Mathematical Modelling of Triple Flame Ring Behaviour

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Abstract

In the present work we study the dynamical properties of lifted round diffusion jet flame, stabilized over the fuel exit. The stabilization mechanism is described in terms of triple flame structure, forming at the edge of the diffusion flame. This “triple flame ring” propagates along the line of stoichiometry and stabilizes the flame at the point, where the local negative velocity of the triple structure compensates the velocity of the jet.

S.Ghosal and L.Vervisch [18] approximated the flame base velocity by local two-dimensional one. The global dependence on the flame base radius was neglected in this study. We introduce this influence at zero order, allowing the triple flame description in the vicinity of iso-stoichiometric surface.

Zero Mach number combustion equations are introduced to describe the flow. Even if the density changes due to the velocity variations are neglected, the variations referred to the temperature increase in the vicinity of the flame front are taken into account; we allow to the small density variations and investigate their impact on the flame velocity.

The flame front is assumed to be parabolic of unknown curvature, which is then found as a function of the chemical properties.

The method of matched asymptotic expansions in parabolic-cylinder coordinates is applied in order to find a global approximative solution for the temperature. The matching procedure also delivers us the closed expressions for the flame velocity as function of the mixture fraction gradient and of small heat release. We compare these theoretical results with direct numerical simulations by J. Boulanger, L. Vervisch, J. Reveillon and S. Ghosal [5].
Kurzfassung


Der Fluss wird mithilfe der Gleichungen im asymptotischen Grenzfall kleiner Mach-Zahlen beschrieben. Wir lassen kleine Dichteänderungen infolge Temperaturänderungen zu und untersuchen deren Einfluss auf die Geschwindigkeit der Flamme.

Es wird angenommen, dass die Flammenfront parabolisch ist. Die Krümmung ergibt sich als eine Funktion von chemischen Eigenschaften.


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Chapter 1

Introduction

We study axisymmetrical triple flame, that is observed at the base of lifted laminar diffusion flame. The dynamics of the flame base is described in terms of laminar flamelet, propagating along the stoichiometric iso-surface in the direction opposite to those of the jet. Due to this "opposed flow" mechanism the round jet flame is stabilized over the fuel exit. The lift-off height, i.e. the distance between the burner and the flame is consequently determined by the jet velocity and the flame response. This "lifted" regime, or triple flame ring, exists only for a limited range of Reynolds numbers: for small values of the jet velocity the flame is attached to the burner, and for velocities exceeding some critical value, blow-out occurs. In its turn, the impact of the mixture fraction gradient on the stabilization over the burner is important: the smaller the gradient, the higher the triple flame propagation velocity is.

Consequently, we are interested in control over the lift-off height in terms of the jet velocity and mixture fraction gradient.

The laminar diffusion jet flame is described with help of axisymmetric zero Mach number combustion equations for unbounded domains. Chemical process is chosen to be a single-step one, with reaction rate described by Arrhenius law.

In the previous studies (see [5], [19]) an approximation for a plane triple flame velocity was used in order to predict the lift-off height for round jet. By this, all the non-local features of the flame base propagation was neglected. We fill up this gap, introducing the leading order dependence on the flame base radius.

The heat released into the flame modifies the flow ahead of the flame front,
increasing the flame propagation velocity. In the present work we consider the situation, where heat release parameter $\alpha$ is small. At the same time the activation energy is large, normalized mixture fraction gradient is small and their product is of order one.

In our analysis, solution to the passive scalar equation for the mixture fraction is approximated by linear profile with gradient, prescribed at the inlet.

Assuming the flame front to be parabolic, we want to determine its curvature. This assumption simplifies considerably the original free-boundary problem and allows us to introduce local parabolic-cylinder coordinates, matching the flame front. Afterwards, standard techniques of the activation-energy asymptotics can be applied.

Dependence on the density changes is incorporated through perturbative analysis of the reactive flow characteristics.

Solutions for both temperature and mixture fraction are found in the form of expansions with respect to small parameter $\alpha$, characterizing the heat released into the flame.

The resulting singular perturbative problems are solved in local parabolic-cylinder coordinates with help of the method of matched asymptotic expansions. The equations for temperature together with the prescribed boundary values define the eigenvalue problems at each order, the eigenvalue is inversely proportional to the square of the triple flamelet propagation velocity.

Closed expressions for the flame curvature and velocity, as well as the temperature field, are given.

Comparison of our theoretical predictions of the lift-off height with direct numerical simulations (DNS) done by J. Boulanger, L. Vervisch, J. Reveillon, S. Ghosal, [5] is presented.

The thesis is organized as follows. In Chapter 2 we introduce the governing equations of the reactive flow, considering them further in the low Mach number limit. General classification in premixed and non-premixed combustion regimes is presented in Chapters 3 and 4 together with different approaches to the flame treatment. We emphasize the importance of the asymptotic methods in combustion modelling and present a perturbative method to find an approximate solution of the singular perturbation problem, appearing in the analysis of the flame zone.
In Chapter 5 we introduce a triple flame model, that is adapted to describe the propagation mechanisms in diffusion flames. The stabilization role of this triple flame, forming at the edge of the lifted round jet, is determined by the velocity of the triple axisymmetric flame, or “triple ring flame” propagation. We consider the idealized situation of the jet with stoichiometric iso-line parallel to one of the axes, so that the flame base radius remains constant. The formulae for the velocity of the flame base as function of this constant, mixture fraction gradient and small heat release are derived.

In Chapter 6 the comparison with Direct Numerical Simulations by Boulanjer, Reveillon, Vervisch and Ghosal, is presented. The cold self-similar solution for the round jet of Darieus and Landau delivers the fluid velocity. We equate both velocities, and obtain the theoretical values of the lift-off height, that are compared with the lift-off heights, got by DNS.

The conclusions are contained in Chapter 7.
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Chapter 2

Mathematics of combustion

2.1 Preliminaries

Combustion is an essential and integral part of our life. The humanity history cannot be imagined without this energy source, that accompanied us since thousands of years. Our civilization, its historical and economical development, are closely related to combustion.

The twentieth century was a period of technological boom, when cars, rockets, and all types of engines became a part of our everyday life. Industry needed the reactors and motors that was more and more elaborated, and in the same time the pollution problems came at the first plan.

All these reasons gave rise to the combustion research development. The first works of S. P. Burke and T. E. Schumann [13] appeared in the twenties, but the real advances in the science of combustion was done in the middle of the twentieth century, with pioneer works of Ya. B. Zeldovich, F. A. Williams, A. Liñán, and others.

When talking about combustion, one cannot separate such fields as fluid dynamics, chemical reactive processes, numerical simulations, asymptotic analysis, turbulence modelling. The complexity of the combustion process demands the complex models to describe it, and this is exactly what makes the combustion science such a challenging and fascinating field.

In the description of the reactive flow the chemical kinetics, driving the reactive processes, has to be coupled with underlying fluid dynamics, because the chemistry is influenced by fluid motion, and vice versa: the chemical reactions,
that are the source of energy, modify the flow.

In order to reduce the complexity of the problem, we introduce a classification of the combustion processes in respect to the underlying fluid field velocity.

We distinguish detonations — reactions at the speed, close to or exceeding the sound velocity, and deflagrations, or combustion at low Mach number. Detonations are described with help of Euler equations. They are characterized by the shock waves propagation.

Second type are deflagrations, that are of special interest in the engineering applications, while the most part of practical combustion processes happen at low speeds. Deflagrations, in their turn, are assigned into two classes: we distinguish premixed and non-premixed low Mach number combustion.

In the case of premixed combustion we suppose fuel and oxidizer to be uniformly mixed. The flame propagates into the fresh gases mixture, leaving the burnt gases behind. This ability to propagate is the main feature of the premixed combustion process. If we consider the reactions to be infinitely fast, the flame front can be viewed as a surface of discontinuity, propagating with a local velocity, that is close to the planar flame velocity. The methods to treat such surfaces are then applied (for example, level-set method for G-equation [6], [21], [41]). The main problem in this case is that in order to couple this purely mathematical approach of propagating interface with reactive flow problem, the local velocity of the flame front propagation has to be determined.

The second deflagration regime is non-premixed combustion, where the gases are separated initially, and the mixing process has to take place before the burning starts. These flames are called diffusion flames, they are dominated by diffusion processes. To describe them we introduce the measure of mixing, or mixture fraction. The equation of the mixture fraction evolution is a passive scalar equation, i.e. the mixture fraction is not modified by reactions. The reaction takes place in the vicinity of the iso-stoichiometric surface of mixture fraction, where reactants are mixed in stoichiometric proportions.

These two approaches dominated the combustion research till 1965 when Philips published the first article about the triple flame that was observed in the laboratory. This flame, appearing at the end of the diffusion flame, consists of two premixed branches: lean and rich, and of a trailing diffusion flame. Its ability to propagate allows us to think, that it is responsible for the flame stabilization processes. The triple flame was investigated by different authors, see for example [15], [19], [27], [34].
2.2 Asymptotical methods in combustion

Asymptotic analysis has been one of the essential analytical tools in combustion research. The first theoretical works about combustion for small Mach number was done by Mikhelson, who described the thermal flame theory in 1889. The notion of deflagration wave appeared for the first time, with the temperature solution, that grows exponentially at the leading edge of the flame.

In 1928 Burke and Schumann presented the theory of diffusion flames for large Damköhler numbers. This work was a first asymptotic treatment of combustion problems, even though wasn’t considered by it’s authors as such. The works of Zeldovich and his school presented an important amount of results in the activation energy asymptotic limit.

In 1970 the activation energy asymptotics analysis was applied by Bush and Fendell to the laminar flame speed problem.

The development of the combustion theory extracted following asymptotic limits:

- hydrodynamic limit;
- small Mach number asymptotics;
- Damköhler number asymptotics;
- activation energy asymptotics.

We discuss these approaches in connection with different combustion regimes below. In the present work we get rid of almost all of these asymptotics: the equation in zero Mach number limit will be considered in order to describe laminar diffusive flame, that is quenching for Damköhler numbers of order unity. We describe the structure of this flame with help of activation-energy asymptotics.

It’s exactly this flame that attracts our attention in the present work, in particular its ability to stabilize the lifted round jet flame over the burner.
2.3 Fundamental equations

The equations driving laminar reactive flow are:

- mass conservation (or continuity equation),

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0; \tag{2.1}
\]

- conservation of momentum,

\[
\rho \frac{D \mathbf{v}}{D t} = \nabla \cdot \mathbf{\Sigma} \tag{2.2}
\]

with stress tensor

\[
\mathbf{\Sigma} = -(p + \frac{2}{3} \kappa \nabla \cdot \mathbf{v}) \mathbf{I} + \kappa [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]; \tag{2.3}
\]

- energy equation,

\[
- \frac{\partial p}{\partial t} + \rho \frac{D h}{D t} - \nabla \cdot (\mathbf{v} \cdot \mathbf{\Sigma}')
\]

\[= \nabla \cdot (\lambda \nabla T) - \sum_{i=1}^{N} h_i^0 \rho_i, \tag{2.4}
\]

where \( h_i^0 \) is the heat formation of the \( i \) th species at the reference temperature \( T_0 \), \( \lambda \) is the coefficient of thermal conductivity and \( \mathbf{\Sigma}' = \mathbf{\Sigma} + \rho \mathbf{I} \).

- for each component of the mixture, the conservation equation of the mass fraction:

\[
\rho \frac{D Y_i}{D t} = \text{div} j_i + \dot{\rho}_i, \quad i = 1, \ldots, N - 1,
\]

\[Y_N = 1 - \sum_{i=1}^{N-1} Y_i; \tag{2.5}
\]
with \( \dot{\rho}_i \) — mass increase per unit volume due to chemical reaction.

In these equations notation \( \frac{D}{Dt} \) is used for material derivative, i.e. 
\[ \frac{D}{Dt} = \frac{D}{Dt} \rho + \mathbf{v} \cdot \nabla. \] 
Quantities \( \rho \) and \( p \) are the mixture density and pressure respectively, \( \mathbf{v} \) is the average fluid velocity, \( T \) is the temperature.

Only the mixture of ideal gases is considered, i.e. the equation of state for ideal fluid is hold:

\[ p = R\rho T \left( \sum_{i=1}^{N} \frac{Y_i}{W_i} \right), \tag{2.6} \]

where \( R \) is the universal gas constant and \( W_i \) are molecular weights of the \( i \)-th chemical species. Also the caloric equation is considered,

\[ h = \sum_{i=1}^{N} h_i Y_i, \quad \text{with} \quad h_i = c_p^i(T - T_0) + h_i^0, \tag{2.7} \]

\( c_p^i \) are the thermal capacities. If we denote by \( c_v^i \) the heat capacity at constant volume, and introduce the new values

\[ c_p = \sum_{i=1}^{N} c_p^i Y_i, \tag{2.8} \]
\[ c_v = \sum_{i=1}^{N} c_v^i Y_i, \]

the \( \gamma \)-gas constant can be defined as

\[ \gamma = \frac{c_p}{c_v}. \tag{2.9} \]

The equation of state will be re-written:

\[ p = \frac{\gamma - 1}{\gamma} \rho c_p T. \tag{2.10} \]

In order to describe the diffusion mechanism, we recall that the sum of diffusive fluxes vanishes,
We suppose that all they satisfy Onsager’s generalization of the Fick’s law:

\[ j_i = \sum_{j=1}^{N} D^{ij} \nabla Y_j, \quad i = 1, \ldots, N. \]  

(2.12)

(here \( D^{ij} \) are diffusion coefficients).

Because the sum of diffusive fluxes is zero, the following conditions for diffusion coefficients hold:

\[ \sum_{j=1}^{N} \left( \sum_{i=1}^{N} D^{ij} \right) \nabla Y_j = 0. \]  

(2.13)

Moreover, the sum of the mass fractions is one, and this gives us the condition

\[ \sum_{j=1}^{N-1} \left[ \sum_{i=1}^{N} (D^{ij} - D^{iN}) \right] \nabla Y_j = 0. \]  

(2.14)

Consequently, the requirement on the diffusion coefficients transforms into

\[ \sum_{i=1}^{N} D^{ij} = \sum_{i=1}^{N} D^{iN} \quad \text{for} \quad j = 1, \ldots, N - 1. \]  

(2.15)

An important simplification is done when we consider a binary reactive mixture. In this case the formulae for reactive fluxes reduce to the well-known Fick’s law \( j_1 = \rho D \nabla Y_1 \) and \( j_2 = \rho D \nabla Y_2 \).

In practice, we often work with the so-called dilute mixtures, where one of the species is presented in much higher quantity than the others, for example in the case of the combustion processes in the air.

Under the assumption of the dilute mixture, the fluxes are described in the analogous way to those of binary mixture situation:

\[ j_i = \rho D^i \nabla Y_i, \quad i = 1, \ldots, N - 1, \]  

(2.16)
and

\[ j_N = \sum_{j=1}^{N-1} \rho (D^N - D^j) \nabla Y_j + \rho D^N \nabla Y_N. \] (2.17)

The complicated expression for \( j_N \) doesn’t play any role for computation of \( Y_N \), because of the relation on the mass fractions \( \sum_{i=1}^{N} Y_i = 1 \), that gives us the possibility to compute \( Y_N \) directly from the other mass fractions.

Since the mass has to be preserved during each of the reactions, the source terms satisfy

\[ \sum_{i=1}^{N} \rho_i = 0. \] (2.18)

If we add up all the equations for mass fractions, considering both facts of the dilution of the mixture and the above condition on the source terms, we get:

\[ \rho \frac{DY}{Dt} = \text{div}(D^M \nabla Y), \quad \text{with} \quad Y = \sum_{i=1}^{N} Y_i. \] (2.19)

We’ve assumed, that

\[ \sum_{i=1}^{N} Y_i = 1 \] (2.20)

initially. This is true for all times, provided the uniqueness of the solution of (2.19).

Let us present the reaction mechanism schematically:

\[ \sum_{i=1}^{N} \nu_{ij}' M_i \Rightarrow \sum_{i=1}^{N} \nu_{ij}'' M_i, \quad j = 1, \ldots, M. \] (2.21)

Here \( M_i \) are the species, and \( \nu_{ij}', \nu_{ij}'' \) are the stoichiometric coefficients of these species as reactant or product respectively.

The mass conservation during the reaction yields to the condition on the stoichiometric coefficients:
The source term $\hat{\rho}_i$ is then defined as

$$\hat{\rho}_i = W_i \sum_{i=1}^{N} (\nu''_{ij} - \nu'_{ij}) R_j,$$

with reaction rate $R_j$. The law of mass action describes the reaction rate as

$$R_j = k_j^f \prod_{i=1}^{N} \left( \frac{Y_i}{W_i} \right)^{\nu'_{ij}} - k_j^b \prod_{i=1}^{N} \left( \frac{Y_i}{W_i} \right)^{\nu''_{ij}}, \quad j = 1, \ldots, M. \quad (2.24)$$

The most common way to define the constants $k_j^f, k_j^b$ is the Arrhenius law, that reflects the fact, that the maximal reaction rate is attained at the maximal temperature:

$$k_j^f = B_j^f T^{\alpha_j^f} \exp\left(-\frac{E_j^f}{RT}\right),$$

$$k_j^b = B_j^b T^{\alpha_j^b} \exp\left(-\frac{E_j^b}{RT}\right), \quad j = 1, \ldots, M. \quad (2.25)$$

The pre-exponential factors are defined from the experiment, and usually supposed to be constant for simplicity.

The set of equations given above is a starting point in the description of the reactive flow. Nevertheless, the equations are already much too complicated to be solved analytically, and considerable simplifications are needed in order to be able to tackle an analytical approach to the laminar flame treatment.

The big part of combustion processes is happening at speeds, that are small compare to the sound speed. For theoretical as well as numerical analysis purposes, it is useful to derive a new set of equations in the limit of low Mach number, $Ma \to 0$. We recall, that the Mach number is defined as fraction of the fluid velocity to the velocity of sound.

In the next section we present the zero Mach number equations for bounded domain with strong heat release. This analysis allows us to exclude the effects of nonlinear acoustic waves. We follow the main lines of the work [8].
2.3.1 Zero Mach number limit equations

We assume the Mach number to be small and the initial pressure $p_0$ to be spatially uniform. The chemical-fluid balance within the first order (with resp. to Mach number) of the initial temperature, mass fractions and velocity, is also assumed.

Further, we use the well-known facts about vector-field orthogonal decomposition and uniqueness of the solution of a suitable boundary problem, see [43]. We formulate both of these theorems below.

**Theorem 1**

Every vector field $v$ in $L^2(\Omega)$ admits a unique orthogonal decomposition into divergence-free vector field $w$ and potential field $\nabla \phi$:

\[
\begin{align*}
v &= w + \nabla \phi, \quad \text{with} \\
\text{div} v &= 0, \quad w \cdot n|_{\partial \Omega} = 0, \\
\Delta \phi &= \text{div} v, \quad \frac{\delta \phi}{\delta n}|_{\partial \Omega} = v \cdot n|_{\partial \Omega}.
\end{align*}
\]

If $P$ is an orthogonal projection of $L^2(\Omega)$ onto the divergence-free vector field, then $Pv = 0$ if and only if $v = \nabla \phi$ for some $\phi$.

