Stellingen
behorende bij het proefschrift
IR Emission Absorption Tomography in Flames
van Robert van den Bercken
Delft, 27 januari 1998


_Dit proefschrift_

2. De invloed van katalyse op het meten van de temperatuur, met een Pt-Rh thermokoppel, in een turbulente diffusievlam, is te verwaarlozen.

_Dit proefschrift_

3. Het toepassen van absorptie-data van verschillende databases kan voor de berekening van de absorptiecoefficient van een gasvolume in een smal golflengtegebied leiden tot aanzienlijke verschillen.

_Dit proefschrift_

4. De concentratie C_2H_2 is geen goede indicator voor de roet-volumefractie in een turbulente diffusie-vlam.

_Dit proefschrift_

5. Aangezien de mens veel leert van zijn fouten, zouden ook mislukte onderzoekseresultaten gepubliceerd moeten worden. Door een gedegen literatuuronderzoek kan dit veel tijd besparen.

6. De vaste termijn van 4 jaar, die staat voor een promotieonderzoek is strijdig met het fundamentele van wetenschappelijk onderzoek; het zoeken naar het onbekende.
7. Bij het schrijven/ontwikkelen van software zou het gebruik van copy en paste vermeden moeten worden.

8. De beste kopieën zijn origineel.

9. De aandacht voor de verschillende sporten op de televisie houdt geen gelijke tred met de special effects in speelfilms.

10. 'De zwakste schakel bepaalt de sterkte van de ketting' gaat meer op voor een volleybalteam dan voor een voetbalelftal.

11. Mazzel is het optimaal benutten van je kansen.
IR Emission/Absorption
Tomography
in Flames

PROEFSCHRIFT

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus Prof. dr. ir. J. Blaauwendraad,
in het openbaar te verdedigen ten overstaan van een commissie,
door het College voor Promoties aangewezen,
op dinsdag 27 januari 1998 te 13.30 uur

door

Robert Eugène Johan VAN DEN BERCKEN

natuurkundig ingenieur
geboren te Venlo
Dit proefschrift is goedgekeurd door de promotor:
Prof. ir. C.J. Hoogendoorn

Samenstelling promotiecommissie:

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Prof.dr.Dipl.-Ing. K. Hanjalić, (Technische Universiteit Delft)
What is there left for me to do in this life,
Did I achieve what I had set in my sights,
Am I a happy man, or is this sinking sand,
Was it all worth it, was it all worth it,
Yeah, now hear my story, let me tell you about it,

........................................

Yes, it was a worthwhile experience,
It was worth it.

From: Was it all worth it, a QUEEN track from The Miracle.
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1 Introduction

1.1 Natural gas combustion

After improving the economy over the last few centuries, mankind is nowadays aware of the environmental consequences this has. The awareness has grown that human behaviour has a negative impact on the environment. Think of terms like acid rain, smog, ozone layer and greenhouse effect. The large energy consumption for industrial and household purposes is one of the major areas of interest. Different energy carriers used are fossil fuels, like oil, coal and natural gas. The latter is the most important type of fuel in the Netherlands, thanks to the discovery and exploration of one of the world’s largest natural gas reserves. With new reserves discovered every year and the combustion processes getting more efficient it is believed that natural gas will remain an important fuel for both the industry and the household appliances for the next 50 years.

One of the products from combustion is CO₂. Because it is believed that this is one of the major contributors to the greenhouse effect, regulations about the environmental emission of CO₂ get stricter. Compared to other fuels, natural gas has a relatively low carbon content and therefore it is a cleaner fuel than for instance oil or coal. Reducing the emission of CO₂ will automatically lead to a more efficient use of the natural gas. Important other products of the combustion of natural gas are nitrogen oxides. These contribute to acid rain. The NOₓ formation is very complex and not yet understood, so a lot of effort has to be made to decrease the formation of NOₓ without loss of efficiency.

For efficient combustion, the ratio of fuel to air is very critical. Therefore the mixing of the fuel and air is very important. Mixing both fuel and air before the combustion makes the process very efficient. The disadvantage of this kind of premixed combustion is the explosive nature of the mixture. For safety reasons the fuel and air are normally supplied separately. The mixing then has to occur by diffusion. The latter can either be laminar or turbulent. This gives respectively a laminar diffusion flame or a turbulent diffusion flame. Turbulent diffusion is much more effective than laminar diffusion. This is why combustion based on turbulent diffusion is much more efficient and of larger interest for research.
1. Introduction

1.2 Background

The description of laminar flames is very well understood for many years now. In a turbulent flow everything is chaotic and velocity, temperature and species concentration strongly fluctuate. To describe all these phenomena, new and complex models are needed. When these models are applied to a turbulent flame, all this is even more complicated because of the interaction with the chemistry. This is why turbulent combustion is challenging for science, both theoretically and experimentally.

In the Section Heat Transfer of the Department of Applied Physics of the Delft University of Technology a project is started to gain more insight in turbulent diffusion flames. The aim of the project is to produce an extensive database with both experimental and numerical results for various relevant quantities. For this, the Delft piloted jet diffusion flame has been designed. The setup has well-defined initial and boundary conditions. The fuel is injected in a central coaxial jet, which is surrounded by an annulus of primary air. This air flow is turbulent. To make sure that the flame is not influenced by the surrounding, the whole is placed inside a burner chamber. To avoid recirculation of combustion products inside this burner chamber, there is a second, low speed coflowing air stream shielding the fuel and primary air from the surroundings. To investigate the effect of turbulence on the combustion, the exit velocities are varied. Because of the high extinction rates for the more turbulent flames, pilot flames are used to prevent the flames from lift-off or even blow-off.

Hitherto three dissertations have appeared with respect to this project. Two of them produced mainly experimental data and the other one presented mainly of numerical simulations. A study on turbulence fluctuations in diffusion flames using Laser Induced Fluorescence is performed by De Vries (1994). Semi-quantitative determination of OH radicals is performed. In addition, NO seeded to the fuel is measured to study the mixing by the shear layer turbulence of a conserved species. The spatial structure of the flame was visualised and length scales of OH and NO concentration fluctuations were derived. Turbulence and OH structures in flames by Stroomer (1995) reports detailed information on the interaction between turbulence and chemistry in combustion. For this, Laser Doppler Anemometry is applied to determine both axial and radial velocities, both mean and fluctuations. Mean temperature is determined with thermo-couples and NO concentrations are again measured with Laser Induced Fluorescence. Despite global stability of the flames, they may be extinguished locally. Comparison of different flame properties has shed some light on the onset of these local extinguitions. Numerical modelling of turbulent natural gas diffusion flames by Peeters (1995) uses assumed PDF modeling to describe this kind of flames. The numerical code validates several simple chemistry models. Furthermore it contains phenomena like radiative heat transfer, turbulent flow and mixing of species as well as the formation of NOx. Next to these three dissertations and the present one, another dissertation will appear, describing numerical simulations based on Monte Carlo simulations. This work is done by Nooren. In addition the paper Coherent Anti-Stokes Raman spectroscopy measurements of temperature fluctuations in turbulent natural gas-fueled piloted jet diffusion flames by Mantzaras and Van der Meer (1997) appeared. They performed CARS measurements to determine mean temperature and temperature fluctuations.
The latter resulted in the rms value of the temperature fluctuations and in temperature PDFs.

1.3 Aims of this study

From the previous discussion it is clear that a lot of data regarding the Delft piloted jet diffusion flame is already available, both experimental and numerical. The aim of this study is to provide more experimental data, for quantities (and locations) still lacking, like soot volume fraction and partial pressure of H$_2$O and C$_2$H$_2$. To do so, an optical measurement technique had to be developed to determine the soot volume fraction and partial pressures. The technique has to be optical because we don't want any interaction between the measurement technique and the flow field. The experimental data will be used to validate numerical simulations, where the soot volume fraction is of interest to improve the radiative heat transfer.

The measurement technique that is applied is Infra-Red Emission Absorption Tomography (IREAT). Combining an absorption and an emission measurement in this technique, it is possible to determine the local species concentration and the local temperature simultaneously. Varying the wavelength in various well chosen intervals, the technique reveals information on different species. This way it is possible not only to measure the soot volume fraction but for instance also the partial pressure of products like H$_2$O or intermediates like C$_2$H$_2$. To calibrate the system and to fine tune some of the parameters involved, the technique is first applied to a laminar premixed flat flame. The latter is known for its extensive and accurate database regarding most quantities of interest. Unfortunately this flame is non-sooting, so it is not possible to calibrate the soot volume fraction part of the technique. For comparison a suction probe will be applied to determine the soot volume fraction at the centreline. This technique can be very simple and cheap, but it is intrusive and not very accurate.

Another simple, cheap but intrusive technique that will be used is a thermocouple. De Vries (1994) reported that it is necessary to correct the thermocouple temperature measurements in the Delft piloted jet diffusion flame not only for radiation, but also for conduction losses. One aim is to develop a new and accurate scheme to perform this conduction correction. Up to now the thermocouples were mostly used to determine the mean temperature. By choosing the right thermocouple it is also possible to determine the temperature fluctuations. Since the latter are also available from CARS measurements these can be validated.

In all the work reported previously, the measurements extended (only) to axial positions of 250 mm or 300 mm. There are two reasons to extend the measurements to larger axial positions. Firstly the flame length is about 900 mm and thus the comparisons made up to now only include about one third of the whole flame. Secondly from visualisation of the Delft piloted jet diffusion flame it is expected that most soot will be found at axial positions larger than 300 mm.
1. Introduction

1.4 Some relevant earlier studies

Flames

As can be concluded from the previous sections, the Delft piloted jet diffusion flame is a research object in the Heat Transfer Section for about 7 years now. This has resulted in several dissertations and related papers. The amount of literature on round jets in a coflow is abundant though. Most of this work has been carried out in forced convection and in vertical wind tunnels. Velocity measurements have been reported by e.g. Stärner and Bilger (1980), Stärner and Bilger (1986), Stärner and Bilger (1987) and Schefer et al. (1987). More recently, these measurements have been extended with single-point measurements, using Raman, Rayleigh and LIF techniques, see e.g. Dibble et al. (1984), Masri et al. (1988), Barlow et al. (1990) and Stärner et al. (1990). The latest measurements regard simultaneous measurements of various species, e.g. Schefer et al. (1990) and Stärner et al. (1992).

The flat flame is produced by a burner manufactured by McKenna. Temperature and OH concentration measurements have for instance been reported by Lucht (1981), Lucht et al. (1985), Kaiser et al. (1986) and De Vries (1994). Reliable numerical results can be obtained from a computer code, PREMIX (Kee et al. (1985)), see e.g. Peeters (1995).

Experimental techniques

Several experimental techniques were mentioned in the previous section, to be employed in both the flat flame and the Delft piloted jet diffusion flame. The main objective is determining the local soot volume fraction in the Delft piloted jet diffusion flame using IREAT. First reports about the determination of concentration or temperature from emission and absorption measurements are from Silverman (1949), Millar et al. (1953) and Freeman and Katz (1960). Tomography was (mostly) not included in the techniques employed, so often the quantities determined were average values over the line-of-sight. With the development of computed tomography in the seventies and eighties, emission and absorption measurements became interesting, because now it was possible to determine the local values. The method was applied for the methane concentration, Emmelman et al. (1980), and for instance nitrogen, Faris and Byer (1987a). Other investigators combined the emission and the absorption measurement to determine both temperature and species concentration, the latter mostly the soot volume fraction, Flower (1983), Hall and Bonczyk (1990) and Shimizu et al. (1990).

For comparison also two other, intrusive techniques are used. First to determine the temperature a thermocouple is applied. There is a lot of literature available about determining the temperature with a thermocouple, see e.g. Bradley and Matthews (1968), Heitor et al. (1985) or Van Maaren (1994). As simple as the measurement technique is, there are some corrections needed to determine the correct gas temperature. First is the radiation correction. This correction is rather straightforward and is applied by most investigators when the thermocouple is applied for high temperatures, e.g. Bradley and Entwistle (1961), Kersten (1992) and Heitor and Moreira (1993). The other correction regards the mismatch in temperature because of conduction through the thermocouple.
1.5. Outline of this thesis

wires. This correction is neglected by most investigators. From De Vries (1994), we
know that this is not correct when measuring the temperature profile in the Delft pi-
looted jet diffusion flame. Some literature is available about the conduction correction,
e.g. Sato et al. (1975) and Van Maaren (1994). Catalytic effects are another reason
why the thermocouple temperature can differ from the gas temperature, e.g. Lucht et
al. (1985) and De Vries (1994). With a properly chosen thermocouple it is possible
to determine not only the mean temperature, but also the fluctuations, see e.g. Ballantyne
and Moss (1977), Yule et al. (1978) or Katsuki et al. (1987).

Next to the thermocouple to validate the temperature measurements, another probe
technique is applied to validate the soot volume fraction. As a comparison also mea-
surements are done with a suction probe. One sophisticated setup is discussed by Prado
et al. (1977) and a general discussion with an extensive list of references can be found
in Heitor and Moreira (1993).

1.5 Outline of this thesis

In Chapter 2 Infra-Red Emission Absorption Tomography is introduced. The chapter
starts with a brief historical overview and some relevant studies in Section 2.1. Then
the theory will be presented. Section 2.2 begins with the derivation of determining
both temperature and species concentration from combined emission absorption mea-
surements. Since our interest is in local values, tomography has to be applied. The
rest of the section deals with the different tomographic techniques. These are split into
transform methods and iterative methods. The main difference between these methods
is the number of times the measured projection is used to calculate the local values.
At the end of the section these methods are evaluated. In Section 2.3 the experimental
setup is introduced that is applied in the experiments. To calculate the species concen-
tration it is necessary to know the absorption coefficient $k$ of the species of interest.
In Section 2.4 the absorption models are presented that are used to calculate these ab-
sorption coefficients. Besides the databases used, also the experimental setup used to
validate some of the parameters is presented. The section is ended with a discussion
about the accuracy of the technique.

After the introduction of the experimental technique employed, the different burner
configurations are introduced in Chapter 3. For calibration of the technique the laminar
premixed flat flame produced with the McKenna burner is used. This configuration is
presented in Section 3.1. After this, in Section 3.2, the Delft piloted jet diffusion flame
is introduced.

In Chapter 4 the other two experimental techniques will be described. First, in
Section 4.2, the thermocouple technique to determine the temperature. After the dis-
cussion of the experimental setup the radiation correction is presented. For the con-
duction correction a special thermocouple is used and three different methods for the
calculation of this correction are introduced. After the discussion about the accuracy
of the mean temperature, the time-resolved measurements are discussed. Then in Sec-
tion 4.3 the suction probe is introduced. This section is split in a description of the
experimental setup, the data reduction and the accuracy of the method.

After the introduction of the experimental techniques and the burner configura-
tions, the results in the flat flame are discussed in Chapter 5. The discussion starts with the thermocouple measurements, both in radial and axial traverses. These are presented in Section 5.2. Then the tomography measurements in the flat flame are presented in Section 5.3, for the two wavelengths that are applicable in the flat flame. The flat flame is non-sooting, so there is no use in measuring the soot volume fraction. Also for this technique we managed to do both radial and axial traverses. The chapter is ended with a summary with the most important conclusions regarding the measurements in the flat flame.

The most important results are presented in Chapter 6. This is the chapter with the experimental results in the Delft piloted jet diffusion flame. After a short introduction, the discussion starts with the thermocouple measurements in Section 6.2. This section is split in a section with the mean temperature and a section with the time-resolved measurements. The latter include both rms values of the temperature fluctuations and PDFs of the temperature. After this the tomography measurements are discussed in Section 6.3. This section begins with the influence of the turbulent fluctuations on the measured values. Then the three different tomographic measurements are discussed, regarding respectively soot, water vapour and acetylene. For all these measurements the emission and absorption are presented, as well line-of-sight as local data. With these profiles both the temperature and the species concentration are determined. Wherever possible, these profiles are compared with numerical simulations. In Section 6.4 the location of the reaction zone and the shear layer are discussed. For this, the flame width is used, based on the different experimental data obtained, also from other investigations. The chapter is ended with a summary of the most important conclusions.

Finally, the most important conclusions with respect to the aims of this study will be given in Chapter 7.
2 IR emission absorption tomography

2.1 Introduction

A lot of effort has been made to get experimental data in combustion processes. The used experimental techniques can be divided into two sorts of techniques. On one hand there are the non-intrusive measurement techniques and on the other hand there exist experimental techniques that are intrusive and do influence the object under investigation. This work describes the determination of temperature and species concentrations in flames. The aim was, to employ a method that is non-intrusive. So methods that use a probe, like thermocouple measurements to determine temperature (Gore et al. (1986), Jeckel and Wittig (1993), Katsuki et al. (1987) and Sato et al. (1975)) or a suction probe to determine species concentration (Dindi et al. (1991), Heitor and Moreira (1993), Seery and Zabielski (1989) and Smyth et al. (1985)) are not suited, because they most often influence the local flow pattern of the flame. Nevertheless, these methods are also used for comparison, because these methods are in principle very simple to implement and not expensive. The methods used in this thesis are discussed in Chapter 4.

Promising methods in combustion science are optical and very often a laser is used, like Coherent Anti-Stokes Raman Spectroscopy (CARS) to determine temperature (Dibble and Hollenbach (1981), Goss et al. (1989) and Mantzaras and Van der Meer (1997)) or Laser Induced Fluorescence (LIF) to determine for instance OH or NO concentrations (Smyth et al. (1985) and De Vries (1994)). A different laser technique is Laser Doppler Anemometry (LDA), but since it is normally needed to seed the flows with scattering particles, this technique is not completely non-intrusive (Goss et al. (1989), Smyth et al. (1985) and Stroomer (1995)). A great advantage of these laser methods is the fact that they lead to point measurements, since normally the main interest is in local values. When the techniques are applied to turbulent systems it is even possible to determine both the mean value and the fluctuations. The latter is important for validation of simulation models, currently extended to turbulent systems (e.g. Peeters (1995)). With most of these methods it is also possible to combine them, so the mean and fluctuation of two or more parameters can be determined at the same location, resulting in a correlation for these parameters. Next to these methods, there is also a technique that uses an optical probe to determine local temperature and con-
centration values (Coppalle and Joyceux (1994) and Mathew and Puri (1995)). The advantage of this method is that it is capable of determining local values directly. The disadvantage is that it is intrusive.

Another promising optical technique, discussed in this chapter, is Infra-Red Emission Absorption Tomography (IREAT). This technique is non-intrusive and measures the thermal emission of and the absorption by the flame. However, these measurements are integrated line-of-sight measurements and a tomographic reconstruction technique has to be used to determine local values. With computers getting faster, just as cameras and detectors, and tomographic reconstruction techniques getting better this demerit gets less important.

First reports about the determination of temperature and/or concentrations, locally or averaged over the line-of-sight, from emission and absorption are from Silverman (1949), Millar et al. (1953), Freeman and Katz (1960), Millikan (1961), Tourin and Krakow (1965), Krakow (1966) and Kuhn and Tankin (1968). Tomography was not often used at that time. Consequently the technique was not very popular and the determined values were mainly path averaged values. With the development of computed tomography in the seventies and eighties, methods like IREAT became interesting again. The method was used to determine the methane concentration (Emmerman et al. (1980) and Santoro et al. (1981)), the concentration of chlorine (Faris and Byer (1986)), nitrogen (Faris and Byer (1987a)) or flame species (Faris and Byer (1987b)). The method was also applied to determine temperature (Uchiyama et al. (1985), Crabol et al. (1990), Fisher and Burkhardt (1990), Bonczyk (1991) and Pattee and Peterson (1992)). Other investigations performed both an emission and an absorption measurement to determine both the temperature and the concentration (Flower (1983), Ray and Semerjian (1983), Flower (1989), Hall and Bonczyk (1990), Shimizu et al. (1990) and Gülder (1992)). Most investigators measured the soot volume fraction for the concentration, although the method is in principle applicable to all species. Next to all these experiments there were also investigators using more or less the same theoretical background, but their measurements were not restricted to a small wavelength region. Instead of a laser as a source or a bandpass filter to define the wavelength region, FT-IR spectra were used to determine the temperature and concentrations, mainly in sooting laminar diffusion flames (Ottesen and Stephenson (1982), Best et al. (1986), Solomon et al. (1986), Solomon et al. (1987), Solomon et al. (1988), Markham et al. (1990) and Best et al. (1991)).

For the work described in this thesis, an experimental setup is used as described in Hall and Bonczyk (1990) and Shimizu et al. (1990). The radiation is measured with an infrared detector. The wavelength is selected by the use of a bandpass filter. In our case we used three different filters to investigate the concentration of soot, water vapour and acetylene. For the absorption measurements a blackbody is used as the radiation source behind the flame. A tomographic reconstruction technique is used to determine the local values from the line-of-sight measurements. These local values are then used to calculate both temperature and species concentration.

The next section will deal with the theoretical aspects to determine the local profiles for both temperature and species concentration. In the same section some schemes to do the reconstruction (different tomographic techniques) will be presented. In Sec-
2.2. Theory

In section 2.3 the experimental setup used to perform the measurements will be presented. In the following section the different absorption models for the various species will be presented, together with the experimental setup used to validate a number of these models. The chapter ends with a discussion about the accuracy of the whole method.

2.2 Theory

This section deals with the theory of tomography, this is the theory about determining a two-dimensional field from one-dimensional measurements. Nowadays, (computed) tomography (CT) is being widely used. It is applied in geology, oceanography, a lot of different industrial applications, but it is best known from its application in medicine, in radiology. The great interest in tomography started with the introduction of X-ray computed tomography by Hounsfield (1972). With his invention he demonstrated that it was possible to reconstruct local values from path integrated measurements with high accuracy. He developed an algebraic algorithm and in 1972 he got a patent on the first CT-scanner. In 1979 he obtained the Nobel price in medicine, together with Cormack, who independently from Hounsfield developed some algorithms regarding CT. From a mathematical point of view, it was already shown by Radon (1917) that it is possible to reconstruct a two-dimensional field from path integrated one-dimensional measurements. To get an unambiguous solution, an infinite number of noiseless projections is needed. A projection is a set of line-of-sight measurements for the same angle, see Fig. 2.1. Tomography as described in this work, all refers to the parallel beam geometry. This in respect to the fan beam geometry mostly used in radiology.

To determine the temperature of a flame, the radiative intensity coming from the flame has to be measured. Assuming that the flame is in local thermodynamic equilibrium, the emitted intensity $I_t$ along a line-of-sight is equal to

$$I_t = \int_{-\infty}^{\infty} \kappa \, B(\lambda, T) \exp \left( - \int_{s}^{\infty} \kappa \, ds' \right) \, ds,$$  \hspace{1cm} (2.1)
where scattering is neglected, $\kappa$ is the local absorption coefficient, $B$ is Planck’s function and where both $\kappa$ and $T$ are dependent on the position $s$. When the absorption is small, the self-absorption may be neglected and Eq. (2.1) can be reduced to

\[
I_t = \int_{-\infty}^{\infty} \kappa B(\lambda, T) \, ds = \int_{-\infty}^{\infty} I_e \, ds, \tag{2.2}
\]

with $I_e$ the local emitted intensity. As will be seen from the measurements, it is allowed to neglect self-absorption in our case. If this is not justified, it is not allowed to use the normal tomographic reconstruction, since Eq. (2.1) does not obey the general tomographic form. Hall and Bonczyk (1990) describe a method how to overcome this self-absorption for a cylinder symmetric case. In Shimizu et al. (1990) a method is described, that solves this problem iteratively.

If $\kappa$ is known and $I_e$ is determined from the measurements, it is possible to calculate the temperature. In a flame, $\kappa$ is a function of wavelength $\lambda$, temperature $T$ and species concentrations. Since the latter two are mostly unknown in a flame, the absorption coefficient is often also not known. To overcome this problem a second measurement has to be performed. A radiation source is placed behind the flame and the absorption of the radiation of this source by the flame is determined. The radiative intensity $I_{f, BB}$ from the flame and from the source through the flame is,

\[
I_{f, BB} = I_f + I_{BB} \exp \left( -\int_{-\infty}^{\infty} \kappa \, ds \right), \tag{2.3}
\]

where $I_{BB}$ is the unattenuated intensity of the radiation source. Rearranging leads to

\[
\alpha \equiv \int_{-\infty}^{\infty} \kappa \, ds = \ln \left( \frac{I_{BB}}{I_{f, BB} - I_f} \right), \tag{2.4}
\]

where $\alpha$ is the path integrated absorption coefficient.

Generally the following will hold

\[
\kappa = k(\lambda, T) \theta, \tag{2.5}
\]

with $k$ the absorption coefficient of a certain species in $\text{m}^{-1} \text{atm}^{-1}$ as a function of wavelength and temperature, and $\theta$ its partial pressure. Using a database for $k(\lambda, T)$ and knowing the wavelength and the temperature, it is possible to determine the partial pressure (or concentration) of the component under investigation. The different absorption models for the various species under investigation are discussed in Section 2.4.

Both Eq. (2.2) and (2.4) are of the general form as presented by Radon (1917)

\[
P(t, \phi) = \int_{-\infty}^{\infty} f(x, y) \, ds, \tag{2.6}
\]

with $t$ the lateral position and $\phi$ the angle of the projection (see Fig. 2.1) and $f(x, y)$ the local field to be determined. The inverse of the Radon transform ($R^{-1}$) is needed to calculate the local field. According to Deans (1983) this is given by

\[
f(x, y) = R^{-1}(P(t, \phi)) = \frac{1}{2\pi} \int_{0}^{\pi} \int_{-\infty}^{\infty} \frac{1}{x\cos\phi + y\sin\phi - t} \frac{1}{r} \, d\phi \, dt. \tag{2.7}
\]
2.2. Theory

Figure 2.2: The backprojection of three projections. The original function is a dot at the centre of the region of interest. The reconstruction is blurred.

Because of the singularity for \( t = x \cos \phi + y \sin \phi \), this equation can normally not be solved. A number of algorithms have been developed, to calculate the local field from the path integrated profiles however. These methods can be divided into two sorts of techniques. The first are the direct or transform techniques, that use every projection just once. Examples are backprojection (BP), filtered backprojection (FBP), convolution backprojection (CBP) and the direct Fourier method (DFM). The other are the indirect or iterative methods, that have an iteration scheme and use every projection more than once. The algebraic reconstruction techniques (ART) are examples. In the next three sections, different techniques will be presented and evaluated.

2.2.1 Transform methods

Backprojection

One of the easiest ways to calculate the local field from the measured projections, is the backprojection. The projections are just smeared out over the original line-of-sight, see Fig. 2.2. In formula this can be written as

\[
f(x, y) = B(P(t, \phi)) = \int_0^{\pi} P(t, \phi) d\phi.
\]  

(2.8)

The figure reveals that the reconstructed image is blurred. To compensate for this effect, the FBP or CBP have to be applied. Another feature that is demonstrated in the figure is the star effect. The reason for this can be found in the insufficient number of projections used to do the reconstruction.

Filtered backprojection

To overcome the blur effect, a more sophisticated technique is needed. Therefore the mathematical derivation for filtered backprojection will be discussed. First the object
function \( f(x, y) \) is written as a two-dimensional inverse Fourier transform

\[
f(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(u, v) \exp(2\pi j(ux + vy)) \, du \, dv,
\]

with \( F(u, v) \) the Fourier coefficients for the frequencies \( u, v \). Transforming the rectangular coordinate system \( (u, v) \) into a polar coordinate system \( (\omega, \phi) \) leads to

\[
f(x, y) = \int_{0}^{\pi} \int_{-\infty}^{\infty} F(u, v) \exp(2\pi j\omega t) |\omega| \, d\omega \, d\phi.
\]

For the Fourier coefficients it holds

\[
F(u, v) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) \exp(-2\pi j(ux + vy)) \, dx \, dy
\]

and after transformation to the polar coordinate system

\[
F(u, v) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) \exp(-2\pi j\omega t) dt \, ds.
\]

Using Eq. (2.6) this becomes

\[
F(u, v) = \int_{-\infty}^{\infty} P(t, \phi) \exp(-2\pi j\omega t) dt.
\]

In this, the Fourier transform of the projections can be recognised,

\[
Q(\omega, \phi) \equiv F(u, v) = \mathcal{F}(P(t, \phi)).
\]

The object function now can be rewritten as

\[
f(x, y) = \int_{0}^{\pi} P^*(t, \phi) \, d\phi,
\]

where

\[
P^*(t, \phi) = \int_{-\infty}^{\infty} Q(\omega, \phi) |\omega| \exp(2\pi j\omega t) \, d\omega = \mathcal{F}^{-1}(Q(\omega, \phi) |\omega|)
\]

is the filtered projection. To get the object function, the backprojection of the filtered projection is taken, where the filtering is a multiplication with \(|\omega|\) in the frequency domain. This filter is known as the rampfilter. The effect of the filtering is demonstrated in Fig. 2.3.

A disadvantage of this method is the use of this rampfilter for noisy data. When the projection contains noise, it is definitely not bandlimited. The Fourier transform of the projection will contain significant values for higher frequencies. Applying the rampfilter will lead to very high components for the higher frequencies, which for a large extent belong to the noise. To overcome this, a different type of filter can be used. First improvement is made by the use of a cutoff frequency. Above this frequency the filter has the value 0, so noise components for frequencies higher than the cutoff frequency will be totally removed. When the filter has the same shape as the rampfilter, but uses a cutoff frequency, it is known as the bandlimiting filter. Further improvements can
be found in using a cutoff frequency and multiplying the original rampfilter with another damping filter, for instance a sinc or a cos filter (Herman (1980)). This way, also frequencies smaller than the cutoff frequency are (partially) eliminated.

One of the things to keep in mind regarding the FBP method is the DC-shift. This shift arises because of the discretisation. The first bin in the frequency domain will have a certain width, larger than 0. Because of this, more than just the zero frequency will be multiplied with 0, the value of the rampfilter in the first bin. Signal will be lost, and the result will shift down a bit, the DC-shift. This problem can be overcome by zero-padding. This means that the projection will be extended with zeros at both sides. As a result, the width of the bins in the frequency domain will decrease and the DC-shift will decrease also.

Convolution backprojection

Starting with Eq. (2.16) and writing it down in the spatial domain, leads to

\[ P^*(t, \phi) = P(t, \phi) \ast \mathcal{F}^{-1}(|\omega|). \]  \hspace{1cm} (2.17)

This shows that it is also possible to get the filtered projection, by calculating the convolution of the original projection with the inverse Fourier transform of the rampfilter. In Ramachandran and Lakshminarayanan (1971) it is demonstrated that in the spatial domain the inverse Fourier transform of the rampfilter in discrete form can be written as

\[ q(k\tau) = \begin{cases} \frac{1}{4\pi^2} & \text{for } k=0 \\ \frac{1}{2\pi k^2 \tau^2} & \text{for } k \text{ odd} \\ 0 & \text{for } k \text{ even,} \end{cases} \]  \hspace{1cm} (2.18)
where $k$ is an integer number and $\tau$ the spatial resolution. A few years later, in Shepp and Logan (1974), it was proven, that accuracy can be improved by using

$$
\hat{q}(k\tau) = 0.4 \cdot q(k\tau) + 0.3 \cdot q((k+1)\tau) + 0.3 \cdot q((k-1)\tau).
$$

(2.19)

For CBP the DC-shift is smaller than for FBP. This is because of the discretisation of the $q$ filters in the spatial domain. If the Fourier transform of this filter is taken, it is expected to give the ramp filter. For all frequencies larger than the DC component this is true, but for the first bin the Fourier transform of $q$ has a value significantly larger than 0. This makes the DC-shift smaller than for FBP and this gives also a minor difference in the results for CBP and FBP (Kak and Slaney (1988)).

