the discontinuity surface and the sum of the two contributions is taken, i.e., we first integrate in the unburned region from \( \xi = \xi_u \) to \( \xi = 0^- \), next in the burned region from \( \xi = 0^+ \) to \( \xi = \xi_b \) and finally add the integrals. This integration computes the integral mean of differences of the hydrodynamic and the reactive model. Integration is used to compute from the three-dimensional fields in the flame layer two-dimensional integral means. We refer to this procedure as *projection*. Thus, the internal structure of the flame layer is projected onto the discontinuity surface and yields the jump conditions for the hydrodynamic variables at the flame surface.

In order to illustrate the procedure we apply it to equation (2.11a). Replacing \( \rho \) and \( m \) by their hydrodynamic counterparts, subtracting the resulting equation from (2.11a) and integrating across the flame, we obtain

\[
\int_{\xi_u}^{\xi_b} \left[ \partial_{\tau} + \chi \right] (\rho - \hat{\rho}) + 2c(m - \hat{m}) \, d\xi + [m - \hat{m}]_{\xi_u}^{\xi_b} = 0. \tag{3.1}
\]

Taking into account that \( m = \hat{m} \) at the unburned and burned sides of the flame, and moreover, that the reactive mass flux \( m \) is continuous at the flame surface, the above relation simplifies to

\[
\int_{\xi_u}^{\xi_b} \left[ \partial_{\tau} + \chi \right] (\rho - \hat{\rho}) + 2c(m - \hat{m}) \, d\xi + [\hat{m}]_{\xi_u}^{\xi_b} = 0. \tag{3.2}
\]

The square bracket \( [\hat{m}] := \hat{m}(0^+) - \hat{m}(0^-) \) denotes the jump of the normal (hydrodynamic) mass flux across the discontinuity surface. Note that in general, the mass flux that enters the flame surface from the unburned mixture differs from the one leaving to the burned side, so that a surface mass must be associated with the discontinuity surface. This surface mass is a function of stretch, curvature and time. The origin of the surface mass is the difference between the densities in the hydrodynamic and reactive models and it is determined by the projection procedure. In [6] it was proposed to define the location of the discontinuity surface by requiring that the surface mass vanishes, i.e., the mass flux entering and leaving the discontinuity surface are identical. Now \( [\hat{m}] = 0 \), which is the case if the integral in
(3.2) vanishes. However, the discontinuity surface defined by this procedure does not coincide with the reaction zone. In fact it is located at a position in the unburned mixture where the temperature is still quite low.

Applying the same projection procedure to the other equations in (2.11), we obtain a set of jump conditions of the following form:

\[ \int_{\xi_1}^{\xi_2} \left[ \left( \frac{\partial}{\partial \tau} + \chi \right) \left( (\rho \nu^i - \hat{\rho} \hat{\nu}^i) \ell_i \right) + 2c \left( (m \nu^i - \hat{m} \hat{\nu}^i) \ell_i + (p - \hat{p}) \ell^1 - (\sigma^{i1} - \hat{\sigma}^{i1}) \ell_j \right) \right] \, d\xi^1 + \\
\left[ \hat{m} \hat{\nu}^i \ell_i + \hat{p} \ell^1 - \hat{\sigma}^{i1} \ell_j \right] = \int_{\xi_1}^{\xi_2} \left( \frac{\partial}{\partial \xi^a} + 2c_a \right) \left( - (p - \hat{p}) \ell^a + (\sigma^{j\alpha} - \hat{\sigma}^{j\alpha}) \ell_j \right) \, d\xi^1, \quad (3.3a) \]

\[ \int_{\xi_1}^{\xi_2} \left[ \left( \frac{\partial}{\partial \tau} + \chi \right) (\rho h - \hat{\rho} \hat{h}) + 2c \left( m h - \hat{m} \hat{h} - (\Phi_h - \hat{\Phi}_h) \right) \right] \, d\xi^1 + \left[ \hat{m} \hat{h} - \hat{\Phi}_h \right] = 0, \quad (3.3b) \]