**Theorem 2**

The boundary value problem

\[
\begin{align*}
\Delta \phi &= f \quad \text{in} \quad \Omega \\
\frac{\delta \phi}{\delta n}|_{\partial \Omega} &= g
\end{align*}
\]

has a solution with $\nabla \phi$ uniquely determined if and only if

\[
\int_{\Omega} f \, dx = \int_{\partial \Omega} g \, ds
\]

Naturally, in the chemical processes energy is associated with the heat, released in the flame during the reaction. That's why we are looking for a new form of energy equation, containing dependence on temperature and chemical reactions. We differentiate the equation of state and the caloric equation, and
derive a new set of equations with help of conservation laws for mass, momentum and energy:

• equation for pressure

\[
\frac{Dp}{Dt} + \gamma p \text{div} \mathbf{v} = (\gamma - 1) \nabla \cdot (\mathbf{v} \cdot \Sigma') + \nabla \cdot (\lambda \nabla T) \\
+ \gamma \sum_{i=1}^{N-1} RT \left( \frac{1}{W_i} - \frac{1}{W_N} \right) \text{div}(\rho D^i \nabla Y_i) \\
+ \gamma \sum_{i=1}^{N-1} \rho (c_p^i - c_p^N) D^i \nabla T \cdot \nabla Y_i \\
+ \sum_{i=1}^{N-1} \left[ \gamma RT \left( \frac{1}{W_i} - \frac{1}{W_N} \right) - (\gamma - 1)(h_i - h_N) \right] \hat{\rho}_i .
\] (2.29)

• equation for temperature

\[
\rho c_p \frac{DT}{Dt} = \nabla \cdot (\lambda \nabla T) + \frac{Dp}{Dt} + \nabla \cdot (\mathbf{v} \cdot \Sigma') \\
+ \sum_{i=1}^{N-1} (c_p^i - c_p^N) D^i \nabla T \cdot \nabla Y_i - \sum_{i=1}^{N-1} (h_i - h_N) \hat{\rho}_i .
\] (2.30)

In order to be able to handle these equations, a non-dimensionalization has to be effectuated first. The reference values are chosen as follow:

1. Characteristic physical length \( L \) is a diameter of the domain, \( L = \text{diam}(\Omega) \).

2. Characteristic velocity \( |v_m| \) is a free space burning velocity.

3. The time scale is \( \tau = L/|v_m| \).

4. The reference pressure is the initial pressure \( p_0 \).

5. The reference temperature \( T_b \) is the adiabatic temperature of the burnt gas.
6. The characteristic heat capacity and molecular weight of the mixture \( c_p^m, \ W_m \).

7. The reference density is defined from state equation for ideal gas:
\[
p_m = \frac{R}{W_m} \rho_m T_b.
\]

With help of these non-dimensional values, different parameters can be composed:

The Reynolds number \( Re = \frac{\rho_m L |v_m|}{\kappa} \),

The Prandtl number \( Pr = \frac{k c_p^m}{\lambda} \),

The Lewis numbers \( Le^i = \frac{\lambda}{\rho_m c_p^m D^i} \),

The Mach number \( Ma = \frac{|v_m|}{\sqrt{\frac{k}{\rho_m}}} \), where \( \Gamma - 1 = \frac{R}{W_m c_p^m} \).

We will develop all the physical quantities in series in respect to the inverse of the parameter \( a = \frac{1}{Ma\sqrt{\Gamma}} \).

Finally, the system of above equations in non-dimensional form is

- equation for non-dimensional pressure, \( \tilde{p} \):
\[
\begin{align*}
\frac{D\tilde{p}}{Dt} + \gamma\tilde{p} \text{div}\tilde{\mathbf{v}} &= \frac{\gamma - 1}{2\alpha^2 Re} \nabla \cdot (\mathbf{v} \cdot \Sigma') + \frac{\gamma - 1}{Pr Re \Gamma - 1} \Delta \tilde{T} \\
&+ \sum_{i=1}^{N-1} \frac{\gamma - 1}{Pr Re \Gamma - 1 Le^i} \left( \tilde{c}_p^{e_N} - \tilde{c}_p^e \right) \nabla \cdot \nabla \tilde{Y}_i \\
&+ \sum_{i=1}^{N-1} \left( \frac{1}{\tilde{W}_i} - \frac{1}{\tilde{W}_N} \right) \text{div}(\tilde{p} \nabla \tilde{Y}_i) \\
&+ \sum_{i=1}^{N-1} \left[ \gamma\tilde{T} \left( \frac{1}{\tilde{W}_i} - \frac{1}{\tilde{W}_N} \right) - \frac{\gamma - 1}{\Gamma - 1} \left( \tilde{h}_i - \tilde{h}_N \right) \right] \tilde{\rho}_i.
\end{align*}
\]
• equation for non-dimensional velocity, $\tilde{v}$:

$$\tilde{\rho} \frac{D\tilde{v}}{Dt} + a^2 \nabla \tilde{p} = \frac{1}{Re} \left[ \Delta \tilde{v} + \frac{1}{3} \nabla (\text{div} \tilde{v}) \right]. \quad (2.32)$$

• equation for non-dimensional temperature, $\tilde{T}$:

$$\tilde{\rho} \tilde{c}_p \frac{D\tilde{T}}{Dt} = \frac{1}{2a^2Re} \frac{\Gamma - 1}{\Gamma} \tilde{\Sigma}_i + \frac{1}{PrRe} \Delta \tilde{T} + \frac{\Gamma - 1}{\Gamma} \frac{D\tilde{p}}{Dt}$$

$$+ \sum_{i=1}^{N-1} \frac{1}{PrReLe} \tilde{\rho} \tilde{c}_p (\tilde{c}_p - \tilde{c}_p^M) \nabla \tilde{T} \cdot \nabla \tilde{Y}_i - \sum_{i=1}^{N-1} (\tilde{\hat{h}}_i - \tilde{\hat{h}}_N) \tilde{\rho}_i. \quad (2.33)$$

• equation for non-dimensional species, $\tilde{Y}_i$:

$$\tilde{\rho} \frac{D\tilde{Y}_i}{Dt} = \frac{1}{PrReLe^i} \text{div}(\tilde{\rho} \nabla \tilde{Y}_i) + \tilde{\rho}_i. \quad (2.34)$$

The new equation of state is

$$\tilde{\rho} = \tilde{\rho} \tilde{T} \left( \sum_{i=1}^{N} \frac{\tilde{Y}_i}{\tilde{W}_i} \right). \quad (2.35)$$

The enthalpy is now governed by equation

$$\tilde{\hat{h}}_i = \frac{h_i}{\tilde{c}_p^M T_b} = \tilde{c}_p^i \tilde{T} + \tilde{h}_i^0, \quad \text{where}$$

$$\tilde{h}_i^0 = (-c_p^i T_0 + h_i^0)/c_p^M T_b. \quad (2.36)$$

The non-dimensional heat capacity of mixture is

$$\tilde{c}_p = \sum_{i=1}^{N-1} (\tilde{c}_p^i - \tilde{c}_p^M) \tilde{Y}_i. \quad (2.37)$$

The source term will be transformed into

$$\tilde{\rho}_i = \frac{L\tilde{\rho}_i}{\tilde{p}} = \tilde{W}_i \sum_{j=1}^{M} (\nu_{ij}^\prime - \nu_{ij}^\prime) \tilde{R}_j, \quad \text{for all species}, \quad (2.38)$$

where the non-dimensional reaction rate $\tilde{R}_j$ is defined as
\[ R_j = D_j \left\{ (\bar{\rho})^{\nu^j} (\bar{T})^{\alpha^j} \exp(-A_j^f / \bar{T}) \Pi_{i=1}^{N_i} \left( \frac{\bar{Y}_i}{\bar{W}_i} \right)^{\nu_i^j} ight\} \]

\[-K_j^{-1} (\bar{\rho})^{\nu^j} (\bar{T})^{\alpha^j} \exp(-A_j^b / \bar{T}) \Pi_{i=1}^{N_i} \left( \frac{\bar{Y}_i}{\bar{W}_i} \right)^{\nu_i^j} \right\}. \]

In the above equations the modulo sign means summation over all species, \( A_j^f \) and \( A_j^b \) are the nondimensionalized activation energies, corresponding to the forward and backward reactions.

The Damköhler constant \( D_j \) is defined as \( D_j = \frac{L}{v_m \tau_j^f} \), and \( K_j^{-1} \) denotes the equilibrium constant, \( K_j^{-1} = \frac{x_j^f}{x_j^b} \).

The chemical characteristic times are

\[ (\tau_j^f)^{-1} = B_j^f T_a^{\alpha^j} \left( \frac{\rho m}{W_m} \right)^{|\nu_j^f|-1}, \]

\[ (\tau_j^b)^{-1} = B_j^b T_a^{\alpha^j} \left( \frac{\rho m}{W_m} \right)^{|\nu_j^b|-1}, \] for \( j = 1, \ldots, M \).

As already mentioned, the domain \( \Omega \) where solution of this problem lives, is supposed to be bounded. In order to solve the set of equations (2.29)-(2.32), we have to prescribe the boundary values of the velocity, as well as the normal gradient components of the temperature and mass fraction:

\[ \bar{v} |_{\partial \Omega} = 0 \quad \text{(no-slip boundary)}, \]

\[ \frac{\delta \bar{T}}{\delta n} |_{\partial \Omega} = 0, \quad \frac{\delta \bar{Y}_i}{\delta n} |_{\partial \Omega} = 0, \] \( i = 1, \ldots, N - 1 \).

The last two conditions simply mean that there are no chemical and thermal quantities escape through the boundary.

Pressure, velocity, temperature and mass fractions will be developed in formal series with respect to the small parameter \( a^{-1} \). The conditions of the spatial uniformity within respective order are used in order to get the following.


Substituting the above expansions into the equations for pressure, velocity, temperature and mass fractions, and using the well-known fact about the uniqueness of the orthogonal decomposition of the velocity vector field \( \mathbf{v}^\infty \) into divergence-free and potential parts

\[
\mathbf{v}^\infty = \mathbf{w}^\infty + \nabla \phi^\infty ,
\]

we get finally zero Mach number combustion equations: (see [8] for details)

- Ordinary differential equation for mean pressure,

\[
\frac{dp^\infty}{dt} = \mathcal{H}(t) = \frac{\int_\Omega \gamma^{-1} \mathbf{G} \, dx}{\int_\Omega \gamma^{-1} \, dx}, \quad \text{with} \quad p^\infty(0) = 1 .
\]

- Equations for divergence-free and potential components of the velocity field:

\[
\Delta \phi^\infty = (\gamma p^\infty)^{-1} (\mathcal{S} - \mathcal{H}(t)),
\]

\[
\frac{\delta \phi^\infty}{\delta n} \big|_{\partial \Omega} = 0 .
\]

\[
\rho^\infty \frac{Dw^\infty}{Dt} + \nabla \pi^\infty = \frac{1}{Re} \Delta w^\infty - \rho^\infty \frac{D \nabla \phi^\infty}{Dt} ,
\]

with \( \pi^\infty \) — a scalar pressure, the existence provided by Theorem 1.

\[
\text{div} \, w^\infty = 0
\]

\[
w^\infty \cdot n|_{\partial \Omega} = 0 , \quad w^\infty \times n|_{\partial \Omega} = -\nabla \phi^\infty \times n|_{\partial \Omega} .
\]
2.3. FUNDAMENTAL EQUATIONS

- Reaction-diffusion equations for the mean temperature $T^\infty$:

$$
\rho^\infty c_p^\infty \frac{DT^\infty}{Dt} = \frac{1}{PrRe} \Delta T^\infty + \frac{\Gamma - 1}{\Gamma} \Theta(t)
+ \sum_{i=1}^{N-1} \frac{\rho^\infty}{PrReLe^i} (\bar{c}_p^i - \bar{c}_p^N)^\infty \nabla T^\infty \cdot \nabla Y_i^\infty
- \sum_{i=1}^{N-1} (h_i^\infty - h_N^\infty) \phi_i^\infty,
$$

(2.47)

with boundary condition

$$
\frac{\delta T^\infty}{\delta n}|_{\partial \Omega} = 0.
$$

(2.48)

- Reaction-diffusion equations for mass fractions $Y_i^\infty$:

$$
\rho^\infty \frac{DY_i^\infty}{Dt} = \frac{1}{PrReLe^i} \text{div}(\rho^\infty \nabla Y_i^\infty) + \dot{\rho}_i, \quad i = 1, \ldots, N - 1
$$

(2.49)

with boundary condition

$$
\frac{\delta Y_i^\infty}{\delta n}|_{\partial \Omega} = 0, \quad i = 1, \ldots, N - 1.
$$

(2.50)

In the above equations $\mathcal{G}$ is a second order differential operator

$$
\mathcal{G}(\rho^\infty, T^\infty, Y^\infty) = \frac{\gamma - 1}{PrRe \Gamma - 1} \Delta T^\infty
+ \frac{\gamma - 1}{PrRe \Gamma - 1} \sum_{i=1}^{N-1} \frac{\rho^\infty}{Le^i} (\bar{c}_p^i - \bar{c}_p^N)^\infty \nabla T^\infty \cdot \nabla Y_i^\infty
+ \sum_{i=1}^{N-1} \frac{\gamma T^\infty}{PrReLe^i} \left( \frac{1}{W_i} - \frac{1}{W_N} \right) \text{div}(\rho \nabla Y_i^\infty)
+ \sum_{i=1}^{N-1} \left[ \gamma T^\infty \left( \frac{1}{W_i} - \frac{1}{W_N} \right) - \frac{\gamma - 1}{\Gamma - 1} (h_i^\infty - h_N^\infty) \right] \phi_i^\infty.
$$

(2.51)

In all above expressions the values with index $\infty$ are defined in an analogous way to the original values.

The expansions (2.42) will be self-consistent, if the initial data for them coincide with those for original values, or
\[
\begin{align*}
\bar{p}(x,0) &= 1 + a^{-2} p_0(x) + O(a^{-3}), \\
\bar{v} &= v_0^\infty + O(a^{-1}), \\
\bar{T}(x,0) &= T_0^\infty(x) + O(a^{-1}), \\
\bar{Y}_i(x,0) &= Y_{i0}^\infty(x) + O(a^{-1}), \quad i = 1, \ldots, N - 1.
\end{align*}
\] (2.52)

The requirement on the approximate chemical-fluid balance for initial data within the terms of order \( a^{-1} \) is
\[
\text{div} \, v_0^\infty = \gamma^{-1}(Y_0^\infty) (S(1, T_0^\infty) - \mathcal{H}_0). \tag{2.53}
\]

The boundary conditions are
\[
\begin{align*}
\frac{\delta T_0^\infty}{\delta n} &= 0, \\
\frac{\delta Y_{i0}^\infty}{\delta n} &= 0, \quad i = 1, \ldots, N - 1, \\
v_0^\infty n|_{\partial \Omega} &= 0, \\
w_0^\infty \cdot n|_{\partial \Omega} &= 0, \\
w_0^\infty \times n|_{\partial \Omega}. 
\end{align*}
\] (2.54)

It is important to note that the chemical-fluid balance condition is posed for the gradient part of the velocity field. The divergence-free component can be chosen in arbitrary manner, if the boundary conditions (2.52) are fulfilled.

### 2.3.2 Further simplifications

The above expressions are derived for bounded domain. In the case of unbounded domain that we will consider herein, the pressure remains constant. The equation for mean pressure then becomes
\[
\frac{dp^\infty}{dt} = \mathcal{H}(t) = 0. \tag{2.55}
\]

From the initial condition on pressure \( p^\infty(0) = 1 \) it follows, that the mean pressure is equal to unity everywhere.
2.3. FUNDAMENTAL EQUATIONS

The next step is the reduction of the number of reactants. We've already mentioned the hypothesis of the dilute mixture, when one component is presented in quantities, that are large compared to the rest of the mixture, and the reaction can be presented as reaction of two species only.

Further, we suppose, that the chain of reactions, leading to the full reactants transformation into the products, can be simply replaced by a one-step irreversible reaction,

\[ F + sO \rightarrow (1 + s)P, \]  

(2.56)

where fuel \( F \) reacts with oxidizer \( O \), forming product \( P \). Hereabove \( s \) is the stoichiometric mass ratio.

Till now, the discussion of this approximation validity is one of the main topics in the combustion community. The methods of reduced chemistry was introduced in order to simulate the "real" combustion processes. Among them we would like specially mention an elegant result of U. Mass (see [29]), who got rid of such a pure mathematical abstraction as a dynamical system attractor.

We further suppose that the heat capacities of both fuel and oxidizer are equal, as well as their molecular weights.

If we introduce these simplifications in the set of zero Mach number equations (2.44)-(2.49), they will take form:

\[
\rho^\infty \frac{DT^\infty}{Dt} = \frac{1}{PrRe} \Delta T^\infty + QR^\infty;
\]

\[
\rho^\infty \frac{DY_1^\infty}{Dt} = \frac{1}{PrReLe} \text{div}(\rho^\infty \nabla Y_1^\infty) - R^\infty;
\]

\[
\Delta \phi^\infty = \frac{1}{PrRe} \Delta T^\infty + QR^\infty;
\]

\[
\rho^\infty \frac{Dw^\infty}{Dt} = \frac{1}{Re} \Delta w^\infty - \rho^\infty \frac{D\phi^\infty}{Dt}.
\]

(2.57)

The density \( \rho^\infty \) is found from the equation of state, and equal \( 1/T^\infty \).

\[
Q = h_1^0 - h_1^0,
\]

\[
R^\infty = \rho^\infty \exp(-T_a/T^\infty)Y_1^\infty
\]

(2.58)
are the heat conduction and reaction rate.

### 2.4 Perturbative methods in combustion

Perturbation theory is a powerful tool to find global approximative solutions for problems, containing a small parameter \( \epsilon \). These methods are very well adapted for theoretical analysis of the reactive flow problems, because they contain a whole palette of parameters that can be considered small in some situations.

The main idea behind these methods is to decompose the function we are looking for into a main part and "perturbed" parts. We get equations at each order of approximation, and all these equations are to be solved in space of the dimension \( n - 1 \) (one of the variables becomes the parameter of expansions now). In this way, the dimension of the problem is reduced by one, and we hope to get soluble equations. Once the solution is obtained at each order, we reconstruct the formal series and get the approximation we are looking for.

This technique could also be applied to the weak turbulent flows, when we are looking for turbulent solution as a perturbation of the laminar flow.

However, in the present work we have to do with laminar flows only.

The gradients of temperature and mass fractions are strongly changing in the narrow region around the flame front. The thickness of this reaction zone is controlled by the inverse of Zeldovich parameter, \( 1/\beta \), where \( \beta \) measures the sensitivity of the reaction to the temperature variations. This region exhibits a typical mixing layer structure, classified mathematically into the singular perturbative problems.

The method of perturbative analysis, applied often to solve this kind of problems, is called asymptotic matching. The method allows the analytical approximation of global solution properties, such as eigenvalues (in our particular case we are talking about burning rate eigenvalue).

The method consists in partition of the domain of the problem definition into overlapping sub-domains. The perturbative analysis is then done in each of these sub-domains independently. The next step is the "matching" itself, i.e. the solution at each of the sub-domains constrained to have the same functional form at each of the overlapping regions. The sequence of asymptotic approxi-
mations is defined in this way. Finally, this collection of solutions satisfies all the boundary conditions in different sub-domains, i.e. we get an approximative solution of the initial boundary value problem, valid in the whole domain.