**Direct Fourier method**

This method starts with the Fourier transform of the different projections. If there were an infinite number of continuous projections, the Fourier space would be completely filled. The object field now is equal to the two-dimensional inverse Fourier transform of this set of transformed projections, see Eq. (2.9) and Eq. (2.14). Unfortunately, the projections are discrete and also the number of projections is finite. To be able to perform the two-dimensional inverse Fourier transform, an interpolation has to be done in the Fourier domain. As reported by Magnusson (1993), the outcome of the reconstruction technique is very sensitive for the kind of interpolation used.

**Application of transform methods**

This section will be ended with some remarks regarding the application of transform methods. One of the things the user has to be aware of is aliasing (see e.g. Kak and Slaney (1988)). Normally an object is not bandlimited. The bandwidth of the projection data can exceed the highest spatial frequency that can be recorded with a given sample distance. This causes aliasing or spectral folding. Following Nyquist the sample frequency must be at least twice the bandwidth of the projection data. Another remark regards the number of projections needed for a good reconstruction. According to Kak and Slaney (1988) the following can be derived. Suppose there are $K$ projections under different angles, all with $L$ rays. The two-dimensional Fourier transform of each projection gives a line in the frequency domain (Fourier Slice Theorem). The angle between 2 of these lines in the frequency domain is $\pi/K$. With the highest possible frequency equal to $W$, the minimum distance between 2 points on neighbouring projections is $W\pi/K$. The distance between 2 neighbouring points in one projection is $2W/L$. To get the frequency domain equally filled, it has to hold that

$$
\frac{W\pi}{K} \approx \frac{2W}{L}
$$

(2.20)

$$
K \approx \frac{\pi L}{2}
$$

(2.21)

The number of projections must be about 1.5 times the number of rays in one projection.

On average the objects of interest in this thesis are assumed to be cylinder symmetric. This means that it is only necessary to record one projection and all the other
projections that are needed for the reconstruction are assumed to be the same. Firstly this gives a considerable speed up in measuring time. Because there is only one projection, this results also in a speed up for calculating the filtered projections. And last the algorithm is speeded up by only calculating the object field as a function of the radius instead of the whole region of interest.

2.2.2 Iterative methods

Another type of methods are the indirect or iterative methods. A description of these methods can be found in e.g. Herman and Lent (1976) and Herman (1980). The description of these methods given here follows the one as presented by Gordon (1974) and Schermer (1996). As opposed to the transform methods, every projection is used more than once. Therefore these methods are normally more time consuming.

The region of interest for the object field is divided into \( n \) different pixels, numbered \( j \), and \( m \) rays, with number \( i \). The value of the estimator of the object field \( f(x, y) \) in a pixel is equal to the average value over the pixel, \( x_j \). Now the projection along one line can be estimated by the following summation,

\[
p_i \approx \sum_{j=1}^{n} m_{i,j} x_j, \tag{2.22}
\]

where \( p_i \) is the (measured) real projection, \( m_{i,j} \) is the weight factor for pixel \( j \) crossed by ray \( i \). The general form of the iterative methods is that the pixel value \( x_j^k \) is estimated, where \( k \) indicates the iteration number. With this the pseudo projection

\[
r_i^k = \sum_{j=1}^{n} m_{i,j} x_j^k \tag{2.23}
\]

is calculated and compared with the real projection \( p_i \). As long as the difference between the two projections is larger than the desired accuracy, the pixel value is corrected and the pseudo projections are calculated again.

In the following, the characteristics of a couple of the iterative methods are presented. The various methods differ in the way that the correction is performed and the actual parameter that is minimised.

Unconstrained ART

The process is started with the initial guess for \( x^0 \), with the \( n \) elements \( x_j^0 \). This initial guess may be chosen freely. For all subsequent iterations, the pixel values are corrected by the weighted difference between the real projection \( p_i \) and the pseudo projection \( r_i^k \),

\[
x_j^{k+1} = x_j^k + \frac{p_i - r_i^k}{||m_i||^2} m_{i,j}, \tag{2.24}
\]

where

\[
||m_i||^2 = \sum_{j=1}^{n} m_{i,j}^2. \tag{2.25}
\]
2. IR emission absorption tomography

Unconstrained ART minimises the variance

\[ V = \sum_{j=1}^{n} (x_j - \bar{x})^2, \]

(2.26)

where

\[ \bar{x} = \frac{\sum_{j=1}^{n} x_j}{n}. \]

(2.27)

Constrained ART

The only difference with unconstrained ART is the fact that now \( X_1 < x_j^k < X_2 \), where \( X_1 \) and \( X_2 \) can be freely chosen. In formula

\[ x_j^{k+1} = \min \left( X_2, \max \left( X_1, x_j^k + \frac{p_i - r_i^k}{||m_{i,j}||^2} m_{i,j} \right) \right). \]

(2.28)

The solution does not necessarily satisfy minimal variance.

ART2

ART2 uses an intermediate estimator \( \hat{x}_j^k \), where

\[ \hat{x}_j^{k+1} = \hat{x}_j^k + \frac{p_i - r_i^k}{||m_{i,j}||^2} m_{i,j} \]

(2.29)

and

\[ x_j^k = \min(X_2, \max(X_1, \hat{x}_j^k)). \]

(2.30)

The pseudo projection \( r_i^k \) is still calculated with \( x_j^k \) and not \( \hat{x}_j^k \). ART2 converges to the solution of minimum variance.

ART3

All the iterative methods presented so far, did not take the accuracy of the measured projection into account. ART3 is one of the methods that does. It is designed to find a solution within a preset error tolerance \( \epsilon_i \), which may vary for every ray,

\[ |p_i - r_i^k| \leq \epsilon_i. \]

(2.31)

Initialisation may again freely be chosen. The algorithm is

\[ x_j^{k+1} = x_j^k + s_i^k \frac{m_{i,j}}{||m_{i,j}||^2}, \]

(2.32)

where

\[ s_i^k = \begin{cases} 0 & \text{if } |p_i - r_i^k| \leq \epsilon_i \\ p_i - r_i^k & \text{if } |p_i - r_i^k| > 2\epsilon_i \\ 2(p_i - \epsilon_i - r_i^k) & \text{if } p_i + \epsilon_i < r_i^k \leq p_i + 2\epsilon_i \\ 2(p_i - \epsilon_i - r_i^k) & \text{if } p_i - 2\epsilon_i \leq r_i^k < p_i - \epsilon_i. \end{cases} \]

(2.33)
2.2. Theory

ART with relaxation

To improve the convergence of the different methods it is possible to use a relaxation factor $\lambda^k$, with $0 < \lambda^k < 2$. For instance for unconstrained ART the algorithm then looks like

$$x_j^{k+1} = x_j^k + \lambda^k \frac{p_i - r_i^k}{||m_i||^2} m_{i,j}. \quad (2.34)$$

Multiplicative ART

Multiplicative ART as presented in Gordon et al. (1970) starts with the initial elements of $x^0$ all 0 or 1, but of course not all 0. Then the algorithm for the other iterations is

$$x_j^{k+1} = \left( \frac{p_i}{r_i^k} \right)^{m_{i,j}} x_j^k. \quad (2.35)$$

The advantage of this algorithm is that once an element is 0, it remains so in all subsequent iterations.

General remarks on ART

Finally some remarks about ART in general. Just as for the transform methods it is useful to perform zero-padding. For the iterative methods the region of interest normally is square, with a width equal to the length of one projection. For projections under $\pm 45^\circ$ not the complete region of interest will be covered. By zero-padding every projection such that the number of elements in that projection is at least $\sqrt{2}$ times the original number of elements, this problem is overcome.

So far it is not discussed in what sequence the projections should be used. In Herman and Meyer (1993) it is suggested to do this as orthogonal as possible. For projections like the ones reported in this thesis it is shown in Schermer (1996) that this indeed improves the reconstruction. First it speeds up convergence and secondly the profiles are more cylinder symmetric. In the last reference it is also revealed that it is not always clear when to stop the algorithm.

2.2.3 Evaluation

There is some extensive literature about the evaluation of the different reconstruction techniques, see e.g. Gordon et al. (1970), Gilbert (1972), Herman and Lent (1976), Censor (1983) and Fisher (1992). The main outcome of most of these evaluations is that it is best to do a specific evaluation for every application, because the reconstruction is strongly dependent on the object field. For our application, this evaluation is extensively described in Schermer (1996) and will be summarised here. Most of the reconstruction techniques presented in the previous section are implemented in the SNARK93 computer code, Browne et al. (1993). However, for FBP we implemented our own code, based on Fast Fourier Transform, see Van den Bercken and Van Broekhoven (1991). For the iterative methods, the permutation method as presented by Herman and Meyer (1993) was added to the SNARK93 system. The object fields under investigation have a top hat, a Gaussian or a double Gaussian shape, see
2. IR emission absorption tomography

![Graphs showing different shapes of object fields](image)

**Figure 2.4:** The different shapes of the object field used in the evaluation, (a) top hat, (b) Gaussian and (c) double Gaussian.

Fig. 2.4. The double Gaussian shape is created by subtracting a smaller Gaussian profile, in width and magnitude, from another Gaussian profile. The projections were contaminated with noise, with a standard deviation from 0 to 15% with respect to the original signal. The number of parallel rays in a single projection was 51. All this in accordance with the profiles as presented in the Chapters 5 and 6. The best results regarding the top hat function are obtained with ART. But for the (almost) noiseless projections the difference with CBP or FBP is not very large. Only the very sharp gradient at the edge is better reconstructed with ART. This difference only results in a discrepancy regarding the width of the reconstructed profile. For the Gaussian and double Gaussian shaped fields, CBP or FBP can be best used. The optimum filter function depends on the exact shape of the field and the noise. For the double Gaussian shape the cos filter is better while the bandlimited filter is better for the Gaussian shape. If the noise level for the latter is high, again the cos filter is preferred. For the results presented in this thesis only FBP is used with a cos² filter, which is not too different from the cos filter, and only the cutoff is varied. The cutoff is selected to obtain the best visual fit between the pseudo projection and the measured projection. Also agreement with traverses for slightly larger and smaller axial positions should exist.

2.3 Experimental setup

The experimental setup used for the tomographic measurements is shown schematically in Fig. 2.5. The intensities are measured with a square 1 mm² PbS detector, from Graseby Infrared. The actual detector area is about 0.75 mm in diameter, determined by an aperture stop mounted on the detector. The bandpass filters used are all from Spectrogon. The specifications of the various used filters are shown in Table 2.1. Since there are no parallel rays between the detector and the flame surface, the position where to put the filter is not obvious and so it is placed on the self-made detector housing, to minimise the amount of scattered light. The field of view of the detector is determined by the aperture on the lens between the detector and the flame surface. The diameter of this aperture is about 3 mm. This value is chosen to insures that the intensity is high enough to detect and the solid angle is so small, that the detection volume at the flame surface may be approximated as a cylinder. The lenses used are special Infrared
2.3. Experimental setup

Table 2.1: The specifications of the different bandpass filters, with \( \lambda_c \) the centre wavelength and FWHM the full width at half maximum.

<table>
<thead>
<tr>
<th>Component of interest</th>
<th>Filter</th>
<th>( \lambda_c ) (( \mu \text{m} ))</th>
<th>FWHM (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>soot</td>
<td>NB-1625-065-B</td>
<td>1.624</td>
<td>67.5</td>
</tr>
<tr>
<td>H(_2)O</td>
<td>NB-2877-053-D</td>
<td>2.877</td>
<td>53.0</td>
</tr>
<tr>
<td>H(_2)O(_4), C(_2)H(_2)</td>
<td>NB-3030-070-D</td>
<td>3.049</td>
<td>64.5</td>
</tr>
</tbody>
</table>

![Diagram](image.png)

Figure 2.5: Schematic view of the experimental setup, with SMR Signal Memory Recorder, Det detector, F bandpass filter, C chopper, A aperture, L lens, S shutter, BB blackbody and TC temperature controller.

Fused silica, with a diameter of 1 inch and a focal length of approximately 200 mm, depending on the selected wavelength. The latter also causes a different position of all the optical components with wavelength. The position of the lenses yields a magnification factor of about 2, resulting in an actual detection volume with a diameter of about 1.5 mm. The aperture between the flame surface and the blackbody radiation source is to make sure that reflections of the flame on the lens are minimised. This is necessary because it is not possible to get lenses with an anti-reflection coefficient sufficiently low for all the used wavelengths. From test measurements it was revealed that this reflection component could be significant and lead to asymmetric profiles. The radiation source employed is a blackbody radiation source from Graseby Infrared, type IR-508, with a standard aperture of 0.1 inch. The temperature of the source during the measurements was set to 1000 °C.

To improve the signal to noise ratio of the detector, the signal is modulated using
a chopper, SRS Inc. model SR540, with a frequency of about 750 Hz. The output voltage of the detector is recorded with the Signal Memory Recorder, transferred to the UNIX system and processed. All the optics are placed on a big translatable mount and the burner is kept at a fixed position. With this system it is possible to adjust the optics relative to the flame in both the axial and radial direction with a resolution of 25 μm. The accuracy for aligning the system is about 1 mm. For measuring one projection, the optics are put at the requested axial height. Then the projection is made by translating the optics relative to the flame from one side of the flame to the other side. At every measuring point measurements are done of both \( I_f \) and \( I_{f, BB} \). Before moving to the next measuring point, the system is traversed outside the flame region and the intensity of the blackbody, \( I_{BB} \), is measured.

The amplitude of the signal is determined with self-developed software. It is not determined with a lock-in amplifier because of the alternating measurement of the intensity of the flame and the intensity of the flame with the intensity of the blackbody transmitted through the flame. This alternating measurement was made possible by the use of a, self-made, shutter in front of the blackbody, which operated at a frequency of about 8 Hz. This frequency is too high to use a lock-in amplifier to determine the amplitude of both the signals with the modulation frequency of the chopper properly. Normally 12 blocks of 8192 measurements at a sampling rate of 62.5 kHz were collected. Because of the discrete sampled signal, this also determined the exact modulation frequency of the chopper. To prevent leakage in the frequency domain from the bin at the modulation frequency into neighbouring bins, the ratio between the sample frequency and the modulation frequency must be an integer. This results in a modulation frequency of the signal of 732.4 Hz.

Not only \( I_f \) and \( I_{f, BB} \) have to be measured, but also \( I_{BB} \). Since only one detector is used it is not possible to do this simultaneously with the \( I_{f, BB} \) measurement. After all the \( I_f \) and \( I_{f, BB} \) measurements at one point from the projection have been recorded, the optics are positioned in such a way, that \( I_{BB} \) can be measured. During all the measurements the thermocouple reading of the temperature controller of the blackbody is used, to correct the measured \( I_{BB} \) to the actual \( I_{BB} \) during the measurement of \( I_{f, BB} \). Including the data transfer to the UNIX system and the measurement of \( I_{BB} \), the data collection for one point in the projection takes about 2 minutes. With typically 51 points in one projection, the time to collect the data for a projection takes about 100 minutes.

Because the aim is to determine the absolute temperature of the flame, the system has to be calibrated. This has been done by placing the blackbody radiation source at the position of the flame. The intensity leaving the blackbody is determined applying Planck’s law and using the temperature of the blackbody and the wavelength of the used bandpass filter as its parameters. Measuring the amplitude of the detector signal as a function of the blackbody intensity it is possible to convert every measured amplitude to an intensity. This is simply done by linearising between two adjacent calibration points. The latter because the detector was not linear over the whole measurement region and the best line, obtained with a linear fit, lead to considerable errors, especially for the absorption measurements.
2.4 Absorption models

In this section the different absorption models, required to calculate the partial pressure or volume fraction of the components from the absorption measurements are presented. The first model regards the parameters with soot as the component of interest. After the discussion regarding soot, different databases regarding gaseous components like H₂O, CO₂ and C₂H₂ will be presented. For validation, some of these parameters are compared with experiments. On one hand measurements in the flat flame are used, see also Chapter 5. On the other hand, for λ = 2.877 μm, measurements with a self-made transmission setup are used to validate the parameters.

Soot

The model described, is the model presented by Lee and Tien (1981). Soot particles can be modeled assuming they have the same optical transitions as graphite. Since the graphite optical transitions involving the π bands are in the visible and the infrared, while the σ transitions are in the ultraviolet, only the π bands have to be considered for accurate optical properties in the visible and infrared. Following Dalzell and Sarofim (1969), the model presented here also assumes two bound and one free electron. This leads to the following dispersion equations

\[ n^2 - k^2 = 1 + \frac{e^4}{m \varepsilon} \sum_{j=1}^{2} \frac{n_j (\omega_{b_j}^2 - \omega^2)}{(\omega_{b_j}^2 - \omega^2)^2 + \omega^2 g_{b_j}^2} - \frac{e^2}{m \varepsilon \omega (\omega^2 + g_f^2)} n_f \]  \hspace{1cm} (2.36)

and

\[ 2nk = \frac{e^2}{m \varepsilon} \sum_{j=1}^{2} \frac{n_j \omega g_{b_j}}{(\omega_{b_j}^2 - \omega^2)^2 + \omega^2 g_{b_j}^2} + \frac{e^2}{m \varepsilon \omega (\omega^2 + g_f^2)} n_f g_f \]  \hspace{1cm} (2.37)

where \( m = n - jk \) is the complex refractive index, \( e \) the electron charge, \( m \) the electron mass in vacuum, \( \varepsilon \) the permittivity, \( n_j \) and \( n_f \) the bound and free electron number densities, \( \omega_{b_j} \) the natural frequency of bound electrons, \( \omega \) the frequency of radiation, \( g_{b_j} \) and \( g_f \) the damping constants of bound and free electrons and \( m^\circ \) the effective electron mass. One difference with the model as presented by Dalzell and Sarofim (1969) is the use of the effective electron mass \( m^\circ \approx m/18 \) instead of the electron mass \( m \) itself. The other differences are demonstrated in Table 2.2. Here \( n_i \) is the total number density. For the model of Lee and Tien (1981) the damping constants must be corrected for the \( T^{1/2} \) dependence, accounting for the Doppler broadening of the absorption bandwidths at flame temperatures. In Dalzell and Sarofim (1969) these damping constants are assumed to be temperature independent. The parameters \( n_i \), \( n_f \) and \( g_{b_1} \) are varied such that the predicted spectral extinction coefficient using the Mie theory gives the best agreement with experimental data in the visible and infrared ranges. A summary of all the dispersion constants used in the model of Lee and Tien (1981) is given in Table 2.3. In Lee and Tien (1981) it is furthermore stated, that the optical properties of soot are relatively independent of the fuel H/C ratio and that \( m \) is rather insensitive to temperature changes at high temperatures. The latter is important because this means that the accuracy of the optical properties is not influenced too much by an uncertainty in the determination of the flame temperature at higher levels.
Table 2.2: The dispersion constants at 300 K, according to (a) Lee and Tien (1981) and (b) Dalzell and Sarofim (1969).

<table>
<thead>
<tr>
<th>Electron</th>
<th>Number density ( n )</th>
<th>Frequency ( \omega ) ((10^{-15} \text{ s}^{-1}))</th>
<th>Damping constant ( g ) ((10^{-15} \text{ s}^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>free</td>
<td>( n_f )</td>
<td>( n_f )</td>
<td>0.54</td>
</tr>
<tr>
<td>bound 1</td>
<td>( n_1 = \frac{1}{12} n_t )</td>
<td>( n_1 )</td>
<td>1.25</td>
</tr>
<tr>
<td>bound 2</td>
<td>( n_2 = n_t - n_1 - n_f )</td>
<td>( n_2 )</td>
<td>7.25</td>
</tr>
</tbody>
</table>

Table 2.3: The dispersion constants at 1450 K, according to Lee and Tien (1981).

<table>
<thead>
<tr>
<th>Electron</th>
<th>Number density ( n ) ((\text{m}^{-3}))</th>
<th>Frequency ( \omega ) ((10^{-15} \text{ s}^{-1}))</th>
<th>Damping constant ( g ) ((10^{-15} \text{ s}^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>free</td>
<td>( 4 \cdot 10^{25} )</td>
<td>—</td>
<td>1.2</td>
</tr>
<tr>
<td>bound 1</td>
<td>( 4.07 \cdot 10^{27} )</td>
<td>1.25</td>
<td>5.9</td>
</tr>
<tr>
<td>bound 2</td>
<td>( 4.47 \cdot 10^{28} )</td>
<td>7.25</td>
<td>5.6</td>
</tr>
</tbody>
</table>

In the Delft pilot jet diffusion flame the soot particles are assumed to be smaller than 20 nm, so the Rayleigh-limit expression holds,

\[
\kappa = \frac{36 \pi n k}{(n^2 - k^2 + 2)^2 + 4n^2k^2} \lambda f_v, \tag{2.38}
\]

where \( f_v \) is the soot volume fraction. This equation is of the form of Eq. (2.5). By creating a database for \( \lambda = 1.624 \mu \text{m} \) with the temperature \( T \) as a parameter it is possible to determine the soot volume fraction from the absorption tomography measurements. Because soot absorbs as a continuum, the measurements at the other wavelengths have to be corrected for soot absorption and emission. For this reason also a database for the other wavelengths has been made.

**Gaseous components**

For the gaseous components there are in general three different band models to describe the radiative properties. The most accurate way to compute these properties is by using Line-By-Line (LBL) calculations, see Taine (1983), Hartmann et al. (1984) or Rothman (1992). This approach is the most accurate but requires large computational times and storage capacities. In most combustion applications a few cm\(^{-1}\) resolution is sufficient so that a Narrow-Band-Statistical (NBS) model, e.g. Ludwig et al. (1973) and Wieringa (1992), or a Cumulative-\( k \) (CK) model, e.g. Rivière et al. (1992) and Rivière (1994), is mostly applied. The parameters of these models are normally derived from LBL calculations. When the interest is only in obtaining heat fluxes or divergences of heat fluxes integrated over the entire spectrum, wide band models can be
used. They average the strength of lines over an entire band. For our tomography setup a bandpass filter is used to determine the wavelength region of interest. The wide band model has a wavelength region that is too coarse, making it not applicable. The NBS models have a resolution that is smaller than the bandwidth of the filters used, making them applicable. The LBL model does the calculation line by line, which means that it can definitely be used. To do this, all the lines within the bandwidth of the filter have to be averaged, just the way it is done for the NBS parameters. The easiest way to get a useful database is by using the NBS parameters and, when necessary, extending the averaging procedure to the bandwidth of the filter in use.

The Rothman (1992) database can be used for LBL calculations. It contains most atmospheric and main combustion products, 32 in total. This database can be used, to check which components absorb at a certain wavelength. For C$_2$H$_2$ no NBS parameters where found, so these are calculated for $\lambda = 3.049 \mu$m with the HITRAN database. The averaging that is used, is the same as described in Hartmann et al. (1984). A disadvantage of HITRAN is that there is still a lack of high temperature values, although the database is being updated for more than 20 years. The reason for this lack of high temperature values is found in the fact that the AFGL database (predecessor of HITRAN, McClatchey et al. (1973)) was made for use in cold atmospheres. In Taine (1983) a method is described how to correct for this lack of high temperature lines. This method is not employed for the calculations regarding the HITRAN database however.

In Fig. 2.6 the absorption coefficient for C$_2$H$_2$ is shown as a function of temperature. The data are calculated using the LBL data from Rothman (1992). The absorption coefficient is strongly non-linear for low temperatures. Consequently, a little bit of cold C$_2$H$_2$ will absorb more than a considerable amount of C$_2$H$_2$ at moderate temperature. As already mentioned, the absorption coefficient for high temperatures may be too low because of the lack of some high temperature lines in the HITRAN database.

One of the first databases regarding NBS parameters for combustion products was
the NASA database presented by Ludwig et al. (1973). For temperatures above 1200 K, these parameters are based on measurements made on long strip-burner H₂/O₂ flames. Data below 1200 K are based on extrapolations from these high temperature data and on analysis of published low temperature H₂O spectra. In Young (1977) it is proven that for H₂O the NASA data for low temperatures are not very accurate. To improve the accuracy, a database is created with the NASA data for high temperatures and the AFGL73 data from McClatchey et al. (1973) for low temperatures. In Hartmann et al. (1984) another set of NBS data for H₂O is presented. This database is based on the data of GEISA83 (1983) and AFGL83, presented by Rothman et al. (1983). Also based on this data is the database presented in Soufiani et al. (1985), for CO₂. Finally, a database regarding both H₂O and CO₂ is being used, from Soufiani (1996).

To validate the different model parameters, experiments are needed. The first set of experiments are the tomographic measurements themselves, performed in the flat flame, for \( \lambda = 3.049 \, \mu m \) and regarding water vapour (H₂O). The flame is simple and simulations in this flame are rather accurate, see Chapter 3 and 5. Assuming that the partial pressure from the simulations is correct and using the measured absorption coefficient \( \kappa \), the absorption coefficient \( k \) can be calculated, using Eq. (2.5).

For \( \lambda = 2.877 \, \mu m \) another experimental setup is used. The optical part of this setup is the same as for the tomographic measurements, see Fig. 2.5. Instead of the flame, a gas tube in a furnace is used. The tube is self-made and of a simpler design than the one described in Hartmann (1986). A schematic view of the furnace with gas tube is shown in Fig. 2.7. The furnace consists of a 180 mm diameter ceramic
tube filled with isolation material and a 82 mm diameter ceramic tube. Inside this tube there are 2 ceramic tubes for optical entrance, with in between a quartz gas tube with an inlet and an outlet. The distance between the two windows is exactly measured. Two other ceramic tubes keep the heating element at position. Near the gas tube a small type B thermocouple is placed to record the temperature of the gas sample under study. The measurements are performed under atmospheric pressure. The gaseous component under study is flushed into the gas tube and the measured value is the equilibrium value reached after about 5 minutes, depending on the component and the gas flow. To measure the absorption coefficient of a gaseous component, three measurements are performed. First the tube is flushed with N₂ and the intensity of the radiation source reaching the detector is measured. Then the tube is flushed with the gaseous component under study and the intensity is measured again. Finally, the tube is flushed with N₂ again. The intensity value for the first and the latter are averaged and are also an indication for the reproducibility. The transmission τ then is the quotient of the intensity with the gaseous component under study and the intensity with N₂. The absorption coefficient is approximated by

\[ k(T) = \frac{-\ln \tau}{pL}, \quad (2.39) \]

where \( p \) is the partial pressure, assumed to be atmospheric and \( L \) is the path length equal to the distance between the two windows of the gas tube. This absorption coefficient holds for the temperature \( T \) recorded by the thermocouple. The assumption is made that the length of the inlet is so long and the gas flow is so small, that the temperature of the gas sample is equal to the temperature of the thermocouple. For the H₂O measurements, a small liquid H₂O flow is used. This flow is so small, that all the H₂O is assumed to be evaporated before it reaches the gas tube. The uncertainty of these measurements is estimated to be 5%.

The validation starts with the H₂O parameters for \( \lambda = 3.049 \ \mu m \). In Fig. 2.8 the temperature dependence of the absorption coefficient is shown for the data of Young (1977), of Hartmann et al. (1984), of Rothman (1992) and of Souffian (1996) together with the experiments from the flat flame and a dataset based on a combination of the data of Hartmann et al. (1984) and the data of Souffian (1996). For temperatures smaller than 600 K the difference between the various database parameters is not significant. For higher temperatures, the absorption coefficient of Rothman (1992) is significantly smaller than all the others. The reason for this is the lack of hot band lines in the database for this wavelength. For high temperatures, the absorption coefficient of Hartmann et al. (1984) is also significantly smaller than for the other two databases, where the absorption coefficient of Souffian (1996) is a bit smaller than the one according to Young (1977). The measurements are about in the middle between the data of Hartmann et al. (1984) and the data of Souffian (1996). In Hartmann et al. (1984) a comparison is made between NBS calculations using the data of Hartmann et al. (1984) or the data of Young (1977) and LBL calculations. These calculations are compared with experiments presented by Burch and Gryvulak (1962). From this comparison it is revealed that for \( \lambda = 3.049 \ \mu m \) these experiments are also in the middle between the calculations done with the data of Hartmann et al. (1984) and the data
of Young (1977). It is concluded, that none of the databases presented regarding \( \text{H}_2\text{O} \) is fully applicable for this wavelength and our temperature range. The measurements and the database of Hartmann \textit{et al.} (1984) and the one of Souffiani (1996) are used to create a new database, that may be used for this specific filter. The absorption coefficient in this new database is 40\% of the absorption coefficient according to Souffiani (1996) and 60\% of the absorption coefficient according to Hartmann \textit{et al.} (1984). As can be seen in the figure, this dataset is equal to all the others for low temperatures and fits the measurements for high temperatures.

For \( \lambda = 2.877 \text{ \mu m} \) and \( \text{CO}_2 \) the absorption coefficient \( k(T) \) is presented in Fig. 2.9. In this figure the data of Ludwig \textit{et al.} (1973), of Souffiani \textit{et al.} (1985), of Souffiani (1996) and of Rothman (1992) are shown, together with the measurements performed in the flat flame. For temperatures smaller than 1300 K there is no significant difference between the data of Souffiani \textit{et al.} (1985) and the one of Souffiani (1996). Above 1300 K the most recent data are a bit higher. The data of Ludwig \textit{et al.} (1973) are smaller for temperatures lower than 1300 K and a bit higher for higher temperatures. For temperatures smaller than 500 K it is conspicuous that these data are significantly smaller than all the other data. This is due to the fact that these data are based on high temperature measurements and extrapolated for low temperatures. For low temperatures the data of Rothman (1992) are smaller than the data of Souffiani \textit{et al.} (1985) and Souffiani (1996), but for temperatures higher than 500 K the data are significantly smaller, where \( k \) is decreasing with temperature. This indicates that the hot band lines are missing in the HITRAN database. The measurements have the same magnitude as the data of Ludwig \textit{et al.} (1973) for temperatures around 1000 K, but are significantly smaller for higher temperatures. The shape of our measured data is about the same as the shape of the data of Souffiani (1996). For \( \text{CO}_2 \) a new database was created equal to 67\% of the absorption coefficient according to the data of Souffiani (1996).
At the same wavelength, \( \text{H}_2\text{O} \) also absorbs. In Fig. 2.10 the absorption coefficient \( k(T) \) according to the data of Young (1977), of Hartmann et al. (1984), of Soufiani (1996) and of Rothman (1992) is compared with the measurements. For low temperatures, the difference between all the databases is just minor. The data of Hartmann et al. (1984) and Rothman (1992) are about the same for the whole temperature range, indicating that hot bands are included in the HITRAN database. The data of Soufiani (1996) are a bit higher for all temperatures and the data of Young (1977) are significantly higher for temperatures around 1000 K and about the same as the others for higher and lower temperatures. The measurements have about the same shape as the data of Hartmann et al. (1984), Soufiani (1996) and Rothman (1992), but are significantly lower. Excluding the hot bands, the data of Rothman (1992) are assumed to be a minimum. Obviously the hot bands are included for this wavelength and component. It is believed that the assumption that the partial pressure of \( \text{H}_2\text{O} \) in the gas tube is atmospheric is not valid. Not all the water is evaporated, or not fast enough. To check this, again the tomographic measurements in the flat flame are used. From the simulations, it is known that \( p_{\text{H}_2\text{O}} = 0.17 \text{ atm, } p_{\text{CO}_2} = 0.08 \text{ atm and } T=1800 \text{ K}. \) For CO\(_2\) the absorption coefficient \( k \) of the corrected dataset will be used. For H\(_2\)O an extrapolated value of the measurements will be applied. The expected measured tomographic absorption coefficient then is \( \kappa \approx 0.17 \cdot 2.5 + 0.08 \cdot 2.3 = 0.61 \text{ m}^{-1}. \) The measured value was \( \kappa = 0.83 \text{ m}^{-1}. \) Now assume that the \( k_{\text{CO}_2} \) is correct and the \( k_{\text{H}_2\text{O}} \) must fully account for this discrepancy. Then the absorption coefficient of H\(_2\)O has to be 3.8 m\(^{-1}\)atm\(^{-1}\), which is between the absorption coefficient \( k = 4.1 \text{ m}^{-1}\text{atm}^{-1} \) according to Hartmann et al. (1984) and the absorption coefficient \( k = 3.6 \text{ m}^{-1}\text{atm}^{-1} \) according to Rothman (1992). In Hartmann et al. (1984) calculations are compared to measurements of Burch and Gryvnak (1962). For \( \lambda = 2.877 \mu\text{m} \) it can be seen that the experiments agree with the NBS calculations using the data of Hartmann et al. (1984) and using the data of Young (1977) leads to too large values. For H\(_2\)O and
\( \lambda = 2.877 \ \mu \text{m} \) the data of Hartmann et al. (1984) will be used. As revealed so far, both \( \text{H}_2\text{O} \) and \( \text{CO}_2 \) absorb at \( \lambda = 2.877 \ \mu \text{m} \). In the combustion products both these components will be present. This way it is not possible to distinguish the two components. In the flat flame and the diffusion flame the combustion is (nearly) complete, as can be seen from the results, so the ratio of the partial pressures is (nearly) constant. For a flame with methane as fuel, this ratio is theoretically 0.5. To calculate the partial pressure of just \( \text{H}_2\text{O} \), a new database is used, in which the absorption coefficient is equal to the sum of the absorption coefficient for \( \text{H}_2\text{O} \) according to Hartmann et al. (1984) and 50% of 67% of the absorption coefficient for \( \text{CO}_2 \) according to Soufiani (1996).