\[ \int_{\xi_1}^{\xi_2} \left[ \left( \frac{\partial}{\partial \tau} + \chi \right) (\rho Y_n - \hat{\rho} \hat{Y}_n) + 2c \left( m Y_n - \hat{m} \hat{Y}_n - (\Phi_n - \hat{\Phi}_n) \right) \right] \, d\xi^1 + \left[ \hat{m} \hat{Y}_n - \hat{\Phi}_Y_n \right] = \int_{\xi_1}^{\xi_2} \omega_n \, d\xi^1, \quad (3.3c) \]

\[ \int_{\xi_1}^{\xi_2} \left[ \left( \frac{\partial}{\partial \tau} + \chi \right) (\rho Z_q - \hat{\rho} \hat{Z}_q) + 2c \left( m Z_q - \hat{m} \hat{Z}_q - (\Phi_q - \hat{\Phi}_q) \right) \right] \, d\xi^1 + \left[ \hat{m} \hat{Z}_q - \hat{\Phi}_Z_q \right] = 0, \quad (3.3d) \]

where \( \sigma^{ij} \) denote the components of the stress tensor and where

\[ \Phi_h := \frac{\lambda}{c_p} \frac{\partial h}{\partial \xi^1} + J^1_h, \quad \Phi_{Y_n} := \frac{1}{\lambda c_n c_p} \frac{\partial Y_n}{\partial \xi^1}, \quad \Phi_{Z_q} := \frac{\lambda}{c_p} \frac{\partial Z_q}{\partial \xi^1} + J^1_{Z_q}. \]

The jump condition for normal momentum states that by replacing the flame structure by a surface we have to include surface forces which usually put the surface under pressure, i.e., the surface is subject to compression. The jump condition for the enthalpy determines the temperature of the reaction zone. The fuel mass fraction \( \hat{Y}_1 \) is constant and known in both the unburned and burned gas mixtures. Complete fuel consumption implies \( [\hat{m} \hat{Y}_1 - \hat{\Phi}_{Y_1}] = -\hat{m} \hat{Y}_{1,u} + \Phi_{Y_{1,u}} \). Finally, the jump condition (3.3c) for the fuel mass fraction \( \hat{Y}_1 \) determines the mass burning rate

\[ \hat{m} = \frac{1}{\hat{Y}_{1,u}} \left[ \int_{\xi_1}^{\xi_2} \left[ \left( \frac{\partial}{\partial \tau} + \chi \right) (\rho Y_1 - \hat{\rho} \hat{Y}_1) + 2c \left( m Y_1 - \hat{m} \hat{Y}_1 - (\Phi_{Y_1} - \hat{\Phi}_{Y_1}) \right) - \omega_1 \right] \, d\xi^1 + \hat{\Phi}_{Y_{1,u}} \right] \quad (3.4) \]

Thus, the projection procedure defines the location of the discontinuity surface, the mass burning rate, and the jump conditions for enthalpy, species mass fractions and momentum, so that the discontinuous hydrodynamic model is closed. The jump conditions for element mass fractions, presented here for the first time, are not independent but the may be used to replace the more complicated jump conditions for species mass fractions.

### 3.2 Integral analysis of the flamelet equations

In this section we will derive an expression for the mass burning rate \( m_h \) at the burned side of the flame from the flamelet equation (2.19). This mass burning rate depends on the state variables \( \psi = (h, Z_q) \) in the burned mixture, which we therefore determine first from the corresponding flamelet equations.
Suppose $\sigma = \sigma(s)$ and $K = K(s)$ are given at a certain location in the flame. Integrating the flamelet equations (2.20a), (2.20b) and (2.20d) across the flame and neglecting the $Q_f$-terms ($f = h, Y, Z_q$), we find the following integral balances

\begin{align}
(\sigma m)_b - (\sigma m)_u &= - \int_{s_u}^{s_b} \sigma(s)\rho(s)K(s)\,ds, \\
(\sigma m)_b (h_b - h_u) &= - \int_{s_u}^{s_b} \sigma(s)\rho(s)\left(K(s)(h(s) - h_u) + \frac{\partial h}{\partial \tau}\right)\,ds, \\
(\sigma m)_b (Z_{q,b} - Z_{q,u}) &= - \int_{s_u}^{s_b} \sigma(s)\rho(s)\left(K(s)(Z_q(s) - Z_{q,u}) + \frac{\partial Z_q}{\partial \tau}\right)\,ds,
\end{align}

where we have assumed that all diffusive/conductive fluxes vanish at the unburned (at $s = s_u$) and burned (at $s = s_b$) sides of the flame. The subscripts $b$ and $u$ denote the value of the corresponding variable in the burned and unburned gas, respectively. For the special case of a steady, stretchless flame, i.e., $\partial h/\partial \tau = \partial Z_q/\partial \tau = 0$ and $K = 0$, we obtain the relations $(\sigma m^0)_b = (\sigma m)_u$, $h^0_b = h_u$ and $Z^0_{q,b} = Z_{q,u}$, where the superscript 0 indicates that the variable is considered to be the solution of the corresponding stretchless flamelet equation.