On the Figure 2.1 the process is presented schematically.

In the boundary-layer theory solution is supposed to be a function of two variables: an independent variable $x$ and a parameter $\delta$, characterizing the boundary layer thickness. The global analysis of the solution in independent variable is then achieved via local analysis in the limit $\delta \to 0$.

The asymptotic expansions are done in the following way. The domain of the solution existence is split into two sub-domains: one, corresponding to the boundary layer itself (the inner domain), and the region outside it, the outer domain.

We are looking for inner and outer solutions in respective domains. The outer solution is get in the limit $\delta \to 0$. This solution also can be calculated, when we put $\delta \to 0$ in the original equation. The outer solution is not the everywhere exact solution of the original problem. This fact indicates its singular perturbative character, and the necessity to treat the problem with the
help of appropriate methods is evident.

We apply the asymptotic matching method described above, with two sub-domains already defined. Once the solution in the outer region is found, we look for the inner one. To this end an appropriate coordinate stretch is needed, namely \( x = \delta X \), where \( X \) is called the inner variable. This solution in the inner region varies slowly as a function of \( X \). The inner solution is then found, as solution of the original equation, re-written in terms of this new variable.

With both these solutions at hand, we carry out the asymptotic matching. This is done in the intermediate limit \( x \to 0, \quad X = x/\delta \to \infty, \quad \delta \to +0 \). The matching condition provides the second boundary condition for the inner problem.

The question, arising when we effectuate this analysis, is those of the overlapping region existence, as well of the agreement between the inner and the outer limits. Sometimes it is possible to prove the existence by perturbative expansions of both inner and outer solutions, when we verify the asymptotic matching at all powers of \( \delta \). In the common case such a procedure is much too complicate. The existence of the overlapping regions will be assumed in the present work.

It is important to distinguish between the solution itself and its approximation, which we get as the result of this analysis. The approximative solution doesn't necessary converge to the exact one. The success of the boundary layer theory consists in the possibility to get the approximations in the cases, where the original equations are not exactly soluble.

The detailed description of singular perturbative methods can be found, for example, in [3].
Chapter 3

Premixed flames

Laminar premixed flames exist in the uniform mixture of gases. First let us consider the basic problem of premixed combustion, the plane flame.

A wavelike one-dimensional flame propagates through the cold fresh gases mixture, converting them into the hot products. The constant speed of propagation of the flame with respect to fresh gases is called burning velocity, or laminar flame speed $S_L$.

The flame thickness $l_F$ is expressed in terms of the burning velocity as

$$l_F = \frac{(\lambda/c_p)T_{ref}}{\rho_u S_L}$$

with the diffusivity $\lambda/c_p$, evaluated at reference temperature $T_{ref}$; $\rho_u$ is the density of the fresh gases.

Because of its similarity with waves' properties, the process of laminar premixed combustion is often also referred to as a deflagration wave.

Let us consider a coordinate system, attached to the deflagration wave with the $x$-axis chosen to be flow oriented; the $y$-axis coincides with the flame front.

We also consider one-step irreversible process:

$$F \rightarrow P.$$
The mass balance through the flame implies
\[ \rho_b u_b = \rho_f u_f = M. \]  
\[ \text{(3.2)} \]
where subscripts \( b \) and \( f \) correspond to the values in burnt and fresh gases respectively.

Under these conditions the equations for temperature and mass fractions take form:
\[
\frac{dT}{dx} = \frac{\lambda}{h^0_1} \left( \frac{dT}{dx} \right) - \frac{h^0_1}{h^0_1} \dot{\rho}_1, \\
M \frac{dY_1}{dx} = \frac{d}{dx} \left( D^{11} \frac{dY_1}{dx} \right) + \dot{\rho}_1. 
\]
\[ \text{(3.3)} \]
We combine both equations in such a way that the reaction term is eliminated, and get:
\[
\frac{M c_p dT}{h^0_1 dx} + M \frac{dY_1}{dx} = \frac{1}{h^0_1} \frac{d}{dx} \left( \frac{dT}{dx} \right) + \frac{d}{dx} \left( D^{11} \frac{dY_1}{dx} \right). 
\]
\[ \text{(3.4)} \]
Integrating this equation over \( x \), together with condition \( Y = 0 \) for \( x \to \infty \), we get the expression for the adiabatic temperature of the burnt gas:
\[ T_b = T_f + \frac{h^0_1}{c_p} Y_1 f. \]
\[ \text{(3.5)} \]
We choose the non-dimensional coordinate system \( x = x/l \), with the characteristic length \( l = \lambda/M c_p \), and the reference temperature is \( T = T c_p/h^0_1 \).

The above equations take the form:
\[
\frac{dT}{dx} = \frac{d^2 T}{dx^2} + \frac{D}{M^2} Y_1, T^{\alpha_1} \exp(-\theta/T), \\
\frac{dY_1}{dx} = \frac{1}{Le} \frac{d^2 Y_1}{dx^2} - \frac{D}{M^2} Y_1, T^{\beta_1} \exp(-\theta/T). 
\]
\[ \text{(3.6)} \]
Here \( \theta \) is the non-dimensional activation temperature, and \( Le = \lambda/c_p D^{11} \) is the Lewis number of fuel. The Lewis number is the inverse of the characteristic fuel length. The fuel concentration profile thickness \( \delta_F \) decreases for fixed
flame thickness $\delta_T$, if $Le > 1$, and increases for $Le < 1$.

Typical temperature and mass fraction profiles are presented on Figure 3.1.

### 3.1 Hydrodynamic limit

From the hydrodynamical point of view, the flame thickness, which is proportional to $\lambda/Mc_p$, is typically small compared to the fluid characteristic lengths. In this case, the flame can be seen as a surface of discontinuity, propagating in the direction normal to itself. (see Figure 3.2) The corresponding jump conditions on the surface are

$$
\rho_f(v_n + V) = \rho_b(v_{nb} + V), \quad v_f = v_{tb},
$$

$$
p_f = \rho_f(v_n + V)^2 = p_b + \rho_b(v_{nb} + V)^2. \quad (3.7)
$$

Here $V$ is the speed of the front propagation into the fresh gases mixture in the normal direction, $T_b$ and $v_n + V$ are the adiabatic temperature and flame speed relative to the fresh gas.

The stationary premixed flame refracts the streamlines of the flow, that is a
direct consequence of the jump conditions across the flame front. We show this process schematically on Figure 3.3. The streamlines turn toward its normal.

Moreover, in the case of non-uniform flame front vorticity is generated, as we can show through the equation of vorticity generation

$$\mathbf{v} \times \mathbf{w} = \frac{1}{\rho} \nabla p + \frac{1}{2} \nabla (v^2),$$  

where $w$ is the vorticity, $v$ the fluid velocity, and $p$ is the pressure.

The equation for the tangential component of the left-hand side is

$$v_n w = -\frac{1}{\rho} \frac{\partial p}{\partial t} - \frac{1}{2} \frac{\partial}{\partial t} (v_n^2 + v_t^2),$$  

with $v_n$ and $v_t$ normal and tangential components of the velocity. If we multiply the above expression with the density $\rho$, we get

$$\rho v_n w = -\frac{\partial}{\partial t} (\rho + \rho v_n^2) + v_n \frac{\partial}{\partial t} (\rho v_n) - \rho \frac{\partial}{\partial t} (v_t^2).$$

We evaluate this expression on both sides of the flame front, subtract them and get

$$\rho_t v_{f_n} (w_t - w_n) = \frac{1}{2} (\rho_t - \rho_n) \frac{\partial}{\partial t} (v_t^2).$$
This is an estimation of the vorticity jump, and in case of the non-planar flame front, the expression on the right-hand side is non-zero; thus the vorticity is produced.

Landau and Darrieu [12], [24] was the first investigated the deflagration wave flame instabilities. They have shown that the planar flame propagating in the uniform mixture is always unstable under perturbations. The kinetic argument justifying this instability is that the flame propagation in the direction, normal to itself, increases its curvature. Self-intersections appear at some moment (see Figure 3.4). Numerical simulations show the break-up into the flame cells.

However, the evidence of the existence of stable planar flame follows from the laboratory experiments. In fact, the diffusive-thermal effects allow the flame to stabilize. Namely, the part of the flame front with large curvature that is advanced in the unburnt mixture, will be surrounded by the gases at low temperature. The diffusive processes have to be completed before the reaction takes place. In the case of reactants with small diffusivities (or $Le > 1$), the heat loss cannot be balanced fast enough by reactants diffusion. This mechanism leads to the flame stabilization.
The flame instabilities can also be caused by chemical kinetics, acoustics, diffusivity, etc.

3.2 Activation-energy asymptotics

In order to perform the analysis of the flame structure, we apply perturbative methods. The boundary-value problem with flame propagation velocity as eigenvalue is defined. The solutions for temperature and this eigenvalue will be found as asymptotic series with respect to the inverse of Zeldovich parameter, defined below.

The main assumption to be done is that the reaction rate is maximal in the immediate vicinity of the maximum temperature, and decreases exponentially elsewhere. In this context, the reaction is supposed to take place in a small vicinity of the maximal temperature, $|T - T_{\text{max}}| < \epsilon$, $\epsilon > 0$, called a flame sheet.

Arrhenius law is a consequence of a strong temperature dependence of the reaction rate. This dependence can be measured with the help of Zeldovich
3.2. ACTIVATION-ENERGY ASYMPTOTICS

The parameter $\beta$, 

$$\beta = \frac{E(T_b - T_0)}{(RT_b^2)}.$$  \hspace{1cm} (3.12)

$E$ is the activation energy, and $\delta/\beta$ characterizes the thickness of the reaction zone. This parameter reflects the fact, that the reaction rate influences the process only in a thin zone around the flame, of order $O(1/\beta)$.

Under these conditions, the problem can be identified as a singular perturbative one, and has to be treated with help of matched asymptotic expansions method, described for example in [3].

In the asymptotic limit $\beta \to \infty$ the normal to the flame sheet is well defined. We choose the $x$-axis to coincide with this normal. We combine the both equations for temperature and mixture fraction in such a way, that the reaction source term is eliminated, prescribing at the boundaries

$$Y_F = Y_{F0}, \quad T = 1 - \alpha \quad \text{for} \quad x = -\infty,$$

$$Y_F = 0, \quad T = 1 \quad \text{for} \quad x = \infty.$$ \hspace{1cm} (3.13)

The temperature can be explicitly expressed in terms of the mass fraction:

$$T = 1 - \alpha(Y_F/Y_0),$$ \hspace{1cm} (3.14)

where the parameter $\alpha$ is defined as

$$\alpha = \frac{T_b - T_0}{T_b}.$$ 

Thus, it is sufficient to consider the equation for mass fraction only. We change the coordinate system $\xi = \rho u x$, normalize the mass fraction $Y = Y_F/Y_0$, and finally get a new equation for mass fraction $Y$:

$$\frac{d^2Y}{d\xi^2} - \frac{dY}{d\xi} = \Lambda Y^n \exp(-\beta Y/(1 - \alpha Y)),$$ \hspace{1cm} (3.15)

where

$$\Lambda = A \exp(-\beta) Y_0^{n-1}/(\rho u)^2$$ \hspace{1cm} (3.16)

is the burning-rate eigenvalue.
We are looking for solution $Y(\xi)$ as well as eigenvalue $\Lambda$.

As already mentioned, in the limit $\beta \to \infty$, the reaction rate is negligible, except for the small values of $Y$. Outside this region the reaction term can be dropped, and the solution is easily found:

$$
Y = 1 - \exp(\xi), \quad \xi < 0, \\
Y = 1, \quad \xi > 0.
$$

(3.17)

In the immediate vicinity of the flame front, $\xi = 0$, a boundary layer forms. We stretch the coordinates in this zone in an appropriate way, introducing

$$y = \beta \xi, \\
\eta = \beta \xi.
$$

(3.18)

We get the new equation

$$
\frac{d^2 y}{d\eta^2} - \frac{1}{\beta} \frac{dy}{d\eta} = \Lambda \beta^{-(n+1)} y^n \exp(-y/(1 - \beta^{-1} \theta y)). 
$$

(3.19)

In order to get a solution valid everywhere, the “inner” solution has to be matched with the “outer” one:

$$
dy \\ d\eta \to -1, \quad \text{for} \quad \eta \to -\infty, \\
y \to 0, \quad \text{for} \quad \eta \to \infty.
$$

(3.20)

Further, the function $y$ and the eigenvalue $\Lambda$ are developed in series in $\beta^{-1}$,

$$
y = y_0 + \beta^{-1} y_1 + \ldots, \\
\Lambda = \beta^{n+1}(\Lambda_0 + \beta^{-1} \Lambda_1 + \ldots).
$$

(3.21)

The sequence of problems $(y_0, \Lambda_0), (y_1, \Lambda_1), \ldots$ to be solved “iteratively”. First we put $\beta^{-1} = 0$ and the equation for $y_0$ is of the form

$$
\frac{d^2 y_0}{d\eta^2} = \Lambda_0 y_0 \exp(-y_0)
$$

(3.22)

together with boundary conditions

$$
y'_0(-\infty) = -1, \quad y_0(\infty) = 0.
$$

(3.23)
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The above equation is easily solved once we've introduced

\[ y_0' = \frac{dy_0}{d\eta}. \]  

(3.24)

Then the new equation

\[ \frac{1}{2} d(y_0')^2 = \Lambda_0 y_0^n \exp(-y_0) \]  

(3.25)

is integrated subject to boundary conditions (3.23), with the eigenvalue \( \Lambda_0 \) defined as

\[ \Lambda_0 = \left( 2 \int_{0}^{\infty} y_0^n \exp(-y_0) dy_0 \right)^{-1}. \]  

(3.26)

If we are interested in a higher order approximations for the burning velocity eigenvalue, the successive values for \( \Lambda_1, \Lambda_2, \) etc. can also be found. With the burning velocity in hand, the comparison with numerics and experiments can be done.

In the above example only one-dimensional flame was considered. This lead us to ordinary differential equations for temperature and mass fraction. The analogous analysis will be done in Chapter 5 in two-dimensional case, where the partial derivatives appear.

We also have to mention here the "ill-possedness" of the burning-velocity eigenvalue problem, or so-called "cold boundary difficulty". The boundary condition \( Y(-\infty) = 1 \) cannot be satisfied, since for the value of \( Y \) equal to one, the reaction term is \( \Lambda \exp(-\beta/(1-\alpha)) \). This value is small for large \( \beta \), but doesn't vanish, what would imply the infiniteness of the burning velocity, that is physically impossible. This fact is a direct consequence of the non-vanisheness of the Arrhenius rate.
Non-premixed combustion is a process, occurring when fuel and oxidizer are separated initially. This type of combustion is especially appropriate for the industrial applications, because it is mixture controlled and moreover, the flame doesn’t propagate dislike in the premixed case.

The non-premixed flame is evidently governed by diffusion mechanisms, we also call such a flame “diffusion flame”.

To characterize the process, the mixture fraction (the proportion of fuel and oxidizer in the mixture) is introduced:

\[ Z = \frac{\nu Y_F - Y_O + Y_{O,2}}{\nu Y_{F,1} + Y_{O,2}} \]  \hspace{1cm} (4.1)

where \( Y_F \) and \( Y_O \) are the fuel and oxidizer mass fractions, corresponding to any state of combustion between burnt and unburnt states. The mass fractions \( Y_{F,1} \) and \( Y_{O,2} \) are the mass fractions of fuel in the fuel stream and of oxidizer in the oxidizer stream respectively, and \( \nu \) is the stoichiometric oxidizer-to-fuel mass ratio.

From the definition of the mixture fraction we see that the mixture fraction varies between zero in the oxidizer stream and one in the fuel stream.

This value is a conserved scalar, which conservation equation has the form

\[ \frac{\partial}{\partial t} (\rho Z) + \nabla \cdot (\rho \nu Z) = \nabla \cdot (\rho \nu \nabla Z). \]  \hspace{1cm} (4.2)
Let us suppose the solution of the equation (4.2) to take a functional form \( Z(x,t) \). Then the stoichiometric iso-surface can be defined as

\[ Z = Z_{st}, \]

In the limit of fast reaction, the reaction zone is associated with a small vicinity of the iso-surface \( Z = Z_{st} \).

The burning velocity in the non-premixed situation depends mainly on the fuel-air equivalence ratio

\[ \phi = \frac{\nu Y_{F,u}}{Y_{O,u}}, \quad (4.3) \]

where \( Y_{F,u} \) and \( Y_{O,u} \) are the fuel mass fractions of fuel and oxidizer in the unburnt mixture.

This value is related to the mixture fraction through

\[ \phi = \frac{Z(1 - Z_{st})}{Z_{st}(1 - Z)}, \quad (4.4) \]

The first solution of the diffusion flame problem was proposed by Burke and Schumann [9]. They associated the flame surface with the zero surface for mass fractions,

\[ Y_F = Y_O = 0. \quad (4.5) \]

The concentrations and temperatures can be then written in terms of the mixture fraction \( Z \). The stoichiometric value of mixture fraction is calculated from the equations for mass fractions and equal to

\[ Z_{st} = (1 + Y_{F,0}W_O/\nu Y_{O,0}W_F)^{-1} \quad (4.6) \]

and the formulae for temperature are obtained:

\[ T(Z) = T_u(Z) + \frac{q^0 Y_{F,1}}{c_p\nu_F W_F} Z, \quad Z < Z_{st}, \]

\[ T(Z) = T_u(Z) + \frac{q^0 Y_{O,2}}{c_p\nu_O W_O} Z, \quad Z > Z_{st}, \]

\[ T_u(Z) = T_2 + Z(T_1 - T_2). \quad (4.7) \]
Here $T_1$ and $T_2$ are the initial temperatures of fuel and oxidizer respectively. The adiabatic temperature solutions are depicted in Figure 4.1. We see that the maximum temperature is reached in the burnt gas along stoichiometric surface $Z = Z_{st}$.

The characteristic time scale of non-premixed combustion is also associated with the mixture fraction. We define the scalar dissipation rate as

$$\chi = 2D|\nabla Z|^2, \quad (4.8)$$

with diffusivity $D$.

The time scale of non-premixed combustion is defined as the inverse of the quenching value of scalar dissipation rate $\chi_q$. This characteristic value can be thought of as a value, corresponding to the situation, where the heat loss cannot be balanced by the chemical reaction heat release, and quenching occurs.

As there is no characteristic velocity, in the contrary to the premixed case,
we define the length scale for diffusion combustion as

\[ l_F = \sqrt{\frac{D}{a}} \]  

(4.9)

where \( a \) is the velocity gradient.

The thickness associated with diffusion flame is

\[ (\Delta Z)_F = \sqrt{\frac{X_{st}}{2a}} \]  

(4.10)

This is the thickness of the reaction zone together with the surrounding diffusive layers. We see that the diffusive flame thickness is not constant, as in the case for premixed combustion, but is a function of the local flow properties.

If we suppose that chemical time scales are small or, in the other words, that chemical reactions are completed much faster then any changes in the underlying fluid flow occur, it makes sense to consider the limit of infinitely fast chemistry. This limit is a common approach in turbulent combustion modelling. The reaction zone can be then associated with infinitely thin layer \( Z = Z_{st} \), or, equivalently, with iso-surface \( \phi = 1 \) in the \( \phi \)-space.