**Correction**

From the discussion in the previous section it is clear that Eq. (2.5) can not always be used directly to calculate the partial pressure of the gaseous component of interest, as several components can have an effect at the same time. This is the case for \( \lambda = 2.877 \ \mu \text{m} \), where \( \text{H}_2\text{O} \), \( \text{CO}_2 \) and soot absorb and \( \lambda = 3.049 \ \mu \text{m} \), where \( \text{C}_2\text{H}_2 \), \( \text{H}_2\text{O} \) and soot absorb. In these cases Eq. (2.5) has to be corrected to calculate the correct partial pressure. For \( \lambda = 2.877 \ \mu \text{m} \) a new database is created that already takes into account the ratio between the partial pressure of \( \text{H}_2\text{O} \) and \( \text{CO}_2 \). The extra correction only involves the absorption by soot. This absorption is estimated using the measurements done for \( \lambda = 1.624 \ \mu \text{m} \). From these measurements the volume fraction of soot is known. By calculating the absorption coefficient of soot for \( \lambda = 2.877 \ \mu \text{m} \) with Eq. (2.38) this absorption by soot for \( \lambda = 2.877 \ \mu \text{m} \) can be estimated. Instead of Eq. (2.5) the following holds for the calculation of the partial pressure of \( \text{H}_2\text{O} \) from the measurements at \( \lambda = 2.877 \ \mu \text{m} \),

\[
p_{\text{H}_2\text{O}} = \frac{\kappa_{\text{H}_2\text{O}} - \kappa_{\text{H}_2\text{O}}(T)}{\kappa_{\text{H}_2\text{O}}(T)},
\] (2.40)
where $\kappa_{\text{H}_2\text{O}}$ is the measured absorption coefficient for $\lambda = 2.877$ $\mu$m, $\kappa_{\text{soot}}$ is the measured absorption coefficient for $\lambda = 1.624$ $\mu$m, $k'_{\text{soot}}(T)$ is the ratio of the absorption coefficient of soot for $\lambda = 2.877$ $\mu$m and $\lambda = 1.624$ $\mu$m and $k'_{\text{H}_2\text{O}}(T)$ is the absorption coefficient of H$_2$O according to the new created database.

For $\lambda = 3.049$ $\mu$m it is a little bit more complicated to calculate the partial pressure of C$_2$H$_2$. Now the correction involves both the absorption of soot and the absorption of H$_2$O for $\lambda = 3.049$ $\mu$m. The principle is the same as the correction for the calculation of the partial pressure of H$_2$O leading to,

$$p_{C_2H_2} = \frac{\kappa_{C_2H_2} - (\kappa_{H_2O} - \frac{\kappa_{\text{soot}}}{k'_{H_2O}(T)}) / k'_{H_2O}(T)}{\kappa_{C_2H_2}(T)},$$

(2.41)

where $\kappa_{C_2H_2}$ is the measured absorption coefficient for $\lambda = 3.049$ $\mu$m, $k'_{H_2O}(T)$ is the ratio of the absorption coefficient of H$_2$O for $\lambda = 3.049$ $\mu$m and $\lambda = 2.877$ $\mu$m, $k'_{\text{soot}}(T)$ is the ratio of the absorption coefficient of soot for $\lambda = 3.049$ $\mu$m and $\lambda = 1.624$ $\mu$m and $k_{C_2H_2}(T)$ is the absorption coefficient of C$_2$H$_2$ according to the Rothman (1992) database.

Of course, if the absorption is not just from one gaseous component this is also the case for the emission. This means that it is necessary to correct the measured emission to get the emission of just the component of interest. The measured emission for $\lambda = 3.049$ $\mu$m is equal to the sum of the emissions of the various species,

$$I_{e,\lambda=3.049\mu m} = \frac{\kappa_{\text{soot}}}{k'^{\mu}_{\text{soot}}(T)} B(T_{\text{soot}}) + \frac{\kappa_{H_2O} - \kappa_{\text{soot}}}{k'_{H_2O}(T)} B(T_{H_2O}) + \kappa_{C_2H_2} B(T_{C_2H_2}).$$

(2.42)

Assuming that the temperature of all the species is the same, the following holds,

$$I_{e,\lambda=3.049\mu m} \approx \left( \frac{k'^{\mu}_{\text{soot}}(T)}{\kappa_{\text{soot}}(T)} + \frac{\kappa_{H_2O} - \kappa_{\text{soot}}}{k'_{H_2O}(T)} + \kappa_{C_2H_2} \right) B(T).$$

(2.43)

With this equation it is possible to calculate the contribution of just C$_2$H$_2$,

$$I_{e,C_2H_2} = \kappa_{C_2H_2} B(T) = I_{e,\lambda=3.049\mu m} - \left( \frac{\kappa_{\text{soot}}}{k'^{\mu}_{\text{soot}}(T)} + \frac{\kappa_{H_2O} - \kappa_{\text{soot}}}{k'_{H_2O}(T)} \right) B(T)$$

$$= I_{e,\lambda=3.049\mu m} - \left( \frac{\kappa_{\text{soot}}}{k'^{\mu}_{\text{soot}}(T)} + \frac{\kappa_{H_2O} - \kappa_{\text{soot}}}{k'_{H_2O}(T)} \right) \frac{I_{e,\lambda=3.049\mu m}}{\kappa_{\text{soot}}/k'_{H_2O}(T) + \kappa_{C_2H_2}}.$$

This finally leads to,

$$I_{e,C_2H_2} = \frac{I_{e,\lambda=3.049\mu m}}{\kappa_{\text{soot}}/k'_{H_2O}(T) + \kappa_{C_2H_2}}.$$

(2.44)

For the emission of H$_2$O at $\lambda = 2.877$ $\mu$m a similar derivation leads to,

$$I_{e,H_2O} = I_{e,\lambda=2.877\mu m} \frac{\kappa_{H_2O}}{\kappa_{\text{soot}}/k'_{H_2O}(T) + \kappa_{H_2O}},$$

(2.45)

where $I_{e,\lambda=2.877\mu m}$ is the measured emission for $\lambda = 2.877$ $\mu$m.
2.5 Accuracy

There are a number of uncertainties involved in the calculation of the temperature and the partial pressure from tomographic measurements. The first uncertainties originate from the measured signals in voltages. Then the calibration used to transform the measured signals to real intensities increases the uncertainty. With these intensities, the integrated emission and absorption are determined. Using a tomographic reconstruction technique, the local quantities are determined and wherever necessary the local profiles are corrected for the emission or absorption of other components. Finally, the temperature and partial pressure are calculated with these local quantities. In this section, the accuracy of this whole process is described. As a reference, the values near the centreline are used, since at the edges of the projections, outside the flame, values are nearly 0 and so relative errors will be insignificant.

First of all, there is the uncertainty in the measured signal. This uncertainty is due to two processes. Firstly it is influenced by the small fluctuations in the chopper frequency because of the way the amplitude of the signal is determined, see Section 2.3. Secondly the fluctuations of the signal being measured will influence the uncertainty of the measured intensity. The latter is either the intensity of the flame, the intensity of the blackbody or a combination of both. For the signal of the blackbody, the estimator of the standard deviation is of the order 0.01%. The estimator of the standard deviation for the signal of the flame is about 2%. For the combination of the intensity of the blackbody and the flame, the estimator of the standard deviation in the measured signal is approximately 0.1%.

To calculate the true intensity values of the three measurements, the calibration is used. The uncertainties in this calibration regard the standard deviation in the measured blackbody signal and in its temperature. The standard deviation in the measured blackbody signal is again 0.01%. The uncertainty in the temperature is 1 K. This results in a 0.5% uncertainty in the intensity for high intensities and 3% uncertainty in the intensity for the lower intensities. After calibration, the uncertainty in \( I_f \) is 3.6%, in \( I_{BB} \) 0.5% and in \( I_{f,BB} \) 0.6%.

With these three intensities, the path integrated absorption coefficient \( \alpha \) is calculated, using Eq. (2.4). From statistics it is derivated that,

\[
\epsilon_\alpha^2 = \left( \frac{\epsilon_{I_{BB}}}{I_{BB}} \right)^2 + \frac{\epsilon_{I_{f,BB}}^2 + \epsilon_{I_f}^2}{(I_{f,BB} - I_f)^2}, \tag{2.46}
\]

where \( \epsilon \) is the absolute uncertainty. From the measurements the following approximations are obtained,

\[
\frac{\epsilon_{I_{BB}}}{I_{BB}} \ll \epsilon_{I_f}, \quad \frac{\epsilon_{I_{f,BB}}}{I_{f,BB}} \approx \epsilon_{I_f}, \quad I_{f,BB} - I_f \approx I_{BB}.
\]

Now it follows that,

\[
\epsilon_\alpha \approx \sqrt{\frac{2}{I_{BB}}} \frac{\epsilon_{I_f}}{I_{BB}}. \tag{2.47}
\]
To decrease the absolute error in the path integrated absorption coefficient, it is best to use a $I_{BB}$ as high as possible and to use an averaging time as long as is practical. For our measurements the absolute error in the path integrated absorption coefficient is about 0.001 for the measurements with $\lambda = 1.624 \, \mu m$ and $\lambda = 3.049 \, \mu m$ and 0.003 for the measurements with $\lambda = 2.877 \, \mu m$. This means that the uncertainty is between 15 and 100% for $\lambda = 1.624 \, \mu m$, between 5 and 30% for $\lambda = 2.877 \, \mu m$ and between 3 and 10% for $\lambda = 3.049 \, \mu m$.

The next step in the process is the tomographic reconstruction, where the local profiles are calculated from the path integrated profiles. This step can be tuned by adjusting the cutoff parameter. For this tuning the knowledge of the flame and the profiles for neighboring axial positions are used. In the local profiles, one value is a non-linear function of several path integrated profiles. All this makes it very hard to derive an exact formula for the uncertainty in the local profiles relative to the uncertainty in the path integrated profiles. Using the results of Schermer (1996) it is estimated that the relative uncertainty in the local profile is the same as the relative uncertainty in the path integrated profile. This is the same as reported by Fisher (1992). For the local emission $I_e$ the standard deviation is 3.5% and for the local absorption coefficient $\kappa$ it depends on wavelength and position and varies between 3 and 100%. For the measurements with $\lambda = 2.877 \, \mu m$ and $\lambda = 3.049 \, \mu m$ these values are corrected because of the emission or absorption of other gaseous components. Using Eqs. (2.40), (2.41), (2.44) and (2.45) this gives additional uncertainties of 1% for $\lambda = 2.877 \, \mu m$ and 5% for $\lambda = 3.049 \, \mu m$.

Calculating temperature from the local emission and absorption coefficient is the following step in the process. This is done by using Planck's law, leading to

$$ T = \frac{c_2}{\lambda \ln(1 + \frac{\kappa}{I_e})}, $$

(2.48)

with $c_1 = 3.7419 \cdot 10^{-16} \, (Wm^2)$ and $c_2 = 1.4388 \cdot 10^{-2} \, (mK)$ the radiation constants and $\Delta \lambda$ the FWHM of the applied filter. The uncertainty in temperature is estimated by varying $\kappa$ and $I_e$ in Eq. (2.48). From this, it followed that for the wavelength and temperature range of interest

$$ \frac{\epsilon_T}{T} \approx \frac{1}{4} \sqrt{\left(\frac{\epsilon_\kappa}{\kappa}\right)^2 + \left(\frac{\epsilon_{I_e}}{I_e}\right)^2}. $$

(2.49)

For low temperatures the relative uncertainty in temperature $\epsilon_T/T$ is somewhat smaller than predicted with this formula. This leads to an uncertainty in temperature of 4.3% for the measurements with $\lambda = 3.049 \, \mu m$ and 2.6% for the other measurements. For measurements in a turbulent system, also a systematic error will be made. This error will be discussed in Section 6.3.2.

Finally, using Eq. (2.5) and the temperature and the local absorption coefficient, the partial pressure of the gaseous component of interest can be calculated. The standard deviation in this partial pressure (or volume fraction) is the same as for the local absorption coefficient, 10-15%, depending on wavelength. In this calculation the uncertainty in the absorption models is neglected, because there are no data available about this uncertainty.
2. IR emission absorption tomography
3 Burner configurations

Experiments in two different burner configurations are performed. The first is a pre-mixed laminar flame produced by a McKenna burner. In Section 3.1 this burner setup is discussed. This flat flame is mainly being used for testing the tomography experiments and calibrating the H₂O partial pressure measurements.

The other setup that is used is the Delft piloted jet diffusion flame burner. With this configuration, a turbulent diffusion flame is created. The main objective in our study for this setup is determining temperature, partial pressure for H₂O and soot volume fraction throughout the whole flame. In Section 3.2 this setup is described.

3.1 Flat flame

The flat flame burner used, is manufactured by McKenna and has already been used in many other investigations, see for example Lucht (1981), Lucht et al. (1985) and Kaiser et al. (1986). Because it is used so much and the configuration is relatively simple, it is well understood. Besides that it is well understood, there is a lot of data available, as well on experimental basis as on theoretical basis, from simulations (see also De Vries (1994) and Peeters (1995)). This makes the setup very appropriate for testing new experimental methods or using it as a calibration source.

In Fig. 3.1 a schematic view of the McKenna burner is given. It consists of a porous disk, 61 mm in diameter, cooled by water flowing through a spiral-shaped tube embedded in the porous disk. The flame is shielded by a nitrogen flow, issuing from a ring with inner diameter of 63 mm and outer diameter of 73 mm. This nitrogen flow is to suppress the entrainment of ambient air. It is impossible to suppress the entrainment of nitrogen though. For our line-of-sight (tomography) measurements this entrainment of nitrogen is of great importance, because this for instance influences the temperature along the measuring path. The entrainment of nitrogen will therefore have its effect on the measured emission. Since the absorption coefficient normally is a function of temperature, the measured absorption will also be influenced by the nitrogen flow. Because of the large diameter of the burner and with a large enough nitrogen flow, the flame can be regarded as a flat 1D flame for small axial positions.

The fuel that is used is methane (99.5 %), oxidiser is air. Fuel and oxidiser are mixed in the internal chamber. The flame produced, is a lean flame, with equivalence
ratio $\phi = 0.845$. The total flow rate for fuel and oxidiser is 1.39 m$^3$/hr. The flow rate for nitrogen is approximately 1.8 m$^3$/hr. The flow rates are measured with variable area mass flow meters (Fisher & Porter) and are corrected for pressure changes. As reported by Peeters (1995) the temperature of the porous disk hardly influences the flame, so the flow rate of cooling water is not critical.

3.2 Piloted jet diffusion flame

The actual measurements have been performed in the Delit piloted jet diffusion flame burner. This burner produces a stabilised axisymmetric turbulent non-premixed flame. The setup consists of a fuel stream inside two air streams, see Fig. 3.2. The fuel pipe has a diameter of 8 mm and its length is about 125 diameters. This is enough to establish a fully developed turbulent flow at the nozzle. For the primary air supply, there is an annulus. Its inner diameter is 35 mm and the outer diameter is 45 mm respectively. This burner setup is mounted on a plate, which can be tilted with respect to another plate, which is fixed to the ground. This is for the vertical alignment of the burner.

There are two stabilising mechanisms for this flame. Firstly, there are pilot flames. Near the nozzle, the inner diameter of the annulus becomes conical with a contraction of 7°, leading to an inner annulus diameter of 15 mm at the burner rim. In the fuel exit the pilot flame insert is placed. This insert is a Molybdenum-made cylindrical tube ending in a ring-shaped thin disk with inner and outer diameter of 6 and 8 mm respectively. This results in an actual fuel jet exit diameter of 6 mm. A consequence of this is that the turbulence of the fuel flow will not be fully developed, as shown in Stroomer (1995). The pilot flames issue from twelve 0.5 mm diameter holes arranged on a 7 mm diameter ring of the disk. An acetylene/hydrogen/air mixture is used for the pilot flames. The mixture has a C/H ratio equal to that of natural gas, to assure the
same basic product composition as of the main fuel (as suggested by Stårner and Bilger (1985)). The pilot flames are rich, because stoichiometric flames appeared to blow off. The Reynolds number of the pilot flames is about 500 and they are initially laminar. Their heat release is maximally about 1 % of that of flame C, which is the standard flame used for all our experiments on the piloted jet diffusion flame (see further). The other stabilising effect comes from a recirculation zone. This is established behind the 4.5 mm thick inner lip between the fuel and the primary air exit.

This burner setup is placed in a throat for a secondary air coflow, see Fig. 3.2. This secondary air flow comes from outside the building and has a temperature of about 285 K. First it flows along a ramp and a flow-straightening blanket and then through the throat, with a contraction-ratio of 4/1 in order to obtain a low velocity (0.35 m/s), low turbulence intensity flow. This coflow is to avoid recirculation of combustion products in the burner chamber, which is placed on top of the throat. The shape of the throat near the blanket is square, but it changes gradually to an octagonal cross section at the beginning of the burner chamber. Unlike the chamber used by De Vries (1994) and Stroomer (1995) our chamber is not octagonal but square. This is to make sure that there is optical access to the flame at all axial locations from one side of the flame to the other side of the flame. The burner chamber is 1.08 m high and 0.57 m side to side. The setup as described so far is designed to avoid draft and recirculation of combustion products. Because of the sharp transition between the exit of the throat.

Figure 3.2: Schematic view of the exit of the axisymmetric piloted jet diffusion flame burner (left) and side view of the throat and burner chamber surrounding this burner (all measures in mm).
3. Burner configurations

Table 3.1: Flow settings for the piloted jet diffusion flames, featuring flow rate \( \phi \), exit velocity \( u \) and Reynolds number \( Re \) of both the gas jet and the primary annular air flow.

<table>
<thead>
<tr>
<th>Flame</th>
<th>( \phi_{gas, jet} ) (g/s)</th>
<th>( u_{gas, jet} ) (m/s)</th>
<th>( Re_{gas, jet} ) (-)</th>
<th>( \phi_{air, ann} ) (g/s)</th>
<th>( u_{air, ann} ) (m/s)</th>
<th>( Re_{air, ann} ) (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.25</td>
<td>11.2</td>
<td>4.6 ( \cdot ) 10^3</td>
<td>3.73</td>
<td>2.2</td>
<td>4.4 ( \cdot ) 10^3</td>
</tr>
<tr>
<td>B</td>
<td>0.34</td>
<td>15.5</td>
<td>6.3 ( \cdot ) 10^3</td>
<td>5.20</td>
<td>3.1</td>
<td>6.2 ( \cdot ) 10^3</td>
</tr>
<tr>
<td>C</td>
<td>0.48</td>
<td>21.9</td>
<td>8.9 ( \cdot ) 10^3</td>
<td>7.40</td>
<td>4.3</td>
<td>8.6 ( \cdot ) 10^3</td>
</tr>
<tr>
<td>D</td>
<td>0.48</td>
<td>21.9</td>
<td>8.9 ( \cdot ) 10^3</td>
<td>13.47</td>
<td>7.9</td>
<td>15.7 ( \cdot ) 10^3</td>
</tr>
<tr>
<td>E</td>
<td>0.48</td>
<td>21.9</td>
<td>8.9 ( \cdot ) 10^3</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

![Images of flames A to E](image-url)

Figure 3.3: Instantaneous video images of piloted jet diffusion flames A to E, covering \( z = -35 \) to \( 400 \) mm and \( y = -95 \) to \( 95 \) mm (see Stroomer (1995)).

and the entrance of the burner chamber, there is a small recirculation zone of secondary air in every corner of the chamber. This was visualised by adding some smoke to the secondary air flow. These recirculations do not seem to influence the flame though. The test section empties into an exhaust hood which also sucks air in from the room.

As fuel, Groningen natural gas is used. Groningen natural gas consists of methane (81.29 %), ethane (2.87 %) and nitrogen (14.32 %) (by mol fraction) and a few higher hydrocarbons, oxygen and carbon dioxide (Geerssen (1980)). The composition can change day to day, but these are just minor differences and the calorific value of the gas remains the same. According to Peeters (1995) there is no significant influence on the jet flame.

In Fig. 3.3 we see instantaneous video images of the piloted jet diffusion flame of the five flames investigated by Stroomer (1995). In Table 3.1 the settings for all these flames are given. Flames A, B and C have a constant ratio of fuel and primary air flow rate with increasing Reynolds number. The primary air excess amounts 15 %.
3.2. *Piloted jet diffusion flame*

In flame D the fuel flow rate is equal to that of flame C, but the primary air excess is 112%. Flame E has again the same fuel flow rate, but has no primary air rate and no pilot flames. This flame demonstrates lift-off. The flow rates are measured with variable area mass flow meters (Fisher & Porter) and are corrected for pressure changes. Since one of our main interests is in soot, those flames that produce enough soot to measure both emission and absorption are investigated in this study. From the video images it can be seen that most of the soot is found in flames A, B and C (the bright areas in the images), with decreasing amount of soot with increasing Reynolds number. Besides that the amount of soot is decreasing, it is clear from the images that the axial position were the soot formation starts increases with increasing Reynolds number. Hitherto most of the experiments performed in these flames are done between the axial positions $x = 50$ and $x = 250$ mm. From the images it is clear that for soot measurements the experiments have to be extended to much larger axial positions. This is why all our experiments extend up to $x = 700$ mm. To capture the whole flame width at all these axial positions, as is necessary for tomography measurements, the measurements also have to be extended to larger radial positions than most of the measurements performed in earlier studies.
3. Burner configurations
4 Experimental methods

4.1 Introduction

In Chapter 2 IREAT has been introduced. This is a non-intrusive method to measure species concentration and temperature simultaneously. For comparison also two simple but intrusive experimental techniques are used. In this chapter both these techniques will be discussed.

First, thermocouples are used to determine the temperature in the flame. This technique will be discussed in Section 4.2. The discussion starts with the advantages and the disadvantages of using thermocouples. Then the used experimental setup will be presented. After this the radiation and the conduction correction, to calculate the correct mean temperature will be explained. The section is ended with the theory about determining the time-resolved temperature.

To determine the soot volume fraction at the centreline, a suction probe is used. In Section 4.3 the experimental setup is presented. This is followed by a description of the data reduction method used to calculate the soot volume fraction. The section ends with a discussion about the accuracy of these suction probe measurements.

4.2 Thermocouple

4.2.1 General

Thermocouples are one of the most widely used experimental instruments in combustion research. They are used to determine local temperatures; mean and fluctuating values (e.g. Bradley and Matthews (1968), Heitor et al. (1985) and Van Maaren (1994)). The advantages of thermocouples are the following. A thermocouple is rather easy to use. They are not so expensive as for example laser techniques. They can have a good time and spatial resolution. Unfortunately, thermocouple measurements do have some limitations. Normally the temperature measured with the thermocouple is different from the actual gas temperature. In general the limitations leading to this systematic error can be summarised as follows.

A probe inside a flow causes local and global field disturbances of either aerodynamic, thermal or chemical nature. The aerodynamic disturbances are considered to be the most serious. They may be minimised by adequate probe design. This means by
4. Experimental methods

choosing a probe as small as possible, so that it is still robust, and by putting the probe in the stream wise direction. The thermal disturbance occurs, when the thermocouple acts as a heat sink. There will be a difference between the measured temperature and the real gas temperature as a result of heat transfer between the thermocouple and its surroundings. This temperature difference is a consequence of convection, radiation and conduction and is much larger than the influence of the other effects discussed in this section, for most practical situations. This error is a function of the temperature difference between the probe and the stream as well as the probe geometry and its parameters. The error due to radiation will be discussed in Section 4.2.3 and the one due to conduction in Section 4.2.4. The chemical disturbances can be catalytic effects on the surface of the thermocouple, which in combustion experiments often is some Pt-Rh alloy. These catalytic effects can also influence the surface of the thermocouple and the properties of the wire can change. Catalysis will speed up the reactions in the flame and this can result in different gas temperatures. To reduce these catalytic effects, a coating can be used, see Heitor and Moreira (1993). However, coatings are often only stable for a few measurements. Furthermore, the composition of the thermocouple can change because of diffusion of coating molecules. Finally, the physical properties of the coatings are poorly known at elevated temperatures. In a laminar flat flame the influence of the catalytic effects can be large (see Lucht et al. (1985), Van Maaren (1994) and De Vries (1994)) especially in the flame front region. In the turbulent jet diffusion flame, with high velocities, catalytic effects will turn out to be negligible, see Section 6.2.

Thermocouples will mostly not be able to fully resolve the spatial or temporal resolution in a turbulent flame. This depends on the dimension of the probe wires and its time constant in comparison with the smallest scales in the turbulent flame, the Kolmogorov micro scale. In a turbulent flame the temperature measured with a thermocouple will therefore be an average. From Heitor and Moreira (1993) it can be concluded that the measured temperature is close to the time averaged temperature.

4.2.2 Experimental setup

In this section the experimental setup for the thermocouple measurements is discussed. In this work, a type B thermocouple has been used. It consists of a Platinum-Rhodium (6%) (Pt-6Rh) wire and a Platinum-Rhodium(30%) (Pt-30Rh) wire. The advantage of these alloys is that they can withstand temperatures up to about 2000 K and that the temperature of the cold junction (see further) is not critical. The latter due to the fact that for this type of thermocouple the difference of the thermo voltage for temperatures between 0 and 50 °C is only 3 μV and this gives only an error of 0.3 K at elevated temperatures. A limitation of the latter is that it is not possible to distinguish temperatures below 400 K.

In Fig. 4.1 the geometry of a conventional thermocouple is shown. A conventional thermocouple consists of two different conducting wires, which are welded at one end (the hot junction). The other ends of the conductors (often referred to as cold junction) have to be kept at a constant temperature. This way a potential is created, known as electro motive force, the value of which depends on the temperature differ-
Figure 4.1: Schematic representation of a conventional type B thermocouple, with two supporting 350 μm wires held by a ceramic tube.

ence between the two junctions and the materials used. For an extensive description of thermocouples the reader is referred to Benedict (1977) or Nicholas and White (1994). The thermocouple consists of two \( D = 50 \, \mu m \) wires with a length of about 5 mm, which are welded together. These are supported by wires of the same material with \( D = 350 \, \mu m \), which themselves are held by a ceramic tube. As already stated by De Vries (1994), in the piloted jet diffusion flame conduction errors appear not to be negligible. To be able to calculate an accurate conduction correction, another thermocouple geometry has been used, a so called triple thermocouple (see also Van Maaren (1994)). The geometry of this thermocouple is shown in Fig. 4.2. Again there is the hot junction between two \( D = 50 \, \mu m \) wires, but now they are supported by four \( D = 350 \, \mu m \) wires, with both alloys on each side. This way three hot junctions are created. In the rest of the thesis, the two additional junctions will be referred to as boundary junctions and the other as hot junction.

The ceramic tube of the thermocouple is placed in a steel holder, which is mounted to the traversing unit of the tomography setup (see Section 2.3). The accuracy of positioning the thermocouple is 1 mm in axial direction, relative to the burner, and 0.5 mm in radial direction. The uncertainty in the steps along the traverse is 0.025 mm. The data are recorded with a DAS-TC, 16 channel input board, from Keithley. The rejection rate used is 400 Hz. The sample frequency is about a factor of 2 lower. For the triple thermocouple the sample frequency even is a factor of 6 lower, because 3 voltages are needed for every measurement. The accuracy for the voltages is 15 \( \mu V \) for the hot junction and 25 \( \mu V \) for the boundary junctions. With a Seebeck coefficient about 10 \( \mu V/K \) this gives an uncertainty of respectively 1.5 and 2.5 K. At every position, the measured value is an average of 1000 measurements.

For the time-resolved measurements, a self-built amplifier is used. The thermocouple voltage of the hot junction is amplified with about a factor of 22. The voltage
of both the boundary junctions is not recorded in this case. The amplified signal is measured with the Signal Memory Recorder when it is digitised by a 12 bit analogue-to-digital converter. The typical sampling rate is 40 kHz, and there are 24 blocks of 32768 measurements stored on a disk of the UNIX system, for post-processing. A traverse is just done from one side of the flame to the centre, with one position doubled at the negative radial position. For \( x = 250 \) mm, the sampling rate is 250 kHz and there were just 12 blocks recorded. In this case a traverse consisted of measurements from one side of the flame to the other side of the flame.

### 4.2.3 Radiation correction

As mentioned in Section 4.2.1, the thermocouple does not read the actual gas temperature. When a thermocouple is positioned in the hot gas, there will be a balance between convective heat transfer from the hot gas to the thermocouple, conduction along the thermocouple wires and radiation. In this section the focus is on the radiation correction and the conduction is disregarded. For an extensive list of references regarding the radiation correction the reader should consult Heitor and Moreira (1993).

The radiation part can be split into radiation emitted by the thermocouple to its surroundings, radiation coming from the hot flame gases absorbed by the thermocouple and radiation originating from the surroundings absorbed by the thermocouple. The second term is often negligible because the emissivity of the gas is very low. The latter term is negligible in the case that the temperature of the surroundings is equal to room temperature. Then the intensity emitted by the surroundings, which is a function of temperature to the power of 4, is negligible compared to the intensity emitted by the (hot) thermocouple. When there is a hot wall or burner in the vicinity of the thermocouple, the latter term may have to be taken into account.

According to Bradley and Matthews (1968) the heat balance for the thermocouple
including convection and radiation, but neglecting conduction leads to

\[ T_g = T_t + \frac{\sigma \varepsilon T_t^4}{h_t}, \]  \hspace{1cm} (4.1)

with \( T_g \) the temperature of the gas, \( T_t \) the measured thermocouple temperature, \( \sigma = 5.67 \times 10^{-8} \text{ W/m}^2\text{K}^4 \) the Stefan-Boltzmann constant, \( \varepsilon \) the emissivity of the thermocouple wire at the hot junction and \( h_t \) the convective heat transfer coefficient. From Eq. (4.1) it follows that the true gas temperature can be determined from the measured thermocouple temperature by adding an extra term, known as the radiation correction. This term depends on the measured temperature to the power of 4 and on some wire and gas parameters which will be discussed below. These parameters are temperature dependent and there is a lot of literature available (see Kersten (1992)). Unfortunately there is some scatter in the data and especially for high temperatures there is a lack of data, certainly for type B thermocouples.