Consider the flamelet equation (2.19) for $Y$, which can be written in the symbolic form

\begin{equation}
A - \frac{\partial D}{\partial s} = S,
\end{equation}

with $A$, $D$ and $S$ the advection, diffusion and chemical source term, respectively, defined by

\begin{equation}
A := \frac{\partial}{\partial s}(\sigma m Y) + \sigma \rho K Y, \quad D := \sigma \frac{1}{\operatorname{Le} \gamma} \frac{\lambda}{c_p} \frac{\partial Y}{\partial s}, \quad S := \sigma \omega Y.
\end{equation}

The first term in $A$ describes advection in $s$-direction and the second term, i.e., the stretch term $\sigma \rho K Y$, advection in the flame surfaces. To find the first integral of equation (3.6a) we multiply it with $D$. Integrating the resulting equation across the flame from $s = s_u$ to $s = s_b$, and taking into account that the diffusion fluxes vanish there, we obtain

\begin{equation}
\int_{s_u}^{s_b} A(s)D(s)\,ds = \int_{s_u}^{s_b} S(s)D(s)\,ds.
\end{equation}

Substituting the appropriate expressions from (3.6b) and taking $Y$ as the integration variable, the second integral can be rewritten as

\begin{equation}
\int_{s_u}^{s_b} S(s)D(s)\,ds = \int_{\gamma_u}^{\gamma_b} \sigma^2 \frac{\lambda}{\operatorname{Le} \gamma} \frac{1}{c_p} \omega Y \,dY.
\end{equation}

In order to determine the first integral in (3.7), we approximate $D$ by integrating equation (3.6a) over the preheat zone and neglecting the source term $S$. This way we obtain

\begin{equation}
\int_{s_u}^{s_b} A(s)D(s)\,ds \approx \int_{s_u}^{s_b} A(s)\left[ \int_{s_u}^{s} A(v)\,dv \right]\,ds = \frac{1}{2} \left[ \int_{s_u}^{s_b} A(s)\,ds \right]^2.
\end{equation}

This approximation of $D$ is justified since the reaction zone is usually much thinner than the preheat zone, so that the major contribution to the integral of $AD$ in equation (3.7) comes from the preheat
zone. In fact, relation (3.9) is exact when the thickness of the reaction layer goes to zero for infinite activation energy, which we therefore assume in the following. Our approach is then equivalent to large activation energy asymptotics to determine the mass burning rate; see [4]. Combining (3.7)-(3.9), using the definition of $A$ in (3.6b) and applying (3.5a), we obtain the following expression for the mass burning rate $m_b$ in the burned gas mixture

$$ (\sigma m)_b + \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) \tilde{Y}(s) \, ds = F(h_b, Z_{q,b}), $$

where $\tilde{Y} := (Y - \gamma_u)/(\gamma_b - \gamma_u)$ is the normalized variable corresponding to $Y$, assuming $\gamma_b \neq \gamma_u$, and where the function $F(h_b, Z_{q,b})$ is defined by

$$ F(h_b, Z_{q,b}) := \frac{1}{\gamma_b - \gamma_u} \sqrt{2 \int_{\gamma_u}^{\gamma_b} \sigma^2 \frac{1}{\text{Le} Y c_p} \omega_Y \, dY}. $$

In [11, 37] we have explained that $F$ should be considered a function of the state vector $\psi_b = (h_b, Z_{q,b})$ in the burned gas mixture. Note that for the special case of a stretchless flame with infinitely thin reaction layer we have $(\sigma m^0)_b = F(h_b^0, Z_{q,b}^0)$.