### 4.1 Flamelet's concept

In the case of turbulent flow, the results from laminar diffusion flames modelling can also be applied through the so-called "flamelet concept".

The hypothesis of the infinitely fast chemistry allows us to associate the flame zone with a surface \( Z = Z_{st} \).

Moreover, we consider the equal diffusivities of fuel and oxidizer, i.e.

\[ L_e_F = L_e_O = 1. \]

The common diffusivity coefficient is introduced,

\[ D = \frac{\lambda}{\rho C_p}. \]
4.1. FLAMELET’S CONCEPT

In this case, the zero Mach number combustion equations for temperature and mixture fraction are

\[
\frac{DZ}{Dt} = \nabla \cdot (\rho D \nabla Z),
\]

\[
\frac{DT}{Dt} = \nabla \cdot (\rho D \nabla T) + QR + \frac{\partial p}{\partial t}.
\]  \hspace{1cm} (4.11)

An orthogonal coordinate system associated with stoichiometric iso-surface is introduced locally. One coordinate is chosen to be perpendicular to \( Z = Z_{st} \), the two others lie on the iso-surface. The next step is to transform this coordinate system into curvilinear coordinates, where the first coordinate is \( Z \) itself, and the former two are kept. The new time is equal to the old one, \( \tau = t \).

In this way, the mixture fraction becomes an independent variable, and equation for \( Z \) is eliminated. With the help of following transformation rules,

\[
\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial Z} \frac{\partial}{\partial \tau},
\]

\[
\frac{\partial}{\partial x_k} = \frac{\partial Z}{\partial Z_k} \frac{\partial}{\partial x_k} \frac{\partial Z}{\partial Z}
\]  \hspace{1cm} (4.12)

for \( k = 2,3 \),

\[
\frac{\partial}{\partial x_1} = \frac{\partial Z}{\partial x_1} \frac{\partial}{\partial Z}
\]

the temperature equation transforms into

\[
\rho \left( \frac{\partial T}{\partial \tau} + v_2 \frac{\partial T}{\partial Z_2} + v_3 \frac{\partial T}{\partial Z_3} \right) - \frac{\partial (\rho D) \partial T}{\partial x_2 \partial Z_2} - \frac{\partial (\rho D) \partial T}{\partial x_3 \partial Z_3}
\]

\[
-\rho D \left[ \left( \frac{\partial Z}{\partial x_1} \right)^2 \frac{\partial^2 T}{\partial Z_2^2} + 2 \frac{\partial Z}{\partial x_2} \frac{\partial Z}{\partial Z_2} \frac{\partial^2 T}{\partial x_1 \partial Z_2} + 2 \frac{\partial Z}{\partial x_3} \frac{\partial Z}{\partial Z_3} \frac{\partial^2 T}{\partial x_2 \partial Z_2} + \frac{\partial^2 T}{\partial Z_2^2} + \frac{\partial^2 T}{\partial Z_3^2} \right]
\]  \hspace{1cm} (4.13)

\[
= QR + \frac{\partial p}{\partial t}.
\]

As in the boundary-layer situation, the derivative in \( Z \)-direction is the dominating one, all the others can be neglected. The time derivative doesn't play big role in the case, where the chemical changes are slow, and finally we get the one-dimensional stationary equation for temperature, describing the laminar diffusion flamelet:
\[ -\rho \chi \frac{\partial^2 T}{\partial Z^2} = QR, \]  

(4.14)

where \( \chi \) is the scalar dissipation rate.

In this case the temperature is a function of the mixture fraction and is described by one-dimensional equation. Thus, the diffusion flame can be considered as a collection of quasi-steady one-dimensional infinitely thin laminar flamelets. This leads to a nice geometrical reactive flow description, where the dynamical properties of flamelets are analyzed.

However, the flamelet's concept is valid only under certain conditions on the scalar dissipation rate.

Let us denote by \( \chi_{st} \) the scalar dissipation rate under stoichiometric conditions,

\[ \chi_{st} = 2D \left( \frac{dZ}{dx_n} \right)^2_{st}, \]  

(4.15)

where only the derivative in the direction, normal to the iso-line \( Z = Z_{st} \) is considered, since the tangential gradient component is zero. For turbulent combustion modelling we replace the mean scalar dissipation rate with its mean value, \( \bar{\chi}_{st} \).

The laminar flamelet exists then only for the values of the stoichiometric scalar dissipation rate, that are smaller than some critical value \( \chi_q \):

\[ \bar{\chi}_{st} < \chi_q, \]  

(4.16)

For the values of \( \bar{\chi}_{st} \), exceeding the critical one, quenching occurs, and the one-dimensional flamelets concept is not valid anymore.

**4.2 Activation-energy asymptotics for diffusive flames**

Let us introduce the Damköhler number, that is the ratio of diffusive and chemical time scales,
4.2. ACTIVATION-ENERGY ASYMPTOTICS FOR DIFFUSIVE FLAME

\[ Da = \frac{\tau_x}{\tau_c} \]  \hspace{1cm} (4.17)

The infinitely fast chemistry corresponds to the limit \( Da \to \infty \). The opposite situation, \( Da \to 0 \) corresponds to the absence of combustion, or pure mixing.

For moderate values of Damköhler numbers, \( Da = O(1) \), the activation-energy asymptotic analysis can be effectuated. We will demonstrate the method on the example of counterflow flame.

We introduce a new variable \( \xi \), representing the stretching around the stoichiometric iso-surface,

\[ \xi = \beta(Z - Z_{st}). \] \hspace{1cm} (4.18)

Here \( \beta \) is Zeldovich number,

\[ \beta = \frac{E(T_{st} - T_{f_{st}})}{2Z_{st}(1 - Z_{st})RT_{st}^2}. \] \hspace{1cm} (4.19)

The non-dimensionalized temperature \( y \) is introduced,

\[ y = \frac{(T_{st} - T)}{RT_{st}^2} - \gamma \xi, \] \hspace{1cm} (4.20)

with

\[ \gamma = 2Z_{st} - 1 - 2Z_{st}(1 - Z_{st}) \frac{T_{f_{st}} - T_{f_{st}}}{T_{st} - T_{f_{st}}}, \] \hspace{1cm} (4.21)

here \( T_{f_{st}} \) is the frozen temperature along the stoichiometric surface, \( Z = Z_{st} \). In terms of these new variables, the equation for temperature takes the form

\[ \frac{d^2y}{d\xi^2} = Da(y^2 - \xi^2) \exp(-(y + \gamma \xi)). \] \hspace{1cm} (4.22)

This equation is integrated numerically together with the matching conditions

\[ \frac{dy}{d\xi} \to \pm 1, \text{ for } \xi \to \pm \infty. \] \hspace{1cm} (4.23)
The Damköhler number $Da$ in our case is defined then as

$$Da = \frac{Y_{O_2}A_F \exp(-E/R_0T_{st})}{2\rho D|\nabla Z_{st}|^2Z_{st}^2\beta^3}.$$  \hspace{1cm} (4.24)

The response of the maximal temperature to the various Damköhler numbers is presented on the Figure 4.2. For small $Da$ there exists a stable solution, corresponding to the cold flow; in the region of large $Da$, i.e. the values, corresponding to the fast chemistry processes, a stable burning solution exists. For the values of $Da$ of order of unity the "catastrophe" scenario can be observed: there are three possible solutions: on the lower, upper, and middle branch. The last one is recognized to be unstable: the situation changes suddenly, once the ignition value of Damköhler number, $Da_I$ is reached, the ignition occurs. By decrease from the large values the extinction limit $Da_E$ is attained, and we are on the lower branch again.

We will come back to this instability phenomena in our description of the triple flames.

The steadiness analysis of the lower and upper branches is demonstrated in
4.3 Steady-state solutions for one-dimensional combustion in stirred reactor

Consider the system of equations in non-dimensional units, describing the combustion process in a stirred reactor:

\[
\frac{dY}{dt} = 1 - Y - DaY \exp(-E/T),
\]

\[
\frac{dT}{dt} = 1 - T + QDaY \exp(-E/T),
\]

with non-dimensional Damköhler number \( Da \), activation energy \( E \) and heat of combustion \( Q \).

In the present context the Damköhler number is defined in a somewhat different way from the previous cases, namely

\[
Da = At_v,
\]

where the pre-exponential factor \( A \) is those from the Arrhenius reaction rate law, and \( t_v \) is a characteristic time length.

By the linear combination of both equations the reaction term can be eliminated, and we get the dependence of temperature on mass fraction

\[
T + QY = 1 + Q.
\]

Thus, the reaction can be described in terms of temperature only,

\[
\frac{dT}{dt} = 1 - T + DaN(T)
\]

with the non-linear operator \( N \) of reactive processes

\[
N = (1 + Q - T) \exp(-E/T).
\]
The maximum and minimum of the temperature are

\[
Y = 1, \quad T_{\text{min}} = 1,
\]

\[
Y = 0, \quad T_{\text{max}} = 1 + Q.
\]  

(4.30)

The steady state of the temperature, \( T_s \) is obtained from the equation

\[
0 = 1 - T_s + DaN(T_s).
\]  

(4.31)

The solution has a typical S-curve profile, with two bifurcation turning points of ignition and extinction, corresponding to the values of Damköhler numbers \( Da_I \) and \( Da_E \). Steady states corresponding to the upper and lower branches of this curve are stable, they are connected by the non-stationary process of ignition-extinction, or vice versa.

We will show this in more details below.

The turning bifurcation points are found from the equation

\[
\frac{dDa}{dT_s} = 0.
\]  

(4.32)

The Damköhler number can be expressed as

\[
Da = \frac{T_s - 1}{N(T_s)}
\]  

(4.33)

and the new equation for the non-linear operator \( N \) is

\[
N(T_s) - (T_s - 1) \frac{dN(T_s)}{dT_s} = 0
\]  

(4.34)

where

\[
\frac{dN(T_s)}{dT_s} = N(T_s) \left( \frac{E}{T_s^2} - \frac{1}{1 + Q - T_s} \right).
\]  

(4.35)

The solutions of the above quadratic equation are
4.3. STEADY-STATE SOLUTIONS FOR ONE-DIMENSIONAL
COMBUSTION IN STIRRED REACTOR

\[
T_{1,E} = \frac{(2 + Q) \pm Q \sqrt{1 - 4(1 + Q)/EQ}}{2(1 + Q/E)}. \tag{4.36}
\]

The solutions exist for the values of activation energy

\[
E > 4(1 + Q)/Q. \tag{4.37}
\]

The approximative expressions in the asymptotic limit of large activation energy \( E \to \infty \), are

\[
T_I = 1 + 1/E, \quad T_E = 1 + Q - \frac{(1 + Q)^2}{E}. \tag{4.38}
\]

To study the upper branch of the steady state solution up to the extinction point, we write down the steady state temperature

\[
T_S = 1 + Q - \epsilon y, \tag{4.39}
\]

with \( \epsilon \) to be determined.

We expand the inverse of the steady state temperature,

\[
\frac{1}{T_S} = \frac{1}{1 + Q} + \frac{\epsilon y}{(1 + Q)^2}. \tag{4.40}
\]

This expression is substituted into those for the steady state temperature (4.31), to get

\[
0 = -Q + \epsilon y + Da \epsilon y \exp \left(-\frac{E}{1 + Q}\right) \exp \left(-\frac{E \epsilon y}{(1 + Q)^2}\right). \tag{4.41}
\]

The second term vanishes in the limit \( \epsilon \to 0 \). In this limit, if we assume \( Q \) to be of order unity, the balance between the first and the third terms requires Damköhler number to be large. Depending on the activation energy, there are two limit cases:
(I) $E = O(1)$. 

This implies $\epsilon = 1/Da$, and consequently the Damköhler number is large. In this case

$$y = Q \exp \left( \frac{1}{1 + Q} \right)$$

(4.42)

and the steady state temperature

$$T_s = 1 + Q - \frac{Q}{Da} \exp \left( \frac{E}{1 + Q} \right).$$

(4.43)

This expression describes the upper branch of the S-shaped curve for small activation energies, and is not able to predict the extinction turning point.

(II) $E$ is asymptotically large.

In this case the expression in the second exponential yields to the expression for $\epsilon$,

$$\epsilon = \frac{(1 + Q)^2}{E}.$$  

(4.44)

The balance of the terms on the right hand side of (4.41) means this time, that

$$\delta = \frac{Da(1 + Q)^2}{EQ} \exp \left( -\frac{E}{1 + Q} \right)$$

(4.45)

is of order of unity. The condition on Damköhler number is then

$$Da \sim \epsilon^{-1} \exp((1 + Q)/\epsilon), \text{ for } \epsilon \to 0.$$  

(4.46)

These limits lead to the new equation

$$1 = \delta y \exp(-y)$$

(4.47)
and $y$ can be determined.

The equation has two solutions for $\delta > e$, one of them corresponds to the upper branch of the S-curve, and the second one to the intermediate branch.

If we want to show the stability of the steady-state solutions, the small temperature perturbation

$$T = T_S + T'(t)$$

has to be introduced into the original temperature equation. This leads us to the equation for perturbation:

$$\frac{dT'}{dt} = -\lambda T',$$

with

$$\lambda = 1 - Da \frac{dN(T_s)}{dT_s} = N(T_s) \frac{dDa}{dT_s}.$$ (4.50)

The solution to (4.49) is

$$T' = T_0' \exp(-\lambda t).$$ (4.51)

The perturbations are decaying for increasing Damköhler numbers, consequently the corresponding solution is stable. This is true for upper and lower branches, and not for the intermediate branch.

4.4 Conclusions

The above analysis concerned with two idealized situations, premixed and non-premixed regimes. However, in the case of non-premixed combustion the processes of quenching lead to the situations, where propagating flames form at the edge of the diffusive flame. The one-dimensional flamelet’s approach fails in this case. A new model is needed, the one unifying the properties of both premixed and diffusive flames. Such a model will be introduced in the next chapter, and the analytical approaches to both regimes will be used to describe this new structure.
Chapter 5

Triple flame

5.1 Introduction

In Chapters three and four we considered two combustion regimes: premixed, where the flame propagates into the fresh gases mixture, leaving totally burnt products behind it; and the non-premixed regime, where fuel and oxidizer are separated initially, so that the diffusion flame forms in a neighborhood of the stoichiometric iso-surface.

During long time these two models dominated combustion research, till in 1965 Phillips observed experimentally propagating structures in non-premixed mixture of gases. This experiment results showed, that the "real" flames are not purely premixed or diffusive. In fact, diffusion flames exhibit the flame propagation property. This regime, where both diffusive and advective processes are present, is called partially premixed combustion.

To model this regime, we suppose that the flame propagation in partially premixed regime happens along the iso-stoichiometric surfaces $Z_s$, where the laminar burning velocity is close to its maximum. This propagation generates a structure, called triple or edge flame, consisting of two premixed brunches, lean and rich, and trailing diffusive flame. (see Figure 5.2) This flame possesses a curved flame front, since the burning velocity attains its maximum at maximum of the reaction rate and decreases away from iso-stoichiometric surface $Z_s$.

The triple flame was assigned to play a significant role in the ignition-extinction mechanism of partially premixed combustion. The round jet flame stabilization over the nozzle was also attributed to the quenching mechanism.
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of the diffusion flame, the triple flame playing stabilizing role in this case.

The two-dimensional flamelet model allows to describe the multidimensional quenching of partially premixed flames. To characterize the quenching process, we introduce the Damköhler number (i.e. the ratio of characteristic diffusion and chemical time scales),

\[ Da = \frac{T_d}{\tau_c}. \]

For small values of \( Da \) the reactive zone is broad. The time needed by reaction to be completed is then so high, that the intermediate step products are able to escape, that leads to non-equilibria.

In chapter four we introduced the S-curve, that is the response of one of the flame characteristics (like maximum temperature, for example) to the Damköhler number variation. We have seen, that there are three regions: two of them, corresponding to very small and relatively large values of Damköhler numbers, are stable. The third one, that was assigned as “middle branch”, is a region of the instability effects, or the region of the partially premixed flames existence. The points \( D_f \) and \( D_t \) on the boundaries of these stability regions are the turning points of the bifurcation from the stable solutions to the intermediate partially premixed solution. If \( Da > D_f \), the hot solution transforms abruptly into the cold one. We see from the Figure 4.2, that the hot flame solution persists through the region of the cold solution existence, that lead to partially burning.

The one-dimensional flamelet approach is not valid anymore in the regions of small Damköhler numbers where quenching occurs.

Once the diffusive flamelet quenched, we observe at the edge of it the triple flame. This flamelet is a two-dimensional one, the lateral diffusion playing essential role in keeping the diffusive flame “alive”.

Mathematically speaking, the triple point is a point of intersection of the iso-stoichiometric surface of the mixture fraction and a zero level set of the G-equation solution for a field variable. (see Figure 5.1)

The triple flames, travelling along stoichiometric iso-surface, \( Z = Z_{st} \), are sketched on the Figure 5.2. The main feature of the triple flame is its ability to propagate, both with positive and negative velocities. The positive propagation downstream of the flow corresponds to the blow-out; negative propagation plays an essential role in the flame stabilization. The propagation velocity, attributed to the triple flame, indicates for example the dynamical behaviour
5.1. INTRODUCTION

Figure 5.1: Triple flame in the non-uniform mixture of gases.

Figure 5.2: Local triple flame propagation along iso-stoichiometric surface.
The free boundary problem of the triple flame propagation was investigated both theoretically and numerically under different assumptions on the mixture fraction gradient and heat release (see for example [14], [15], [17], [19], [27], [39]). The analytical approaches furnished us the expressions for the triple flame propagation, that was compared with results from direct numerical simulations.

In their theoretical studies J. Dold [11], L. Hartley and J. Dold [19] derived the analytical expressions for the triple flame velocity under the assumption of zero heat release. They also observed the relationship between the mixture fraction gradient and velocity of the triple flame propagation. The small gradients of the mixture fraction increase the velocity, and vice versa.

Ruetsch, Vervisch and Liñán [39] investigated numerically the effects of heat release on the triple flames. They showed, that the mixture fraction is not independent from the heat release, but that the mixture fraction gradient is modified in front of the flame.

Consequently, these effects of the heat release have to be included in the analytical description of the flame propagation.

S. Ghosal and L. Vervisch [17] introduced small, but non-zero heat-release in their analysis of two-dimensional symmetric triple flamelet. They considered the flame in the moving frame, the x-axis was associated with diffusion flame and y-axis was chosen to be tangent to the flame front. (see Figure 5.3) The flame front in this work was approximated by a hyperbolic profile of unknown curvature, that allowed to overcome the difficulty of the original free-boundary problem.

The triple flames play also an essential role in the stabilization of lifted round jets. When inflow velocity exceeds some critical value, the flame detaches from the burner and moves downstream. It was observed, that this situation doesn't necessary lead to blow-out of the flame, but the flame can be stabilized at some distance from the fuel exit, called lift-off height.(see Figure 5.4)

In their paper Müller, Breitenbach and Peters [33] investigated this stabilization property in case of the lifted turbulent jet. They derived an expression for turbulent burning velocity, accounting the partially premixed flame propagation along the iso-surface of stoichiometric mixture, as well as the flamelet
5.1. INTRODUCTION

They noted the importance of the flamelet quenching for the stabilization of lifted flames.