The wire emissivity is estimated to be equal to the values given by Bradley and Entwistle (1961). For temperatures above 1250 K these values are fitted to the following equation:

\[ \varepsilon_t = 9.35 \cdot 10^{-5} T_t + 0.06. \]  \hspace{1cm} (4.2)

The accuracy of this fit is 1.5%. The reported data are valid for Pt-10Rh. The data agree with the data reported by Touloukian and DeWitt (1970). The data for pure Pt give a lower emissivity at the same temperature, indicating that emissivity increases with Rh percentage. The values from Eq. (4.2) will be an overestimation for Pt-6Rh and an underestimation for Pt-30Rh. Assuming a constant emissivity for the hot junction, using the data that are valid for Pt-10Rh in case of the type B thermocouple will probably lead to an underestimation of the emissivity. For 1800 K this difference is estimated to be 8%, based on an extrapolation of the data for Pt and Pt-10Rh.

The convective heat transfer coefficient can be found from the following equation of the Nusselt number,

\[ Nu = \frac{h_t D}{\lambda_g}, \]  \hspace{1cm} (4.3)

with \( \lambda_g \) the thermal conductivity of the gas and \( D \) the diameter of the thermocouple. The thermal conductivity of the gas can be estimated from flue gas properties (see Geerssen (1980)),

\[ \lambda_g = 3.75 \cdot 10^{-5} T_f + 0.04, \]  \hspace{1cm} (4.4)

with \( T_f \) the film temperature, assumed to be equal to the average of the gas temperature and the thermocouple temperature. Photos taken from several hot junctions, revealed that the hot junction comes closest to a cylinder and not to a sphere (Van der Eerden (1994)). The diameter of the hot junction is estimated to be \((70 \pm 10) \mu m\). As quoted by Hinze (1959), the expression of Kramers (1946)

\[ Nu = 0.42 Pr^{0.2} + 0.57 Pr^{0.33} Re^{0.5}, \]  \hspace{1cm} (4.5)
which holds for $0.01 < \text{Re} < 10^4$, is valid. The dimensionless numbers $\text{Pr}$ and $\text{Re}$ also have to be evaluated at the film temperature. The Prandtl number is given by

$$\text{Pr} = \frac{\nu}{a}, \quad (4.6)$$

where $\nu$ is the kinematic viscosity and $a$ the thermal diffusivity. From Geerssen (1980) they are assumed to be

$$\nu = 2.50 \cdot 10^{-7} T_l - 1.43 \cdot 10^{-4} \quad (4.7)$$

and

$$a = 2.89 \cdot 10^{-7} T_l - 1.22 \cdot 10^{-4}. \quad (4.8)$$

The Reynolds number is defined as

$$\text{Re} = \frac{uD}{\nu} \quad (4.9)$$

with $u$ the mean velocity. The value of the mean velocity follows either from LDA measurements or numerical simulations.

Now it is possible to correct the measured thermocouple temperature for radiation effects, with an accuracy of 25% in the correction. This inaccuracy is mainly due to the uncertainty in the emissivity and the diameter of the thermocouple.

### 4.2.4 Conduction correction

In the previous section only the radiation correction has been treated. In this section the focus will be on the conduction correction. For this, the heat balance of Eq. (4.1) extended with the conduction term leads to (e.g. Van Maaren (1994)),

$$T_g = T_i + \frac{\sigma \varepsilon_i T_i^4}{h_t} \frac{\lambda_t}{4h_t} \frac{d^2 T_i}{dx^2}, \quad (4.10)$$

with $\lambda_t$ the thermal conductivity of the thermocouple wire and $x$ the direction along the thermocouple wire. Except for the thermal conductivity all the other parameters are already evaluated in the previous section. For the thermal conductivity the following formula is used

$$\lambda_t = 1.00 \cdot 10^{-2} (T_i - 1400) + 74.8. \quad (4.11)$$

This is the fitted thermal conductivity for a Pt-40Rh alloy according to Touloukian and DeWitt (1970), which is recommended for all Pt-Rh alloys. From Eq. (4.10) it is seen that the second derivative of the thermocouple temperature is needed to calculate the conduction correction, defined as the latter term on the right hand side of that equation. Since only the thermocouple temperature at the hot junction is known, this derivative can only be approximated.

A first attempt to calculate this second derivative assumes that the temperature distribution in the thermocouple is independent of the position of the thermocouple in the flame. This means that the temperature of the wire 1 mm away from the hot
4.2. Thermocouple

junction is equal to the temperature of that same hot junction when it is traversed 1 mm. In this case the second derivative of the thermocouple temperature at one position may be evaluated by calculating the second derivative of the measured hot junction temperatures. To get better results a smoothed temperature profile is used to calculate the second derivative. Because of the large influence of the (thicker) supporting wires, they have a larger radiation correction, this method will give only a rough indication of the conduction correction. This calculation is referred to as method a.

When a second-order equation, like Eq. (4.10), has to be solved, two boundary conditions are needed. With a conventional thermocouple these boundary conditions are unknown, but with a triple thermocouple these boundary values are measured simultaneously. Labelling these boundary junctions w(est) and e(ast), the second derivative of the thermocouple temperature can be approximated by

$$\frac{d^2 T_i}{dx^2} = \frac{T_w + T_e - 2T_i}{\Delta x^2},$$  \hspace{1cm} (4.12)

where $\Delta x$ is the length of the 50 $\mu$m thermocouple wire between the hot junction and a boundary junction, which is in this case assumed to be equal for both sides. This correction will give an overestimation of the conduction correction at most positions. The temperature profile is assumed to be parabolic. At most positions, with the temperature gradient of the flame over the thermocouple not too large, the temperature profile will be flatter near the hot junction and the biggest temperature gradient is found near the boundary junction. This correction method is referred to as method b.

A better estimation of the conduction correction is possible when the thermocouple wire between the two boundary junctions is divided into multiple smaller volumes. Then the 1-D thermal diffusion equation is solved for all these volumes using a numerical difference scheme. This calculation is referred to as method c. Suppose there are $N$ measurements in a traverse. So the gas temperature $T_g$ has to be determined for $i = 1$ to $i = N$. For every $i$ there is the hot junction temperature $T_{sc}(i)$ and there are the two boundary conditions $T_w(i)$ and $T_e(i)$. The thermocouple wire now is divided into $2M + 1$ volumes with pointer $j$, so that $j = 0$ is the volume at the hot junction. For every volume $j$ it holds

$$T_g(i, j) = T_{sc}(i, j) + \frac{\sigma e_i T_{sc}^4(i, j)}{h_t} - \frac{\lambda_i D}{4h_t} \frac{d^2 T_{sc}(i, j)}{dx^2},$$ \hspace{1cm} (4.13)

with

$$\frac{d^2 T_{sc}(i, j)}{dx^2} = \frac{T_{sc}(i, j - 1) + T_{sc}(i, j + 1) - 2T_{sc}(i, j)}{\Delta^2},$$ \hspace{1cm} (4.14)

where $\Delta$ is the length of a volume, equal to the resolution of the measurement and the index $sc$ referring to a thermocouple volume. Linearising the radiation term, this can be rewritten as

$$\left(h_t + \sigma e_i T_{sc}^3(i, j) + \frac{\lambda_i D}{2\Delta^2}\right) T_{sc}^{k+1}(i, j) =$$

$$h_t T_g(i, j) + \frac{\lambda_i D}{4\Delta^2}\left(T_{sc}^k(i, j - 1) + T_{sc}^k(i, j + 1)\right),$$ \hspace{1cm} (4.15)
where $k$ is the iteration number. In a simpler notation this leads to

$$a_P T_{P}^{k+1} = S_P + a_{WE}(T_W^k + T_E^k),$$

(4.16)

where $S_P$ is a source term and $P$ stands for the point $(i, j)$, $W$ for $(i, j - 1)$ and $E$ for $(i, j + 1)$. To speed up convergence, the method of Gauss Seidel is used instead of the method of Jacobi. The following equation is solved iteratively,

$$a_P T_{P}^{k+1} = S_P + a_{WE}(T_W^k + T_E^{k+1}).$$

(4.17)

The algorithm for the whole process is as follows:

1. estimate the gas temperature $T_g(i)$, this is the measured temperature $T_t(i)$ corrected for radiation and a conduction term according to method a,

2. calculate the temperature profile inside the thermocouple by solving Eq. (4.17) for every $i$,

3. compare the smoothed measured profile $T_t(i)$ with the calculated profile $T_{tc}(i, 0)$,

4. if no convergence, then correct the gas temperature $T_g(i)$ with $T_t(i) - T_{tc}(i, 0)$ and go to step 2.

This way the temperature profile in the thermocouple is determined and this will give a better approximation of the temperature profile in the thermocouple around the hot junction than the parabolic profile that is assumed when just the two boundary values are used to estimate the second derivative, like in method b. A disadvantage of this method is that the resolution of the measurement has to be very good so that $M$ is not to small. Also the length of the thermocouple should fit to the resolution of the measurement. The total width of the traverse must be so large that the conduction correction is negligible for the outermost measurements. This means that there is no problem extrapolating the gas temperature with $M$ points of the last determined temperature at each side of the traverse. The latter is needed to solve Eq. (4.17) for the boundary elements.

Now the three conduction correction methods will be compared for two different shapes of the measured temperature profile. In Fig. 4.3 and 4.4 two measured temperature profiles are shown, together with the conduction correction as calculated with the three different methods. The thermocouple diameter used in these calculations is $D = 70 \, \mu m$ and its length is $l = 4 \, mm$. From Fig. 4.3 it is revealed that especially for method a and c there can be a significant scatter in the calculated corrections particularly at the exterior of the flame. Both figures also demonstrate that there are significant differences between the three methods. For both used temperature profiles it holds that the correction from method a is the smallest by far and the correction with method b is the largest. Using method a seems to give a large underestimation of the conduction correction, whether the temperature gradient is considerable (Fig. 4.4) or not. Fig. 4.4 shows that this correction even can have the opposite sign in comparison with the other two correction methods. The higher correction according to method b and c indicates that the heat loss through the supporting wires is considerable. Comparing

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4.2. Thermocouple

Figure 4.3: (a) Measured temperature profile (flame C, z = 550 mm), (b) calculated conduction corrections using a diameter \( D = \) 70 \( \mu \)m and length \( l = 4 \) mm according to method a (\( \ldots \times \ldots \)), method b (\( \ldots \circ \ldots \)), method c (\( \ldots \triangle \ldots \)).

In these two methods it is demonstrated that method b indeed gives a higher correction than method c, indicating that for the used temperature profiles the assumption of a parabolic temperature profile inside the thermocouple is not correct.

In Fig. 4.5 method b and c are compared for different assumed lengths \( l \) of the thermocouple, for one measured temperature profile. With larger assumed thermocouple length, the correction with method b becomes smaller, as is expected from Eq. (4.12) and from Bradley and Matthews (1968). For method c there seems to be an asymptotic value for increasing length of the thermocouple, not necessarily equal to zero. Because of the influence of the thick wires, which radiate more than the thin wires, so that the end of the thin wires always will be cooler than the rest of the wire, there always will
be some conduction. This asymptotic value seems to agree with the correction according to method a. Only for extremely long thermocouples, method a seems to give a good approximation for the conduction correction.

The method giving the most reliable results is expected to be method c. The accuracy of the conduction correction is estimated to be 25%, mainly due to parameter uncertainty. When the conduction correction is compared to the radiation correction, they are comparable, for \( l = 4 \text{ mm} \). So for this kind of thermocouple in this type of flames, the conduction correction is not negligible.

Because of the large velocity in the Delft piloted diffusion flame the total correction, including both radiation and conduction, normally is smaller than 100 K. The
4.2. Thermocouple

Figure 4.5: Conduction correction according to method b (· · · o · · ·) and method c (· · · Δ · · ·) compared with each other for diameter \( D = 70 \) μm and different length \( l \) of the thermocouple (measurement profile of flame C, \( x = 250 \) mm). (a) \( l = 4 \), (b) \( l = 6 \) and (c) \( l = 8 \) mm.
total accuracy is estimated to be 40 K, due to the radiation and conduction correction and the statistical uncertainty in the measured temperature. For the flat flame the velocities are significantly smaller and the total correction has a maximum of about 200 K. This leads to a total accuracy of 60 K.

4.2.5 Time-resolved measurements

Time-resolved measurements done with a thermocouple suffer from the thermal inertia of the thermocouple. This means that the thermocouple normally will damp the temperature fluctuations. Neglecting the radiation and the conduction heat losses from the thermocouple, the measurements normally are compensated using the following equation (which can easily be derived from a heat balance of the thermocouple bead):

\[ T_g = T_t + \tau \frac{dT_t}{dt}, \tag{4.18} \]

where

\[ \tau = \frac{\rho C_p V}{Ah} = \frac{\rho C_p D^2}{4\lambda_g Nu} \tag{4.19} \]

is the characteristic time constant of the thermocouple, \( \rho \) the density of the thermocouple wire and \( C_p \) its specific heat at constant pressure (see Ballantyne and Moss (1977), Yule et al. (1978), Heitor et al. (1985), Katsuki et al. (1987) or Heitor and Moreira (1993)). Including the radiation losses in the heat balance leads to:

\[ T_g = T_t + \tau \frac{dT_t}{dt} + \frac{\sigma \epsilon T_t^4}{h_t}. \tag{4.20} \]

The time constant of the thermocouple depends on the heat transfer coefficient. Therefore it is a function of the local velocity, temperature and composition. To know the temporal local velocity, it is necessary to perform for instance LDA measurements simultaneously, see Heitor et al. (1985). Since no LDA measurements are done simultaneously, the mean velocity from simulations has been used. The local temperatures can be taken from the time-resolved measurements themselves. To include these temporal fluctuations of the temperature, the time constant has to be determined iteratively. Typically convergence is reached after only a few iterations. Another variable that can influence the time constant is the composition. No experimental data are available regarding the composition of the piloted jet diffusion flame. Therefore results from simulations are used again. From Heitor et al. (1985) it is known, that the composition does not have a large influence on the time constant. Only when the probe is in a methane rich area, the time constant will drop with about 65%, which is mainly due to the large difference in the thermal conductivity. Since most of the measurements are not done in a fuel rich area, the parameters are just the ones that hold for the products and do not differ to much from those of pure air, as used by Heitor et al. (1985). For this reason, the time constant also is not corrected with the factor \( F = 0.65 \) as suggested by Heitor et al. (1985).

The linearised profiles for \( \lambda_g, \nu \) and \( a \) as presented in Section 4.2.3 were only valid for temperatures larger than 1100 K. Now the parameters are also needed for lower
4.2. Thermocouple

Table 4.1: The thermocouple time constant in ms for a thermocouple with a diameter of 65 \( \mu \text{m} \) as a function of the temperature \( T \) and the velocity \( u \).

<table>
<thead>
<tr>
<th>( T ) (K)</th>
<th>( u ) (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>10</td>
</tr>
<tr>
<td>500</td>
<td>40.1</td>
</tr>
<tr>
<td>1000</td>
<td>32.3</td>
</tr>
<tr>
<td>1500</td>
<td>30.3</td>
</tr>
</tbody>
</table>

temperatures. For this reason also a linear fit for the lower temperatures has been made, resulting in:

\[
\lambda_k = 6.96 \cdot 10^{-5} T - 4.69 \cdot 10^{-3},
\]

\[
\nu = 1.55 \cdot 10^{-7} T - 3.85 \cdot 10^{-8}
\]

and

\[
a = 2.34 \cdot 10^{-7} T - 6.15 \cdot 10^{-5}.
\]

With these parameters it is possible to reproduce the dependence of the time constant on temperature and velocity as reported by Heitor et al. (1985). This means that it is not necessary to determine the time constant of the thermocouple from for instance, a forced convection decay of the temperature of the thermocouple bead after the removal of a direct-current overheating pulse as described in Lockwood and Moneib (1981).

The accuracy of this method depends on the following errors: inaccuracies in the value of \( \tau \), the response of the thermocouple which is not exactly first-order and the inability to compensate for all frequencies. The value of \( \tau \) will be inaccurate because of an uncertainty in the temperature and its fluctuation, an uncertainty in the velocity and its fluctuation and because the composition is not known. As stated before, the latter will not lead to a large error as long as the measurements are not in a flame rich part. Looking at Table 4.1 it can be concluded that an uncertainty of 50 K in the temperature also will not lead to a significant error in \( \tau \). Also it follows that the influence of the temperature fluctuations up to 500 K even will not lead to an error in \( \tau \) that is larger than about 7%. Using the fluctuating temperature instead of the mean temperature will probably not lead to very different results. From Stroomer (1995) it is known that the largest rms value for the velocity in the Delft piloted jet diffusion flame is about 4 m/s. The location where the largest velocity fluctuations occur, coincides with the location of the highest mean temperature. From Table 4.1 it is seen that in that case the influence of the velocity fluctuations will lead to an error in \( \tau \) of about 20%. From Eq. (4.18) it can be seen that this uncertainty in the thermocouple time constant will hardly influence the mean temperature, but that it mainly will affect the temperature fluctuations. Further comment on this will be given in Section 6.2.2, where the measurements will be compared with CARS measurements and simulations.
4. Experimental methods

From Heitor et al. (1985) it is clear, that the response of the thermocouple is higher than first-order. As a consequence this will lead to an overcompensation for low temperatures. As stated before, it is impossible to distinguish temperatures below approximately 400 K with a type B thermocouple and as will be shown in Section 6.2.2 this thermocouple will not suffer from this overcompensation.

Ballantyne and Moss (1977) used a 50 \( \mu \text{m} \) thermocouple also and claimed that the thermocouple bandwidth was DC-2 kHz. Heitor et al. (1985) used a 15 \( \mu \text{m} \) thermocouple, with a bandwidth of DC-5 kHz. They also did some experiments with a 40 \( \mu \text{m} \) thermocouple and claimed that its bandwidth was DC-2 kHz. Using a thermocouple with a diameter of about 65 \( \mu \text{m} \) it is expected that the frequency response will be distinguishable from the noise for frequencies up to 1 kHz. From Stroomer (1995) and Peeters (1995) it is known that typical time scales in the piloted jet diffusion flame are of the order of 1 ms, so with our thermocouple it should be possible to determine all or most of the temperature fluctuations. With the data of Table 4.1 it is expected that the thermocouple time constant is so large, that it is not possible to resolve all the turbulent fluctuations. We will come back to this subject in Section 6.2.2 where the results of the measurements are discussed.

4.3 Suction probe

4.3.1 General

One of the easiest ways of obtaining the soot volume fraction, is using a suction probe. In Fig. 4.6 a schematic representation of the experimental setup is given. A gas sample is extracted from the flame, with a pump (TSI, model 3105). The flow is monitored by a variable area mass flow meter (Fisher & Porter). To prevent leakage of water into the flow meter and pump a small water tank is placed before the flow meter. The soot is collected on a filter placed in a self made enclosure that is being kept at a constant temperature of about 100°C. This temperature ensures that no water is collected on the filter. The filter is a Teflon coated paper filter (Pallflex products corporation, type: T60A20). A water reservoir between the probe and the filter enclosure collects all the water that is condensed in the first part of the tube system in which the gas sample cools from flame temperature to about room temperature. The actual probe is a quartz tube with inner diameter 3.7 mm and outer diameter 5.4 mm. The probe is placed horizontally in the flame. The flow used, is chosen so that the velocity at the tip of the probe is just smaller than the mean axial velocity component of the flame. Because the flame is highly turbulent it is not possible to measure isokinetic (i.e. the sampling velocity matches the stream velocity), see Heitor and Moreira (1993).

4.3.2 Data reduction

Regarding the mass flows it holds that:

\[
m_{\text{total}} = \Phi_V \cdot t \cdot \rho_{\text{air}} + m_{\text{soot}} + V_{\text{H}_2\text{O}} \cdot \rho_{\text{H}_2\text{O}},
\]

(4.24)

where \( m_{\text{total}} \) is the total mass extracted from the flame, \( \Phi_V \) the volumetric flow of gas in the flow meter, \( \rho_{\text{air}} \) the density of air, \( t \) the time, \( m_{\text{soot}} \) the soot mass collected on the
filter. $V_{H_2O}$ the volume of water collected in the reservoir and $\rho_{H_2O}$ the density of water. Because the exact composition of the gas in the flow meter is unknown and changes from position to position, the density is approximated with a (constant) density of air. From Eq. (4.24) the soot mass fraction $f_m$ is obtained,

$$f_m = \frac{m_{soot}}{\Phi_V \cdot t \cdot \rho_{air} + m_{soot} + V_{H_2O} \cdot \rho_{H_2O}}. \quad (4.25)$$

The purpose of the probe measurements is to use them as a rough check for the tomography measurements. This means that the soot volume fraction $f_v$ is needed and not the soot mass fraction $f_m$. The latter can be of importance for model simulations though. To get the soot volume fraction $f_v$, the volumetric flows are used. This leads to the following expression for the total volume,

$$V_{total}(T) = V_{gas}(T) + V_{soot}(T) + V_{H_2O}(T)$$

$$= \Phi_V(T) \cdot t + \frac{m_{soot}}{\rho_{soot}} + V_{H_2O}(T_{room}) \cdot \frac{\rho_{H_2O}(T_{room})}{\rho_{H_2O}(T)}$$

$$= \Phi_V(T_{room}) \cdot \frac{T}{T_{room}} \cdot t + \frac{m_{soot}}{\rho_{soot}}$$

$$+ V_{H_2O}(T_{room}) \cdot \frac{\rho_{H_2O}(T_{room})}{\rho_{H_2O}(T)} \quad (4.26)$$

where $\rho_{soot} = 1900 \text{ kg/m}^3$ is taken as an average, constant soot density and $T$ is the temperature of the gas extracted from the flame. For the soot volume fraction it holds:

$$f_v = \frac{m_{soot}/\rho_{soot}}{\Phi_V(T_{room}) \cdot \frac{T}{T_{room}} \cdot t + \frac{m_{soot}}{\rho_{soot}} + V_{H_2O}(T_{room}) \cdot \frac{\rho_{H_2O}(T_{room})}{\rho_{H_2O}(T)}}. \quad (4.27)$$

This equation reveals that the temperature $T$ of the gas extracted from the flame has to be known to determine $f_v$. Together with the assumption of the constant soot density, this results in a larger uncertainty for $f_v$ than for $f_m$.  

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4.3.3 Accuracy

Generally speaking, probe measurements in a flow can cause local and global field disturbances of either an aerodynamic, thermal or chemical nature, see also Section 4.2.1. The aerodynamic disturbances are likely to be the most serious, although they will be minimum for an adequate probe geometry in parabolic flows, like the Delft piloted jet diffusion flame. Because of the size of the probe there will be some influence on the flow though. The thermal disturbances may arise from the probe acting as a heat sink. Since the probe is not cooled these disturbances are assumed to be negligible. The errors arising from catalytic effects will also be negligible, since our probe is a quartz probe.

The type of averaging of probe techniques is not very well understood (Heitor and Moreira (1993)). Density and concentration fluctuations in turbulent flames complicate the interpretation of the results due to the inability of the sampling system to follow these fluctuations. As suggested by Bilger (1977) it is assumed, that the measured volume fraction falls between the time and density weighted average.

Effectively quenching the chemical reactions is also of major concern when using a probe for concentration measurements (Heitor and Moreira (1993)). Since the probe is not cooled, the temperature gradient inside the probe will not be as large as it is for (water-)cooled probes. For probe measurements determining gas composition this will usually give a large uncertainty, but since the activation energy regarding soot reactions is much higher than for gas reactions, quenching is already effective at higher temperatures. If the quenching is not sufficiently effective, this will give rise to an error, equivalent to a corresponding positional error in the stream wise direction.

One of the most serious problems with probe measurements is the deposition of soot along the walls of the tube system. A solution for this problem is injecting water in the tip of the probe, see Prado et al. (1977). However, this results in a probe design that it is not simple anymore. Instead of avoiding the deposition of soot along the walls, the soot is scraped from these walls every 3 samples. This amount of soot is dried and weighted and the 3 samples are corrected corresponding to the soot mass that is collected on the filter. For the measurements this correction factor is approximately 1.6 with an error of about 15% because of soot not scraped from the wall and inadequate drying of the soot.

In the current setup it is not possible to keep the temperature above the dew point of water, so there will always be condensation. This water is collected in the water reservoir and will contain some soot also. A minor part of the soot is lost this way. To ensure that no water is collected on the filter, the filter holder is placed in a furnace with a temperature of approximately 100 °C to avoid condensation.

The same traversing unit is used as for the tomography measurements (see Section 2.3). The accuracy of positioning the probe is 1 mm in axial direction, relative to the burner, and 0.5 mm in radial direction. The uncertainty in the steps along the traverse is 0.025 mm. The accuracy in the axial direction can be worse in the case that quenching is not effective enough as discussed above.

For determining the soot volume fraction $f_v$ it is necessary to know all the volumetric flows at the temperature of the extracted gas sample, see Eq. (4.27). The temperature from the thermocouple measurement is taken as the temperature of the
gas sample. The uncertainty for the temperature is thus 40 K. This results in a relative uncertainty for the soot volume fraction of 3%.

Another unknown quantity in Eq. (4.27) is the density of soot, \( \rho_{\text{soot}} \). Assuming that the soot in the piloted jet diffusion flame does not differ much from soot in other flames and is approximately the same for all the measured positions, the density is taken to be a constant average, \( \rho_{\text{soot}} = (1900 \pm 100) \text{ kg/m}^3 \) (Boerstoel (1996)). This results in an uncertainty of 5% for \( f_v \).

To calculate the gas flow, the density of the gas has to be known. This changes from position to position and is also a function of time because of the turbulent fluctuations. Because of these changes of the flow it is not possible to correct the flow settings. The best flow that can easily be estimated is a mean flow. For this, the density of the gas is approximated with the density of air for room temperature. This gives rise for another uncertainty in \( f_v \) of 15%.

In total it can be concluded that the uncertainty for \( f_v \) is 25%, with the possibility that due to ineffective quenching the value of the soot volume fraction corresponds to an axial position larger than the axial position where the gas sample is taken.
4. Experimental methods
5 Flat flame results

5.1 Introduction

In this chapter results of measurements in the flat flame will be discussed. The measurements consist of thermocouple measurements to determine the temperature and tomography measurements to determine both temperature and partial pressure of H$_2$O. The flat flame, produced by the McKenna burner, is a good study or calibration object. Many researchers have used it for experiments, see for example Lucht (1981), Lucht et al. (1985), Kaiser et al. (1986) and De Vries (1994). For validation of the temperature, recent CARS measurements of Mantzaras (1996) are used. There is also a reliable computer code for this type of flame, PREMIX (Kee et al. (1985)), using the Warnatz chemistry model (Warnatz (1984)), see for example Peeters (1995). With this extensive amount of available data the flat flame is a useful object to tune the parameters for the experiments described in this work. Next to this it will also provide an indication of the accuracy of the methods. For both measurement techniques the experiments exist of an axial traverse as well as radial traverses. The thermocouple measurements will be discussed in Section 5.2 and the tomography measurements in Section 5.3. The chapter ends with a summary of the most important conclusions.

5.2 Thermocouple measurements

In this section the thermocouple measurements performed in the flat flame, described in Section 3.1, will be discussed. The purpose of these measurements is twofold. First they are done to see how accurate the thermocouple measurements are and whether the parameters have to be tuned. Secondly these measurements will give an indication about how flat the flat flame really is. To do so, first a radial traverse is done. These measurements are corrected with all the three methods described in Section 4.2.4. The measurements demonstrate that there is a big difference between the results using method a and the results from the other two methods. With the assumption that the small difference between method b and c is equal for all the positions measured, it is possible to correct an axial traverse with method b and compensate it to get the results that would have been obtained when method c was applied. These last measurements than are compared with CARS measurements and predictions from PREMIX. With
5. Flat flame results

Figure 5.1: Measured thermocouple temperature in the flat flame at \( x = 10 \, \text{mm} \), uncorrected (\( \times \)) and, corrected with method c (\( \cdots \circ \cdots \)).

Figure 5.2: The radiation correction (\( \triangle \)) and the conduction correction (\( \cdots \times \cdots \)) for the measurement in the flat flame at \( x = 10 \, \text{mm} \).

In this comparison it is possible to tune the parameters used in the methods.

Radial traverse

In Fig. 5.1 the measured and corrected temperature profile for \( x = 10 \, \text{mm} \) are shown. From this figure it is clear that the flat flame indeed is rather flat. The uncorrected temperature at \( y = 15 \, \text{mm} \) is about 40 K lower than the temperature at \( y = -25 \, \text{mm} \). For the temperature corrected with method c this difference is about 50 K. The relative difference is respectively 2.4 and 2.7%. Also it can be seen that the temperature gradient in the radial direction is less than infinite at the exterior of the flame. From this it is concluded, that at this axial position the nitrogen coflow does influence the profile.

The radiation and the conduction correction for the measurement in the flat flame
5.2. Thermocouple measurements

![Graph showing ΔT (K) vs y (mm) with symbols indicating different methods.]

Figure 5.3: The conduction correction for the thermocouple measurement in the flat flame at \( z = 10 \) mm, method a (△), method b (×) and method c (○).

for \( x = 10 \) mm can be seen in Fig. 5.2. The radiation correction is 0 K outside the flame, as expected, and inside the flame this correction is approximately constant, with a value of about 87 K. The conduction correction is nearly 0 K outside the flame. These small values, larger than zero, are due to the fact that there is some statistical fluctuation in the measured temperatures leading to a certain change in derivative of the temperature. In the core of the flame the conduction correction is fairly constant, with a value of about 110 K. At the exterior of the flame, where the temperature (and its derivative) changes significantly, there is a peak in the conduction correction, with a maximum value of about 180 K. So even in a flame without a radial temperature gradient, using a thermocouple with supporting wires that are significantly thicker than the thermocouple wires, the contribution of the conduction correction to the total correction can be significant and in this case it even is the major contribution to the whole correction.

Most measurements regarding the flat flame are done for \( y = 0 \) mm and varying \( x \), a so called axial traverse (see Schoenung and Hanson (1981), Cattolica (1982) and Kaiser et al. (1986)). Because the calculations done with PREMIX are also 1D all the variables are just a function of the axial position. When an axial traverse is done with the thermocouple, it is not possible to correct the measurements for conduction using either method a or method c. To know what is the systematic error in case an axial traverse is corrected with method b, the radial traverse is corrected for all the three methods. In Fig. 5.3 the conduction correction for all the methods applied to the measured radial profile for \( x = 10 \) mm is given. As can be expected, method a gives a conduction correction close to zero inside the core region. This method underestimates the conduction correction completely, in this case for about 110 K. When method b and method c are compared, it can be seen that the first overestimates the correction with about 30 K, independent of the radial position, for positions inside the core region.
5. Flat flame results

![Graph showing temperature gradient](image)

**Figure 5.4:** The radiation (\(\triangle\)) and the conduction correction (\(\cdots \times \cdots\)) calculated with method b for the axial traverse in the flat flame.