We like to compare the mass burning rates for a stretched and a stretchless flame. Applying equation (3.10) for $K \neq 0$ and $K = 0$, respectively, we can derive the following relation

$$ m_b(\psi_b) + \frac{1}{\sigma_b} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) \tilde{Y}(s) \, ds = m_b^0(\psi_b), $$

where we have explicitly emphasized the dependence of $m_b$ and $m_b^0$ on the state vector $\psi_b = (h_b, Z_{q,b})$. Note that the variable $m_b^0(\psi_b)$ in the right hand side of (3.12) is the mass burning rate of a stretchless flame, as defined in (3.11), however to be evaluated as a function of the state vector $\psi_b$ of a stretched flame. Relation (3.12) can be rewritten as

$$ \frac{m_b(\psi_b)}{m_b^0(\psi_b)} = 1 - \frac{\text{Kay}}{\text{Le} Y}, $$

where the Karlovitz integral $\text{Kay}$ is defined by

$$ \frac{\text{Kay}}{\text{Le} Y} := \frac{1}{\sigma_b m_b^0(\psi_b)} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) \tilde{Y}(s) \, ds, $$

i.e., $\text{Kay}/\text{Le} Y$ is the weighted mass flow rate $\int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) \tilde{Y}(s) \, ds$ along the flame surfaces scaled with the mass flow rate $\sigma_b m_b^0(\psi_b)$ normal to these surfaces. Summarizing, we can compute the mass burning rate $m_b$, from (3.13), with the Karlovitz integral $\text{Kay}$ and the state vector $\psi_b = (h_b, Z_{q,b})$ given in (3.14) and (3.5b)-(3.5c), respectively.

Next, we introduce several approximations for the Karlovitz integral. First, if we assume that $\sigma(s) = \text{const}$ in the flame, i.e., we consider a flat flame, we have

$$ \frac{\text{Kay}^{(1)}}{\text{Le} Y} := \frac{1}{m_b^0(\psi_b)} \int_{s_u}^{s_b} \rho(s) K(s) \tilde{Y}(s) \, ds. $$

Second, if we instead assume that $\sigma(s) K(s) = \sigma_b K = \text{const}$ in the flame, relation (3.14) reduces to

$$ \frac{\text{Kay}^{(2)}}{\text{Le} Y} := \frac{K}{m_b^0(\psi_b)} \int_{s_u}^{s_b} \rho(s) \tilde{Y}(s) \, ds. $$
Both integrals in (3.15a) and (3.15b) have to be computed numerically. Finally, if we apply the weak stretch approximation to the second case, i.e., we replace \( \rho(s) \) and \( Y(s) \) by their steady, stretchless counterparts \( \rho^0(s) \) and \( Y^0(s) \), respectively, take \( \sigma(s) = 1 \) and \( \lambda/c_p = \text{const} \), we can derive an analytical expression. Assuming moreover \( \text{Le} = 1 \), i.e., \( \mathcal{Y} = T \), we have

\[
\frac{\text{Ka}^{(3)}_{\mathcal{Y}}}{\text{Le}_Y} := \text{Ka}_b(\theta + 1) \frac{\ln(\theta + 1)}{\theta},
\]

(3.15c)

where \( \theta := (T_b^0 - T_u)/T_u \) is the thermal expansion coefficient and where \( \text{Ka}_b := K \rho_b^0 \delta_t/m_b^0 \) is Karlovitz number at the burned side of the flame; see [13] for more details.

Finally, we also give the mass burning rate \( m_{\text{il}} \) at the inner layer. We think that \( m \) at the inner layer describes the propagation of the flame best, since most chemical reactions take place there. Moreover, Groot et al. [15] have shown that only \( m_{\text{il}}^0 \) is independent of \( \sigma \), whereas \( m^0 \) at all other locations in the flame does depend on \( \sigma \). Integrating the flamelet equation (2.20a) from \( s_{\text{il}} \) to \( s_b \), we obtain

\[
(\sigma m)^{\text{il}} = (\sigma m)^{b} + \int_{s_{\text{il}}}^{s_b} \sigma(s) \rho(s) K(s) \, ds.
\]

(3.16)

Obviously, for a stretchless flame we have \((\sigma m)^{\text{il}} = (\sigma m)^{b}\). In Section 5 we will compute \( m_{\text{il}}/m_{\text{il}}^0 \) for a spherically expanding flame, and validate the model (3.13)-(3.14) for \( m_b \), as well as the approximations for the Karlovitz integral defined in (3.15).