Favier and Vervisch [14] also studied the lift-off mechanism of turbulent non-premixed flames, indicating the benefit of the triple flame from the vorticity, as well as two different behaviours of the triple flame, that of stabilization and that of blow-out.

Boulanger, Réveillon, Vervisch and Ghosal [5] applied the results from the two-dimensional laminar triple flamelet modelling to the lifted jet flame, which is in fact axisymmetric. They effectuated the direct numerical simulations of the lifted round diffusion flame base and compared their theoretical results with those they got from DNS.

In order to get an idea how does the triple flame on the base of lifted round jet look like, we present on Figure 5.5 the contour lines for temperature and reaction rate from these simulations. The parabolic form of triple flame is associated with the iso-lines of reaction rate. The maximum temperature is attained close to the maximum of the reaction rate.
Figure 5.4: Round lifted diffusion jet flame.
Figure 5.5: Iso-contours of temperature (left) and reaction rate (right) from DNS by Boulanger et al..
5.2 Problem formulation

We investigate the dynamical behaviour of the triple (or edge) flame, forming on the base of the lifted laminar jet flame, over the fuel exit. In practice we would like to stabilize the lifted flame over the burner, in order to avoid the damages caused by the high temperatures on the burner itself. We'd like to be able to control the propagation velocity (and, consequently, the lift-off height), by given mixture fraction and velocity of the gases on the fuel exit.

The goal of the present paper is to derive the expressions for velocity in dependence on mixture fraction gradient and small density variations, similar to those of [17], with the flame base radius taken in account. We will introduce the dependence on the radius of the flame base in a parametric way. The results we obtain are compared with those of the planar case, as well as the numerical simulations of the round jet. We will see, that the jet radius makes flame propagate faster, and the under-prediction of the lift-off height is corrected.

To derive the formulae for triple flame propagation velocity, the method of asymptotic expansions in the vicinity of the flame front is applied. In order to keep the 'non-local' influence of the jet radius, we introduce this radius as a fixed constant in the two-dimensional axisymmetric equations, which are then reduced to the planar case. This procedure allows us to treat the problem as a perturbative one in the vicinity of the flame, keeping at the same time the correction that is due to the axisymmetrical nature of the problem.

Surprisingly, we get a very good agreement with numerical experiments, even though the radial component dependence replaced by its approximation in the vicinity of the triple point.

The flame shape in our work is considered to be parabola of unknown curvature, following Ghosal and Vervisch [17], who showed the validity of such an approximation in the planar case. The curvature is found then as a part of the solution by matching procedure.

We also obtain the closed expressions for temperature and velocity in dependence on the flame curvature and flame base radius.

The triple flamelet in partially premixed regime, consisting of two premixed (lean and rich) branches and of a trailing diffusion flame, propagates along the stoichiometric iso-surface of the mixture fraction. The flame is stabilized at a point, where velocity of the outcoming jet equals the propagation triple flame velocity.
The chemical processes are described by a one-step reaction: \( n_0 \) molecules of fuel (molecular mass \( m_0 \)) react with \( n_1 \) molecules of oxidizer (molecular mass \( m_1 \)) to form \( n_p \) molecules of product (molecular mass \( m_p \)). We also suppose the reaction to be infinitely fast, that allows us to think about the premixed flame front as a surface.

### 5.3 Mathematical modelling

The main goal of the present work is to keep at leading order the influence of the flame base radius on the triple flame ring propagation. For this purpose, we consider the "idealized" situation, where the line of the iso-stoichiometry stays parallel to the mean flow direction. (see Figure 5.6)

This assumption allows us to introduce local coordinate frame, attached to
the triple flame and keep the dependence on the flame base radius in the same time. The \( x \)-axis is chosen in the direction of the flow and coincides with stoichiometric iso-surface \( Z = Z_{st} \), the radial component \( r \) is perpendicular to it, with \( r = r_0 \) determining the position of the diffusive flame for positive \( x \). In the frame, where the triple flame is stationary, the velocity of interest is those of the jet, issuing from infinity, \( U = U_\infty \).

The low Mach number equations, derived in the previous chapter, are rewritten in cylinder coordinates \((r, x, \phi)\).

We write down the transport equations for species and mixture fraction, as well as energy equation. We consider the laminar flow, so that the viscosity effects can be neglected, and the velocity components are described by the continuity equation only.

By definition of the triple flame, both characteristics of the diffusive and premixed behaviours are exhibited by these flames. Consequently, in order to analyze the flame structure, both methods from premixed and non-premixed flame analysis have to be applied.

We write down the equations in cylindrical coordinates, and after pass to the local analysis, introducing the local parabolic-cylinder coordinates, matching the form of the flame (supposed to be parabola of a curvature to be determined), in the flame vicinity.

The perturbative methods for mixing layers are applied in order to find an approximative solution of our problem. All the quantities are developed in series with respect to the small parameter \( \alpha \), characterizing the heat release. Solutions are presented as asymptotical series with the terms up to the first order.

We consider the diffusivity of reactants and to be equal, i.e. a unique diffusion coefficient \( k \) can be introduced.

### 5.3.1 Governing equations

The equations of zero Mach number combustion for unbounded domains of the chapter two will be used here with some modifications, due to the new scaling and axisymmetrical nature of the problem.

First of all, the following non-dimensionalization is done:
• the reference velocity is chosen to be $U_\infty$, which is the unknown velocity of the triple flame propagation.

• appropriate length scale is given by diffusion length $k/U_\infty$.

All the equations are transformed in the dimensionless cylinder coordinates

$$(r, X) = (rU_\infty/k, xU_\infty/k)$$

(5.1)

where the $(r, x)$ are the coordinates in physical space.

We recall here, that both equations for mass fractions $Y_0$ and $Y_1$ can be combine in order to get the passive scalar equation in physical space for the mixture fraction $Z$:

$$\rho \frac{DZ}{Dt} = k\rho_\infty \nabla^2 Z.$$  

(5.2)

The mass fractions can be also expressed in terms of the mixture fraction:

$$Y_0 = (T_0 - T) \frac{m_0\nu_0 c_p}{Q} + Z,$$

(5.3)

$$Y_1 = (T_0 - T) \frac{m_1\nu_1 c_p}{Q} + Z + 1.$$  

(5.4)

The maximum temperature $T_s$ is reached just behind the flame surface, along the stoichiometric line, where the combustion is complete. We can find this value $T_s$, putting $Z = Z_s = 1/(1 + \bar{\tau})$ (here $\bar{\tau} = (\nu_1\mu_1)/(\nu_0\mu_0)$) and $Y_0 = 0$ in the equations above:

$$T_s = T_0 + \frac{Q}{m_0\nu_0 c_p} \frac{1}{1 + \bar{\tau}} = T_0 + \frac{Q}{(m_0\nu_0 + m_1\nu_1)c_p}.$$  

(5.5)

This value $T_s$ is then used in order to construct the non-dimensional temperature $\Theta$:

$$\Theta = \frac{T - T_0}{T_s - T_0},$$

(5.6)

that characterizes the thermal changes across the flame. $T_0$ is the temperature far upstream.
Moreover, we introduce two parameters, that will be useful for our asymptotical analysis. The first one, $\alpha$, characterizes the amount of heat, released into the flame,

$$\alpha = T_s - T_0 = \left[1 + \frac{(m_0 \nu_0 + m_1 \nu_1)c_p T_0}{Q}\right]^{-1}. \quad (5.7)$$

The second parameter we introduce is the already well-known Zeldovich parameter $\beta$, that is used in the description of the inner structure of the flame surface,

$$\beta = \frac{T_a}{T_s}. \quad (5.8)$$

In practice, Zeldovich parameter is moderately large. We will analyse the problem in the useful activation energy asymptotic limit, $\beta \to \infty$.

The equations, describing reactive flow, will be transformed into:

- reactive-diffusive equation for non-dimensional temperature,

$$\bar{\omega} \left( u \frac{\partial \Theta}{\partial r} + v \frac{\partial \Theta}{\partial X} \right) =$$

$$= \frac{1}{r} \frac{\partial \Theta}{\partial r} + \frac{\partial^2 \Theta}{\partial r^2} + \frac{\partial^2 \Theta}{\partial X^2} + \lambda \bar{\omega}^{\nu_0+\nu_1} \Sigma(Z/Z_s, \Theta) \exp \left[ -\frac{\beta(1-\Theta)}{1-\alpha(1-\Theta)} \right], \quad (5.9)$$

where

$$\Sigma(x, y) = (x - y)^{\nu_0} [(1 - x) + r(1 - y)]^{\nu_1} \quad (5.10)$$

and the burning rate eigenvalue $\lambda$ is defined by

$$\lambda = \frac{k Q A}{c_p T_s \alpha} \frac{\rho_0^{\nu_0+\nu_1-1}}{(1 + r)^{\nu_0+\nu_1}} \exp(-\beta/\alpha) \frac{1}{U_\infty^2}. \quad (5.11)$$

- passive scalar equation for mixture fraction,

$$\bar{\omega} \left( u \frac{\partial Z}{\partial r} + v \frac{\partial Z}{\partial X} \right) = \frac{1}{r} \frac{\partial Z}{\partial r} + \frac{\partial^2 Z}{\partial r^2} + \frac{\partial^2 Z}{\partial X^2}, \quad (5.12)$$
5.3. MATHEMATICAL MODELLING

- continuity equation

\[ \frac{\partial}{\partial r} (\bar{w}ur) + \frac{\partial (\bar{w}v)}{\partial x} = 0. \tag{5.13} \]

As density is related to the temperature through \( \rho = \frac{m_{p0}}{k_B T} \), we write down the new expression for dimensionless density as function of heat release:

\[ \bar{\rho} = \frac{1 - \alpha}{1 - \alpha (1 - \Theta)}. \tag{5.14} \]

The above set of equations is to be solved prior to boundary conditions

\[ \Theta(r, -\infty) = 0, \tag{5.15} \]

and

\[ \Theta(r, \infty) = \begin{cases} \frac{(1 - Z)(1 - Z_s)}{(1 - Z_s)}, & r \leq r_0 \\ \frac{Z}{Z_s}, & r \geq r_0 \end{cases}. \tag{5.16} \]

Together with these boundary conditions, equation (5.9) defines an elliptic boundary eigenvalue problem in \( \lambda \), that is related to the flame speed through (5.11).

The boundary conditions for mixture fraction are:

- \( Z = 1 \) in the fuel stream,
- \( Z = 0 \) in the oxidizer stream
- \( Z = Z_s = \frac{1}{1 + r} \) under stoichiometric conditions.

Several remarks have to be done on the equation (5.12) for mixture fraction. As we noted in the introduction, there is a strong dependence of the flame propagation velocity on the mixture fraction gradient. For this reason, we are interesting in the mixture fraction gradient rather than in the exact solution for \( Z \). Following this idea, we develop the solution for \( Z \) in Taylor series in the vicinity of the stoichiometric surface, \( r = r_0 \), and keep the linear part only. This local approximation of the mixture fraction will be considered further in our analysis.
5.3.2 Perturbative analysis

In our new formulation we recognize the mixing layer equations, that define a singular perturbative problem. The temperature undergoes the crucial changes in the vicinity of the flame front, so that two different solutions have to be found. We apply the asymptotic matching methods, discussed in chapter two, in order to match both solutions and to determine the burning rate eigenvalue $\lambda$.

We consider the case of small, but finite heat release,

$$\alpha \ll 1.$$  \hspace{1cm} (5.17)

By this, the original equations are linearized, and the initial problem is simplified considerably.

We start with the Ansatz:

$$\begin{align*}
\Theta &= \Theta^{(0)} + \alpha \Theta^{(1)} + O(\alpha^2), \\
Z &= Z^{(0)} + \alpha Z^{(1)} + O(\alpha^2), \\
\tilde{w} &= 1 + \alpha \tilde{w}^{(1)} + O(\alpha^2), \\
u &= u^{(0)} + \alpha u^{(1)} + O(\alpha^2).
\end{align*}$$  \hspace{1cm} (5.18)

These expansions will be substituted into the respective equations for temperature, mixture fraction and velocity. The linearity of differential operators allows us to equal the terms of the corresponding order on the left with those on the right hand side. At the first step, the zero-order approximations are found, then the first-order terms. In both cases the problems we get are the singular perturbative problems, associated with mixing layers. As discussed in chapter two, the matched asymptotic expansions are effectuated in the limit of high activation energy.

The Theorem 1 of the previous chapter is used once again here, when we want to decouple the divergence-free component of the velocity field from the potential one. We recall, that the divergence-free component can be chosen in arbitrary way, for example:

$$u = u^{(0)} + u^{(1)},$$  \hspace{1cm} (5.19)

with $u^{(0)} = (0,1)$.

From (5.14) the immediate development of the non-dimensional density $\tilde{w}$ has form:
\[ \dot{w} = 1 - \alpha \Theta^{(0)} + O(\alpha^2). \] (5.20)

For \( \alpha = 0 \) the density is equal to unity, i.e. \( \dot{w}^{(0)} = 1 \), and in this case velocity decouples from density, that allows us for arbitrary choice of the solenoidal velocity part.

The simplified equations for temperature and mixture fraction are:

\[ \frac{\partial \Theta}{\partial X} = \frac{1}{r} \frac{\partial \Theta}{\partial r} + \frac{\partial^2 \Theta}{\partial r^2} + \frac{\partial^2 \Theta}{\partial X^2} + \lambda \Sigma(Z/Z_s, \Theta) \exp(\beta(1 - \Theta)), \] (5.21)

and

\[ \frac{\partial Z}{\partial X} = \frac{1}{r} \frac{\partial Z}{\partial r} + \frac{\partial^2 Z}{\partial r^2} + \frac{\partial^2 Z}{\partial X^2}. \] (5.22)

Due to the coordinate choice and problem formulation, only transversal gradients "survive" in the equation of the mixture fraction:

\[ 0 = \frac{1}{r} \frac{\partial Z}{\partial r} + \frac{\partial^2 Z}{\partial r^2}. \] (5.23)

We consider the flame to be symmetric with respect to \( r = r_0 \) (here \( r_0 \) is the radius of the flame base), so that the stoichiometric value is fixed at \( 1/2 \).

We develop solution of the equation (5.23) in the vicinity of \( r = r_0 \) in Taylor series, and get, prior to boundary conditions \( r \to \infty, \ Z \to 0 \), and \( r = r_0, \ Z = 1/2 \):

\[ Z = \frac{1}{2} \left[ 1 + \mu(r - r_0) + O((r - r_0)^2) \right] \] (5.24)

where

\[ \mu = \frac{1}{Z_s} \frac{\partial Z}{\partial r} \bigg|_{r=r_0} \] (5.25)

is the value of the mixture fraction gradient, prescribed at the inlet.

In the present work we handle the case of small mixture fraction gradient,
\[ \mu = O(1/\beta) \]

in the limit \( \beta \to \infty \).

From the equation (5.23) for mixture fraction we can calculate the coefficients in the Taylor expansion of \( Z \), taking the derivatives on both sides and evaluating them at the surface \( Z = Z_{st} \):

\[ \left. \frac{1}{r_0} \frac{\partial Z}{\partial r} \right|_{r=r_0} = - \left. \frac{\partial^2 Z}{\partial r^2} \right|_{r=r_0}. \] (5.26)

It is evident, that all the coefficients of the Taylor's series for \( Z \) are of the order \( \mu = O(1/\beta) \). In particular, the second coefficient in the expansion (5.24) is

\[ \left. \frac{1}{r_0} \mu = - \left. \frac{\partial^2 Z}{\partial r^2} \right|_{r=r_0}. \] (5.27)

If we consider a narrow region close to \( Z = Z_s \), defined by

\[ |r - r_0| < \frac{1}{\sqrt{\beta}}, \] (5.28)

that is the region of thickness higher then those of the reactive zone, we can re-write the solution for mixture fraction as

\[ Z = \frac{1}{2} [1 + \mu(r - r_0)] + O(1/\beta^2). \] (5.29)

### 5.4 Activation-energy asymptotics

We study the basic equations in the activation-energy asymptotics (AEA) limit, \( \beta \to \infty \), already described for the one-dimensional planar diffusive flame in previous chapter. Only "well-developed" triple flames are considered, i.e. the flames with \( \beta \mu \sim O(1) \).

In the limit of large activation anergy, \( \beta \to \infty \), there is a narrow zone of thickness \( \sim O(1/\beta) \), forming in the vicinity of the flame zone. This zone is
of a mixing-layer character, i.e. the components of the reactive flow undergo abrupt changes within it, meaning the singularities formation for large $\beta$. The problem is then recognized to be a singular perturbative one.

The method of matched asymptotic expansions is applied to find the solution, consisting of two parts: the “outer solution”, valid everywhere except in the vicinity of the flame front, and the “inner solution”, that connects smoothly two branches (one in front and the other behind the flame), of the outer solution.

While we consider the reaction zone to be infinitely small, the temperature just behind the flame front may be obtained by setting $Y_1 = 0$ (in the fuel stream, $r < r_0$), or $Y_0 = 0$ (in the oxidizer stream, $r > r_0$), since the deficient component is completely consumed.

The expression for temperature is obtained then from (5.3) and (5.4),

$$\Theta = 2(1 - Z) = 1 - \mu |r - r_0| - O(1/\beta^2). \quad (5.30)$$

Ahead of the premixed flame the reaction-diffusion equation for temperature is those of the cold flow,

$$\frac{\partial \Theta}{\partial X} = \frac{1}{r \partial r} \frac{\partial \Theta}{\partial r} + \frac{\partial^2 \Theta}{\partial r^2} + \frac{\partial^2 \Theta}{\partial X^2}. \quad (5.31)$$

Under the coordinate transformation

$$\Theta = \exp(X/2) F$$

equation (5.31) transforms into

$$\left( \frac{\partial^2}{\partial r^2} + \frac{1}{r \partial r} \right) F + \frac{\partial^2}{\partial X^2} F = \frac{1}{4} F. \quad (5.32)$$

The next transformation

$$F = \frac{1}{\sqrt{r}} f$$
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delivers us the equation similar to those of the planar case, with the potential force \( \left( -\frac{1}{r^2} + 1 \right) \):

\[
\frac{\partial^2 f}{\partial r^2} - \frac{1}{4} f \left( -\frac{1}{r^2} + 1 \right) + \frac{\partial^2 f}{\partial x^2} = 0. 
\] (5.33)

In this equation the "non-local" forces are described as potential through \( -\frac{1}{r^2} + 1 \). We'd like to keep only parametric dependence on this force, reducing afterwards the equations to the two-dimensional case in the vicinity of the flame. We achieve this, keeping only the leading term of the potential in the vicinity of \( r = r_0 \), i.e. replacing potential force by constant \( c = 1 - \frac{1}{r_0^2} \).

This constant is supposed to be positive, that is equivalent to the condition \( r_0 > 1 \) (i.e. the radius of the flame base in large enough). In the opposite case of the small radial components the term \( \frac{\partial}{\partial r} \) is simply approximated by \( \frac{\partial^2}{\partial r^2} \), i.e. we are back to the 2-D case.

Once the parabolic-cylinder coordinates

\[
X = \frac{\sqrt{c}}{2} [\xi^2 - \eta^2 + \eta_0^2],
\]
\[
r - r_0 = \sqrt{c} \xi \eta
\] (5.34)

are introduced, the problem is completely reduced to the local one, keeping nevertheless the parametric dependence on radius of the flame base \( r = r_0 \). In this new coordinates \( \eta = \eta_0 \) corresponds to the flame surface, \( \eta < \eta_0 \) is the zone behind the flame front, and \( \eta > \eta_0 \) – ahead of it.