**Axial traverse**

In Fig. 5.4 the radiation and the conduction correction for the axial traverse in the flat flame are shown using method b. From this figure it is revealed that both the corrections are almost constant for axial position larger than 5 mm. It now is assumed that this will also hold when method c would have been applied and that the difference between the two correction methods is not a function of the axial position, for \(x > 5\) mm. To calculate the correct temperature for the axial traverse, this measurement is corrected with method b and additionally the temperature for the whole traverse is corrected with another 30 K. The discrepancy for axial positions smaller than 5 mm is due to catalytic effects (Lucht *et al.* (1985) and De Vries (1994)). The thermocouple used was not coated and so the Pt and the Rh will act as a catalyst inside the reaction zone. For the flat flame used in these experiments, this reaction zone is situated at about 2 mm above the burner surface and nearly all the reactions are ended within 10 mm above the burner (De Vries (1994) and Peeters (1995)). This is consistent with the shape of the measured axial thermocouple profiles.

In Fig. 5.5 the corrected measurements are compared with numerical calculations performed with the PREMIX code and with CARS measurements also performed in this flame. To investigate the influence of the settings of the different parameters, the measurements have been corrected varying the value of the diameter of the thermocouple bead or the length of the thermocouple wire. The major uncertainty in the thermocouple correction measurement is the value of the diameter of the thermocouple bead. This diameter is varied between 70 and 50 \(\mu m\). Besides this, also one correction is done with the length of the thermocouple 5 instead of 4 mm.

The agreement between the CARS measurements and the simulations is good. Only the axial temperature gradient of the simulations is a little bit steeper, leading to a maximum discrepancy of about 20 K. The difference in the gradient is probably due to slightly different flow settings. The axial temperature gradient can be derived
from the following equation:

$$\rho u C_p \frac{dT}{dx} = Q_{\text{rad}},$$  \hspace{1cm}(5.1)$$

where $Q_{\text{rad}}$ is the radiation source term. The latter is a function of the composition and the radiation parameters of the radiating gaseous components. These parameters are merely constant and the composition does not change a lot as long as the region of interest is in the product zone. Consequently this radiation source term can be assumed to be constant. When the flow settings will be different during the experiment, compared to the settings in the calculation, the $\rho u$ term also will have a different value.

As already stated, the radiation source term is constant, so this automatically leads to a change in the axial temperature gradient too. When the velocities are larger than assumed in the simulations, the axial temperature gradient in the experiments will be smaller than follows from the predictions.

For all the thermocouple measurements it is clear that for small axial positions ($x < 7 \text{ mm}$) catalytic effects do play a significant role. For comparison with the CARS measurements and the simulations, only the region $10 < x < 40 \text{ mm}$ is used. First it can be seen that the gradient of the thermocouple measurements is even smaller than the gradient of the CARS measurements. This difference in gradient is so large, that it probably is not only due to different flow settings. For the correction with the standard dimensions ($l = 4 \text{ mm}, D = 70 \mu \text{m}$) the thermocouple temperature is higher for the whole traverse. For $x = 10 \text{ mm}$ the difference is just 2 K with the simulations and 20 K with the CARS measurements, whereas for $x = 40 \text{ mm}$ this difference is respectively 67 K and 62 K. For decreasing diameter or increasing length of the thermocouple it can be seen, that the corrected temperature decreases. For the calculation with $l = 4 \text{ mm}, D = 65 \mu \text{m}$ the differences for $x = 10 \text{ mm}$ are respectively -20 K and -2 K and for $x = 40 \text{ mm}$ respectively 47 K and 42 K. Since the length of the thermocouple is measured to be (4.0 ± 0.2) mm and from photos the diameter of the thermocouple is not expected to be smaller than 65 $\mu \text{m}$ the combination $l = 4 \text{ mm}, D = 65 \mu \text{m}$ is used for all the further measurements. Taking into account the accuracy of the thermocouple measurement and the radial gradient of the flat flame, the thermocouple measurement corrected with $l = 4 \text{ mm}, D = 65 \mu \text{m}$ is in good agreement with both the simulations or the CARS measurement.

5.3 Tomography measurements

The flat flame is not just a good calibration object for the thermocouple measurements, but also for the IREAT measurements. To test the accuracy of this latter method and the used parameters, measurements are done for $\lambda = 3.049$ and $2.877 \mu \text{m}$. It is no use to perform measurements for $\lambda = 1.624 \mu \text{m}$ in this flame because no soot is formed in this laminar premixed methane flame. The measurements are performed at the axial positions $x = 4, 10, 20$ and $30 \text{ mm}$ above the burner surface. These positions were chosen, to be sure that the entrainment of nitrogen does not influence the measurements significantly and a substantial part of the path length is inside the potential core. The discussion starts with an extensive discussion of the measurements for $x = 4 \text{ mm}$ and
5. Flat flame results

\[ \lambda = 3.049 \, \mu m, \text{ after which the results at the other heights for the same wavelength follow.} \]

Since the tomographic reconstruction of the measurements for \( \lambda = 2.877 \, \mu m \) is nearly the same, just the final results of these measurements are presented.

In Fig. 5.6 the measured intensity profiles \( I_s, I_{BB} \) and \( I_{L, BB} \) are shown. The first and the latter are projections of a cross section of the flame, see Fig. 2.1. The \( I_{BB} \) profile is not perfectly flat as is expected. This is due to small temperature changes of the blackbody radiation source (< 1 K). By measuring this intensity frequently, it is possible to take these temperature changes into account. The local emitted intensity profile \( I_o \), given in Fig. 5.7, is calculated with the FBP technique described in Section 2.2. The profile has a very steep gradient and is nearly flat inside the flame region. By integrating the local profile, like in Eq. (2.2), it is possible to check whether the reconstruction has given a good solution. This profile is also shown in Fig. 5.6a and it can be seen that the reconstruction is quite satisfactory.

The line-of-sight absorption profile \( \alpha \) is calculated using the three measured profiles and Eq. (2.4). In Fig. 5.8 this integrated profile is shown as well as the integrated local absorption coefficient. This local absorption coefficient is presented in Fig. 5.9 and also calculated with the FBP technique described in Section 2.2. For this local profile it also holds that there is a steep gradient at the flame edge and inside the flame region the value is nearly constant. The measured absorption also reveals that self-absorption may be neglected.

From the two local profiles in Fig. 5.7 and 5.9 and using Planck's law it is possible to calculate the mean local temperature, see Fig. 5.10. In this figure also the temperature measured with CARS and calculated with PREMIX is shown. These temperatures coincide at this axial position. The reader should keep in mind that both the CARS measurement and the calculations with PREMIX are 1D, so the radial profiles shown in the figure (the dotted and the dashed line) are just an extension of the centre-line value for easier visual comparison. The tomography temperature is 150 to 300 K.
Figure 5.6: The line-of-sight intensities for the flat flame and \( \lambda = 3.049 \ \mu m \), at \( z = 4 \ mm \), (a) \( I_t \), measured (---) and integrated from Fig. 5.7 (---) and (b) \( I_{t, \text{BB}} \) (---) and \( I_{\text{BB}} \) (---).

higher, where the largest differences are found at the exterior of the flame and near the centreline of the flame. The higher values at the centreline are due to the dip of the local absorption coefficient at this position. This dip is attributed to the fluctuations in \( \alpha \) near the centreline. The line-of-sight absorption profile in Fig. 5.8 seems to be flat or even have a small dip near the centreline, leading to a considerable dip in the local absorption coefficient profile. The higher values of the temperature at the exterior of the flame are due to the difference in the width of the local emission and the local absorption profile, see Fig. 5.7 and Fig. 5.9. Because the absorption coefficient profile is smaller than that of the emitted intensity, due to the less steep gradient, the temperature will be larger at the positions where the local absorption coefficient is already decreasing, while the local emission profile still has the same value. For the other radial positions the difference in temperature is at least 150 K and so significantly larger than the uncertainty in the measurement. To improve the results the reconstruction will be done differently. Some a-priori knowledge will be used.

Because the flame is supposed to be 1D, the sensitivity of the results can be tested
5. Flat flame results

**Figure 5.7:** The reconstructed local emission profile for the flat flame and $\lambda = 3.049 \, \mu m$, at $x = 4 \, mm$.

**Figure 5.8:** The line-of-sight absorption profile for the flat flame and $\lambda = 3.049 \, \mu m$, at $x = 4 \, mm$, measured (---) and integrated from Fig. 5.9 (---).

by assuming a local profile with a certain width and height and integrating this profile to see if it fits the measurements. In Fig. 5.11 and Fig. 5.13 the assumed profiles of respectively the local emission and the local absorption coefficient are shown, that result in a satisfying reconstruction. In Fig. 5.12 and Fig. 5.14 the corresponding integrated profiles and the measurements are given. From these figures it is clear that the assumed flat profiles also give a good reconstruction. This is also an indication that the flat flame indeed may be assumed as a 1D flame. In Fig. 5.15 (a)-(c) the measurements and the integrated profiles of the emission profile are given for the other three heights, $x = 10, 20$ and $30 \, mm$. This figure demonstrates that the flame width decreases with increasing height. This results also in a decrease of the measured intensity profile. For these axial positions an assumed flat profile leads to good results, although with increasing height the fit at the exterior of the flame is more and more too small. It
is concluded that the gradient gets less steep with increasing height. Also it must be stated that the difference between the width of the emission profile and the width of the absorption profile increases with increasing height. This leads to an absorption profile that is wider than the emission profile for the larger axial positions, where it was smaller for $x = 4$ mm. The explanation for this can be found in the Lewis number. This is a non-dimensional number comparing thermal diffusion with particle diffusion. In Smooke (1991) it is stated that for $\text{H}_2\text{O}$ in a stoichiometric premixed methane flame $\text{Le}<1$, which means that the diffusion of heat is smaller than the diffusion of $\text{H}_2\text{O}$ molecules. Consequently $\text{H}_2\text{O}$ will be spread over a wider radial region than the temperature profile. As a result, the $\text{H}_2\text{O}$ furthest away from the centreline will be cooler than $\text{H}_2\text{O}$ closer to the centreline. This cooler $\text{H}_2\text{O}$ will contribute to absorption, but because the temperature is lower its contribution to the emission will be less or even
5. Flat flame results

Figure 5.11: The assumed local emission profile for the flat flame and \( \lambda = 3.049 \, \mu m \), at \( x = 4 \, mm \).

Figure 5.12: The line-of-sight emission profile for the flat flame and \( \lambda = 3.049 \, \mu m \), at \( x = 4 \, mm \), measured (—) and integrated from Fig. 5.11 (— — —).

negligible. A second explanation for the difference in the width of the emission and the absorption profile can be found in the entrainment of nitrogen at the exterior of the flame. Cold nitrogen and hot products mix at the exterior of the flame, resulting in the cooling of the hot products. These cooler products will still be able to absorb, but their contribution to the emission will be negligible.

In Fig. 5.16 the partial pressure of \( H_2O \) is shown as a function of the axial position. It is calculated using Eq. (2.5), the assumed \( \kappa \) value and the absorption coefficient data for \( k \) of Hartmann et al. (1984), Soufiani (1996), Young (1977) and the corrected dataset, all presented in Section 2.4. Also given in the figure is the partial pressure as predicted by PREMIX. The partial pressure calculated with the data of Hartmann et al. (1984) is approximately 70% higher than the predictions. The data of Soufiani (1996) and the data of Young (1977) are nearly the same and they give partial pressures that are
5.3. Tomography measurements

Figure 5.13: The assumed local absorption coefficient profile for the flat flame and $\lambda = 3.049 \text{ m} \mu \text{m}$, at $x = 4 \text{ mm}$.

![Graph showing absorption coefficient profile](image)

Figure 5.14: The line-of-sight absorption profile for the flat flame and $\lambda = 3.049 \text{ m} \mu \text{m}$, at $x = 4 \text{ mm}$, measured (--) and integrated from Fig. 5.13 (-- --).

![Graph showing absorption profile](image)

about 25% lower. These findings are in agreement with what was seen in Section 2.4, the data of Hartmann et al. (1984) leading to a partial pressure that is far too high and the other two resulting in a partial pressure that is somewhat too low. To be able to calculate the partial pressure in the diffusion flame, a new dataset is created from the data of Hartmann et al. (1984) and the data of Soufiani (1996). For low temperatures the difference between these two datasets is negligible and for high temperatures the measurements in the flat flame are used as a calibration. This results in a corrected dataset which is equal to 60% of the absorption coefficient according to the data of Hartmann et al. (1984) and 40% of the absorption coefficient according to the data of Soufiani (1996). This dataset gives excellent agreement between the predicted and measured partial pressure of H$_2$O.

With the local emitted intensity, the local absorption coefficient and Planck's law
5. Flat flame results

Figure 5.15: The line-of-sight emission profile for the flat flame and $\lambda = 3.049 \mu m$, at (a) $x = 10$, (b) $x = 20$ and (c) $x = 30$ mm, measured (–) and integrated from an assumed flat profile (— — —).
5.3. Tomography measurements

Figure 5.16: The calculated partial pressure of H₂O in the flat flame, as a function of the axial position for \( \lambda = 3.049 \mu m \), using the different databases, Hartmann et al. (1984) (\( \triangle \)), Soufiani (1996) (+), Young (1977) (\( \times \)) and the corrected dataset (\( \circ \)). Also the values predicted with the PREMIX code are given (\( \square \)).

Figure 5.17: The calculated temperature in the flat flame, as a function of the axial position for \( \lambda = 3.049 \mu m \), measured with the tomography setup (\( \circ \)), compared with the CARS measurement (\( \times \)), the thermocouple measurement (\( \cdot \cdot \cdot \)) and the simulation (\( \cdot \cdot \cdot \cdot \)).

The temperature at the centreline is calculated, for the four different heights. In Fig. 5.17 this temperature is given as a function of the axial position. For these calculations the assumed local profiles are used. The calculated temperatures are 15 to 50 K higher than the CARS measurements and the predictions from PREMIX and again the temperature gradient is less steep, just as was the case for the thermocouple measurements. Despite this small difference in the temperature gradient, the tomography setup gives temperatures that are comparable with other measurements and predictions taking into account the uncertainties.

The same measurements are also performed for \( \lambda = 2.877 \mu m \). Because the results
5. Flat flame results

![Figure 5.18: The calculated temperature in the flat flame, as a function of the axial position for λ = 2.877 μm, measured with the tomography setup (◦), compared with the CARS measurement (×), the thermocouple measurement (· · ·) and the simulation (—).](image)

for these measurements are nearly the same, only the final results will be presented. Again the measurements are reconstructed with assumed local profiles. From these local profiles the temperature is calculated. This temperature as a function of the axial position is displayed in Fig. 5.18. In this figure also the temperature from the simulation and from both the CARS and the thermocouple measurements is shown. The temperature calculated from the tomography measurements is about 130 K higher than the other temperatures. Because the temperature from the tomography measurement is far too high and the absorption coefficient is temperature dependent, both the temperature from the tomography measurement and a temperature 130 K lower are used to calculate the partial pressure of H₂O as a function of the axial position. These partial pressure values are presented in Fig. 5.19 together with the expected values following from the simulations. The partial pressure using the tomography temperature is too high while the partial pressure using the reduced temperature is too low. The differences are however within 1% absolute pressure. In this work it is preferred to use the true temperature to calculate the partial pressure of H₂O, which is the corrected tomography temperature.

Using the assumed local profiles, it is possible to determine the width of the flame as a function of the axial position. This width is shown in Fig. 5.20 for both the investigated wavelengths. This figure demonstrates that the width of the flame is a linear function of the axial position. This is also revealed from Fig. 5.21, which is an IR-image of the same flame. The light triangle shape indicates the linear function of the width of the flame with height. The area inside the triangle is darker. In the color image this is red, indicating that intensity is higher. This means that the temperature is higher, or the path length is larger. From the other results it is known that mainly the latter is the case. Just above the burner the temperature is lower, leading to a smaller intensity, although the path length is larger, resulting in the brighter color.

Hitherto all the measurements were radial traverses at a certain axial position, lead-
5.3. Tomography measurements

Figure 5.19: The calculated partial pressure of $\text{H}_2\text{O}$ in the flat flame, as a function of the axial position for $\lambda = 2.877 \, \mu\text{m}$, using the calculated temperature (○) and this temperature reduced with 130 K (+) compared with the predicted values from PREMIX (□).

Figure 5.20: The width of the flat flame as a function of the axial positions, from the measurement with $\lambda = 2.877$ (+) and with $\lambda = 3.049$ (△).

...ing to a 1D slice or projection of the flame, like is needed for a regular tomographic reconstruction. Knowing the function that describes the width of the flame as a function of height and assuming that the local properties inside the flame are not dependent on the radial position, it is possible to determine the local properties from an axial traverse. Knowing both the local absorption coefficient and the local emitted intensity, the temperature and the partial pressure of $\text{H}_2\text{O}$ can be calculated as a function of the axial position. Fig. 5.22 gives the temperature as a function of the axial position. The figure displays the temperature from the axial traverse for both $\lambda = 3.049 \, \mu\text{m}$ and $\lambda = 2.877 \, \mu\text{m}$, as well as the temperature from the thermocouple measurements and the CARS measurements. The latter two just for the axial positions where also a radial traverse is done. From this figure it is clear that again the temperatures for
\[ \lambda = 2.877 \, \mu m \] are about 130 K higher than the measurements with \( \lambda = 3.049 \, \mu m \) indicate. The latter results are in good agreement with the temperatures of both the other measurement techniques, including the slope. Knowing the temperature as a function of the axial position it is possible to determine the partial pressure of H\(_2\)O as a function of the axial position. In Fig. 5.23 this partial pressure is shown for the measurements at \( \lambda = 3.049 \, \mu m \) and the measurements at \( \lambda = 2.877 \, \mu m \). The latter uses both the temperature calculated from the measurements and this same temperature decreased with 130 K. For comparison also the partial pressure of H\(_2\)O calculated with the simulations is given. From the figure it is obvious that using the correct temperature to calculate the partial pressure, gives a significant difference with the profile for \( \lambda = 2.877 \, \mu m \) and the temperature according to the tomography measurement. The calculations with the measured tomography temperature lead to values that are too high. With the reduced temperature, the partial pressure is in agreement with the values of the measurement for \( \lambda = 3.049 \, \mu m \) and the predictions from PREMIX. Using the temperature from the measurement itself, the partial pressure is about 0.01 too high, which is about 6\% in this case and thus not significant.
5.4 Summary

Thermocouple measurements

In section 4.2.4 three methods were presented to correct the thermocouple measurements for radiation and conduction. Only method b is applicable for an axial traverse. In this chapter it is shown that with one (or more) radial traverse(s) it is possible to correct the axial traverse as if method c were used. The measurements in the flat flame make it further possible to tune the parameters needed in the different correction models. The tuning differences in these parameters were just minor and smaller than the uncertainty in these parameters. The difference between the measurements and the
simulations was about 40 K, which is about the estimated uncertainty of the measuring technique. The axial traverse showed that the uncoated thermocouple measurements suffered from catalytic effects in the small reaction zone region. Regarding the thermocouple measurements it can be stated that for the very large region outside the reaction zone, method c is the best correction method for radial traverses, method b can be used in the case of an axial traverse. With the new parameters the accuracy of the technique is 50 K, depending a little bit on the flame the measurements are performed in.

**Tomography measurements**

Next to the thermocouple measurements this chapter focused on the tomography measurements in the flat flame. The conclusions regard the technique itself but also information about the flame. Because the flat flame is supposed to be 1D, the radial profile of both the emission and the absorption are supposed to be flat. The local profiles determined with the reconstruction are indeed rather flat and when used to calculate the projections again, they compare very well with the measured projections. The calculated temperatures from these profiles are, for $\lambda = 3.049 \, \mu m$, about 150 to 300 K higher than the temperatures from the simulations or CARS measurements. Instead of calculating the local profiles, also assumed flat profiles can be used. These profiles also lead to good projections and the temperature belonging to these profiles is between 0 and 50 K too high, depending on the axial position of the radial traverse. As long as the entrainment of nitrogen is negligible, the flat flame is indeed flat. Comparing the width of the absorption and the emission profiles, it was seen that the first increased more with axial position than the latter. This shows that $Le < 1$, which means that the diffusion of $H_2O$ molecules is larger than the diffusion of heat. With the local absorption coefficient profile it is also possible to calculate the partial pressure of $H_2O$ profile. Comparison with the simulations made clear that there were large deviations. It was concluded that there was no good dataset available for the absorption coefficient at $\lambda = 3.049 \, \mu m$ and a new dataset was created, which produced results comparable with the predictions. For $\lambda = 2.877 \, \mu m$ the temperature was about 130 K too high, even for the assumed flat profiles. Calculating the partial pressure of $H_2O$ for these measurements it was concluded that it is best to use the correct (reduced) temperature and that the dataset of the absorption coefficient for this wavelength is accurate enough for a good comparison with the simulations. The radial traverses also showed that the width of the flame decreased linear with the axial position. This was confirmed by an IR-image of the flame. Knowing the width as a function of the axial position and assuming that the flat flame is perfectly flat, it is possible to do an axial traverse with the tomography setup and calculate the local values. The results are comparable with those of the radial traverses. Finally we conclude that we have a tomography setup, that gives comparable results for the radial and the axial traverses, produces partial pressures comparable with the simulations and temperatures that are within the uncertainty for $\lambda = 3.049 \, \mu m$ and are about 130 K too high for $\lambda = 2.877 \, \mu m$. 

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6 Piloted jet diffusion flame

6.1 Introduction

The main interest of the work described in this thesis regarded the measurements in the Delft piloted jet diffusion flame. This, to extend the amount of data already available from measurements (De Vries (1994), Stroomer (1995) and Mantzaras and Van der Meer (1997)) or simulations (Peeters (1995)). The measurement techniques used here are thermocouples and IR Emission Absorption Tomography.

A thermocouple is a widely used, relatively good understood and cheap measurement device. For the thermocouple measurements the extension of the database for the Delft piloted jet diffusion flame regarded mean temperature profiles. This because there was a lack of measurements done for axial positions larger than 250 mm. Therefore most of the radial traverses are for positions higher in the flame. Only for flame C, the measurements have been done in the whole flame. This is the flame with the highest velocities and is marked as standard flame in all the measurements and simulations. Flame A and B have the same fuel to air ratio as flame C, but the velocities are smaller. In the next section, the average temperature measurements are discussed.

In that section the average thermocouple temperature measurements are compared with model calculations and CARS measurements. For a detailed description of the simulations performed by Peeters, the reader is referred to his thesis (Peeters (1995)). The model used is based upon the Favre-averaged transport equations for mass, momentum (including buoyancy) and enthalpy. Turbulence is modelled by a standard $k-\epsilon$ model, with a correction for round jet development. A four-flux radiation model is used to simulate radiative heat losses, excluding the formation (and radiation) of soot. In the limit of high Damköhler number, the chemistry attains equilibrium even within the smallest turbulent eddies, before the turbulent mixing process will disturb this chemical equilibrium. All thermo-chemical variables are related to the mixture fraction $\xi$, which is a conserved scalar. Hence, by assuming a Probability Density Function for $\xi$, the mean values of all dependent properties can be determined. In the present calculations, the assumed PDF is a $\beta$-function.

The Monte Carlo simulations used a 2D elliptic Monte Carlo algorithm to solve for the joint probability density function of velocity and composition. The Monte Carlo solver is used in combination with a $k-\epsilon$ mean flow model. The laminar flamelet
concept is used (Peters (1984)), so the turbulent diffusion flame is seen as an ensemble of laminar diffusion flamelets. The strain rate is based on the Kolmogorov time scale. The PDF for the strain rate has a Gaussian shape, as suggested by Bradley et al. (1992), with the mean and variance following Yeung et al. (1990). The laminar flamelet library did not contain extinguished flamelets, thus local extinction is not described. Radiation is not included in the model yet.

In Section 6.2.2, the time-resolved measurements in flame C are compared to CARS measurements and simulations. The main objective of these measurements was to see whether a simple and cheap experimental technique such as thermocouples can give reliable results for the probability density function of temperature in this type of flame.

The last 10 years, a couple of articles have been written about using tomography in flames to determine both temperature and species concentration, see Fisher and Burkhardt (1990), Hall and Bonczyk (1990) and Wakai et al. (1992). In this thesis it is determined what is possible with a relatively simple tomographic setup in a turbulent diffusion flame.

In Section 6.3.2 the influence of turbulence is predicted by performing some simulations, with the model used by Peeters. These findings are checked with the results from the measurements as presented in the next three sections. Section 6.3.3 shows the results regarding soot. These data are completely new and can only be compared with measurements done with a suction probe, at the centreline of the flames. When soot formation is included in the simulation models, these data can be used to validate these models. In Section 6.3.4 the measurements to determine the partial pressure of H₂O are presented. For these measurements there are no experimental data to compare with, only simulated data are available. In Section 6.3.5 measurements regarding the partial pressure of C₂H₂ are discussed. There are no other experimental data available in this flame and the modelling is also in its early stages. C₂H₂ is interesting because it is believed to be a precursor of soot (Leung et al. (1991) and Boerstoel (1997)). The chapter is ended with a summary with the most important conclusions.

6.2 Thermocouple measurements

6.2.1 Average temperature measurements

In this section the averaged thermocouple temperature measurements are compared with model calculations and CARS measurements. The model calculations consist of simulations done by Peeters (1995) and Monte Carlo simulations performed by Nooren (1996). The CARS measurements have been done by Mantzaras and a description of the measurement technique and the measurements can be found in Mantzaras and Van der Meer (1997). The accuracy of these measurements is approximately 50 K, depending slightly on radial position and temperature gradient. The accuracy of the thermocouple measurements in the diffusion flame is 40 K, as reported in Section 4.2.4. All the results presented in this section reflect data for flame C.

In Fig. 6.1 (a)-(f), temperature profiles are presented for respectively x = 50, 100, 150, 200, 250 and 300 mm. For x = 50 mm the maximum measured temperature
6.2. Thermocouple measurements

Figure 6.1: Comparison of the measured and simulated mean temperature for flame C, with thermocouple measurement (•), CARS measurement (×), Peeters' simulation (−) and Monte Carlo simulation (⋯), for (a) \(x = 50\), (b) \(x = 100\), (c) \(x = 150\), (d) \(x = 200\), (e) \(x = 250\) and (f) \(x = 300\) mm.

for thermocouple and CARS is nearly equal. They agree considering the measuring inaccuracies. The differences in the minimum temperature, at the centreline, are not significant as this type of thermocouple can not accurately measure temperatures below 400 K. The maximum temperature for the simulations is not significantly lower than for the measurements and the minimum temperature, at the centreline, is also in agreement with the CARS and the thermocouple measurements. The width of the temperature profile is a bit wider for the thermocouple measurement than for the CARS measurement. In view of the accuracy of the measurement techniques, the agreement is excellent. The profiles according to the simulations are comparable and slightly wider than the profiles from the measurements.

For \(x = 100\) mm both the minimum and the maximum temperature as well as the width of the profiles, for all the experiments as well as the simulations are the same, taking the accuracy of the techniques into account. For \(x = 150\) mm the agreement for all these parameters between the measurements and the simulations is excellent. For \(x = 200, 250\) and \(300\) mm, these parameters are also within the accuracy of the measurement techniques. For \(x = 200\) mm and larger axial positions the width of the flame is under predicted by both simulations, where the difference in flame width increases with axial position. The width of the profiles for \(x = 200, 250\) and \(300\) mm for the thermocouple measurements and the CARS measurements is
Figure 6.2: Comparison of the measured and simulated mean temperature for flame C, with thermocouple measurement (.), CARS measurement (×), Peeters’ simulation (−) and Monte Carlo simulation (···), for (a) \( x = 400 \), (b) \( x = 450 \), (c) \( x = 500 \), (d) \( x = 550 \), (e) \( x = 600 \) and (f) \( x = 700 \) mm.

in agreement, taking into account the accuracy in the measured temperatures and the large temperature gradient.

In Fig. 6.2 (a)-(f) the temperature profiles are given for respectively \( x = 400 \), 450, 500, 550, 600 and 700 mm. For \( x = 400 \) mm the Monte Carlo simulations agree within the accuracy for both the maximum and the minimum temperature with the thermocouple measurements. There is also no significant difference between the CARS measurements and Peeters’ simulations, however they are some 150 K higher than the thermocouple measurements. For axial positions larger than 400 mm Peeters’ simulations give a largest temperature difference with the thermocouple measurements of about 160 K, where the measured temperature is higher, resulting in a smaller profile for the simulations. For the Monte Carlo simulations, the profile is a little bit smaller, but the temperatures are within the accuracies, for axial positions up to 550 mm. For higher axial positions this difference in temperature increases to 220 K for \( x = 700 \) mm.

Taking into account the measurements and the simulations at all the heights, the following conclusions can be drawn. First of all, the width of the flame is not correctly predicted by both simulation models. Regarding the simulations of Peeters this was also seen by De Vries (1994), Stroomer (1995) and Peeters (1995). For small axial positions, the predicted flame width is somewhat too large. Then around \( x = 150 \) mm
Figure 6.3: The radial thermocouple temperatures for (a) flame A, (b) flame B and (c) flame C, with \( z = 200 \) (--), \( z = 300 \) (——), \( z = 400 \) (———), \( z = 500 \) (—), \( z = 600 \) (—*) and \( z = 700 \) mm (—△—).

the flame width of the measured profiles and from the simulations is comparable. For larger axial positions the width of the flame is underestimated by the simulations. The
second conclusion regards the prediction of the flame length. Both the simulations predict the length of the flame too large, where the Monte Carlo simulations show the largest difference. Regarding the minimum and the maximum temperature the following can be stated. For axial positions smaller than 300 mm, all the measurements and the simulations are mostly within 50 K. These differences are not significant, considering the accuracies of 50 K for the CARS measurements and 40 K for the thermocouple measurements. For $x = 400$ mm there is a discrepancy between the two measurement techniques. There is also a difference between the two simulation techniques and the thermocouple measurements for larger axial positions. The latter is probably caused by the difference in both the predicted flame width and flame length.

In Fig. 6.3 (a)-(c) the radial temperature profiles of the thermocouple measurements are given for flame A, B and C for the axial positions $x = 200, 300, 400, 500, 600$ and 700 mm. The main features of the three flames are the same. Starting with the reaction zone between the fuel and the air flow, shown in the double peaked profiles for the lower axial positions, diffusion gets more important for larger axial positions, leading to more Gaussian profiles at those positions. Further it holds that the higher the flow velocities, the wider the radial temperature profiles. Except that the radial profile is wider, the maximum temperature is also higher. This maximum temperature at the axis is attained at a higher axial location. The explanations for these are the following. The higher the velocities, the higher the turbulence level, because flame A and B are not fully developed, since the flame length increases with velocity, see also Stroomer (1995). When the turbulence level is higher, the mixing of the two flows is better. The total diffusion coefficient will be larger because the turbulent diffusion is larger, leading to a wider flame and thus a wider temperature profile. Because the mixing is better also the soot formation is expected to be smaller. When there is less soot in the flame, the radiation losses will also be smaller, leading to a higher temperature in the flame. Because of the higher axial velocity the temperature maximum will occur at a larger axial position. Another reason for this longer flame can be found in the fact that with increasing velocity ratio between jet and annulus, the deformation of the reaction zone decreases, resulting in a smaller reaction zone area and leading to a slower burnout of the reactants and an overall longer flame. Better mixing also can lead to a lower temperature maximum in a radial profile, because the same amount of energy or a bit more will have to heat up more gas. This only leads to minor temperature differences.