4 Comparison of both descriptions

We have introduced two moving, curvilinear coordinate systems attached to the flame (flame coordinates), one based on a specific flame surface (uniform flame coordinates) and one based on iso-surfaces of a progress variable (iso-scalar flame coordinates). The conservation equations for premixed flames, rewritten in terms of flame coordinates, reduce to a quasi-one-dimensional system of differential equations, since variations along the flame surface(s) are usually much smaller than variations across the flame and hence can be neglected. The quasi-one-dimensional system is referred to as the Intrinsic Disturbed Flame Equations (IDFE) for the uniform flame coordinates and Strongly Stretched Flamelets Equations (SSFE) for the iso-scalar flame coordinates. Both IDFE and SSFE contain parameters describing the geometry of the flame.

Comparing both formulations, we note the following:

1. Uniform flame coordinates are by definition based on a single flame surface, whereas for iso-scalar flame coordinates we have infinitely many flame surfaces.

2. In the uniform flame coordinate system, the coordinate \( \xi^1 \) can be interpreted as a distance and therefore coordinate surfaces \( \xi^1 = \text{const} \) are parallel. In fact it is identical to the level set function \( G \); see Section 5. In the iso-scalar coordinate system, these coordinate surfaces are iso-surfaces of the variable \( \mathcal{Y} \) and are in general not parallel.

3. The IDFE contain the mean curvature \( c \) and the stretch rate \( \chi \) as parameters and the SSFE contain the area parameter \( \sigma \) and the mass based stretch rate \( K \).

4. For uniform flame coordinates, \( c \) and \( \chi \) change only weakly due the geometry of the coordinate system. For iso-scalar flame coordinates \( \sigma \) and \( K \) are fields in the flame zone.
5 Applications

The two descriptions of premixed flames presented in this paper have a lot in common, but their application is different. The basic idea in the application of the IDFE is to derive a numerical method based on the level set approach, where the expression for the burning speed is used to determine the local propagation of the flame surface. The jump conditions give the increments of fluid velocity, pressure, element and species mass fractions across the flame surface. The major advantage of this approach is that the detailed structure of the flame in the reaction layer need not be resolved, so that fast computations are possible. Also the model can be used for analytical studies of flame behaviour as in the stability analysis in [7] or to investigate the mass burning rate for complex reaction kinetics in [17]. The SSFE are both the basis for numerical methods and are also the underlying model to analyse flame stretch in (partially) premixed laminar and turbulent flames. Groot et al. [15] derived a G-type kinematic formulation from the system of flamelet equations (2.20) to simulate spherically expanding laminar flames. However, since
this kinematic formulation has to be solved for a series of independent flame surfaces, this method is difficult to extend to more general flames. For this reason, van Oijen et al. [25, 26, 27, 28] derived the so-called Flamelet Generated Manifold (FGM) method from the flamelet equations introduced above. In the FGM method, the multi-dimensional conservation equation for $\mathcal{Y}$ is solved, instead of the kinematic condition for $\mathcal{Y}$, together with the flamelet system (2.20). The source term $\omega_\mathcal{Y}$ is tabulated and precomputed from the flamelet system. Application of the FGM method requires the computation of the chemical source terms, but only one (or a few) of these suffice. This approach is not as efficient as the (numerical) method based on the IDFE, however, it is more widely applicable. As an example, it is possible to model strongly stretched (turbulent) flames. Furthermore, this approach has proven to be very successful for the computation of (partially) premixed flames [29]. Extensive comparisons with detailed chemistry computational results have been carried out as well. Burner-stabilised Bunsen flames, partially-premixed triple flames and ceramic burner stabilised flames in a furnace have been investigated with success [27].

In the following, we apply the IDFE and SSFE theories to simulate and analyse premixed flames. First, we solve the IDFE to simulate a low pressure Bunsen flame and compare the numerical results with experiments; see also [3]. Parameters of the flame are the pressure $p = 69 \, \text{mbar}$, equivalence ratio $\varphi = 0.88$, unburned gas temperature $T_u = 310 \, \text{K}$ and the Reynolds number $Re = 25$. Figure 1 shows a chemoluminescence picture as observed in the experiment. The burner consists of a porous ring where a very stable pilot flame is established. In the centre of the burner a Bunsen flame develops, which is effectively stabilised by the pilot flame. The structure of the flame is measured by Raman spectroscopy and compared to the simulations.