Equation (5.33) is then transformed into

\[
\frac{\partial^2 f}{\partial \xi^2} + \frac{\partial^2 f}{\partial \eta^2} - \frac{1}{4} c^2 (\xi^2 + \eta^2)^2 f = 0. 
\] (5.35)

By variables separation

\[
f(\xi, \eta) = M(\xi)N(\eta)
\] (5.36)
The ordinary differential equations for functions \( M \) and \( N \) are
\[
\frac{d^2M}{d\xi^2} + \left(p - \frac{1}{4}c^2\xi^2\right)M(\xi) = 0,
\]
with \( p > 0 \), that is dictated by boundary conditions on temperature, and
\[
\frac{d^2N}{d\eta^2} + \left(-p - \frac{1}{4}c^2\eta^2\right)N(\eta) = 0.
\]

In the first equation we recognize the Schrödinger equation for one-dimensional quantum harmonic oscillator. It is was shown (see [23]), that this equation possesses solutions, limited at infinity, if the quantization condition for energy levels \( p \) is fulfilled:
\[
p = \left(n + \frac{1}{2}\right)c, \quad n = 0, 1, 2, \ldots
\]
The eigenfunctions \( M_n \) of Schrödinger equation are
\[
M_n(\xi) = \exp\left(-\frac{c\xi^2}{4}\right) H_n\left(\sqrt{\frac{c}{2}}\xi\right),
\]
where \( H_n \) are the Hermite polynomials, defined as
\[
H_n(\xi) \exp(-\xi^2) = (-1)^n \frac{d^n}{d\xi^n} \exp(-\xi^2).
\]
The eigenfunctions \( N_n \) to the second equation for \( p = \left(n + \frac{1}{2}\right)c \) are the parabolic-cylinder functions, with following asymptotic approximations for large argument \( \xi \):
\begin{align*}
U(a,z) &\sim \exp(-z^2/4)z^{-a-1/2} \left\{ 1 - \frac{(a+1/2)(a+3/2)}{2z^2} + \ldots \right\}, \\
V(a,z) &\sim \sqrt{\frac{2}{\pi}} \exp(z^2/4)z^{-a-1/2} \left\{ 1 + \frac{(a-1/2)(a-3/2)}{2z^2} + \ldots \right\}. \quad (5.43)
\end{align*}

The functions \( V(a,z) \) growth exponentially at infinity, that is in contradiction with boundary condition on temperature. Thus, only the functions \( U(a,z) \) will be kept in order to construct an appropriate solution for temperature:

\[ N_n(\eta) = U \left( \left( n + \frac{1}{2} \right), \sqrt{c}\eta \right). \quad (5.44) \]

The general solution to (5.31) in the vicinity of \( r = r_0 \) will be of the form

\[ \frac{1}{\sqrt{r_0}} \exp \left( \frac{\sqrt{c}}{4}\left( \xi^2 + \eta^2 + \eta_0^2 \right) \right) \sum_{n=0}^{\infty} a_n M_n(\xi) N_n(\eta) \quad (5.45) \]

with coefficients \( a_n \) to be determined.

Regrouping the terms, we get the solution for temperature \( \Theta \):

\[ \Theta = \exp \left[ \frac{\sqrt{c}}{4}(\xi^2 + \eta_0^2 - \eta^2) \right] \exp \left( -\frac{1}{4} \xi^2 \right) \times \]

\[ \sum_{n=0}^{\infty} a_n H_n \left( \frac{\sqrt{c}}{\sqrt{2}} \xi \right) U(n + 1/2, \sqrt{c}\eta). \quad (5.46) \]

In order to determine the coefficients \( a_n \), we use the orthonormality property of Hermite polynomials,

\[ \int_{-\infty}^{+\infty} H_n(z)H_m(z) \exp(-z^2) = \left\{ \begin{array}{ll} 0, & nm \\
2^n n! \sqrt{\pi}, & n \neq m \end{array} \right. \quad (5.47) \]

as well as the boundary condition

\[ \Theta(\xi, \eta_0) = 1 - \mu|\xi|\eta_0 - O(1/\beta^2) \quad (5.48) \]
(which follows from the continuity of the temperature across the flame surface).

The scalar product multiplication will be applied on both right and left hand sides of (5.4), and the coefficients $a_n$ are calculated:

$$a_n = \frac{\int_{-\infty}^{+\infty} (1 - \mu \eta_0) \xi H_n \left( \sqrt{\frac{c}{2}} \exp \left( -\frac{c}{4} \xi^2 - \frac{1}{4} \xi^2 \right) \right) d \left( \sqrt{\frac{c}{2}} \eta \right)}{2^n \sqrt{\pi U (n + 1/2, \sqrt{\sigma_0})}}. \quad (5.49)$$

The integrals in (5.49) are zero for odd $n$, because the integrand function is symmetric with respect to $\xi = 0$ in these cases. The integrals for even $n$ are convergent, provided exponential decreasing of integrands at infinity. They contain the factor $\mu$ and consequently are of the order $O(1/\beta)$. The only non-zero coefficient at leading order is $a_0$. The factor

$$\exp \left( \frac{c - \sqrt{c}}{4} \xi^2 \right)$$

is small compared to the order of $c$ and will be neglected in further analysis. (It is also possible to consider the estimation for temperature we get without this factor as an upper bound for the temperature ahead of the premixed front.)

Thus, the following estimation can be done for the coefficient $a_0$:

$$a_0 = \frac{\sqrt{r_0}}{U(1/2, \sqrt{\sigma_0})} + O(1/\beta) \quad (5.50)$$

When we substitute the expressions for $a_n$ in (5.45), we get the approximation for temperature at leading order in $1/\beta$:

$$\Theta^{(0)} = \frac{\text{erfc} \left( \frac{\sqrt{c}}{\sqrt{2} \sqrt{\sigma_0}} \right)}{\text{erfc} \left( \frac{\sqrt{c}}{\sqrt{2} \sqrt{\sigma_0}} \right)} \exp \left[ \left( \frac{\sqrt{c}}{4} - \frac{1}{4} \eta_0^2 - \eta^2 \right) \right] + O(1/\beta). \quad (5.51)$$

Once again, we neglect the factor $\exp \left[ \left( \frac{\sqrt{c}}{4} - \frac{1}{4} \eta_0^2 - \eta^2 \right) \right]$ decaying from unity much slowly, then the erfc-function.

The parabolic function can be written down in terms of error complementary function,
erfc(x) = \int_x^\infty \exp(-y^2)dy,

U(1/2, \sqrt{\eta}) = \frac{\text{erfc}\left(\frac{\sqrt{\eta}}{\sqrt{2}}\right) \sqrt{\pi}}{\exp\left(-\frac{1}{2} \frac{\eta^2}{\eta_0^2}\right)} \quad (5.52)

Finally, we write down the approximation for temperature in the form:

\Theta^{(0)} = \frac{\text{erfc}\left(\frac{\sqrt{\eta}}{\sqrt{2}}\eta_0\right)}{\text{erfc}\left(\frac{\sqrt{\eta}}{\sqrt{2}}\eta_0\right)} + O(1/\beta). \quad (5.53)

Behind the flame front, along the diffusion flame, the first derivative \( \partial \Theta / \partial r \) becomes singular. The heat losses are balanced by lateral diffusion, \( \partial^2 \Theta / \partial r^2 \). Thus, the \( X \)-derivatives vanish, and the boundary condition for the temperature behind the partially premixed front is

\Theta(r_0, X) = 1. \quad (5.54)

The temperature solution \( \Theta = 1 - \mu|r - r_0| \) is the first order approximation behind the flame front in the vicinity of \( r = r_0, \ X > 0 \). This solution satisfies the boundary condition (5.48), and the expression for temperature can therefore be written up to the first order in \( r - r_0 \) as

\Theta = 1 - \mu|r - r_0| - O(1/\beta^2). \quad (5.55)

The mixture fraction gradient \( \mu \) in our analysis was chosen to be of order \( O(1/\beta) \), thus the above equation at leading order in \( 1/\beta \) is

\Theta(r, X) = 1 + O(1/\beta). \quad (5.56)
5.4. ACTIVATION-ENERGY ASYMPTOTICS

5.4.1 The inner solution and the asymptotic matching

The above formulae (5.51), (5.55) was derived in the outer region of the temperature definition, that doesn’t contain the singularities. In the immediate vicinity of the flame front, where \( \Theta \) is very close to one, the reaction term cannot be neglected anymore. We have to “stretch” this zone, and effectuate the activation energy asymptotic analysis, described in previous chapter.

First of all, equation for temperature is re-written in parabolic-cylinder coordinates:

\[
\left( \xi - \frac{\eta}{\xi \eta + r_0} \right) \frac{\partial \Theta}{\partial \xi} - \left( \eta - \frac{\xi}{\xi \eta + r_0} \right) \frac{\partial \Theta}{\partial \eta} =
\]

\[
= \frac{\partial^2 \Theta}{\partial \xi^2} + \frac{\partial^2 \Theta}{\partial \eta^2} + \lambda c(\xi^2 + \eta^2)\Sigma(1 + \mu \xi \eta + O(1/\beta^2), \Theta) \exp(-\beta(1 - \Theta)). \tag{5.57}
\]

The stretch variable is chosen to be \( \tau = \beta(\eta - \eta_0) \), and the temperature in this region is measured with a help of the new variable \( \theta \), which is the deviation of the temperature from those on the flame surface, scaled to order of unity:

\[
\Theta = 1 - \mu \eta_0 |\xi| - \frac{\theta}{\beta} - O(1/\beta^2). \tag{5.58}
\]

For further use, we denote by \( B \) the product \( \mu \beta \), \( B = O(1) \). We re-write (5.21) in terms of these scaled variables, expand \( \theta \) in asymptotic series in \( 1/\beta \), and get at the leading order:

\[
\theta_{rr} = c \Lambda_0 (\xi^2 + \eta_0^2) \theta \nu (\nu + 2B \eta_0 |\xi|) \exp(-\theta) \exp(-B \eta_0 |\xi|), \tag{5.59}
\]

where \( \Lambda_0 \) is the first term in the expansion \( \lambda = \beta^{2\nu+1}(\Lambda_0 + \ldots) \).

We integrate this equation prior to boundary conditions

\[
\theta_r(\tau = 0) = 0, \quad \theta_r(\tau = \infty) = 0,
\]

and get:

\[
\theta_r^2(\tau \to +\infty) = 2c \Lambda_0 (\xi^2 + \eta_0^2) \exp(-B \eta_0 |\xi|) F_{\nu}(2B \eta_0 |\xi|). \tag{5.60}
\]
Here the function $F_n$ is defined by

$$F_n(\alpha) = \int_0^\infty \theta^n (\theta + \alpha)^n \exp(-\theta) d\theta. \quad (5.61)$$

To determine $\Lambda_0$, we reinforce the asymptotic matching condition:

$$\Theta_\eta(\xi, \eta \to \eta_0) = -\Theta_\tau(\xi, \tau \to \infty), \quad (5.62)$$

where $\Theta_\eta$ corresponds to the outer, and $\Theta_\tau$ to the inner solution. We write down the expressions for the coefficients $a_n$ in temperature expansion with the help of Kronecker symbols $\delta_{n,0}$ as

$$a_n = \frac{\delta_{n,0}}{U(1/2, \sqrt{\nu \eta_0})} + O(1/\beta). \quad (5.63)$$

Making use of the following property of parabolic cylinder functions,

$$\frac{dU(n + 1/2, y)}{dy} = U(n - 1/2, y), \quad (5.64)$$

we calculate the derivative of the temperature with respect to $\eta$,

$$\Theta_\eta(\xi, \eta_0) = -\sqrt{c} \sum_{n=0}^{\infty} a_n U(n - 1/2, \sqrt{c \eta_0}) H_n \left( \frac{\sqrt{c}}{2} \right) =$$

$$= \sqrt{c} \frac{U(-1/2, \sqrt{c \eta_0})}{U(1/2, \sqrt{c \eta_0})} + O(1/\beta). \quad (5.65)$$

The expression above is replaced by those containing error complementary functions. The use is done of the fact that

$$U(-1/2, z) = \exp \left( -\frac{1}{4} z^2 \right), \quad \text{and}$$

$$U(1/2, z) = \frac{\text{erfc} \left( \frac{z}{\sqrt{2}} \right)}{\sqrt{\pi}} \exp \left( -\frac{1}{2} \frac{z^2}{2} \right).$$
The matching condition (5.62) then takes the form:

\[
\sqrt{c} \frac{U(-1/2, \sqrt{c\eta_0})}{U(1/2, \sqrt{c\eta})} = \sqrt{c} \frac{2}{\pi} \exp(-c\eta_0^2/2) \text{erfc}(\sqrt{c\eta_0}/\sqrt{2}) = [2cA_0(\xi^2 + \eta_0^2) \exp(-B\eta_0|\xi|)F_\nu(2B\eta_0|\xi|)]^{1/2}.
\] (5.66)

In order the parabolic flame front approximation to be consistent, we have to enforce the matching condition up to the second order only.

Equating the coefficients by term \( \xi^0 \) gives us the expression for the burning-speed eigenvalue:

\[
\sqrt{2A_0}\Gamma(2\nu + 1) = \sqrt{2} \frac{\exp(-c\eta_0^2/2)}{\eta_0 \text{erfc}(\sqrt{c\eta_0}/\sqrt{2})},
\] (5.67)

here \( \Gamma \) is the Gamma-function. The coefficients by \( \xi \) are zero, and at the order \( \xi^2 \) we get the equation for the curvature of the parabola, \( \eta_0 \),

\[
\eta_0 = \frac{(4\nu - 2)^{1/4}}{\sqrt{B}}.
\] (5.68)

The stoichiometric planar flame speed in physical variables is (Líñán and Williams)

\[
U_\infty^S = \left[ \frac{2mkA\nu\Gamma(2\nu + 1)}{\beta^{2\nu+1}} \left( \frac{\rho_\infty}{\beta} \right)^{2\nu-1} \exp(-\beta/\alpha) \right]^{1/2}.
\] (5.69)

The velocity of the triple flame base propagation, \( U_\infty \), is equal to the stoichiometric velocity in the limit \( r_0 \to \infty, \mu \to \infty \).

Using the above expressions, we get the formulae for the normalized velocity, expressed in terms of the mixture fraction gradient:

\[
\frac{U_\infty}{U_\infty^S} = \sqrt{\frac{\pi}{2}} \eta_0 \exp \left( \frac{c\eta_0^2}{2} \right) \text{erfc} \left( \sqrt{\frac{c}{2}} \eta_0 \right),
\] (5.70)
Here $U_\infty$ is the flame velocity in physical units, $U_\infty^S$ is the stoichiometric planar flame speed, $\kappa$ is the flame curvature. We note the dependence of the velocity on the global characteristics, $r_0$, through the coefficient $c = 1 - 1/r_0^2$. In the limit $r_0 \to \infty$ we get the formulae of the planar case.

The normalized velocity as a function of normalized mixture fraction gradient presented on the Figure 5.7. We observe the increase of the velocity flame propagation due to the global curvature effects.
Figure 5.7: The normalized velocity plotted as a function of the normalized mixture fraction gradient with and without correction, due to the radius of the flame base. Line: planar case, asterisks: corrected solution.
5.5 Effects of heat release

As it was shown by several authors, [19], [39], the velocity field in front of the flame is modified by heat release. This effect is clearly seen on the Figure 5.8, that presents the plot of the iso-lines of heat release together with underlying flow field velocities (from DNS by Boulanger and others, [5]).

When the premixed flame front propagates through the gas mixture, it deviates the streamlines of the flow in front of it. To consider this mechanism in detail, we have to go back to the description of the flame front as a surface of discontinuity in temperature, velocity and density. The fluid flow equations are solved on the both sides of the flame front, and the jump conditions are defined:

\[ \rho_f (v_{nf} + V) = \rho_b (v_{nb} + V), \]
\[ p_f + \rho_f (v_{nf} + V)^2 = p_b + \rho_b (v_{nb} + V)^2. \]  

Hereabove \( V \) is the velocity of the flame front in the direction, normal to itself. \( v_{nf}, v_{nb}, v_{nf} \) and \( v_{nb} \) are the fluid velocity normal and tangential components in fresh and burnt gas respectively. Adiabatic flame temperature \( W \) is given by \( W = v_{nf} + V \).

In the frame, where the flame front is stationary, these jump conditions are transformed into

\[ u_f = W, \quad u_b = \sigma W, \quad \sigma = \frac{\rho_f}{\rho_b}, \]
\[ \rho_f W^2 (1 - \sigma). \]  

As illustrated on Figure 5.9, the tangential component remains the same, and the normal component of the velocity vector increases, what makes the streamlines refract towards the centerline.

This impact of the density changes across the flame front was also confirmed by numerical simulations in [39].

These effects make it important to distinguish between two flame velocities: local and far-field velocity. The local speed is related to the chemical reaction rate, and close to the velocity of the planar diffusion flame along the stoichiometric surface \( Z = Z_s \). The far-field speed is assigned to be those of the triple flame propagation \( U_\infty \). From the jump conditions (5.74) it is easy to see, that both velocities are equal, when the density changes are neglected.
Figure 5.8: Deviation of the velocity vector field through the flame due to heat release effects (from DNS by Boulanger et al.)
Therefore, a correct prediction of the triple flame propagation requires the incorporation of the heat release effects in our analysis. This is the subject of the present section.

The vector field decomposition into divergence-free and potential parts of chapter two is only legitimate when the chemical-fluid balance is hold. However, the propagating flame front is a source of energy and able to break down this balance. Thus, the conditions of the low Mach number fluid field velocity decomposition are not fulfilled in general. We will show that the vorticity production can be neglected, when heat release and mixture fraction gradient are small. In this case, the velocity perturbation due to density changes is potential in the whole domain.

The amount of the vorticity, produced by the temperature variations across the flame surface, can be calculated from the vorticity generation equation,

$$\frac{d}{Dt}\left(\frac{\mathbf{w}}{\tilde{\rho}}\right) = \frac{1}{Ma^2} \left(\nabla \frac{\tilde{\rho}}{\tilde{\rho}^2}\right).$$

(5.75)

The jump conditions across the flame are those for the tangential and normal component of gradient of pressure and density respectively,

$$(\nabla p/p)_t \sim Ma^2 \mu, \quad (\nabla \rho/p)_t \sim \mu,$$

$$(\nabla p/p)_n \sim Ma^2 \alpha, \quad (\nabla \rho/p)_n \sim \alpha.$$  

(5.76)

In the limit of small Mach number and small heat release, the vorticity gener-
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ated by the flame front can be neglected. The velocity perturbation can then be described by a potential $\psi$, namely:

\[
\begin{align*}
    u &= \alpha \psi_r + \ldots, \\
    v &= 1 + \alpha \psi_x + \ldots
\end{align*}
\]  

(5.77)

We introduce these expressions for the velocity into the temperature equation (5.9), and get at leading order in $\alpha$:

\[
\frac{1}{r} \psi_r + \psi_{rr} + \psi_{XX} = \Theta_X^{(0)}. 
\]  

(5.78)

Re-written in local parabolic-cylinder coordinates $(\xi, \eta)$, this equation takes form:

\[
\frac{1}{r_0} \left( \eta \frac{\partial}{\partial \xi} + \xi \frac{\partial}{\partial \eta} \right) \psi + \psi_{\xi\xi} + \psi_{\eta\eta} = -\eta \Theta_H^{(0)}. 
\]  

(5.79)

Behind the premixed front the right hand side of (5.79) vanishes,

\[
\frac{1}{r_0} \left( \eta \frac{\partial}{\partial \xi} + \xi \frac{\partial}{\partial \eta} \right) \psi + \psi_{\xi\xi} + \psi_{\eta\eta} = 0, 
\]  

(5.80)

and ahead of the premixed front is equal to

\[
\sigma \eta \exp \left( \frac{c(r_0^2 - \eta^2)}{2} \right), 
\]  

with $\sigma = \frac{\sqrt{c}}{\sqrt{2\pi}} \exp \left( -\frac{c \eta_0^2}{2} \right) / \text{erfc} \left( \frac{\sqrt{c}}{\sqrt{2 \eta_0}} \right)$. 