Besides the radial traverses with the thermocouple, also some axial traverses are performed. In Fig. 6.4 these measured temperatures for the various traverses are presented. First thing that is revealed by the figure is the fact that we found not just one smooth line, but there seem to be two profiles. More measurements in one profile reproduce very good. The profile with the lowest temperatures for the larger axial positions is in error and probably due to contamination of the thermocouple by soot. Because of the soot on the thermocouple, its parameters will change and this will affect the heat balance. The time constant of the thermocouple will increase and this results in less fluctuations measured. This is very plausible, since not only the mean temperature dropped, but also the rms value of the fluctuations. Also the convective heat transfer coefficient $h_c$ and the emissivity $\epsilon_\ell$ will be changed. This will result in a change of the mean temperature. This effect is not seen for flame B and C. The tem-

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temperature difference between the two traverses is significant. It is easy to detect if there is soot on the thermocouple in a radial traverse. When this is the case, it is possible to clean the thermocouple by just moving it to a hot region with enough oxidiser.

6.2.2 Time-resolved temperature measurements

In the previous section the averaged thermocouple temperatures as measured in the Delft piloted jet diffusion flame with a standard triple thermocouple were discussed. In this section the time-resolved thermocouple measurements in the Delft piloted jet diffusion flame will be presented. The results shown in this section include radiation correction and use the fluctuating temperature for calculating the correction, see Section 4.2.5. Also calculations without the radiation correction and using just the mean temperature are performed. From these calculations it was concluded that including the radiation correction just shifts the temperature to a higher level. Although this correction is not linear, the influence on the rms value and the shape of the temperature PDF is not significant. Also the influence of using the fluctuating temperature instead of the mean temperature was of minor importance. Because they both had also no large influence on the processing time the calculations were done including both.

For the rms value of the temperature fluctuations, \( T'_{\text{rms}} \), the agreement between the thermocouple measurement and the Monte Carlo simulation is reasonable, while the CARS measurement and the simulation done by Peeters are in agreement too, but the latter two differ significantly from the first two for most measured locations.

For \( x < 300 \text{ mm} \), near the centreline, the agreement of the rms value between both the simulations and the CARS measurement is good, while the thermocouple measurement gives a rms value that is smaller than 30 K, see Fig. 6.5. This also leads to a PDF for the thermocouple measurement that is too heavily peaked, see Fig. 6.6 and Fig. 6.7. It seems, that in this region, the thermocouple is not capable of following all the temperature fluctuations, leading to a correct mean value with a too small rms value. The fact that with a thermocouple these fluctuations are not seen for these axial positions,
Figure 6.5: The $T'_{\text{rms}}$ in flame C as a function of the radial position, for thermocouple measurement (×), CARS measurement (×), Peeters’ calculation (—) and the Monte Carlo simulation (· · ·), for (a) $x = 100$, (b) $x = 250$, (c) $x = 400$, (d) $x = 500$, (e) $x = 600$ and (f) $x = 700$ mm.

is in agreement with the findings of Ballantyne and Moss (1977). They did the same kind of measurements with a 50 μm thermocouple in a methane turbulent diffusion flame. They also found no temperature fluctuations for small axial and radial positions. From the fact that they measured no temperature fluctuations, they concluded that the temperature indeed did not fluctuate. However from the CARS measurements and Peeters’ simulations it is clear that this is definitely not the case in the Delft piloted jet diffusion flame. The turbulent time scales are smaller than 1 ms (Stroomer (1995) and Peeters (1995)), and the time constant of the thermocouple is larger than 20 ms (Table 4.1). We conclude that in this region the time scales in the flame are much smaller than the time constant of the thermocouple. As a result, the mean temperature will be correct, but the temperature fluctuations will be underestimated. This leads to a PDF that is too heavily peaked, but with a mean temperature that is correct.

For locations near the centreline but for larger axial positions, the rms value of the thermocouple measurements is a little bit smaller than the value from the Monte Carlo simulations and much smaller than the value from either the CARS measurements or Peeters’ simulations. Looking at the PDF for these locations, see Fig. 6.8 and 6.9, it is seen that the thermocouple measurements largely lack the range of the PDF where $1700 < T < 2100$ K. These temperatures will mainly occur near the reaction zone. From this it can be concluded that the reaction zone fluctuates with the smallest time
6.2. Thermocouple measurements

Figure 6.6: The temperature PDF in flame C for $x = 100$ mm, with thermocouple measurement (---), CARS measurement at nearest location (bars, radial value between brackets) and Peeters’ calculation (- - -), for (a) $y = 3.0$ [3.5], (b) $y = 6.0$ [6.2], (c) $y = 9.0$ [9.5] and (d) $y = 10.5$ mm.

Figure 6.7: The temperature PDF in flame C for $x = 250$ mm, with thermocouple measurement (--- for $y \geq 0$ and - - - for $y < 0$), CARS measurement at nearest location (bars, radial value between brackets) and Peeters’ calculation (- - -), for (a) $y = 0.0$, (b) $y = \pm 12.0$ [11.0], (c) $y = \pm 15.0$ [16.5] and (d) $y = \pm 18.0$ [18.5] mm.

scales, which are so small, that the thermocouple is not capable of resolving these temperature fluctuations. The lack of these higher temperatures was also seen by Heitor et al. (1985). They contributed this to radiation or mixing with the (colder) surroundings. Since radiation is included in the model, this can not be the reason in our case. This lack of higher temperatures is seen at the burner axis where, for not too large axial positions, it is not likely that there will be entrainment of the surrounding gases. Also the PDF of the CARS measurements and Peeters’ simulations clearly show these higher temperatures leading to the conclusion that they do really exist.
Figure 6.8: The temperature PDF in flame C for \( z = 400 \) mm, with thermocouple measurement (---), CARS measurement at nearest location (bars, radial value between brackets) and Peeters' calculation (--), for (a) \( y = 0.0 \), (b) \( y = 15.0 \) [13.0], (c) \( y = 20.0 \) [22.0], (d) \( y = 25.0 \) [25.0], (e) \( y = 30.0 \) [31.0] and (f) \( y = 45.0 \) mm.

Figure 6.9: The temperature PDF in flame C for \( z = 500 \) mm, with the thermocouple measurement (---) and Peeters' calculation (--), for (a) \( y = 0.0 \), (b) \( y = 20.0 \), (c) \( y = 30.0 \) and (d) \( y = 35.0 \) mm.
At higher locations, but away from the burner axis, the rms value of the thermocouple measurements is about 80% of that of the CARS measurements, where the maximum rms value is found at the same radial position. The simulations both have the maximum of the rms value at a position too close to the centreline, which was also seen for the mean temperatures. The maximum value of the simulations of Peeters is almost twice the maximum value of the thermocouple measurements. For \( x = 400 \) and 500 mm the maximum rms value of the Monte Carlo simulations is about the same as the one from the thermocouple measurements. For \( x = 600 \) and 700 mm the rms value of the Monte Carlo simulations is higher than from the thermocouple measurements. The latter again is in agreement with the results seen for the mean temperatures, where one of the conclusions was that the flame length as predicted by the Monte Carlo simulations was too large. Taking a closer look at the temperature PDF for \( x = 400 \) mm, it is seen that in both the measurement techniques the peak near room temperature is not present, where this is more pronounced for the thermocouple measurement. The latter again is due to the fact that the used thermocouple can not significantly measure temperatures below 400 K.

In Fig. 6.9 the temperature PDFs are given for \( x = 500 \) mm. The shape of the PDFs for higher locations are nearly the same as for this location and they all lead to the same conclusion. We know that the thermocouple has a bias effect for low temperatures because of the materials used for the thermocouple. There is also a bias effect for high temperatures because those temperatures coincide with the smallest time scales which can not be followed by the thermocouple. Taking these two effects into account, we conclude that the agreement in PDF shape is always reasonable. Secondly the results also demonstrate, that our thermocouple does not suffer from overcompensation, as reported in Section 4.2.5.

For \( x = 250 \) mm the traverse extended both the negative and the positive side. In Fig. 6.7 the thermocouple temperatures for both these sides are given. From this figure it can be concluded that the measurement reproduces and that the diffusion flame is symmetric.

It is revealed that the thermocouple used is not capable of following the turbulent fluctuations near the reaction zone. This leads to a PDF that lacks the highest temperatures and to mean temperatures that are too small. This can be overcome by using a thermocouple with a smaller diameter, at least one order smaller in diameter. Although it is possible to make such a small thermocouple, it is probably not robust in our flames. This leads to a compromise when a lot of (mean) temperature measurements have to be done.

In Chapter 4 one of the reported disadvantages of the used thermocouple was the possibility of catalysis. In Chapter 5 it was shown that the thermocouple used in these investigations suffered from catalytic effects when applied in the laminar flat flame. From the results presented in the last two sections it can be concluded that this is not the case, when the thermocouple is used to measure the temperature in the Delft piloted jet diffusion flame.
6.3 Tomography measurements

6.3.1 Introduction

The Delft piloted jet diffusion flame is a highly turbulent flame. This means that temperature and species concentrations will strongly vary in time, as already shown in the previous section regarding temperature. Since radiative emission is not a linear function of temperature it is important to know the influence of these turbulent fluctuations on the tomographic measurements. This will be discussed in Section 6.3.2. It will be shown that there is not much influence on the concentration measurements, but that one has to be very careful when temperature has to be determined.

Then the measurements performed in the Delft piloted jet diffusion flame will be presented. These measurements have been done for three different wavelength regions, to determine three different species concentrations. This differs from the tests in the flat flame (Chapter 5), because in the Delft piloted jet diffusion flame soot is present. In Section 6.3.3 measurements at $\lambda = 1.624 \, \mu m$ will be presented. With these measurements it is possible to determine the soot volume fraction. This is done for the first three flame settings, for axial positions larger than or equal to 300 mm, where most of the soot is expected (see Section 3.2). Since soot radiates at all wavelengths these measurements are also used to correct the measurements at other wavelengths. To determine the partial pressure of H$_2$O the bandpass filter with $\lambda = 2.877 \, \mu m$ is used, just as was done for the measurements in the flat flame. Measurements with this filter are also done for the three flames under investigation in this thesis. The last set of measurements regard $\lambda = 3.049 \, \mu m$. With measurements at this wavelength it is possible to determine the concentration of C$_2$H$_2$. The measurements have to be corrected for the soot volume fraction and the partial pressure of H$_2$O, since both soot and H$_2$O also absorb at this wavelength. This last set of measurements has been done in flame A and in flame C. The latter because there were some data available for comparison. The first because the largest concentrations are expected to be found in this flame, because it also produces the highest volume fraction of soot and C$_2$H$_2$ is known to be a precursor of soot, see Leung et al. (1991) and Boerstoel (1997).

6.3.2 Influence of turbulence

It is well known that the emission of a gas volume is not a linear function of temperature (see also Eq. (2.1)). Measuring instantaneous emissions and calculating temperature directly from such measurements would give accurate results. Since the tomographic technique applied is both averaging in space and time, this can lead to temperatures that are not correct. In this section an estimation will be given of the systematic error that will be made when the time averaged line-of-sight radiative emission is used to determine the mean local temperature in a turbulent flame. It will be shown that this error is wavelength dependent.

The line-of-sight radiative emission can be approximated by a linear summation of the local emission in all the volumes along the path. This is a digitised form of Eq. (2.2). In that case the self-absorption is neglected and the transmission from each volume to the detector is unity. The turbulent flow field is assumed to consist of a
number of eddies that have uniform properties and are statistically independent. It is furthermore assumed that a volume has at least the size of such an eddy. This means that all the volumes are statistically independent. Now the line-of-sight emission is a linear summation of statistically independent variables. This leads to the conclusion that the time averaged line-of-sight emission is just a linear summation of the average local emission of each volume along the path. To study the influence of turbulence on the tomographic measurement technique it is sufficient to pay attention to the local emission (and its relation to temperature).

To get an idea about the influence of the fluctuations on the measurement technique, the model from Peeters was extended with an extra feature. From this simulation the temperature and the species concentrations are known. Not just the mean values, but also the fluctuation of all these parameters are determined. The latter because the model uses PDFs. This is enough information to give an estimation of the influence of the turbulence on the determination of temperature. Eq. (2.2) shows that the local emission is a function of the wavelength and temperature, according to Planck's law, and of the absorption coefficient. The absorption coefficient is a function of the species concentration and indirectly also a function of the temperature. The latter dependence is normally not very large (see Section 2.4) and for this part of the research assumed to be negligible. It is also assumed that the influence of the fluctuation of the species concentration has a marginal effect and can be neglected. This is true when the temperature fluctuations and the species concentration fluctuations are not correlated. Then the fluctuating emission coefficient may be replaced with the mean emission coefficient. The latter can be calculated using the mean temperature and species concentration. This results in a local emission as a function of temperature. With the mean and the fluctuations of the temperature known from the model and assuming a (constant) emissivity of 1, the PDF of the local emission and its mean value are calculated. Because wavelength is a parameter in Planck's law, this mean local emission will be different for different wavelengths \( \propto B(\lambda, T) \). Since mean temperature is known from the model, it is also possible to determine the local emission belonging to this mean temperature. This will lead to a different, also wavelength dependent, local emission \( \propto B(\lambda, T) \). For each wavelength this leads to two different profiles for the local emission.

In Fig. 6.10 (a)-(l) all the results regarding the local emission are shown for different axial positions. From these figures it is revealed that the difference between the results with \( \lambda = 2.877 \, \mu m \) and those with \( \lambda = 3.049 \, \mu m \) is small. This can be expected since the difference in wavelength is also not too large. The figures also show that, assuming an equal emission coefficient, the emission for \( \lambda = 1.624 \, \mu m \) is larger with respect to the emission for the other two wavelengths. This follows directly from Planck's law. The figures also demonstrate that, whatever the shape of the profile, the calculated mean local emission is always higher and the profile is wider compared to the local emission calculated with the mean temperature. The latter is the result of the non-linearity of Planck's law on temperature. It must not be forgotten that a simplification has been made by creating the data in Fig. 6.10, since these calculations are done without taking into account the fluctuations of the emission coefficient or its wavelength dependency.
Figure 6.10: The calculated mean local emission in flame C, for $\lambda = 1.024\mu m$ (- - -), $\lambda = 2.877\mu m$ (---) and $\lambda = 3.049\mu m$ (---), and the calculated local emission of the mean temperature (the same line types, but with a o), for the following axial positions: (a) $x = 25$, (b) $x = 50$, (c) $x = 100$, (d) $x = 150$, (e) $x = 250$, (f) $x = 400$, (g) $x = 450$, (h) $x = 500$, (i) $x = 550$, (j) $x = 600$, (k) $x = 650$ and (l) $x = 700$ mm.
6.3. Tomography measurements

The main purpose of the emission measurement is the determination of the mean local temperature. Our interest is knowledge about the error made calculating the temperature from the emission measurement. The local emission obtained with the tomographic reconstruction from the measurement is comparable with the mean local emission calculated including the temperature fluctuations. For the determination of the temperature the assumption is made that the local emission from the measurement is comparable with the emission calculated using the mean temperature. This will lead to a systematic error in the temperature determined from the measured local emission. In Fig. 6.11 (a)-(l) three lines and one line with symbols are given, for the same axial positions as in Fig. 6.10. The line with symbols is the mean temperature as calculated by Peeters' model. The other three lines represent the three different wavelengths. The temperatures are the temperatures calculated according to Planck's law, using the corresponding mean local emission.

First thing demonstrated by the figure is the fact that the difference between the mean temperature and the temperature from the mean emission is wavelength dependent. The higher the wavelength the smaller the difference between the two temperature profiles. This means that the temperature as determined from the tomography measurements regarding soot, at the lowest wavelength, will give higher temperatures than the other two measurements. Since the wavelength difference between the latter two is small, the difference between these measurements is again of minor importance.

Next thing revealed is the fact that the temperature, including the fluctuations, is always higher and the temperature profile is always wider. Depending on the shape of the profile and thus on the axial position in the flame, there is a region in the flame where this difference is not significant. For \( x = 25 \) and 50 mm the temperature from the mean emission is always higher than the mean temperature. Since it is very hard to perform tomography measurements at the wavelengths of interest in this region, this does not influence the experiments described in this thesis. For the axial positions between 100 and 550 mm the figure shows that around the centreline of the flame, between the two maxima, the difference between the two temperature profiles is nearly constant and fairly small. For \( \lambda = 1.624 \mu m \) this difference is about 120 K for \( x = 150 \) mm and for the other two wavelengths this difference is approximately 60 K. For \( x = 400 \) mm they are respectively 50 K and 20 K. For axial positions larger than 500 mm, the temperature profile is more and more Gaussian. The region where the temperature from the mean emission is close to the mean temperature is just a small region near the centreline. For \( x = 700 \) mm the difference at the centreline is respectively 115 K and 55 K.

In the exterior of the jet flame turbulent fluctuations are largest and consequently the temperature difference is larger. The temperature calculated using the mean local emission is about 350 K too high at 750 K true mean temperature, about 300 K too high at 1000 K and approximately 225 K too high at 1250 K, for the highest two wavelengths. As a consequence of this too high predicted temperature, the width of the flame will also be over predicted.

Regarding the determination of the temperature from the tomographic measurements the following can be summarised. The temperature and the width of the temperature profile will always be overestimated. Near the centreline the temperature
difference is about 100 K for \( \lambda = 1.624 \mu m \) and 50 K for the other two wavelengths. In the exterior this temperature difference increases with decreasing true temperature.

6.3.3 Soot

In the next three sections the tomographic results for the piloted jet diffusion flame will be presented. First the measurements for \( \lambda = 1.624 \mu m \) will be presented in this section. Since soot is the only component inside the flame that absorbs radiation in this wavelength region, it is possible to determine the local soot volume fraction with a measurement at this wavelength. The discussion starts with a qualitative comparison of the measured local emission with the expectations as presented in the previous section. At first the discussion will only reflect to the measurements in flame C. Next to this discussion, the measurements in the other flames will be presented. After the discussion about the local emission, there is a discussion about the local absorption coefficient. Combining these two quantities the local temperature can be calculated. Wherever calculated, these values are compared with the expectations from the simulations. Using the local absorption coefficient and the temperature, it is possible to calculate the mean local soot volume fraction. Comparing the three different flames the soot volume fraction is expected to increase going from flame C to B to A, because of the decrease in velocity and the decreasing level of turbulence. At the end of the section, the measured soot volume fraction at the centreline will be compared to the soot volume fraction as measured with the suction probe experiment. The next two sections first discuss measurements at \( \lambda = 2.877 \mu m \) and then measurements at \( \lambda = 3.049 \mu m \). For these latter two there are no other measurements to compare with, so the comparisons are only done with simulations.

Emission profiles for flame C

For flame C the tomographic measurements regarding soot have been done for axial positions equal to and larger than 400 mm. This flame contains not enough soot to perform reliable absorption measurements for lower axial positions. Even for the traverses done the uncertainty in the local absorption coefficient is about 100%. Regarding the emission measurement, the uncertainty is just about 3%, so the latter measurements are fairly trustworthy. Although the absorption measurements are not very accurate they still give a good idea about the presence of soot in this flame and the influence of turbulence on the tomographic measurements.

To get a better feeling for the accuracy of the emission measurements, the line-of-sight emission profiles are shown in Fig. 6.12. This figure contains both the measured emission profile and the profile calculated by integrating the local emission profile determined with the tomographic reconstruction technique. The figure demonstrates that the fluctuation in the measured profile indeed is not too large and that the integrated profile is a rather good fit of the measured profile. Due to the use of a cutoff, the local profile used to calculate the integrated profile may loose some energy during the filtering, resulting in an integrated profile that is a little bit too low. Looking at the sequence where the axial position increases from 400 to 700 mm the figure reveals that the width of the flame is nearly constant. However, the magnitude increases. The
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![Figure 6.11](image)

Figure 6.11: The calculated temperature in flame C using the mean local emission, for $\lambda = 1.624\mu m$ (---), $\lambda = 2.877\mu m$ (---) and $\lambda = 3.049\mu m$ (····) and the mean temperature as calculated by Peeters (--o--) for the following axial positions: (a) $x = 25$, (b) $x = 50$, (c) $x = 100$, (d) $x = 150$, (e) $x = 250$, (f) $x = 400$, (g) $x = 450$, (h) $x = 500$, (i) $x = 550$, (j) $x = 600$, (k) $x = 650$ and (l) $x = 700$ mm.
increase of the integrated emission is probably due to an increase in the local emission, since the integration path does not change significantly.

In Fig. 6.13 (a)-(g) the local emission reconstructed from the measurements is displayed for axial positions equal to 400, 450, 500, 550, 600, 650 and 700 mm. The profiles can be compared with the local emission profiles from the calculations shown in Fig. 6.10. The width of the profile from the measurements is much larger than the width of the profile calculated with the mean temperature and a bit larger than the width of the mean local emission profile. The large mismatch in width with the profile calculated with the mean temperature is the first experimental indication that there is influence from turbulence on the tomographic measurements. The small mismatch in width with the profile of the mean local emission is due to the underestimation of the width of the flame by the simulations done by Peeters, see Section 6.2.1. With the assumption that the influence of the turbulence on the absorption measurement is
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![Graphs showing emission profiles](image)

Figure 6.13: The reconstructed local emission for flame C and \( \lambda = 1.624 \, \mu m \), (a) \( x = 400 \), (b) \( x = 450 \), (c) \( x = 500 \), (d) \( x = 550 \), (e) \( x = 600 \), (f) \( x = 650 \) and (g) \( x = 700 \, mm \).

negligible, the tomographic measurement will result in a mean temperature that is too high and a temperature profile that is too wide.

Next the shape of the reconstructed local emission profiles in Fig. 6.13 (a)-(g) can be compared with the shape of the calculated mean local emission profiles in Fig. 6.10. For \( x = 400 \, mm \) both the profiles have a double Gaussian shape. The plateau near the centreline seems to be wider in the measurements. Also the position of the maximum is at larger radial positions. This can be expected since in Section 6.2.1 it was already concluded that the simulations from Peeters underestimate the width of the flame for these axial positions. The ratio between the emission at the centreline and the maximum emission is quite comparable for the measurement and the simulation. However one has to be very careful with this comparison, because this ratio also depends on the emission coefficient of the radiating soot. For the simulations the emission coefficient was assumed to be constant, while in the measurement it is very likely to be dependent of radial position, since temperature varies with both radial position and soot volume

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fraction. For \( x = 450 \) mm both shapes are also double Gaussian and again the measurement profile is wider than the profile from the simulations. Comparing both these profiles with the profiles for \( x = 400 \) mm it can be seen that the value at the centreline for \( x = 450 \) mm is larger than for \( x = 400 \) mm, but the difference for the maximum value of the emission is much larger for the measurement than for the simulation. The reason for this can not be found in the temperature difference. As in Fig. 6.2 it is revealed that the difference between the temperature from the simulations and the temperature from the thermocouple measurements is nearly constant. This implies that the emission coefficient has to be larger. This is an indication that the soot volume fraction for \( x = 450 \) mm is larger than for \( x = 400 \) mm. Beside this increase in magnitude, the width of the profile of the soot volume fraction for \( x = 450 \) mm will also be larger. For \( x = 500 \) mm the double Gaussian shape of the profile seems to change into a single Gaussian shape, for both the measurement and the simulations. Again the measurement profile is wider and also the increase in comparison with the profiles for \( x = 450 \) mm is larger for the measurement than for the simulation. The latter again indicating that the soot volume fraction has increased for \( x = 500 \) mm in comparison with \( x = 450 \) mm. For \( x = 550 \) mm both the profiles are Gaussian and the width of the measurement is still larger than for the simulation. Now the difference with the profiles for \( x = 500 \) mm is much larger for the measurement than for the simulation, so the soot volume fraction for \( x = 550 \) mm will be much larger than it is for \( x = 500 \) mm. For \( x = 600 \) mm the shapes are both Gaussian again, with the width of the measurement larger than for the simulation, but the magnitude has increased about the same amount for both the measurement and the simulation. The minor difference that occurs can be caused by an increase in temperature for the thermocouple measurement relative to the temperature from the simulation, but the soot volume fraction will hardly change between \( x = 550 \) and 600 mm. For \( x = 650 \) mm the shapes are both Gaussian. The measurement profile is wider than the profile from the simulations. Compared with the profiles for \( x = 600 \) mm the magnitude for the measurement did increase a bit, while the simulation leveled or even decreased a little. So the soot volume fraction is expected to increase slightly between \( x = 600 \) and 650 mm. For \( x = 700 \) mm both the Gaussian profiles have decreased due to a decrease in temperature and a decrease in soot volume fraction.

**Local emission profiles for flame A and B**

The local emission for flame A and B is given in Fig. 6.14 (a)-(f). Because there is more soot in these flames, the measurements are already reliable at lower locations in the flame. This is the reason why the measurements in these two flames start at \( x = 300 \) mm. The first thing that can be noticed is the fact that the shape of the profile is more pronounced double peaked for this lower location, with respect to the higher axial positions. This is also shown by the profiles from the simulations done for flame C, see Fig. 6.10. The next thing that is revealed by comparing Fig. 6.13 and Fig. 6.14 is the fact that for most axial positions, the local emission is highest for flame A and lowest for flame C. There is just one exception to this, \( x = 700 \) mm. Here the local emission for flame A is lower than the one for flame B and even for
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![Graphs showing local emission for flame A and flame B for different x positions.](image)

Figure 6.14: The reconstructed local emission for flame A (---) and flame B (---) for \( \lambda = 1.624 \, \mu m \), (a) \( x = 300 \), (b) \( x = 400 \), (c) \( x = 450 \), (d) \( x = 500 \), (e) \( x = 600 \) and (f) \( x = 700 \, mm \).

flame C. The reason for this can be found in the fact that the flame length of the three flames is not the same. The thermocouple measurements showed already that flame C is the longest and flame A the shortest. Consequently both the temperature and the soot volume fraction will start to decrease at a lower axial position for flame A with respect to the other two flames. As a result, also the local emission will decrease at a lower position. The thermocouple measurements also demonstrated that the flame width for flame C was the largest and for flame A the smallest. In addition to this, the absolute temperature for flame A was the lowest and for flame C the highest, while the absolute difference was not too large. This holds for axial positions clearly smaller than the flame length. When the temperature profile decreases and the emission increases, this indicates that the soot volume fraction indeed increases in the sequence of flame C to B to A. The two figures also reveal that the width of the local emission increases in the sequence of flame A to B to C. This is due to the fact that the turbulence level of the flame also increases in this sequence. A higher turbulence level results in better mixing and this improves the combustion. This results in a higher temperature and consequently the temperature profile will be wider. In Section 6.2.1 it was already seen that the width of the temperature profile increased in respect with this flame order. Secondly, turbulence will influence the width of the emission profiles because of the non-linear dependence on temperature, as reported in Section 6.3.2. This influence increases with turbulence level resulting in the widest emission profile for the most
turbulent flame, flame C.

For the profiles at \( x = 500 \text{ mm} \) the following can be stated. For flame A the profile has a Gaussian shape. For flame B this emission profile is more flat near the centreline. For flame C the emission profile is more double Gaussian as already stated before. The discussion of the profiles for flame C showed that with increasing axial position the emission profile changed from double Gaussian to Gaussian. This again reveals that flame A is the shortest flame and flame C the longest. Performing the same analysis for flame A and B as is done for flame C leads to the conclusion that the maximum soot volume fraction for these two flames also occurs around \( x = 600 \text{ mm} \).

**Absorption profiles for flame A**

Next parameter under investigation is the absorption. Because there is no direct link with the calculations on the influence of turbulence and because of the large uncertainty in the absorption measurements, first the results for the flame with most absorption, flame A, will be presented. The discussion starts with the measured integrated absorption, after which the local absorption coefficient will be discussed. In Fig. 6.15 the line-of-sight absorption profile is given for axial positions between 300 and 700 mm. The scatter in the measured line-of-sight profile shows that the uncertainty in these measurements is considerable with respect to the magnitude. The absorption is also that small, that self-absorption may be neglected. Still it is possible to give some char-
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Figure 6.16: The local absorption coefficient for flame A and $\lambda = 1.624 \mu m$, from the measurement (---) and the (maximum) local absorption coefficient, calculated using the measured local emission and the thermocouple temperature (-- --), for (a) $x = 300$, (b) $x = 400$, (c) $x = 450$, (d) $x = 500$, (e) $x = 600$ and (f) $x = 700$ mm.

acteristic features of this type of measurement in these flames. One thing that is very clear from Fig. 6.15 is the fact that the integrated absorption increases with height, with its maximum around $x = 600$ mm. The figure also demonstrates that the integrated local absorption coefficient profile gives a reasonable fit through the measurements. For more detail, Fig. 6.16 is needed. This figure shows the local absorption coefficient as calculated with the tomographic reconstruction technique, from the measurements. When the local absorption coefficient profile is compared with the local emission profile (Fig. 6.14), it can be seen that the width of the emission profile is larger than the width of the absorption coefficient profile. Comparing the widths of these two profiles with the profiles in Fig. 6.10, the emission profile agrees best with the calculated mean local emission profile, while the absorption coefficient profile agrees best with the profile of the calculated local emission of the mean temperature. This is an indication that the absorption is hardly influenced by turbulence, because of the small dependence of the absorption coefficient on temperature. The assumption that the emission is only influenced by temperature, through Planck's law and not via the emission coefficient, seems to be valid.

From Fig. 6.16 it is also revealed that there is a small peak in the absorption coefficient at the exterior of the flame. This effect is also present in the profiles of the other two flames. Striking is the fact that the magnitude of this effect is nearly the same for
all the different flames and axial positions. One possible explanation is that this is due to the reconstruction technique. When the cutoff is chosen too small, the reconstruction disregards too much high frequencies and some signal can be found in regions where there should not be any signal. Counter arguments for this are the fact that there is nothing like this in the emission profiles and the fact that it is not likely that these peaks have the same height. Another explanation can be found when it is assumed that these peaks are also present in the absorption measurement. The physical explanation for this effect is not absorption, but diffraction. At the exterior of the flame there often is a substantial temperature gradient. This temperature gradient leads to a gradient in the refraction index. Because of this gradient in the refraction index it is possible that rays at the exterior of the flame will not be straight and will not reach the detector. This results in a loss of intensity and will be interpreted as absorption. We have already seen something like this during the first tests of this experiment: where a smaller blackbody aperture was used and absorption peaks were revealed at the exterior of the flame.

There is a second line type, a dashed line, in Fig. 6.16. This local absorption coefficient is calculated using the local emission from the tomographic measurement and the temperature from the thermocouple measurement. Since the measured local emission is larger than the local emission calculated using the mean temperature, this local absorption coefficient gives a maximum value for the local absorption coefficient. The figure reveals that indeed the latter absorption coefficient is larger than the one from the absorption measurement. Since this local absorption coefficient is a maximum, this also leads to the conclusion that the soot volume fraction calculated using the measured absorption coefficient has a maximum that is about 2 or 3 times as large as the calculated value. One very striking thing in the figure is the difference in value for $x = 700$ mm. The absorption is nearly zero, but the emission is still significant. Turbulence is a possible cause for this. Fig. 6.10 shows that the difference between the mean local emission and the emission from the mean local temperature increases with axial position. So for $x = 700$ mm, where the turbulent length scales are the largest (De Vries (1994) and Peeters (1995)), the difference between these emissions is expected to be the largest. The second cause can be found in the large uncertainty in the absorption measurement. The absorption is so low that it is not significant and the local absorption coefficient can be completely wrong. Because of the large uncertainty in the measurement, it is very likely that the cutoff for the filtering in the tomographic reconstruction technique is chosen too small. As a result the width of the local profile is overestimated, because of the lack of high frequencies. Consequently the local absorption coefficient, near the centreline, will be underestimated.