In the simulations, the model of Section 3.1 extended for inhomogeneous mixtures is used. At the flame surface methane is converted into carbon monoxide. The oxidation of carbon monoxide to carbon dioxide is computed from simplified chemistry. Thus the jump conditions replace only part of the flame structure. The flow on either side of the flame is computed from the incompressible Navier-Stokes equations coupled with a Poisson equation for the pressure, which is obtained by taking the divergence of the momentum equations. The velocity and pressure are computed using a fractional step method; see [3] for more details. Both flow fields are coupled through the jump conditions. The flame surface is represented by a level set function $G$, defined in the entire domain, and satisfying the equation

$$\frac{\partial}{\partial t} (\rho G) + \nabla \cdot (\rho v G) = m |\nabla G|.$$  \hspace{1cm} (5.1)

The iso-surface $G(x, t) = 0$ implicitly represents the surface. The mass flux $m$ follows from the methane mass fraction jump condition. The jump condition contains integrals depending on the detailed structure of the flame. Quantitative values of these integral are computed using the INSFLA code [18]. We employ WENO schemes for space discretisation and the third order TVD Runge Kutta method for time integration [34]. The total computation is very inexpensive, comparable to the numerical simulation of nonreactive, incompressible flow.

Figure 1 shows the location of maximum chemoluminescence in the experiment and the simulation. The maximum occurs slightly downstream the flame surface. The corresponding location is computed from the maximum production rate of OH, which can be expressed in terms of an integral relation. The numerically computed height agrees well with the experimental observations.

Finally, we apply the SSFE to analyse DNS simulations of turbulent premixed flames [24]. As an example, the propagation of spherically expanding fire balls in a 3D cube of size $5 \times 5 \times 5 \, \text{mm}$ is explored, and we assume that all Lewis numbers are equal to 1. For space discretisation we use a sixth order compact finite difference scheme [20] on a $127 \times 127 \times 127$ grid and for time integration we
take the (compact) third-order Runge-Kutta method. Navier-Stokes Characteristic Boundary Conditions (NSCBC) are applied on all (outflow) boundaries [31, 32]. The FGM method used in this research is a one-dimensional manifold computed using the GRI 3.0 reaction mechanism, using the mass fraction of CO$_2$ as single controlling variable $Y$. Results of these computations (after one turbulent eddy turn over time) with $u'/s_L = 4.1$ and turbulent Reynolds number $Re_t := u'\ell_t/(s_0^2\delta_t) = 3.7$ are presented in Figure 2. Combustion takes place in the thin-reaction zones regime. Velocity vectors are presented together with the isotherms $T = 305$ K (unburned boundary), $T = 1698$ K (inner layer) and $T = 1849$ K (burned boundary). Flamelets are also constructed by following several paths from the burned towards the unburned flame boundaries (thick lines), perpendicular to the local isotherms. We use the numerical data of the spherically expanding flame to validate the models for $n_b$ presented in the previous section. Since all Lewis numbers are assumed to be 1, this means that there is no preferential diffusion and that the equilibrium state is not perturbed, i.e., $\psi_b = \psi_b^0$. As a result, relation (3.13) only describes the influence of stretch on the local mass burning rate in the turbulent flame. Figure 3 shows a scatter plot of $m_{i3}/m_{i1}^0$ versus $K$ for the four different expressions of the Karlovitz integral, given in (3.14) and (3.15). Clearly, only the expression in (3.14) for the Karlovitz integral reproduces the theoretical result (3.13), which means that the detailed structure of $\sigma(s)$ and $K(s)$ has to be taken into account for strongly stretched flames. The weak stretch limit is clearly not valid in this case.