(5.81)

This leads to the equation

\[
\frac{1}{r_0} \left( \eta \frac{\partial}{\partial \xi} + \xi \frac{\partial}{\partial \eta} \right) \psi + \psi_{\xi\xi} + \psi_{\eta\eta} = \sigma \eta \exp \left( \frac{c(r_0^2 - \eta^2)}{2} \right). 
\]  

(5.82)

The boundary conditions are derived from the symmetry requirement on the radial velocity component,

\[
v = 0 \quad \text{for} \quad r = r_0. 
\]  

(5.83)
In terms of the velocity perturbation $\psi$ the boundary conditions are written as

$$
\psi_T(0, \eta) = 0, \\
\psi_\eta(\xi, 0) = 0.
$$

(5.84)

We are looking for solution in the vicinity of $r = r_0$, that corresponds in new coordinates to the axes $\xi = 0$ or $\eta = 0$. Together with the boundary conditions, introduced above, and due to the fact, that velocity perturbation stays limited even at infinity, we conclude, that the first term on the left hand side of (5.79) can be suppressed.

Therefore, the equations for velocity perturbation reduce to those of the planar case,

$$
\psi_{\xi \xi} + \psi_{\eta \eta} = 0 \quad (5.85)
$$

for $0 < \eta < \eta_0$, and

$$
\psi_{\xi \xi} + \psi_{\eta \eta} = \sigma \eta \exp \left( \frac{\eta_0^2 - \eta^2}{2} \right) \quad (5.86)
$$

for $\eta \geq \eta_0$.

These two equations, considered together with the boundary conditions (5.84), deliver the only physically relevant solution $\psi_0 = \psi(\eta)$.

The solution of the first equation prior to the boundary conditions is constant, and without loose of generality we set this constant to be equal to zero,

$$
\psi_0(\eta) = 0. \quad (5.87)
$$

The solution of the second equation is

$$
\psi_0(\eta) = \frac{\text{erfc} \left( \frac{\sqrt{2} \eta}{\sqrt{\sigma \eta_0}} \right)}{\text{erfc} \left( \frac{\sqrt{2} \eta_0}{\sqrt{\sigma \eta_0}} \right)} + \sigma \sqrt{\epsilon} (\eta - \eta_0) - 1 \quad (5.88)
$$
for $\eta > \eta_0$, and
\[ \psi_0(\eta) = 0 \] (5.89)
for $\eta < \eta_0$.

The local expressions for the velocity components along the axes $r = r_0$ and $X = 0$ are:

\[ u(r,0) = \frac{\alpha \sigma \xi}{\eta_0^2 + 2 \xi^2} \left[ 1 - \exp \left( -\frac{c \xi^2}{2} \right) \right], \quad \text{and} \quad (5.90) \]

\[ v(X,r = r_0) = \begin{cases} 
1 - \frac{\alpha \sigma}{\sqrt{\eta_0^2 - 2X}} [1 - \exp(\sqrt{c}X)], & X < 0 \\
1, & \text{otherwise} \end{cases} \] (5.91)

### 5.5.1 Reduction of the mixture fraction gradient near the flame tip

In this section we are looking for the second term $\zeta$ in the perturbative expansion of the mixture fraction,

\[ Z = \frac{1}{2} (1 + \mu (r - r_0)) + \alpha \zeta + \ldots \] (5.92)

We substitute this expression into the equation for mixture fraction gradient (5.12), and retaining the leading terms only (up to the first order in $\alpha$), we get:

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\partial \zeta}{\partial r} + \frac{\partial \zeta}{\partial X} \right) + \frac{\partial^2 \zeta}{\partial r^2} + \frac{\partial^2 \zeta}{\partial X^2} = \frac{1}{2} \mu r \] (5.93)

Once transformed into local parabolic-cylinder coordinates $(\xi, \eta)$, the above equation takes form

\[ \frac{1}{\xi \eta + r_0} \left( \xi \frac{\partial \zeta}{\partial \eta} + \eta \frac{\partial \zeta}{\partial \xi} \right) - \xi \frac{\partial \zeta}{\partial \xi} + \eta \frac{\partial \zeta}{\partial \eta} + \frac{\partial^2 \zeta}{\partial \xi^2} + \frac{\partial^2 \zeta}{\partial \eta^2} = \frac{1}{2} \mu \psi_r \] (5.94)
The right-hand side is given by the function $\psi_0(\eta)$, calculated above. As we are interesting in the modification of the mixture fraction gradient, only the factor by $\xi\eta$ is essential.

Thus, we are looking for solution of (5.94) in form:

$$\zeta(\xi, \eta) = \xi F(\eta) + \phi(\xi, \eta).$$  \hfill (5.95)

Substituting everything in the original equation (5.94) we see, that the function $F$ has to satisfy the equation

$$F'' - F + \eta F' = \frac{1}{2} \mu \psi_0'(\eta),$$  \hfill (5.96)

which is the same equation as in two-dimensional case.

Behind the premixed flame, the boundary conditions are once again found from the symmetry argument to be

$$\zeta(0, \eta) = 0,$$
$$\zeta(\xi, 0) = 0.$$ \hfill (5.97)

These conditions in terms of the function $F$ is simply

$$F(0) = 0.$$ \hfill (5.98)

Thus, the initial problem is well-defined.

The right hand side of (5.96) is zero behind the flame front, and the initial problem (5.96), (5.98) has the solution

$$F(\eta) = a\eta$$ \hfill (5.99)

with unknown constant $a$.

This constant will be determined when we analyze the solution behaviour in front of the flame front.

In order to calculate the expression on the right-hand side of (5.96), we write down the expression for the derivative of the function $\psi_0(\eta)$,
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\[ \psi_0(\eta) = -\sqrt{\frac{c}{2\sqrt{\pi}}} \frac{\exp\left(-\frac{c}{2}\eta^2\right)}{\text{erfc}\left(\sqrt{\frac{c}{2}\eta_0}\right)} + \sqrt{\alpha}. \] (5.100)

In the equation above we used the fact that

\[ \frac{d}{dz} \text{erfc}z = -\frac{2}{\sqrt{\pi}} \exp(-z^2). \] (5.101)

Thus, equation (5.96) takes form

\[ F'' - F + \eta F' = \frac{1}{2} \mu \sqrt{\alpha} \left[ 1 - \exp\left(\frac{c(\eta_0^2 - \eta^2)}{2}\right)\right]. \] (5.102)

The discussion in the previous section pointed out, that in our model there is no vorticity generation up to the first order, i.e. the mixture fraction is continuous together with its first derivative. The initial conditions for the equation (5.102) are then

\[ F(\eta_0) = a \eta_0, \]
\[ F'(\eta_0) = a. \] (5.103)

We are looking for the solution of the form

\[ F(\eta) = \eta f(\eta). \] (5.104)

The equation for this new function \( f \) is

\[ f'' + \left(\eta + \frac{2}{\eta}\right) f' = \frac{1}{2\eta} \mu \sqrt{\alpha} \left[ 1 - \exp\left(\frac{c(\eta_0^2 - \eta^2)}{2}\right)\right]. \] (5.105)

This equation can be integrated directly,

\[ f(\eta) = a + \frac{1}{2} \mu \sqrt{\alpha} \left[ \left(\frac{1}{\eta_0} - \frac{1}{\eta}\right) - \right]. \]
\[ - \int_{\eta_0}^{\eta} \frac{dt}{(t^2 + \frac{\eta_0^2}{2t^2})} \exp\left(\frac{c(\eta_0^2 - \eta^2)}{2}\right). \]  

From the pair of conditions

\[ f \text{ is finite for } \eta \to \infty \]
\[ \zeta \to 0, \quad \eta \to -\infty, \quad r \text{ fixed} \]  

we conclude, that

\[ f(\infty) = 0. \]

The expression for the constant \( a \) is found, integrating (5.106) in the limit \( \eta \to \infty \):

\[ a = \frac{\mu}{4}(\sigma_0^2 - \sigma \sqrt{\sigma_0} - 1). \]  

The new expression for the mixture fraction taking into consideration the density changes, is

\[ Z = \frac{1}{2}(1 + \mu')(r - r_0), \]

with modified mixture fraction gradient

\[ \mu' = \mu + 2\alpha a. \]

We see, that the gradient on the top of the edge flame will be reduced firstly by the premixed flame front curvature and secondly, by the radius of the flame base.

### 5.5.2 Modified solution for temperature

The goal of the present section is to find the derivative of the temperature along the flame surface rather than the approximative solution of temperature itself. Once the derivative is found, it delivers us the necessary matching condition to
First of all, the perturbed equation for the temperature is written down:

\[
\psi_r \Theta_r^{(0)} + \frac{1}{r} \psi_r \Theta^{(0)} - \Theta^{(0)} \Theta_X^{(0)} + \psi_X \Theta_X^{(0)} =
\]

\[
= \left( \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} \right) \Theta^{(1)} + \frac{\partial^2}{\partial X^2} \Theta^{(1)} - \Theta_X^{(1)}. \tag{5.112}
\]

As in the previous section, we introduce local coordinates \((\xi, \eta)\) and all the non-local influences in the above equation will be neglected. The equation is thus reduced to those of the planar case, and afterwards we follow the analysis of [17].

The equation for temperature perturbations in local coordinates \((\xi, \eta)\) is

\[
\xi \Theta^{(1)}_\xi - \eta \Theta^{(1)}_\eta - \Theta^{(1)}_{\xi \xi} - \Theta^{(1)}_{\eta \eta} =
\]

\[
\sqrt{c} \sigma \exp \left( \frac{c(\eta_0^2 - \eta^2)}{2} \right) \left[ \text{erfc}(\sqrt{c} \eta / \sqrt{2}) + \text{erfc}(\sqrt{c} \eta_0 / \sqrt{2}) \right]
\]

\[
\sqrt{c} \sigma \left( 1 - \exp \left( \frac{c(\eta_0^2 - \eta^2)}{2} \right) \right)
\]

ahead of the flame, and

\[
\xi \Theta^{(1)}_\xi - \eta \Theta^{(0)}_\eta - \Theta^{(1)}_{\xi \xi} - \Theta^{(1)}_{\eta \eta} = 0 \tag{5.114}
\]

behind it.

The boundary condition

\[
\Theta(\xi, \eta_0) = \begin{cases} 
2(1 - Z(\xi, \eta_0)), & \text{for } \xi \geq 0, \\
2Z(\xi, \eta_0) & \text{for } \xi < 0.
\end{cases} \tag{5.115}
\]

is a consequence of the fuel and oxidizer mass fractions vanishing on the flame.
Substituting the expression (5.110) for the mixture fraction into (5.115), we get the boundary condition for the first order perturbative solution for the temperature:

$$\Theta^{(1)}(\xi, \eta) = -2a_0|\xi|^2. \quad (5.116)$$

We are looking for solution of the boundary problem, defined above, as a sum of two functions:

$$\Theta^{(1)}(\xi, \eta) = T_0(\eta) + T_1(\xi, \eta). \quad (5.117)$$

As the right-hand side of the original equation is only $\eta$-dependent, $T_1$ satisfies the homogeneous equation

$$\partial_\xi T_1 + \eta \frac{\partial T_1}{\partial \eta} - \frac{\partial^2 T_1}{\partial \xi^2} - \frac{\partial^2 T_1}{\partial \eta^2} = 0, \quad (5.118)$$

accompanied with the boundary condition

$$T_1(\xi, \eta_0) = -2a_0|\xi|. \quad (5.119)$$

The equation for the $\eta$-dependent function $T_0$ is

$$T_0'' + \eta T_0' = -\sqrt{\sigma} \exp \left( \frac{c(n_0^2 - \eta^2)}{2} \right) \left\{ \text{erfc} \left( \frac{\sqrt{c} \eta_0 / \sqrt{2}}{\sqrt{\sigma}} \right) + \sqrt{\sigma} \left( 1 - \exp \left( \frac{c(n_0^2 - \eta^2)}{2} \right) \right) \right\} \quad (5.120)$$

This function vanishes at the flame surface, as well as at the infinity:

$$T_0(\eta_0) = 0, \quad T_0(\infty) = 0. \quad (5.121)$$

This last equation is solved, using the method of parameters variation from the theory of ordinary differential equations. First, the homogeneous equation for $T_0$ is solved. Afterwards, the unknown coefficients in the solution of the
homogeneous equation are supposed to be the functions of \( \eta \). They are found by substitution of the solution of the homogeneous equation into the original one.

The solution of the homogeneous equation is

\[
T_0(\eta) = -\sqrt{\pi/2} \text{erfc}(\sqrt{c\eta}/\sqrt{2}) + B, \tag{5.122}
\]

where the coefficients \( A \) and \( B \) satisfy

\[
A'(\eta) = -g(\eta), \quad B'(\eta) = -\sqrt{\pi/2} \text{erfc}(\sqrt{c\eta}/\sqrt{2}) g(\eta). \tag{5.123}
\]

Hereabove \( g(\eta) \) is defined as

\[
g(\eta) = \sigma \exp(c\eta_0^2/2) \left[ \frac{\text{erfc}(\sqrt{c\eta_0}/\sqrt{2})}{\text{erfc}(\sqrt{c\eta_0}/\sqrt{2})} + \sqrt{c\sigma} \left( 1 - \exp \left( \frac{c(\eta_0^2 - \eta^2)}{2} \right) \right) \right]. \tag{5.124}
\]

The boundary conditions on \( T_0 \) imply that the coefficient \( B \) vanishes at infinity,

\[
B(\infty) = 0, \tag{5.125}
\]

that determines the boundary condition for \( A \):

\[
A(\eta_0) = \sqrt{\frac{\pi}{2}} \frac{B(\eta_0)}{\text{erfc}(\sqrt{c\eta_0}/\sqrt{2})}. \tag{5.126}
\]

The value of the coefficient \( B \) at the flame surface is found by integration and equal to

\[
B(\eta_0) = \sqrt{\frac{\pi}{2}} \int_{c\eta_0}^{\infty} \text{erfc} \left( \frac{\sqrt{c\eta}}{\sqrt{2}} \right) g(\eta)d\eta. \tag{5.127}
\]
As mentioned in the beginning of this section, only the derivative along the flame surface is essential for our analysis. The derivative \( T'_0(\eta_0) \) is easily calculated with help of the above expressions,

\[
T'_0(\eta_0) = \sqrt{\sigma} B(\eta_0).
\] (5.128)

The equation for the function \( T_1(\xi, \eta) \) is exactly the same as the equation (5.31) for \( \Theta^{(0)} \) considered in the previous section, only the boundary condition is different. By analogy, the solution is written down as

\[
T_1(\xi, \eta) = \exp \left[ \frac{\sqrt{c}}{4} (\xi^2 + \eta_0^2 - \eta^2) \right] \exp \left( -\frac{1}{4} c \xi^2 \right) \times \sum_{n=0}^{\infty} \frac{b_n}{\sqrt{\eta_0}} H_n \left( \frac{\sqrt{c}}{\sqrt{2}} \xi \right) U(n + 1/2, \sqrt{c} \eta),
\] (5.129)

with coefficients \( b_n \) defined by

\[
b_n = -2a\eta_0\sqrt{\eta_0} \frac{\int_{-\infty}^{+\infty} |\xi| H_n \left( \frac{c}{2\xi} \right) \exp \left( -\frac{c}{4} \xi^2 \right) d \left( \frac{c}{2} \xi \right)}{2^n n! \sqrt{\pi} U(n + 1/2, \sqrt{c} \eta_0)}.
\] (5.130)

From these expressions it is easy to see, that the derivative is of the order

\[
\partial_\eta T_1 \sim \mu \sim O(1/\beta)
\] (5.131)

and it can be neglected at leading order.

Finally, this analysis delivers us the necessary matching condition for temperature:

\[
\Theta_1^{(1)}(\xi, \eta_0) = T'_0(\eta_0) + O(1/\beta).
\] (5.132)

If we calculate the integral expression for \( B(\eta_0) \), we get

\[
\Theta_1^{(1)}(\xi, \eta_0) = \sqrt{\sigma} \mathcal{L}(\eta_0) + O(1/\beta),
\] (5.133)
with
\[
\mathcal{L}(\eta_0) = \sigma^2 \left[ \pi \exp(\sigma \eta_0^2) \int_{-\infty}^{\infty} \text{erfc}^2(x \sigma) dx - \frac{\sqrt{\eta_0}}{\sigma} + 1 - \frac{1}{2\sigma^2} \right].
\] (5.134)

### 5.5.3 The inner solution

This time the matched asymptotic expansions are done for the temperature approximation
\[
\Theta = \Theta^{(0)} + \alpha \Theta^{(1)},
\] (5.135)

with both \(\Theta^{(0)}\) and \(\Theta^{(1)}\) already found in the previous sections. The density doesn’t decouple from the velocity anymore, and the expression for it to be used in the temperature equation is
\[
\tilde{\omega} = 1 - \alpha \Theta^{(0)}.
\] (5.136)

The expression for the mixture fraction \(Z = 1 + \mu \rho |r - r_0|\) is substituted in the source term in the temperature equation (5.21).