Next there is the shape of the profile inside the flame. It is conspicuous that the shape of all the profiles is Gaussian. Further on when the soot volume fraction is discussed we come back to the shape of the profile. Taking a closer look at the peak level near the centreline, it is obvious that the absorption coefficient increases until $x = 600$ mm after which it drops very sharply to almost zero for $x = 700$ mm.
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![Graphs showing temperature profiles](image)

Figure 6.17: The temperature for flame A from the tomography measurements at $\lambda = 1.624 \mu m$ (—) and from the thermocouple measurements ($\circ$) for (a) $x = 300$, (b) $x = 400$, (c) $x = 450$, (d) $x = 500$, (e) $x = 600$ and (f) $x = 700$ mm.

Absorption profiles for flame B and C

For flames B and C no results are shown, but almost the same conclusions can be drawn. The small differences are the following. The absorption is smaller for flame B and even smaller for flame C. With this the uncertainty in the conclusions for these flames increases. Especially for the lowest axial positions the absorption is not significantly larger than zero. Still both for flame B and C the maximum local absorption coefficient appears around $x = 600$ mm, where the decrease of this coefficient with height, for larger axial positions, is largest for flame A and smallest for flame C. The latter again corresponds with the fact that flame A is the shortest and flame C the longest flame.

Temperature profiles for flame A

When both the local emission and the local absorption coefficient are known, temperature can be determined. Since only for flame A the local absorption coefficient is reliable for most of the performed traverses this flame is discussed extensively. The temperature profiles for flame A are shown in Fig. 6.17, for both the tomography and the thermocouple measurements. This figure reveals that the temperature determined from the tomography measurements is higher and the profile is wider. This figure also demonstrates that the temperature from the tomography measurements always has a
double Gaussian shape. Especially for \( x = 500 \) mm the peak temperatures are extremely high.

The simulations regarding the influence of turbulence on the tomographic measurements done for flame C showed that the temperature profile determined from the tomographic measurement will be both too wide and too high. This overestimation will not be as significant near the centreline as it is for positions away from the centreline. However for the two measurements techniques the difference in temperature near the centreline is significant. There are three possible explanations for this. First the influence of turbulence is larger than calculated from the simulations, indicating that not all the assumptions are correct. One possible candidate is the assumption of the constant emissivity. When the temperature fluctuations and the species concentration fluctuations are correlated it can be expected that the influence of turbulence will be larger then now calculated. Another explanation is that there is something wrong in the temperature as determined from the tomography measurements. This can be due to the fact that the local emission or the local absorption is not correct. Knowing the uncertainties in the measurement the latter is more likely the case. This would mean that the local absorption coefficient is too low and the calculated soot volume fraction would also be too low. It is also possible that the reconstruction technique is the cause of this effect. Especially near the centreline the value of the local profiles does not influence the integrated profiles that much. Depending on the step between two measurements in one traverse, the local profile near the centreline can change considerably while the integrated profile does not change significantly. One has to be very careful with this explanation. If this happens for the absorption it probably also takes place for the emission and a large part of the effect will be canceled. The third explanation can be found in the fact that the mean thermocouple temperature is too low, as reported in Section 6.2.2.

The other effect that is noticed in the figure is the fact that the tomographic temperature profile always is double Gaussian, with extremely high peak temperatures for \( x = 500 \) mm. This is due to the fact that the turbulence only influences the emission and not the absorption. Turbulence makes the emission profile wider. The influence on the absorption profile will be negligible, resulting in an absorption profile as wide as expected. At the exterior of the flame, the emission has a certain value, while the absorption is nearly zero. The temperature is a function of the fraction of the local emission and the absorption coefficient, see Eq. (2.48), and the temperature will increase to a maximum at the exterior of the flame, where this fraction reaches zero. For flame B and C these effects are even bigger because the absorption is lower and the turbulence level is higher for these flames. The consequence of all this is that it is not possible to determine the correct temperature with this tomographic reconstruction technique in the very strongly fluctuating turbulent parts of the flame.

The soot volume fraction in flames A, B and C

Since the temperature determined from the tomographic measurements is not fully correct, the temperature from the thermocouple measurements is used to calculate the soot volume fraction from the local absorption coefficient. In Fig. 6.18 (a)-(c) this soot
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Figure 6.18: The soot volume fraction for (a) flame A, (b) flame B and (c) flame C, with $x = 300$ ($-$), $x = 400$ ($-$), $x = 450$ ($-$), $x = 500$ ($-$), $x = 550$ ($-$), $x = 600$ ($-$), $x = 650$ ($-$) and $x = 700$ mm ($-$).
Figure 6.19: The soot volume fraction at the centreline, measured with the tomography setup (---) and with the suction probe (· · ·), for flame A (○), flame B (□) and flame C (△).

Volume fraction is shown for the three different flames for axial traverses where the maximum value of the soot volume fraction is larger than $1 \cdot 10^{-8}$. From Fig. 6.18 (a) it is seen that the soot formation starts near the centreline. Then the soot region widens with axial position and the amount of soot also increases. The maximum soot volume fraction is reached for $x = 600$ mm and almost all the soot has disappeared for larger axial positions (for $x = 700$ mm the soot volume fraction is smaller than $1 \cdot 10^{-8}$). For flame B and C only the values for the larger axial positions are reliable so nothing can be said about the soot formation region, but it is clear that the maximum soot volume fraction occurs around $x = 600$ mm. Both flame B and C are longer than flame A, so the decrease of soot volume fraction for larger axial positions is less than for flame A. As already stated in the discussion of the local absorption coefficient the shape of all the profiles is Gaussian. This is not what is expected. To form soot it is necessary that there is fuel and insufficient oxidiser to burn all the fuel. The temperature has to be high enough to start the chemical reactions. This results in the first soot formation at the fuel rich side of the reaction zone. In the diffusion flame this reaction zone is where the fuel and the air mix, and this is not at the centreline. Consequently either the shape of the measured profiles or our assumption is not correct.

Now that the soot volume fraction is obtained from the absorption measurement, it can be compared with the expectations that are made in the discussion of Fig. 6.10 and Fig. 6.13 regarding flame C. Between $x = 500$ and $550$ mm an increase in the soot volume fraction was expected. That is also seen from the absorption measurement. For $x = 500$ mm the soot volume fraction is so low that it is not possible to measure it, while for $x = 550$ mm the soot volume fraction gives a significant amount of absorption. Increasing the axial position to $600$ mm, the soot volume fraction is expected to stay at the same level and that is also what follows from the absorption measurements. Going to $x = 650$ and $700$ mm an increase in soot volume fraction is seen, followed by a decrease, just as was expected. Concluding it can be stated that there is a fairly good agreement between the emission and the absorption measurements.
6.3. Tomography measurements

![Figure 6.20: The average OH concentration measured by De Vries (1994) for (a) flame A, (b) flame B and (c) flame C, with $x = 50$ (- - -), $x = 100$ (---), $x = 150$ (--), $x = 200$ (—), $x = 250$ (—Δ—) and $x = 300$ mm (—+—).](image)

In Fig. 6.19 the soot volume fraction at the centreline of the three different flames is given as a function of the axial position in the flame. The soot volume fraction is measured with both the tomographic technique and the suction probe. The agreement between the two measurement techniques is fairly good, considering the uncertainty in both the measurements. The only discrepancy between the two techniques can be found in the axial position where the maximum soot volume fraction occurs. For all flames this is at a lower position for the probe measurements. This is probably caused by ineffective quenching. The temperature in the tip of the probe is still high enough so that reactions can take place and depending on the composition of the sample, soot will be formed or will be oxidated. The latter will be surely the case when the gas sample is taken at the axial position where the soot volume fraction is at its maximum. This can lead to a maximum at a lower axial position than is really the case. Another thing that can be seen from the comparison is the extremely high peak for the soot volume fraction from the tomographic measurement at $x = 600$ mm in flame A. Taking a closer look at the original measurement and its reconstruction, it can be said that the local absorption coefficient profile can be taken a bit wider and less high, without effecting the reconstruction and the measurement. This peak is probably due to an imperfect reconstruction, caused by a not good enough chosen cutoff and/or filter.

**Influence on OH measurements**

In Fig. 6.20 the average OH concentration, as measured by De Vries (1994), is shown for the three different flames. The results shown are from LIF measurements. The average concentrations are somewhat larger for the positive values of $y$, with respect to the negative values of $y$. This is due to a small effect of laser absorption in combination with not fully saturated fluorescence. The concentration of OH is a good indicator for the reaction zone. Therefore it is not expected to find a significant amount of OH near the centreline for flame A. Puri et al. (1992) and De Vries (1994) attributed this average centreline signal to soot scattering or PAH fluorescence. In Fig. 6.21 the average OH concentration at the centreline is presented for flame A. This can be compared with the soot volume fraction at the centreline as shown in Fig. 6.19.

The soot volume fraction measured with the tomography setup is not expected to be
significant for axial positions smaller than 300 mm. This is definitely true for flame B and C. The soot volume fraction measured with the suction probe is significant for flame A for \(x = 200\) mm. Extrapolating the measured values to smaller axial positions leads to the conclusion that the soot formation starts even at about \(x = 100\) mm. Comparing this with the OH profile at the centreline leads to the conclusion that soot scattering can be a cause for the fluorescence signal at the centreline. For \(x = 300\) mm the soot volume fraction for flame B is significant and somewhat smaller than the soot volume fraction for flame A at \(x = 200\) mm. The average OH concentration for flame B at \(x = 300\) mm is significantly smaller than the average OH concentration for flame A at \(x = 200\) mm. This makes it questionable whether soot scattering is the cause for the fluorescence signal at the centreline. For flame C definitely no soot is present for axial positions smaller than \(x = 300\) mm. Therefore no OH signal is expected at the centreline in that flame.

In Puri et al. (1992) LIF measurements in laminar diffusion flames are discussed. Methane and ethene were the studied fuels. The main interest was in three flames, designated as non-smoking, incipient smoking and smoking. The OH signal contained three peaks. Going from the centreline to the exterior of the flame, these peaks were attributed to PAH, soot and OH respectively. The latter two peaks have about the same magnitude. The reported OH concentrations are comparable with the average OH concentrations measured in our Delft piloted jet diffusion flames. For flame A at \(x = 300\) mm, the signal attributed to soot is about 10% of the signal attributed to OH. For consistency in the measurements this leads to the conclusion that the soot volume fraction in flame A has to be about 10% of the soot volume fraction as reported in Puri et al. (1992). The latter is about \(3 \cdot 10^{-6}\). This results in an expected soot volume fraction of about \(3 \cdot 10^{-7}\) in flame A at \(x = 300\) mm. The soot volume fraction measured with the suction probe is about \(3 \cdot 10^{-8}\) and thus about 1 order of magnitude smaller. This leads to the conclusion that the OH signal at the centreline is not due to soot scattering.
6.3. Tomography measurements

![Graphs showing emission intensity vs. distance for different wavelengths and locations](image)

Figure 6.22: The local emission for flame C for the measurements with $\lambda = 2.877 \, \mu m$, measured (—), and corrected for the emission of soot (— — —), for (a) $x = 100$, (b) $x = 150$, (c) $x = 250$, (d) $x = 400$, (e) $x = 500$, (f) $x = 600$ and (g) $x = 700 \, mm$.

6.3.4 Water vapour

In this section the results for the tomographic measurements at $\lambda = 2.877 \, \mu m$ will be presented. The main aim is to measure the partial pressure of H$_2$O in the Delft piloted jet diffusion flame. The arrangement of this section will mainly be equal to the one of Section 6.3.3. There are two major differences when these measurements are compared with the measurements regarding soot. The first and most important is the fact that the measured absorption is much higher, leading to an uncertainty that is smaller. A disadvantage is that soot also absorbs at $\lambda = 2.877 \, \mu m$. The measurements first have to be corrected for either the emission or the absorption of soot, to find the emission or the absorption of just the water vapour. As will be seen in this section, these corrections are mostly negligible. In flame A around $x = 600 \, mm$, where the highest soot volume fraction was found, this correction reaches its maximum of about 30%.
Local emission profiles for flame C

In Fig. 6.22 (a)-(g) the local emission is shown for the axial positions 100, 150, 250, 400, 500, 600 and 700 mm. This emission is corrected for the emission from soot wherever the latter has been measured. This corrected emission is the local emission regarding H$_2$O and can be compared to the emission from the calculations as shown in Fig. 6.10. Just as for the soot measurements, the width of the measured profile is best comparable with the mean local emission and not with the emission of the mean local temperature.

Now the focus will be on all the separate axial positions. For $x = 100$ mm the comparison between the profiles of the measurement and the mean local emission is fairly good. At the centreline the emission is nearly zero. Proceeding to larger radial positions a maximum is reached just before $y = 10$ mm and the width of the total profile is about 15 mm. For $x = 150$ mm the conclusions are the same, only the radial locations have shifted slightly. The maximum now occurs just outside $y = 10$ mm and the total width is about 20 mm. For both the measurement and the simulation the local emission has increased a bit, resulting in a partial pressure of H$_2$O that will be nearly the same for $x = 150$ and 100 mm. The local emission near the centreline is for $x = 150$ mm clearly larger than zero. Probably the amount of H$_2$O here will be larger. For $x = 250$ mm the local emission near the centreline is about half its maximum. This indicates that there will be a significant amount of H$_2$O near the centreline. For this location and higher in the flame, the measurement also is wider than the profiles from the simulations. Taking a closer look at the maximum local emission for $x = 250$ mm, this is about the same as for $x = 150$ mm for both the measurement and the simulation. This means that the $p_{H_2O}$ will be about the same. For $x = 400$ mm both the measurement and the simulation profiles are still double Gaussian. Also the increase of both profiles is about the same, again indicating that there is not a large change in partial pressure of H$_2$O. For $x = 500$ mm both the profiles are Gaussian with a very flat top. Compared with the profiles for $x = 400$ mm the measurements have increased more than the simulations, indicating that the partial pressure of H$_2$O must have increased too. For $x = 600$ mm the profiles are both Gaussian and they both have about the same maximum level as the profiles for $x = 500$ mm. Now the partial pressure will be comparable to its value for $x = 500$ mm. For $x = 700$ mm the profile from the simulation is Gaussian, but the measurement has a small double Gaussian profile. The latter is probably due to an imperfect cutoff and/or filter in combination with the high inaccuracy. Taking a closer look at the integrated emission profile and the reconstruction, it can be seen that near the centreline the reconstruction is a fit through the minima of the measurement. The local profile near the centreline can be higher without influencing the reconstruction negatively. The magnitude of the profiles has decreased when compared with the profiles for $x = 600$ mm, for both the measurement and the simulation. This is caused by a decreasing temperature. A lower temperature gives a decrease in blackbody radiation. The absorption coefficient $k$ of H$_2$O (in m$^{-1}$atm$^{-1}$) increases with decreasing temperature for this temperature range (see Fig. 2.10). A lower temperature, thus a higher absorption (and emission) coefficient, together with a lower emission must be caused by a decrease in partial pressure of H$_2$O.
6.3. Tomography measurements

![Graph showing local emission for flame A at x = 600 mm for the measurement with λ = 2.877 μm, measured (--) and corrected for the emission of soot(---).]

Figure 6.23: The local emission for flame A at x = 600 mm for the measurements with λ = 2.877 μm, measured (--) and corrected for the emission of soot(---).

Next the local emission of the measurements regarding soot, Fig. 6.13, and those regarding H₂O, Fig. 6.22, will be compared. For the latter it can be seen that the maximum emission is nearly constant for all the axial positions. For the first, there is a difference in maximum emission of about a factor of 6 for the measured radial profiles. The soot formation is much slower and a global feature, while the formation of H₂O is rather fast and a more local feature.

In Fig. 6.22 not just the measured local emission is shown, but also the corrected one. In most of the graphs, the difference of these two profiles is very hard to see. This can be expected since the amount of soot in flame C is rather low and the correction for the emission of soot will also be low. Knowing the soot volume fraction in all the three flames, the largest correction is expected in flame A for x = 600 mm. In Fig. 6.23 this measured and corrected local emission are displayed. This figure reveals that the maximum correction is approximately 30%.

**Local emission profiles for flame A and B**

The corrected local emission for flame A and B is given in Fig. 6.24 (a)-(g). The first thing that is demonstrated by Fig. 6.22 and Fig. 6.24 is the fact that the shape of the profiles changes from double Gaussian to Gaussian with increasing height, just as was the case for the soot measurements. Again this transition takes place at the lowest axial position for flame A and the highest axial position for flame C, indicating that flame A is the shortest and flame C the longest flame. The magnitude of the emission profile for the three different flames is not very dissimilar. The thermocouple temperature profiles for every axial position show that temperature is just a little bit lower for flame A and a bit higher for flame C. The partial pressure of H₂O is expected to be about the same for all three flames. The width of the profiles slightly increases in the sequence of flame A to B to C. This is in agreement with what was seen for the thermocouple temperature measurements and the tomographic measurements regarding soot.

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Absorption profiles for flame C

In Fig. 6.25 (a)-(g) the line-of-sight absorption is shown for flame C. When this is compared to the absorption for the soot measurements in Fig. 6.15, it can be seen that the absolute deviation in the measurements is the same. Because the absorption for the H₂O measurements is much larger than for the soot measurements, about a factor of 10, the relative uncertainty in the H₂O measurements is much smaller than for the soot measurements. Although the absorption is much larger with respect to the soot measurements, still neglecting self-absorption will not lead to a significant increase in uncertainty. Again the reconstruction gives a reasonable fit through the measurements, but even with a much better signal to noise ratio, it still is not possible to resolve structures in the flame with a mm order spatial resolution. From Fig. 6.25 it is also clear that the absorption increases with increasing axial position. Since the width of the profile also increases it is not possible to say anything about the local absorption
6.3. Tomography measurements

Figure 6.25: The line-of-sight absorption for flame C and λ = 2.877 μm, measured (—) and integrated from Fig. 6.26 (— —) for (a) x = 100, (b) x = 150, (c) x = 250, (d) x = 400, (e) x = 500, (f) x = 600 and (g) x = 700 mm.

The local absorption coefficient is presented. In this figure the local absorption coefficient is approximately constant until x = 400 mm, has its maximum between 500 and 600 mm and decreases again for x = 700 mm. Comparing the width of the local absorption coefficient and the local emission, the profile of the first is slightly smaller than the profile of the latter. This is again an indication that the emission, through temperature, is influenced by turbulence, but that the absorption is hardly influenced by turbulence.

When the local absorption coefficient of the soot measurements was discussed, some peaks at the side of the flame were revealed. In Fig. 6.26 it is seen that for H₂O these peaks are not present. One possible explanation is that the physical phenomenon producing these peaks is not present in these measurements. When diffraction is the cause of these peaks, it is not very likely that it is not present in the measurements regarding H₂O. More likely is the fact that it is present, but negligible. This is possible
since the absorption of the H₂O measurements is about 1 order of magnitude larger than of the soot measurements and the peaks in the latter measurements were already smaller than the signal. Thus it is very likely that the peaks are present in the measurement, but negligible in comparison with the absorption signal from H₂O. The latter was expected, because after the first tests done, where the blackbody aperture was varied, this effect disappeared with the largest aperture. Also in the measurements in the flat flame nothing like this was encountered.

For the soot measurements also the local absorption coefficient was presented, calculated from the local emission and the thermocouple temperature. This absorption coefficient was also calculated for the H₂O measurements, but since this local absorption coefficient was at least a factor of 3 larger than the measured absorption coefficient this was not very meaningful. Neglecting the influence of turbulence, the maximum partial pressure calculated from the local absorption coefficient will be much higher than the actual calculated partial pressure from the measurements.
6.3. Tomography measurements

![Graphs showing temperature profiles](image)

Figure 6.27: The temperature for flame C from the tomography measurements with $\lambda = 2.877 \, \mu m$ (---) and from the thermocouple measurements (o), for (a) $x = 100$, (b) $x = 150$, (c) $x = 250$, (d) $x = 400$, (e) $x = 500$, (f) $x = 600$ and (g) $x = 700$ mm.

Absorption profiles for flame A and B

For flame A and B, the conclusions regarding the local absorption coefficient are about the same as for flame C. Also the magnitudes of the local absorption coefficient for all the three flames are comparable. The only major difference is the length of flame A. This flame is clearly shorter than the other two. This is demonstrated by the fact that the maximum in the local absorption coefficient for this flame occurs between $x = 300$ and 400 mm instead of between $x = 500$ and 600 mm as for the other two flames.

Temperature profiles for flame C

With the local emission and the local absorption coefficient, temperature can be calculated. In Fig. 6.27 the temperature for flame C is presented together with the temperature from the thermocouple measurements. Just like is seen for the soot measurements,
the tomographic temperature profile is higher and wider than the thermocouple temperature profile. This is expected, since this was one of the conclusions regarding the influence of turbulence on the tomographic measurements, see Section 6.3.2. Taking a closer look at the results from Fig. 6.11 it is seen that the discrepancy between the two measurement techniques is wavelength dependent. The higher the wavelength, the lower the discrepancy. Comparing Fig. 6.17 and Fig. 6.27 it is demonstrated that this is also the case for the tomography measurements. Even though Fig. 6.17 demonstrates the temperature for flame A and Fig. 6.27 for flame C, the discrepancy with the thermocouple measurements is even bigger for the soot measurements in flame C. Also here it shows that the influence of turbulence on the tomographic measurements is wavelength dependent. Another prove for this fact can be found in the shape of the temperature profile. For the soot measurements most of the temperature profiles, shown in Fig. 6.17, were double Gaussian because of the emission profile that was too wide and the absorption coefficient profile that was not influenced by turbulence. The tomographic temperature profiles in Fig. 6.27 are wider than the thermocouple temperature profiles, but the peaks at the exterior of the flame are not as distinguishing as for the soot measurements. The discrepancy between the tomographic and thermocouple temperature profiles is also expected to be the least near the centreline. As is displayed in Fig. 6.27 this is also the case for the H$_2$O measurements. Just as for the soot measurements, this discrepancy is larger than expected from the simulations. In the previous section three explanations were given. Each of them also holds for the H$_2$O measurement. The first was that the influence of the turbulence is larger than calculated from the simulations. As expected the influence is smaller for a larger wavelength, but this says nothing about the accuracy of the calculated influence of the turbulence. Also the explanation that it is due to the wrongly determined tomographic temperature can not be refuted. The accuracy of the measurements regarding H$_2$O is better than the soot measurements. This means that it can be expected that a discrepancy in temperature will be smaller for the H$_2$O measurements. Finally it still holds that the thermocouple temperature is systematically somewhat too low.

The partial pressure of H$_2$O in flames A, B and C

The absorption at $\lambda = 2.877 \, \mu m$ is due to H$_2$O and soot, just as is the case for the emission. Therefore the local absorption coefficient has to be corrected, before the partial pressure of H$_2$O can be calculated. This correction will be the largest for the measurement for $x = 600 \, mm$ in flame A, just as for the emission. In Fig. 6.28 the partial pressure of H$_2$O is presented, both with and without this correction for the absorption of soot. Again the maximum correction is about 30%. In most traverses the soot volume fraction is much smaller than for $x = 600 \, mm$ in flame A. This correction will then be much smaller and often negligible. All the partial pressures presented in this section are corrected for the absorption by soot.

In Fig. 6.29 (a)-(c) the corrected partial pressures are shown for the different axial traverse in the three flames. From the discussion of the local emission in flame C some expectations were given about the influence of the axial position on the partial pressure of H$_2$O. Going from $x = 100$ to 150 mm the profile is expected to get
6.3. Tomography measurements

![Graph](image)

Figure 6.28: The partial pressure of H$_2$O for flame A at $x = 600$ mm for the measurements with $\lambda = 2.877$ μm, measured (---) and corrected for the absorption of soot (−−−).

slightly wider. The magnitude is expected to be the same, but near the centreline the partial pressure can be larger. This is revealed in Fig. 6.29 (c). For $x = 250$ mm there surely is some H$_2$O expected near the centreline and its magnitude is expected to be about the same as for 150 mm. The non-zero value at the centreline follows also from the absorption measurements, but the magnitude of the partial pressure of H$_2$O is a bit higher for $x = 250$ mm than for 150 mm. This is probably a temperature effect. For $x = 250$ mm the temperature is little higher than for 150 mm, resulting in an absorption coefficient $k$ that is slightly lower. The same amount of absorption must be caused by a higher partial pressure. For $x = 400$ mm the profile is expected to be double Gaussian and about the same as for $x = 250$ mm. The shape of the profile is between Gaussian and double Gaussian and the magnitude is definitely larger. The first can be due to an imperfect reconstruction. The latter is again due to an increase in temperature. For $x = 500$ mm, as expected, a Gaussian profile is seen, with an increase in magnitude. For $x = 600$ mm no big difference is seen with the profiles for $x = 500$. For $x = 700$ mm the partial pressure of H$_2$O starts to decrease. So in general the emission and the absorption measurements lead to the same conclusions.

From a comparison of the profiles in Fig. 6.29 (a)-(c) the following can be stated. The width of the flame does not change significantly with the turbulence level. Comparing the profiles for $500 < x < 700$ mm it is revealed that flame A is the shortest and flame C the longest flame. With increasing axial position the profiles change from double Gaussian to Gaussian. For flame A this transition occurs again at the lowest position and for flame C at the highest. This transition of the profiles shows that H$_2$O is formed near the reaction zone and then spreads by diffusion. The turbulence level influences the magnitude of the partial pressure of H$_2$O. The mixing is better for a higher turbulence level. Better mixing results in a better combustion and thus in more products like H$_2$O and CO$_2$. For flame C the partial pressure of H$_2$O is the highest, with the maximum about the maximum reachable for complete combustion of natural gas. For flame A the maximum is significantly lower, indicating that combustion is not
Figure 6.29: The partial pressure of H$_2$O measured with the tomography setup, corrected for soot, for (a) flame A, (b) flame B and (c) flame C, for $x = 100$ (---), $x = 150$ (--), $x = 250$ (···), $x = 300$ (——), $x = 400$ (→→), $x = 500$ (−−−), $x = 600$ (−×−) and $x = 700$ mm (−△−).
6.3. Tomography measurements

Figure 6.30: The volume fraction of H$_2$O calculated by Peeters, for flame C, with $x = 100$ (---), $x = 150$ (---), $x = 250$ (---), $x = 400$ (---), $x = 500$ (---), $x = 600$ (---), and $x = 700$ mm (Δ-Δ).

The volume fraction of H$_2$O can also be compared with the simulations from Peeters. In Fig. 6.30 the volume fraction, which differs not significantly from the partial pressure, calculated by these simulations is displayed. First thing that is noticed is the fact that the magnitude of the partial pressure (from the measurements) and the magnitude of the volume fraction (from the simulations) are comparable. For the lower axial positions the measured partial pressure is about 20% lower. Around $x = 500$ and 600 mm, where the partial pressure reaches its maximum, the measurements and the simulations are within a few percent. For larger axial positions in the flame, the measured partial pressure is again some 20% lower than the calculated volume fraction. For one axial position, the radial profile of the partial pressure has a significantly different shape than the radial profile of the volume fraction. For $x = 150$ mm the calculated profile is double Gaussian, while the measured profile tends to be Gaussian. The double Gaussian profile is also what is expected from the emission profile and it is also strange that the profiles of the partial pressure for 100 and 250 mm are double Gaussian and the profile in between is not. It is very likely that something is wrong with the absorption measurement in combination with the reconstruction, for $x = 150$ mm. For all the other profiles, there is a good agreement regarding the shape of the profiles.

The width of the calculated profiles is about the same as the width of the measured profiles. This is not expected. Comparing the temperature profiles it was seen that the width of the calculated profiles, for axial positions larger than 150 mm, was smaller than the width of the measured profiles. This was also the case for the LDA measurements (Stroomer (1995)) and the CARS measurements (Mantzaras and Van der Meer (1997)). For more details, the temperature profile measured with a thermocouple and the profile of the partial pressure of H$_2$O will be compared. These profiles are displayed in Fig. 6.31 for the axial positions 150, 400 and 600 mm. Regarding only the
width of the profile, the figure reveals that for \( x = 150 \) mm the profiles have about the same width. For larger axial positions, the width of the temperature profile is significantly larger than the width of the profile for the partial pressure. The figure also reveals that \( \text{H}_2\text{O} \) is formed near the reaction zone, which is indicated by the temperature peaks, but at the fuel rich side. In Chapter 5 it was shown that for the laminar flame the diffusion of \( \text{H}_2\text{O} \) was larger than the diffusion of heat. For the turbulent diffusion flame the figure demonstrates that this is also true (see also Section 6.4).

6.3.5 Acetylene

Finally, tomography measurements are performed in the Delft piloted jet diffusion flame at a wavelength of \( \lambda = 3.049 \) \( \mu \)m. At this wavelength soot as well as \( \text{H}_2\text{O} \) and \( \text{C}_2\text{H}_2 \) absorb. Correcting the measurements for the absorption of soot and \( \text{H}_2\text{O} \), information about the partial pressure of \( \text{C}_2\text{H}_2 \) can be obtained. As in the last two sections, the discussion will start with the local emission. The main interest is in (the standard) flame C, but also results of flame A will be presented. After the local emission the measured absorption profile will be discussed. This again to get an idea about the accuracy of the absorption measurements. Then the discussion will proceed with the local absorption coefficient for flame C. With the two local parameters the temperature can be calculated which will be compared with the thermocouple measurements. The final step is the calculation of the partial pressure of \( \text{C}_2\text{H}_2 \) with the correction for soot and \( \text{H}_2\text{O} \). It will be demonstrated that for the measurements at this wavelength the correction is significant. This corrected partial pressure will be compared with the results of the Monte Carlo simulations. At the end of the section, the partial pressure of \( \text{C}_2\text{H}_2 \) will be compared with the soot volume fraction. This will give an indication about \( \text{C}_2\text{H}_2 \) being a precursor of soot.
6.3. Tomography measurements

Figure 6.32: The local emission for flame C for the measurements with $\lambda = 3.049 \mu m$, measured (--), and corrected for the emission of soot and H$_2$O (---), for (a) $x = 100$, (b) $x = 150$, (c) $x = 250$, (d) $x = 400$ and (e) $x = 500$ mm.

Local emission profiles for flame C

Both the corrected and the uncorrected local emission for flame C are given in Fig. 6.32, for the axial positions 100, 150, 250, 400 and 500 mm. Different from the H$_2$O measurements, the corrections for the measurements regarding C$_2$H$_2$ are not negligible. This is not because of the correction for the presence of soot, but mainly because of the correction for the presence of H$_2$O. In the previous two sections it was revealed that there is not a large amount of soot in the flames, especially in flame C, but the amount of H$_2$O is considerable for most axial traverses done in all three flames. The following discussion about the local emission reflects the corrected values.

First the profiles at the different axial positions will be compared. From this comparison, some expectations will be presented about the amount of C$_2$H$_2$ at these heights. To do so, the measurements shown in Fig. 6.32 will also be compared with the mean local emission from the simulations as presented in Fig. 6.10. For $x = 100$ mm the emission at the centreline is small, but significant. The maximum is reached at radial positions just smaller than 10 mm. The half width of the whole profile is about 15 mm. Except for the non-zero values at the centreline, the measured profile is in accordance with the profile from the simulations. The non-zero values near the centreline might be due to a small amount of C$_2$H$_2$. For this low axial position the temperature is still rather low near the centreline. The absorption coefficient of C$_2$H$_2$ (in m$^{-1}$atm$^{-1}$) is strongly not linear for low temperatures, see Fig. 2.6. A fairly small amount of
C₂H₂ at low temperature can result in a considerable emission. For \( x = 150 \text{ mm} \) the width of the profile increases a bit in comparison with the width of the profile for \( x = 100 \text{ mm} \). The magnitude of the maximum also increases slightly, while the value near the centreline increases significantly. This is also the case for the calculations. It is expected that the partial pressure of C₂H₂ will be nearly the same for these two axial positions. Furthermore, because of the strong non-linearity of the absorption coefficient of C₂H₂, it is not possible to say anything about the partial pressure near the centreline. For \( x = 250 \text{ mm} \) and for higher axial positions, the width of the measured profiles is larger than the width of the calculated profiles. In fact, the width of the measured profiles is about the same as the width of the profiles from the H₂O measurements. Near the centreline the emission is close to the maximum value, so with the temperature at a moderate level this means that there is a considerable amount of C₂H₂ at the centreline. At the radial position where the maximum value occurs, the partial pressure will be about the same as the maximum level for the profile for \( x = 150 \text{ mm} \). For the profiles for \( x = 400 \text{ mm} \), the maximum value is approximately the same again and the value near the centreline has increased again, both for the measurement and the calculation. The profiles are still double Gaussian. The partial pressure of C₂H₂ is expected to be about the same again. For \( x = 500 \text{ mm} \) the local emission profile is Gaussian and the maximum value has again not changed. This will lead to a partial pressure profile that is Gaussian too, with a maximum value that is again about the same level as for all other axial positions.