6 Discussion on combined methods

A premixed flame represents a thin layer of high activity separating the burned and unburned gas mixtures. In the present paper we reviewed the properties of two flame coordinate systems, which allows us to describe flame behaviour in terms of a quasi-one-dimensional system of differential equations. The IDFE are based on one flame surface and weak curvature asymptotics. At each order of the asymptotic series expansion, the differential operator is one-dimensional, yet, convection and diffusion along the surface is accounted for by source terms containing lower order terms. In the SSFE, advantage is taken of the fact that diffusion vanishes along iso-surfaces resulting in a quasi-one-dimensional system of equations. A feature which is common to both approaches is that the quasi-one-dimensional equations

Figure 1: Steady state flame surface of part of the low pressure methane Bunsen flame. Left: OH-chemoluminescence picture, right: numerical simulation; see [3]
are analyzed by integral analysis to determine the change of a variable across the flame layer. The IDFE account for transverse diffusion, but requires perturbations like stretch, curvature and frequencies to be small, while SSFE does not impose a restriction on perturbations, but it neglects transverse diffusion. Since transverse diffusion may not be neglected in the momentum equations, the corresponding integral balances are presented for the IDFE only. In the SSFE approach, the flow equations have to be solved numerically.

In an application of IDFE, we demonstrated that integral analysis not necessarily must be applied to the whole flame structure but rather can be restricted to the fuel consumption layer and the inner layer. Jump conditions relate the state just behind the inner layer to the one in the unburned mixture. In the oxidation layer, which proceeds the flame inner layer, the reactions are computed employing multidimensional transport equations. Obviously, the IDFE and SSFE can be applied to any layer of high activity. To construct IDFE for nonreactive layers the physical effect that creates the layer must be excluded from the discontinuous model. IDFE is advantageous for those layers that are weakly perturbed. Jump conditions replace the whole layer, yet the asymptotic approach may account for weak transverse diffusion processes. SSFE is advantageous when substantially perturbed layers are considered. If multiple layers are considered, fluxes at the interface between different layers have to be taken into account in the integrals involved. For the layers governed by the SSFE, relations for the momentum jump across the layer cannot be provided, so that numerical simulation of the flow field becomes necessary. At the same time perturbations like stretch and curvature dominate transverse diffusion effects. Thus SSFE and IDFE have distinct but overlapping regions of applicability.

We propose to construct numerical algorithms that combine IDFE, SSFE and full multi-dimensional equations to construct adaptive hierarchical schemes, that provide accurate solutions at low computa-

Figure 2: Cross sections through the center of the flame at $t/\tau = 1$ for $u'/s_L = 4.1$ and $Re_t = 3.7$. The bold lines are isotherms corresponding to the position of the unburned side, the inner layer and the burned side of the flame ($T = 305, 1698$ and $1849$ K). The vectors represent the gas velocity. Six flame paths (thick lines) are projected on the plane $z = 0$. The spatial coordinates are given in mm; see [24].
Figure 3: Scaled mass burning rate $m_{il}/m_{il}^0$ at the inner layer as a function of the Karlovitz integral $K_{ay}$ and its approximations $K_{ay}^a (a = 1, 2, 3)$. Top left: $K_{ay}$. Top right: $K_{ay}^{(1)}$. Bottom left: $K_{ay}^{(2)}$. Bottom right: $K_{ay}^{(3)}$. 
tional cost. Recall that typical hydrocarbon premixed flames have a structure consisting of multiple layers. In particular, a thin preheat zone, where diffusion balances convection is followed by a yet thinner inner layer, where reaction balances diffusion, which is possibly followed by an oxidation layer, where reaction balances convection. The oxidation layer might be the widest of all, as in our application [3], or of intermediate size as in [33]. Due to the separation of length scales it is possible to combine numerical implementations of these methods for each layer. In Table 1 we have compiled a list of combined models, which can be expected to be potential candidates for highly effective numerical schemes, as the curvature, stretch rate or frequency of perturbations is increased. The numerically most efficient model of a flame as a gasdynamic discontinuity (IDFE) can be applied to all layers as long as perturbations are sufficiently small. With increasing amplitude of perturbations the jump conditions, which actually represent a zero-dimensional model, must successively be replaced by the more complex one-dimensional model (SSFE) and eventually by the full multi-dimensional equations. The more complex models are first applied to the widest layer and finally to the thinnest layer. We speculate that the reaction layer can be described by the one or zero-dimensional models as long as extinction/ignition phenomena are not observed.