The equation (5.21) for the temperature in non-dimensional units up to the first order in \(\alpha\) then takes the form
\[
(1 - \alpha \Theta^{(0)}) \left( (1 + \alpha \psi_X \frac{\partial \Theta}{\partial X} + \alpha \psi_r \frac{\partial \Theta}{\partial r} \right) = \frac{1}{\eta} \frac{\partial \Theta}{\partial \eta} + \frac{\partial^2 \Theta}{\partial r^2} + \frac{\partial^2 \Theta}{\partial X^2}
\] (5.137)
\[+ \lambda (1 - \alpha \Theta^{(0)}) \Sigma(Z/Z_0, \Theta) \exp(\beta(1 - \Theta) - \alpha \beta (1 - \Theta)^2).
\]

When we transform everything into local parabolic-cylinder coordinates, we get
\[
(1 - \alpha \Theta^{(0)}) \left( (1 + \alpha \psi_X) \left( \frac{\xi \partial \Theta}{\partial \xi} - \eta \frac{\partial \Theta}{\partial \eta} \right) + \alpha \psi_r \left( \eta \frac{\partial \Theta}{\partial \xi} + \xi \frac{\partial \Theta}{\partial \eta} \right) \right)
\] = \frac{\eta}{\xi + r_0} \frac{\eta}{\xi + r_0} \frac{\xi}{\xi + r_0} \frac{\partial \Theta}{\partial \eta}
\]
\[+ \frac{\partial^2 \Theta}{\partial \xi^2} + \frac{\partial^2 \Theta}{\partial \eta^2} + \lambda (1 - \alpha \Theta^{(0)})^{2\nu} (\xi^2 + \eta^2) \Sigma(1 + \mu \xi \eta, \Theta) \exp(-\beta(1 - \Theta)^2).
\] (5.138)
Further, we introduce the stretching coordinate \( \tau = \beta(\eta - \eta_0) \) and the inner measure for temperature, \( \theta \):

\[
\Theta = 1 - \mu'\eta_0|\xi| - \frac{\theta}{\beta}.
\]

(5.139)

The equation (5.138), re-written in terms of \( \theta \), takes the form (at leading order in \( \frac{1}{\beta} \)):

\[
\theta_{rr} = \Lambda_0(\xi^2 + \eta_0)^2\theta(\theta + 2B\eta_0|\xi|)^\nu(1 - \alpha)^{2\nu}\exp(-\theta)\exp(-B\eta_0|\xi|),
\]

(5.140)

with the constant \( B \) is now defined as

\[
B = \mu'\beta = O(1)
\]

(5.141)

with the mixture fraction gradient \( \mu' \) as defined in (5.111). We integrate the above equation prior to the boundary condition

\[
\theta_r(r = 0) = 0
\]

(5.142)

and get the new matching condition

\[
\theta^2_r(r \to \infty) = 2\Lambda_0|\xi^2 + \eta_0|^2\exp(-B\eta_0|\xi|)F\nu(2B\eta_0|\xi|),
\]

(5.143)

with \( F \) defined as

\[
F\nu(x) = (1 - \alpha)^{2\nu}\int_0^\infty \theta^\nu(\theta + x)^\nu\exp(-\theta)d\theta.
\]

(5.144)

The matching asymptotic condition

\[
\Theta\eta(\xi, \eta \to \eta_0) = -\theta_r(\xi, \tau \to \infty)
\]

(5.145)

will be used in order to define the burning rate eigenvalue \( \Lambda_0 + \alpha\Lambda_1 \). The outer derivative was calculated in the previous section and is equal

\[
\Theta\eta(\xi, \eta \to \eta_0) = \Theta^{(0)}\eta(\xi, \eta_0) + \alpha\Theta^{(1)}\eta(\xi, \eta_0).
\]

(5.146)
Equating the correspondent terms by $\xi^0$ and $\xi^2$, we get the new formulae for velocity in dependence on mixture fraction gradient and curvature, including pressure changement effects.

**5.5.4 Expressions for velocity in dependence on mixture fraction gradient, effects of heat release included**

Results for velocity and mixture fraction gradient in dependence on radius heat release $\alpha$, and radius of the flame base $r_0$ through $c = 1 - \frac{1}{r_0}$:

$$\frac{U_\infty}{U_\infty^s(\alpha)} = \frac{\eta_0}{\sigma} [1 + \alpha L(\eta_0)], \quad (5.147)$$

(here flame velocity is normalized by $U_\infty^s(\alpha)$, stoichiometric planar flame velocity),

$$U_\infty^s(\alpha) = (1 - \alpha)U_\infty^S. \quad (5.148)$$

$$\frac{k}{U_\infty^s(\alpha)} \frac{1}{Z_s} \left( \frac{\partial Z}{\partial r} \right)_0 = \frac{\sqrt{4\nu - 2}}{\beta} \frac{1}{\eta_0^2} \frac{U_\infty}{U_\infty^s(\alpha)}. \quad (5.149)$$

with $\left( \frac{\partial Z}{\partial r} \right)_0$ the mixture fraction gradient, evaluated at the triple point, related to it upstream value through

$$\left( \frac{\partial Z}{\partial r} \right)_0 = \left( \frac{\partial Z}{\partial r} \right)_\infty \left[ 1 + \frac{\alpha}{2} \frac{\sqrt{4\sigma\eta_0 - \sigma_0^2}}{1 + \sqrt{4\sigma\eta_0 - \sigma_0^2}} \right]^{-1}. \quad (5.150)$$

$$\frac{k}{U_\infty^s(\alpha)} \kappa = \frac{1}{\sqrt{\sigma_0^2}} \frac{U_\infty}{U_\infty^s(\alpha)}. \quad (5.151)$$

From the above equations we see, that both heat release and flame base curvature play role in the increasing of the triple flame velocity. This also demonstrated on the Figure 5.10, where the normalized velocity is depicted versus normalized mixture fraction gradient.
Figure 5.10: Velocity as function of mixture fraction gradient with corrections due to heat release and radius of the flame base.

In the limit \( \alpha \ll 1 \), and \( \kappa \ll 1 \) the above formulae reduce to the expressions

\[
\frac{U_\infty}{U_\infty^*(\alpha)} = 1 + \frac{\alpha}{\sqrt{c}} - \frac{k}{U_\infty^*(\alpha)^\kappa},
\]

(5.152)

\[
\kappa = \frac{\beta}{\sqrt{4\nu - 2\sqrt{c}Z_S}} \left( \frac{\partial Z}{\partial r} \right)_0,
\]

(5.153)

with

\[
\left( \frac{\partial Z}{\partial r} \right)_0 = \frac{1}{1 + \alpha} \left( \frac{\partial Z}{\partial r} \right)_\infty.
\]

(5.154)

These formulae will be used in the next chapter in order to compare our theoretical results with the DNS by J. Boulanger, J. Reveillon, L. Vervisch, S. Ghosal.
Chapter 6

Comparison with DNS of round jet

The triple flame as the mechanism of the round jet stabilization over the burner was discussed by several authors [14], [18], [33], [35]. Lifted diffusion flames are rather observed in turbulent regime, but the idealized model of the laminar lifted flame can be produced in laboratory conditions. In the present chapter we will consider the Landau-Squire solution for round jet to be the far-field velocity for the lifted round jet. Equating the triple flame ring velocity to those of the round jet, we find the distances between the burner and the base of the lifted flame, called lift-off heights. These results then compared to the simulations of round jet, effectuated by J. Boulanger, J. Reveillon, L. Vervisch and S. Ghosal. (see [5])

S. Ghosal and L. Vervisch [18] considered a lifted laminar diffusion flame with the far-field velocity delivered by a self-similar Landau-Squire solution for round jet, that we discuss in details below.

Let us introduce the spherical coordinates \((r, \theta, \phi)\) with polar axis in the direction of the jet, with emergence point as origin.

The continuity equation for submerged jet, issuing into the infinite space filled with the fluid in spherical coordinates \((r, \theta, \phi)\) is

\[
\frac{1}{r^2} \frac{\partial (r^2 u_r)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial (u_\theta \sin \theta)}{\partial \theta} = 0. \tag{6.1}
\]

The velocity components in the limit of small \(\theta\), or relative high Reynolds
number, are

\[
\begin{align*}
v_r &= \frac{8\nu\alpha^2}{(\alpha^2 + \theta^2)^2} \\
v_\theta &= -\frac{4\nu}{\alpha^2 + \theta^2},
\end{align*}
\]

(6.2)

here \( \nu \) is the kinematic viscosity, and \( \alpha \) is related to the jet momentum through

\[
\alpha = \frac{32\pi\nu^2 \rho}{3P}.
\]

(6.3)

We introduce the streamline function

\[
\psi(r, \theta) = \nu r f(\theta)
\]

(6.4)

with

\[
f(\theta) = \begin{cases} 
\frac{4\theta}{\theta^2 + \theta_0^2} & \text{for } \theta \leq \theta_0, \\
2(1 + \cos \theta) & \text{otherwise},
\end{cases}
\]

(6.5)

where \( \theta_0 \) is the opening angle of the jet,

\[
Re = \frac{32\theta_0^{-2}}{3}.
\]

(6.6)

The length scale is chosen to be

\[
l = k/U_s
\]

(6.7)

with \( U_s \) the flame velocity along the stoichiometric iso-surface.

The expressions for non-dimensional velocity components can be re-written in terms of the stream-function

\[
\begin{align*}
v_r &= \frac{1}{r^2 \sin \theta} \frac{\partial \psi}{\partial \theta} \\
v_\theta &= -\frac{1}{r \sin \theta} \frac{\partial \psi}{\partial r}, \\
\psi(r, \theta) &= Sr f(\theta)
\end{align*}
\]

(6.8)
here $S = \nu/k$ is the Schmidt number.

The triple laminar flame propagates along the stoichiometric iso-line, and stabilizes the round jet at the point, where the velocity of this flamelet equals those of the round jet, given by (6.8). In order to calculate the point of the stabilization we need to know the shape of the stoichiometric iso-surface. From the results of Squire [42], the mixture fraction can be described in context of the round jet solution by

$$Z = \frac{C}{r} \left( \frac{\theta_0^2}{\theta^2 + \theta_0^2} \right)^{2S}$$

(6.9)

with constant $C$ to be determined from the boundary conditions on the mixture fraction.

As we see, this solution has singularity at $r = 0$. To avoid this difficulty, we introduce the “virtual origin” at distance $r_0 = a/\theta_0$ below the jet exit. The constant $C = a/(l\theta_0)$ is then found, provided $Z = 1$ at $r = r_0$.

The expression for mixture fraction (6.9) enables us to calculate the shape of the stoichiometric iso-surface. We consider the stoichiometric value of mixture fraction to be equal to 0.0625. The equation

$$Z = Z_s$$

(6.10)

delivers us the path of the triple flame propagation,

$$r = \frac{1}{Z_s l \theta_0} \left( \frac{\theta_0^2}{\theta^2 + \theta_0^2} \right)^{2S}$$

(6.11)

here $l = l/a$ is the new length scale, with $a$ the nozzle diameter.

The expression for mixture fraction gradient and fluid velocity along the stoichiometric surface is

$$\mu = \left| \frac{1}{Z_s r} \frac{\partial Z}{\partial \theta} \right| = \frac{1}{Z_s} \frac{Sl}{\theta_0} \left( 1 + \frac{\theta^2}{\theta_0^2} \right)^{2S-1}$$

(6.12)

The flow velocity along stoichiometric surface is
The results for the triple flame ring velocity of the previous chapter can be used now for theoretical prediction of the lift-off height.

We recall, that this velocity is approximated by

$$U = S_L^0 \frac{(1 + \alpha)}{\sqrt{c}} - \frac{1}{\sqrt{c}} \mathcal{F}_a(\chi_s).$$

(6.14)

(here $S_L^0$ is the laminar velocity of the planar flame), with

$$\mathcal{F}_a(\chi_s) = A_a \chi_s^{1/2}$$

the correction due to the curvature of the flame.

Here

$$A_a = \frac{\beta}{(Z_s^0 \sqrt{4 \nu - 2}) (\lambda/\rho C_p)^{1/2} / (1 + \alpha)},$$

and $\chi_s$ is a mixture fraction dissipation rate.

With all these expressions in hand, the lift-off height is calculated with help of following algorithm:

- calculate the coefficients $A$ and $B$, with

$$A = \frac{\beta \theta_0}{2 \sqrt{4 \nu - 2} \sqrt{c} (1 + \alpha)},$$

(6.15)

and

$$B = \frac{\theta_0 \alpha (1 + \alpha)}{8 Z_s S_s k \sqrt{c} S_L^0}.$$  (6.16)

- solve the transcendental equation

$$(1 + x^2)^{2 S_e - 2} [1 + A x (1 + x^2)] = B,$$  (6.17)
with respect to \( x = \theta / \theta_0 \) with help of Newton method.

- compute the lift-off height \( h \)

\[
h = r(x \theta_0) \cos(x \theta_0) - \frac{a}{\theta_0}.
\]  

Here the subscript \( s \) denotes the value on the stoichiometric line.

This algorithm was effectuated for two different values of heat release, \( \alpha = 0.3 \) and \( \alpha = 0.8 \).

The value of Schmidt number is chosen to be \( S = 1.3 \) in both cases. We would like to note here, that as was discussed in [18], the choice of the Schmidt number has an impact on the stability of the lift-off solution. For values of Schmidt numbers, smaller then unity, there exists a critical value \( S_c \), such that for \( S < S_c \) the lifted flame solution can become unstable, and is subject to sudden bifurcations to blow-out. We avoid this region of instability by the choice of \( S > 1 > S_c \).

In their paper Boulanger, Vervisch, Réveillon and Ghosal [5] applied three different approximations for triple flame velocity in order to estimate the lift-off height. They compared the results with numerical simulations of full compressible axisymmetrical Navier-Stokes equations. The results show, that the best theoretical description is naturally those taking into consideration the heat release effects.

We would like to compare our results with these numerical simulations of fully compressible Navier-Stokes equations. The compact sixth order PADE numerical scheme [25] to approximate the space derivatives and Runge-Kutta method for the time derivatives was used. This allowed to the high resolution in the vicinity of the flame zone. However, the precision of these calculations demanded a sacrifice in the jet stream resolution. Only limited region around the flame base was simulated, the velocity field on the inlet delivered by the cold Landau-Squire solution. As this solution is valid only far enough from the jet exit, the simulations was done only for the lifted flames with high enough Reynolds numbers.

The boundary was treated with help of the Characteristic Navier-Stokes boundary conditions. [37]

The corrections to the lift-off heights due to the heat release effects was
The results of the two sets of simulations are presented below, compared to the new theoretical predictions we obtained in previous chapter.

The highest values of lift-off height are got for Reynolds numbers, close to the blow-up condition. As the velocity of the triple flame ring is increased by the heat release, the lift-off heights in the theory without heat release effects are over-predicted. As we see on the Figures 6.2 and 6.3, the blow-out in these cases is reached for the values of $Re$, smaller then those from DNS.

We use the new velocity approximation to calculate the lift-off heights for different values of $Re$, until the blow-out is reached.

The schematic development of the lifted flame is presented on the Figure 6.1, where the iso-contours of the reaction rate are calculated for the different values of Reynolds numbers $Re$. The values of lift-off height are also presented.

As we see, the radial component of the iso-stoichiometric surface is not constant, as was assumed in our model. In order to apply our results, we choose the parameter $r_0$ of the flame base radius to be the mean value of the axial component on the interval $(1,r_{max})$. The maximum value is found with help of the expression for the iso-stoichiometric line (6.11), maximizing it for different opening angles of the jet.

The constant $c$, corresponding to the DNS, done in [5], is $c = 0.426$.

The comparison with DNS shows us, that in both cases an important amelioration in theoretical prediction of the lift-off heights is achieved.
Figure 6.1: Lift-off heights (H) and flame base radius (R) in units of nozzle radius for different values of Re (from DNS by Boulanger et al.). The contour lines are those of the reaction rate.
Figure 6.2: Comparison of our theoretical results for lift-off heights (in units of nozzle radius) as function of Reynolds number with DNS and theoretical approximation by J. Boulanger, L. Vervisch, J. Reveillon and S. Ghosal for $\alpha = 0.3$. Line: plane case, diamonds: DNS results, asterisks: results with correction due to the radius of the flame base.
Figure 6.3: Comparison of our theoretical results for lift-off heights (in units of nozzle radius) as function of Reynolds number with DNS and theoretical approximation by J. Boulanger, L. Vervisch, J. Reveillon and S. Ghosal for $\alpha = 0.8$. Line: plane case, diamonds: DNS results, asterisks: results with correction due to the radius of the flame base.
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Chapter 7

Conclusions

In the present work dependence of the triple flame velocity on the radius of the flame base was introduced in a parametric way. The mixture fraction was treated as a function of radial component only, that allowed us to introduce the coordinate frame, where the stoichiometric iso-surface is parallel to one of the axes. The triple flame ring propagates along the stoichiometric iso-surface, and the radius remains unchanged.

This simplified model allows us to handle the original axi-symmetric equations in the analogous way to the two-dimensional case, described in [17].

The assumption of the mixture fraction linearity was done in the vicinity of the diffusion flame. This enabled the specification of the value of temperature along stoichiometric line as a linear function of the mixture fraction gradient.

Further, asymptotic analysis of the triple “ring” flame in the limit of large activation energy $\beta \to \infty$ was done and the approximative solution for temperature was found by elimination of the terms of order $O(1/\beta)$ and higher.

The comparison with high-order DNS results showed the validity of the this new laminar triple ring velocity approximation, even though the expressions we've derived are not valid in the whole domain of the triple flame existence (the approximation of the mixture fraction by a linear profile valid only when we are close enough to the diffusion flame; all the formulae was derived for the radial distances big enough, $r > 1$).
Notations

\[ c_p^i \quad \text{thermal capacity of } i\text{-th chemical species} \]
\[ c_v^i \quad \text{heat capacity at constant volume of } i\text{-th chemical species} \]
\[ h \quad \text{enthalpy} \]
\[ k \quad \text{common diffusivity coefficient} \]
\[ p \quad \text{mean pressure} \]
\[ Q \quad \text{heat release} \]
\[ R \quad \text{universal gas constant} \]
\[ t \quad \text{time} \]
\[ T, \Theta \quad \text{temperature} \]
\[ T_0 \quad \text{initial temperature} \]
\[ u, v \quad \text{mean velocity} \]
\[ w \quad \text{vorticity} \]
\[ \lambda \quad \text{coefficient of thermal conductivity} \]
\[ \rho \quad \text{density} \]
\[ Da \quad \text{Damköhler number} \]
\[ D^{ij} \quad \text{diffusivity coefficients} \]
$j_i$  
\text{diffusive fluxes}

$Le$  
\text{Lewis number}

$Ma$  
\text{Mach number}

$R_j$  
\text{reaction rates}

$r_0, c = 1 - \frac{1}{r_0^2}$  
\text{flame base radius and characteristic constant}

$S_L$  
\text{laminar flame speed, or burning velocity}

$U_\infty$  
\text{velocity of triple flame propagation}

$W_i$  
\text{molecular weight of } i\text{-th chemical species}

$Y_i$  
\text{mass fraction of } i\text{-th chemical species}

$Z$  
\text{mixture fraction}

$\alpha$  
\text{parameter of heat release}

$\beta$  
\text{Zeldovich parameter}

$\mu$  
\text{normalized mixture fraction gradient, evaluated at stoichiometric iso-surface}

$\nu_{ij}', \nu_{ij}''$  
\text{stoichiometric coefficients of species } i \text{ as reactant and product respectively}

$\dot{\rho}_i$  
\text{mass increase per unit volume due to chemical reaction}

$\chi$  
\text{scalar dissipation rate}

$(r, x, \phi)$  
\text{cylinder coordinates}

$(\xi, \eta)$  
\text{local parabolic-cylinder coordinates}
Bibliography


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Curriculum vitae

Sept. 10, 1972
Born in Sosnovy Bor, Leningrad region, Russia.

1979 – 1986
Primary and secondary school at Sosnovy Bor.

1986 – 1989
Specialized Physics and Mathematics school attached to Leningrad University.

1989 – 1994
Study at Mathematical-mechanical faculty of St. Petersburg State University, Russia, first class diploma of this University in Mathematics and Pedagogy.

1994 – 1995
Postgraduate courses in economics at Institute of Mathematical Economics of Russian Academy of Science. Diploma in economics.

1995 – 1998
Research and teaching assistant at St. Petersburg State University.

1997
Grant of the French Government for three months practical work at University Paris-Orsay, France.

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Research and teaching assistant at Seminar for Applied Mathematics, ETH Zürich.