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Table 1: Hierarchy of combined models for a multi-layer description of premixed flames. Note that if the same model is used for both layers they are treated as a single layer.

In conclusion we state, that conservation equations formulated in flame coordinates represent a useful model, both for theoretical and numerical studies of premixed flames. In fact, flame coordinates allow us to study quite general flames, so that the prior necessary restriction to very simple flame configurations, such as stagnation point flames or spherical flames no longer applies.

### A Tensor calculus

This appendix is based on [38]; see also [1] for a detailed account on tensor calculus. Consider the (time-dependent) coordinate transformation

$$ T : (x, t) \mapsto (\xi, \tau), $$

(A.1)

where $x := (x_1, x_2, x_3)$ denotes the Cartesian and $\xi := (\xi^1, \xi^2, \xi^3)$ the curvilinear, flame coordinate system. Moreover, $t$ and $\tau$ denote the time in the Cartesian and curvilinear coordinate systems, respectively. Obviously, $\xi = \xi(x, t)$ and $\tau = t$. The covariant and contravariant base vectors $a_i$ and $a^j$ are defined by, respectively,

$$ a_i := \frac{\partial x}{\partial \xi^i}, \quad a^j := \nabla \xi^j, \quad (i, j = 1, 2, 3), $$

(A.2)
where the gradient operator is taken w.r.t. the Cartesian coordinates \( \mathbf{x} \). The properties of these base vectors are determined by the (symmetric) covariant and contravariant metric tensors \((g_{ij})\) and \((g^{ij})\), defined by, respectively,

\[
g_{ij} := a_i \cdot a_j, \quad g^{ij} := a^i \cdot a^j, \quad (i, j = 1, 2, 3).
\] (A.3)

These tensors are each other's inverse, having determinant

\[
g = \det(g_{ij}) = 1 / \det(g^{ij}) = (\det(a_1, a_2, a_3))^2 > 0.
\] (A.4)

Using the Einstein summation convention, i.e., terms or products containing indices repeated once in the upper position and once in the lower position should be summed over the appropriate range of this index, we have for the differential operators in this paper the following expressions:

\[
\nabla q = \frac{\partial q}{\partial \xi^i} a^i,
\] (A.5a)

\[
\nabla \cdot \mathbf{u} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^i} \left( \sqrt{g} u^i \right), \quad u^i := a^i \cdot \mathbf{u},
\] (A.5b)

\[
\nabla \cdot (s \nabla q) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^i} \left( \sqrt{g} s g^{ij} \frac{\partial q}{\partial \xi^j} \right),
\] (A.5c)

\[
\frac{\partial q}{\partial t} = \frac{\partial q}{\partial \tau} - \mathbf{x} \cdot \nabla q, \quad \dot{x} := \frac{\partial \mathbf{x}}{\partial \tau},
\] (A.5d)

\[
\frac{\partial q}{\partial t} + \nabla \cdot (q \mathbf{u}) = \frac{1}{\sqrt{g}} \left( \frac{\partial}{\partial \tau} \left( \sqrt{g} q \right) + \frac{\partial}{\partial \xi^i} \left( \sqrt{g} q U^i \right) \right), \quad U^i := a^i \cdot (\mathbf{u} - \dot{x}),
\] (A.5e)

where \( q \) and \( s \) are arbitrary scalar fields and \( \mathbf{u} \) an arbitrary vector field. Moreover, \( u^i \) and \( U^i \) are the contravariant component and the contravariant component relative to the moving coordinate system, respectively, and \( \dot{x} \) is the velocity of the moving coordinate system. Finally, we need the so-called internal differential operators:

\[
\nabla_t q = \frac{\partial q}{\partial \xi^\alpha} a^\alpha,
\] (A.6a)

\[
\nabla_t \cdot \mathbf{u} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^\alpha} \left( \sqrt{g} u^\alpha \right), \quad u^\alpha := a^\alpha \cdot \mathbf{u},
\] (A.6b)

\[
\nabla_t \cdot (s \nabla_t q) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^\alpha} \left( \sqrt{g} g^{\alpha \beta} \frac{\partial q}{\partial \xi^\beta} \right),
\] (A.6c)

where \( \alpha, \beta = 2, 3 \). The subscript \( t \) indicates that these operators only contain derivatives in directions tangent to the flame surfaces.

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