Local emission profiles for flame A

The local emission for flame A is given in Fig. 6.33 (a)-(f). Comparing the profiles for flame A and C roughly leads to the same conclusions as for the measurements at \( \lambda = 2.877 \mu \text{m} \). First of all it is seen that the profiles change from a double Gaussian shape to a Gaussian shape. The axial position where the transition between these two shapes occurs is again smaller for flame A, indicating that this flame has a smaller flame length. The magnitude of the local emission for flame A is slightly higher than for the measurements in flame C. Because temperature is little lower in flame A, this will probably lead to partial pressures that are approximately the same for both flames. The width of the local emission profiles for both flames are nearly equal. For flame A the width is a minor fraction smaller. This is probably caused by the lower turbulence level for this flame, as already discussed in Section 6.3.3.

Absorption profiles for flame C

The line-of-sight absorption for flame C is presented in Fig. 6.34 (a)-(e). The magnitude of the absorption and its uncertainty are comparable to the magnitudes for the H₂O measurements, as shown in Fig. 6.25. Also for these measurements, there is a reasonable signal to noise ratio, but again not sufficient to expect a small spatial resolution. In the figure it can also be seen that the absorption increases with height, but also does the width of the profile. Because of this and the fact that the absorption is not just from C₂H₂, but also from soot and H₂O, it is not possible to give a forecast regarding the partial pressure of C₂H₂. This implies that it is also not possible to give
a forecast about the partial pressure of $C_2H_2$ using the local absorption coefficient as shown in Fig. 6.35. Comparing the local absorption coefficient for the $C_2H_2$ measurements and the $H_2O$ measurements (Fig. 6.26) the following can be stated. The width of the profiles is about the same. The magnitude is smaller for the $C_2H_2$ measurements, indicating that the absorption coefficient $k$ for $H_2O$ is smaller for $\lambda = 3.049 \mu m$ than for $\lambda = 2.877 \mu m$. The transition between a double Gaussian and a Gaussian profile is at a lower axial position for the $C_2H_2$ measurements. This means that the formation of $C_2H_2$ takes place not only in the reaction zone, but also in the fuel rich zone, assuming that it is not $C_2H_2$ from the pilot flames. This seems in agreement with what was seen for the soot measurements in flame A. For these measurements it was seen that the soot formation also seemed to start near the centreline and not in the fuel rich side of the reaction zone.

In the discussion of the $H_2O$ measurements two more comparisons with the soot measurements were made. The first one was about the peaks at the side of the flame. These were present in the soot measurements, but not detected in the $H_2O$ measurements. For the measurements at $\lambda = 3.049 \mu m$ these peaks are also not present in the profiles of the local absorption coefficient. This supports the statement that these peaks are probably detected because of the small absorption in the soot measurements and negligible to the relatively large absorption in the $H_2O$ and $C_2H_2$ measurements. The second part of that discussion was about the local absorption calculated from the local
emission and the thermocouple temperature measurement. This is not very meaningful in this case, since the absorption and the emission are both depending on the partial pressure of C₂H₂ and H₂O. For H₂O it was seen that the maximum local absorption coefficient was at least a factor of three larger than the measured one, so this will not lead to any information about the local absorption coefficient of C₂H₂.

**Absorption profiles for flame A**

For flame A the conclusions are not very different from the conclusions for flame C. The local absorption coefficient has nearly the same magnitude and its profile the same width as for flame C. For the lower axial positions the profile has a different shape though, it is already Gaussian and not double Gaussian. Another difference is the fact that for the higher axial positions, something like the peaks at the exterior of the flame, seen in the soot measurements, is also present in these profiles. Although these peaks are not as distinct as for the soot measurements. More and accurate research, specifically dealing with the diffraction problem, has to be done.

**Temperature profiles for flame C**

In Fig. 6.36 the temperature profiles are presented for the tomography measurements at λ = 3.049 μm and λ = 2.877 μm and for the thermocouple measurements. The
6.3. Tomography measurements

Figure 6.35: The local absorption coefficient for flame C and \( \lambda = 3.049 \, \mu\text{m} \), for (a) \( x = 100 \), (b) \( x = 150 \), (c) \( x = 250 \), (d) \( x = 400 \) and (e) \( x = 500 \) mm.

difference between the two tomography measurements is not significant, at most radial positions. Where it is significant, this is definitely due to a systematic error in one of the measurements at that radial position, since this is at the exterior of the flame or near the centreline, for \( x = 100 \) mm. Most of the observations made discussing the temperature profiles of the tomography measurement for H\(_2\)O also hold for the profiles of the measurement of C\(_2\)H\(_2\). The temperature profile is higher and wider than the one from the thermocouple measurement. The difference is smaller than for the soot measurement and about the same as for the H\(_2\)O measurement. The latter is probably due to the small difference in wavelength and the uncertainty in the tomography measurement. The smaller influence of the turbulence on temperature is also seen from the double Gaussian profile, which is less than for the soot measurement, and from the smallest discrepancy with the thermocouple measurements near the centreline.

The partial pressure of C\(_2\)H\(_2\) for flame A and C

As already mentioned, both the absorption and the emission at \( \lambda = 3.049 \, \mu\text{m} \) are due to C\(_2\)H\(_2\), H\(_2\)O and soot. To calculate the partial pressure of C\(_2\)H\(_2\) a correction has to be made for the partial pressure of H\(_2\)O and the soot volume fraction. The latter correction is expected to be negligible at most positions just as it was for the H\(_2\)O measurements. The first will turn out not to be negligible. In Fig. 6.37 the partial pressure of C\(_2\)H\(_2\) is presented for the arbitrary axial position \( x = 250 \) mm, both with
Figure 6.36: The temperature for flame C from the tomography measurements at $\lambda = 3.049 \mu m$ (---), at $\lambda = 2.877 \mu m$ (---) and from the thermocouple measurements (○), for (a) $x = 100$, (b) $x = 150$, (c) $x = 250$, (d) $x = 400$ and (e) $x = 500$ mm.

Figure 6.37: The partial pressure of $C_2H_2$ for flame C for $x = 250$ mm for the measurements with $\lambda = 3.049 \mu m$, measured (---) and corrected for the absorption of soot and $H_2O$ (---).
6.3. Tomography measurements

Figure 6.38: The partial pressure of $C_2H_2$ measured with the tomography setup, corrected for soot and $H_2O$, for (a) flame A and (b) flame C. for $x = 100$ (---), $x = 150$ (---), $x = 250$ (---), $x = 300$ (---), $x = 400$ (---), $x = 500$ (---) and $x = 600$ mm (---).

and without correction for the partial pressure of $H_2O$ and the soot volume fraction. In this figure it is demonstrated that the maximum correction is about 40% and that it has a strong dependence on radial position. Because of the latter, the shape of the profile can substantially change due to the correction. It has to be concluded that for this measurement the correction is insuperable. All the partial pressures of $C_2H_2$ presented further, are corrected for the partial pressure of $H_2O$ and the soot volume fraction.

This corrected partial pressure of $C_2H_2$ is shown in Fig. 6.38 (a) and (b), for respectively flame A and C. The partial pressure of $C_2H_2$ is about the same for both flames, both qualitative and quantitative. The partial pressure of $C_2H_2$ in flame C will first be compared with the conclusions that were made in the discussion of the local emission. Then it will be compared to results of the Monte Carlo calculations performed by Nooren. Finally the partial pressure of $C_2H_2$ will be coupled to the measured soot volume fraction.

From the profiles of the local emissions, a double Gaussian profile with the max-
ima at radial positions just smaller than 10 mm and a total width of about 15 mm is expected. This is also seen for the partial pressure profile. Even the non-zero values at the centreline can be detected in the profile. For $x = 150$ mm the profile is a bit wider and the maximum value is about the same as for the profile for $x = 100$ mm. For $x = 250$ mm the maximum value is again about the same, where the width has increased again. At the centreline there is a considerable amount of $C_2H_2$. For $x = 400$ mm the value near the centreline has increased, and the maximum value is again about the same. In the absorption measurements the profile is flat Gaussian, while the profile from the local emission has a more double Gaussian shape. For $x = 500$ mm both the profiles are Gaussian. The partial pressure of $C_2H_2$ has decreased, while this was not expected from the local emission measurements. In general, just as for the soot and the $H_2O$ measurements, the agreement between the absorption and the emission measurements is good. A difference with the measurements regarding soot and $H_2O$ is that for the $C_2H_2$ measurements it is essential to correct for the emission or absorption of the other components.

The next comparison that will be made is between the measurements in flame C and the Monte Carlo simulations done by Nooren. The volume fraction of $C_2H_2$ calculated by the latter are shown in Fig. 6.39. First thing that is noticed is the large difference, about a factor of 10, in magnitude. There are two possibilities for this. Either the absorption coefficient used to calculate the partial pressure of $C_2H_2$ is not correct, or the simulations are wrong. From Section 2.4 it is known that the first is possible. Regarding the simulations it can be stated that it is not likely that all the (chemistry) models used in the Monte Carlo simulations are correct yet. The shapes of all the profiles in the measurements and the simulations are the same. The transition between the double Gaussian and the Gaussian profile is at the same axial position. Also the width of the profiles is comparable for the lower axial positions. For larger axial positions the profiles from the simulations have again a somewhat smaller width than the profiles from the measurements. Besides the factor of 10 difference in magni-
6.3. Tomography measurements

Figure 6.40: The soot volume fraction (—) and the partial pressure of C_{2}H_{2} (· · ·) at the centreline for flame A (○) and flame C (△).

Figure 6.41: The soot volume fraction (—) and the partial pressure of C_{2}H_{2} (· · ·) for flame A, for x = 300 (+), x = 400 (●), x = 500 (○) and x = 600 mm (x).

The magnitude between the measurements and the simulations, also the mutual relation between the profiles at different axial positions is not the same. For the measurements the maximum magnitude is about the same for all the profiles, while for the simulations there is a maximum between x = 400 and 500 mm, which is higher than the maximum for all the other profiles. For the measurements this maximum (near the centreline) is located around x = 400 mm. Again the flame length is larger for the simulations than for the measurements. This is in agreement with what was seen for the thermocouple temperature measurements.
Comparing the soot volume fraction and the partial pressure of \( \text{C}_2\text{H}_2 \)

In Fig. 6.40 and Fig. 6.41 both the partial pressure of \( \text{C}_2\text{H}_2 \) and the soot volume fraction are presented. In Fig. 6.40 the value at the centreline is given as a function of the axial position for both flame A and C. In Fig. 6.41 radial profiles are displayed for flame A, for axial positions where the soot volume fraction is significant. From the figures it can be concluded, that a considerable amount of \( \text{C}_2\text{H}_2 \) is needed near the centreline, before soot formation starts. Since \( \text{C}_2\text{H}_2 \) is assumed to be a precursor of soot, it is expected that \( \text{C}_2\text{H}_2 \) is formed before the production of soot. This is confirmed by the measurements. But the measurements also show that soot is formed near the centreline to a substantial extent, whereas it is expected to occur mostly between the centreline and the reaction zone. Furthermore, the amount of \( \text{C}_2\text{H}_2 \) slowly decreases, when the soot volume fraction increases. This indicates that the formation of soot is a relatively slow process. From the values at the centreline, it is seen that the partial pressure of \( \text{C}_2\text{H}_2 \) is nearly independent of the flame type. This, while there is a huge difference in the soot volume fraction produced in both flames. A certain level of \( \text{C}_2\text{H}_2 \) is necessary to start the formation of soot, but there are more parameters involved. Temperature must be high enough, but not too high and the amount of oxidiser must be below a certain value.

6.4 Reaction zone and shear flows

In this section we will take a closer look to the reaction zone and the shear flows in the Delft piloted jet diffusion flame. First the theoretical location of the reaction zone and the shear layers will be discussed. After that, the location of the reaction zone and the inner shear layer will be identified from several measurements. The latter include tomography measurements regarding \( \text{H}_2\text{O} \) and \( \text{C}_2\text{H}_2 \), thermocouple measurements for the temperature profiles, LDA measurements from Stroomer (1995) regarding mean axial velocity and in particular its fluctuations and LIF measurements from De Vries (1994) regarding both \( \text{OH} \) and \( \text{NO} \).

Theoretical approach

The most important source of turbulence in turbulent jet flames is from turbulent shear layers. In our three-flow system with a central fuel jet and a primary air annulus jet issuing in a secondary air coflow, there is one shear layer mixing fuel and primary air and one layer mixing primary and secondary air. They both influence the reaction zone. The latter is the narrow region in the flame where the reactions mainly occur. In this region the fuel to air ratio is near stoichiometric. A mixture is stoichiometric when fuel and air are mixed on a molecular scale so that there is sufficient, but not more, air to react with all the fuel. In Fig. 6.42 the centre of the reaction zone is indicated with the solid line. For an extensive discussion about the location of the reaction zone and its shape, the reader is referred to De Vries (1994). The broken lines in the figure indicate the two shear layers. On the inside the inner shear layer invades to the uniform velocity jet. On the outside it penetrates into the primary air and causes the jet to entrain fluid from the surroundings. The entrainment of air causes the shear layer to grow. Close
to the nozzle, the centreline velocity is not yet influenced by the shear layer and no air is entrained. This small region is cone-shaped and is known as the potential core. All turbulence found in this region is from the turbulent pipe flow. Downstream of the potential core the inner shear layer causes the flow to develop turbulence. Further downstream the turbulence becomes fully developed because of the influence of the outer shear layer. The latter is the shear layer between the primary and the secondary air. On the inside it spreads into the primary air and further downstream into the mixing of the primary air and the fuel jet. On the outside it penetrates into the ambient air.

**Experimental verification**

Next we will try to identify the location of the reaction zone and the shear layers from measurements. For this the measured profiles of OH, T, NO, $u'_{rms}$, H$_2$O and C$_2$H$_2$ will be used. For NO the full distance at half maximum is used to determine $d_{NO}$. For all other quantities $d$ represents the distance between the two radial locations with maximum value. To identify the reaction zone, OH concentration and thermocouple temperature measurements will be used. In Fig. 6.43 the distance $d_{OH}$ based on the LIF measurements regarding OH, reported in De Vries (1994), is shown. Unfortunately these measurements only extend to an axial position of 300 mm. Near the nozzle, for small axial positions, the distance of the flame is mainly determined by the burner geometry, which can be seen from the distance that is independent of the flame settings. Further downstream there is a significant difference in the distance of the three flames, where flame C has the largest distance and thus is the widest.

Another indicator for the reaction zone is the temperature. In Fig. 6.44 the distance based on the thermocouple temperature measurements is presented. For the smaller axial positions this distance is determined from thermocouple measurements performed by De Vries (1994), further downstream the distance is based on the ther-
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Figure 6.43: The distance between the two radial locations with maximum value based on the OH measurements from De Vries (1994), for flame A (– – – • • • •), flame B (– – – × × × ×) and flame C (– – – △ △ △ △).

Figure 6.44: The distance between the two radial locations with maximum value based on the thermocouple temperature measurements from De Vries (1994) (– – – –) and the thermocouple temperature measurements presented in this thesis (– – – –), for flame A (○), flame B (×) and flame C (△).

mocouple measurements as presented in this thesis. The figure reveals that there is a good connection between the measurements at the smaller axial positions and the ones further downstream. Again it is demonstrated that the distance increases in the sequence flame A, B and C. The shape of the profiles is also comparable with the shape of the reaction zone as presented in Fig. 6.42. The length of this cigar-shaped zone is between 500 and 600 mm. This is in agreement with the value of about 540 mm reported by De Vries (1994).

Next to the LIF measurements regarding OH, De Vries (1994) also reports LIF measurements regarding NO. For the latter the NO is seeded to the fuel jet. The
distance $d_{NO}$ is assumed to indicate the shear layer between the fuel and the primary air. In Fig. 6.45 the distance based on the NO measurements is presented. The figure shows that flame C is the widest again and flame A the most narrow flame.

From the LDA measurements reported in Stroomer (1995) the distance based on the axial rms velocity is calculated. This distance is again the distance between the two radial locations with maximum value and is presented in Fig. 6.46. This distance is also an indication of the position of the shear layer. The distance reflects the inner shear layer only, because not all the radial traverses extended so far that the outer shear layer could be resolved. However the measurements that included the outer shear layer revealed that the turbulent intensity of the outer shear layer is larger than the turbulent intensity of the inner shear layer (Stroomer (1995)). If $d_{NO}$ and $d_{u'rms}$ are compared to
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**Figure 6.47:** The distance between the two radial locations with maximum value based on the H$_2$O tomography measurements, for flame A (· · · o · · ·), flame B (· · · x · · ·) and flame C (· · · Δ · · ·).

**Figure 6.48:** The distance between the two radial locations with maximum value based on the C$_2$H$_2$ tomography measurements, for flame A (· · · o · · ·) and flame C (· · · Δ · · ·).

d$_{OH}$ and d$_{r}$, it is revealed that the reaction zone is located on the fuel lean side of the inner shear layer for axial positions smaller than about 250 mm. Further downstream the shear layer and the reaction zone coincide and the turbulence strongly interacts with the chemistry. For even higher axial positions also the outer shear layer interacts with the reaction zone and the turbulence is fully developed, see Fig. 6.42.

Now the reaction zone and the shear layer are more or less located, the focus will be on the distance based on the tomography profiles regarding H$_2$O and C$_2$H$_2$. The first is given in Fig. 6.47 and the latter in Fig. 6.48. For H$_2$O the profile of the distance for flame B has a completely different shape and is not in between the profiles of the distance for flame A and C. Therefore this profile is not taken into account in the following discussion. Comparing d$_{H_2O}$ with d$_{r}$, the first is smaller than the latter and
consequently the radial profile of $p_{H_2O}$ is Gaussian at a smaller axial position than the temperature profile. This means that $H_2O$ is formed at the fuel rich side of the reaction zone. The distance based on the $H_2O$ measurements demonstrates that for small axial positions most $H_2O$ is formed near the shear layer, where diffusion of the products is not yet important. The distance based on the $C_2H_2$ profiles is comparable with the distance based on the $H_2O$ profiles. This means that most $C_2H_2$ is formed on the fuel rich side of the reaction zone near the shear layer. This is expected because this is the side where there is not sufficient oxidiser to burn all the fuel, completely. That is the region where some intermediate products will exist.

In Fig. 6.49 the distance for flame C according to the calculations from Peeters is shown. This distance is based on the $T$, the OH and the $H_2O$ profile. As we know from the measurements, the flame width and the flame length of the calculations and the experiments differ. Therefore the profiles will only be compared qualitatively. The figure reveals that for the calculations also $d_{OH}$ is larger than $d_T$. However, for the calculations the difference is larger than for the experiments. Just as for the experiments, also for the calculations, $d_{H_2O}$ is smaller than $d_T$. Not only is the magnitude smaller, but $d_{H_2O}$ is also zero for a smaller axial position. Concluding, it can be stated that the qualitative comparison between the measurements and the calculations is fairly good.

This chapter started with the discussion of the average temperature measurements, performed with a thermocouple. These results are compared with simulations with assumed PDFs from Peeters (1995), Monte Carlo simulations performed by Nooren (1996) as well as with CARS measurements done by Mantzaras and Van der Meer (1997). For axial positions smaller than 500 mm the average temperature profiles are all double Gaussian. For axial positions smaller than 300 mm the maximum temperatures and the minimum temperature at the centreline of all the measurements and simulations are within the inaccuracies equal and thus show within their significance a good agreement. The flame width based on the two measurement techniques is com-
parable. For \( x = 150 \) mm this is also comparable with the flame width predicted with both simulations. For smaller axial positions the flame width according to the simulations is somewhat too large. For larger axial positions the flame width is predicted significantly too small. For \( x = 400 \) mm it is seen that the thermocouple measurements are not significantly different from the Monte Carlo simulations and that the CARS measurements are in agreement with the simulations with assumed PDF. The difference between the two measurement techniques is significant. Unfortunately just one radial CARS measurement traverse is available for these larger axial positions. For axial positions larger than 500 mm the difference between the thermocouple measurements and the Monte Carlo simulations also becomes significant. The reason for this can be found in the prediction of the flame length. For both the simulations the latter is significantly too large. In to the simulations, the flame width is under predicted and the flame length is over predicted. Probably the \( k - e \) turbulence model includes not all the features to describe the mixing behaviour in flame C correctly.

Next to the radial traverses also some axial traverses were done in the flames. From these measurements it is seen that for axial positions smaller than 550 mm two temperature readings are possible. For temperatures above 700 K, the lower temperature reading is not correct and due to the deposition of soot on the thermocouple.

Not only the average temperature was determined with the thermocouple, but also the temperature fluctuations. For the rms value of the temperature fluctuation, the agreement between the thermocouple measurements and the Monte Carlo simulations is good. For most measured locations these two differ significantly from the CARS measurements and the assumed PDF simulations though, where the agreement between the latter two is good again. For axial positions larger than 300 mm, the thermocouple is believed to produce reliable rms measurements. For smaller axial positions the measurements are influenced by the following defects. With the 65 \( \mu m \) type B thermocouple used in the piloted jet diffusion flame it is not possible to determine temperatures below 400 K or temperatures above 1700 K. The first because of the thermo electric properties of the thermocouple material used. The latter because of the smaller time scales present in the flame in comparison with the time constant of the thermocouple. As a result the largest temperature fluctuations will be averaged by the thermocouple. The fact that these high temperatures were not measured also lead to the conclusion, that the measurement technique did not suffer from catalytic effects in the turbulent flames, like they were seen in the thermocouple measurements in the flat flame.

The second technique, which is the main aim of this study is the Infra-Red Emission Absorption Tomography technique. The first interest was in determining the influence of the turbulence on the measurement technique. To investigate this influence, the assumed PDF simulation was extended with an extra feature, to calculate local emission, based on Planck's law and a constant emission coefficient of the gas. From these simulations done, it was seen that the mean temperature as determined with this technique, will be too high. This also leads to temperature profiles that are too wide. This difference in temperature proved to be wavelength dependent, where the temperature difference was the largest for the smallest wavelength. This follows directly from Planck's law. For axial positions of 150 and 700 mm, this discrepancy was estimated
to be 60 and 120 K for respectively $\lambda = 3.049 \, \mu m$ and $\lambda = 1.624 \, \mu m$. The smallest deviations were calculated around \( x = 400 \, mm \), with values of respectively 20 K and 60 K. Compared to the errors in the thermocouple and the CARS measurements this is quite good.

Three different types of measurements were done with the tomographic technique. The first one, with $\lambda = 1.624 \, \mu m$, to determine both temperature and soot volume fraction. The second one, with $\lambda = 2.877 \, \mu m$, to determine both temperature and partial pressure of H$_2$O. The latter was possible by correcting the measurements with the emission and absorption of soot. This correction was negligible in most traverses, but was about 30% for the highest soot volume fraction measured. The last type of measurements were done with $\lambda = 3.049 \, \mu m$. After correcting for the emission and the absorption of both soot and H$_2$O it was possible to determine both temperature and partial pressure of C$_2$H$_2$. In this case, the correction, mainly the one regarding H$_2$O, was significant.

The absorption measurement regarding soot is not very accurate. Although the accuracy of both the H$_2$O and the C$_2$H$_2$ absorption measurement is better, it is still difficult to determine a local absorption coefficient profile with high spatial resolution. Comparing the tomographic temperature profiles with the thermocouple temperature profiles it is clear that turbulence indeed leads to a tomographic temperature that is too high. This temperature difference was between 130 and 350 K for the regions where it was predicted to be between 20 and 120 K. The influence of turbulence indeed proved to be wavelength dependent. For soot it is also visible, that the influence of turbulence is not the same for the local emission and the local absorption. The width of the first is clearly larger than expected, while the width of the latter is hardly influenced. This leads to a temperature peak there where the absorption is low and the emission not. This effect is also seen in the other two measurements, but not as clear as in the soot measurements. With the tomographic technique as described in this thesis, it is possible to determine the correct temperature in a strongly fluctuating flame, when the absorption is so strong that it can be accurately measured and the measurements can be corrected for the fluctuations.

All three measurements show that flame A is the smallest and shortest flame and flame C the widest and longest. Taking the temperature difference of the different axial positions in the flames into account, qualitatively the emission and the absorption lead to the same amount of the absorbing species, for all the three measurements. The soot volume fraction determined with the tomographic technique is comparable to the soot volume fraction at the centreline determined with the suction probe. The agreement regarding the partial pressure of H$_2$O measured with the tomographic technique and calculated by Peeters also is good. For the partial pressure of C$_2$H$_2$ there is a difference of about a factor of 10 between the measurements and the Monte Carlo simulations, where the the Monte Carlo simulations give the lowest values. The reason for this is twofold. First the absorption coefficient $k$, from the HITRAN database, is not accurate, leading to a large uncertainty in the measurements. On the other hand the chemistry modelling leads to a considerable uncertainty in the predictions. Regarding the width of the C$_2$H$_2$ profiles, it is revealed that the measurements and the simulations are similar. This is remarkable since for most other measurements done so far, there always
is a difference in the width of the profiles. Probably the simulations have not the right chemistry model regarding the prediction of intermediate products.

For the soot measurements, some absorption peaks are seen at the exterior of the flame. These peaks are attributed to diffraction, which was also seen in some early test measurements. These peaks are visible in neither the H₂O nor the C₂H₂ measurements. The latter is probably due to the higher absorption present in these measurements, masking the diffraction effect. Comparing the soot volume fraction and the partial pressure of C₂H₂ it is concluded that C₂H₂ is, as expected, a precursor of soot, but there are more requirements to form soot, since the concentration of C₂H₂ is about the same for all the three flames, while there is a clear difference in soot volume fraction. Effects of temperature and the amount of oxidiser are important parameters in the soot forming and oxidation reactions.

The location of the reaction zone and shear layer is determined using the distance between the radial locations with maximum value determined from several experiments. For axial positions smaller than about 250 mm, the inner shear layer is located inside the reaction zone. Further downstream the reaction zone and the shear layer coincide and here the turbulence strongly interacts with the chemistry. The distance \( d_{OH} \) is a good indicator for the reaction zone, where the distance \( d_T \) only is a good estimator for the location for the reaction zone for lower axial positions. This is also seen from the simulations with assumed PDF. The distance \( d_{OH} \) is a good indicator for the reaction zone because OH is a short living intermediate, which is not strongly influenced by diffusion. The latter gets more and more important for the temperature with increasing axial position.

The water vapour is formed at the fuel rich side of the reaction zone near the inner shear layer. The distance based on the measured H₂O profiles is comparable with the \( d_{H₂O} \) calculated from the simulation. Acetylene is formed at approximately the same location. This can be expected since this is the fuel rich side, with some oxidiser to start some reactions, but not enough to complete all the reactions. As a result intermediates can exist in this region.
7 General remarks

This chapter is devoted to a discussion about the main conclusions and findings of the described work, with respect to the aims of this study presented in Chapter 1. First aim was to extend the database regarding the Delft piloted jet diffusion flame. For an improvement of the modelling of the radiative heat transfer, the soot volume fraction had to be determined with an optical technique. The optical technique applied is Infra-Red Emission Absorption Tomography (IREAT). For comparison the soot volume fraction is also measured with a suction probe. Varying the wavelength, the optical technique can determine the species concentration of other species than soot, like water vapour and acetylene. The first is an end product of combustion and the latter an intermediate product, which is believed to be a precursor of soot. The database regarding parameters in this flame is also extended by measuring up to axial positions of 700 mm, instead of the maximum of 300 mm used in other investigations, where a lot of effort was made to validate the initial conditions of the process.

Besides the species concentration, IREAT simultaneously determines the temperature. These measurements are validated with thermocouple measurements. The thermocouple measurements are done with a triple thermocouple instead of a conventional thermocouple. With the triple thermocouple we are able to correct the thermocouple temperature not only for radiation, but also for conduction. The temperature profile is calculated numerically, using both the measured hot junction temperature and the temperature of the boundary junctions. For a thermocouple with practical dimensions (a length of about 10 mm) the conduction correction is considerable (50 to 100 K), even in a flame with no temperature gradient like the flat flame. The total accuracy of the thermocouple average temperature measurements is 40 K in the piloted jet diffusion flame and 60 K in the flat flame.

Next to the determination of the mean temperature, we used the 65 μm Pt-Rh thermocouple for time-resolved measurements. In the piloted jet diffusion flames the time constant of the thermocouple is between 20 and 40 ms. Following the discussion in Ballantyne and Moss (1977) we expected the thermocouple bandwidth to be DC-1 kHz. This should be sufficient to resolve most frequencies in the piloted jet diffusion flame. This was not the case, since a lack of high temperatures is found in the PDFs for small axial positions. A thermocouple with a diameter of about 5 μm has to be used to resolve all frequencies. The disadvantage of such small diameter is that the thermocouple then (probably) is not strong enough.
The soot volume fraction measurements are validated with simple suction probe measurements. The accuracy of the latter is 25%. One disadvantage of the method is the fact that due to ineffective quenching the measured soot volume fraction can regard another axial position than the one the sample is taken.

Calculating the species concentration from the absorption measurement of IREAT, the absorption coefficient $k$ has to be known. Several databases have been evaluated, for the various species under investigation. The maximum difference between the various databases and experimental data is a factor of 3, mainly for high temperatures. For reliable measurements it is best to determine the absorption coefficient $k$ for the experimental setup, with a calibration of that setup. The results regarding the flat flame reveal that the flat flame is a possible calibration object. The gas tube, presented in Chapter 2, proved to be another one.

Since it is very hard to find a wavelength region where the absorption is due to just one (gaseous) component, the measurements normally have to be corrected for either absorption or emission by these other components. The results regarding the measurement of the partial pressure of $\text{H}_2\text{O}$ show that it is possible to correct for the absorption by $\text{CO}_2$ with the assumption that the ratio of the concentration of these two species is a (constant) factor of 2. The corrections with respect to soot proved to be negligible for most axial positions, with a maximum of 30% at the centreline for $x = 600$ mm. The corrections for the acetylene measurements regarding water vapour are significant for all measurements, with a maximum of approximately 40%. The latter correction affected not only the magnitude, but also the shape of the profile.

First measurements were performed in the flat flame. The conduction correction for the thermocouple measurements was about 100 K and the total correction about 200 K, where the corrected mean temperature was between 1500 and 1900 K. Comparing the mean temperature with the temperature from CARS measurements and calculations, no significant differences were found. The axial traverse revealed that the type B thermocouple suffered from catalytic effects near the flame front. This resulted in a temperature rise of 150 K near the flame front. For the measurements with IREAT the a-priori knowledge of a flat profile was used in the reconstruction technique. For $\lambda = 3.049$ $\mu$m this resulted in a temperature that was not significantly different from the thermocouple measurements. For $\lambda = 2.877$ $\mu$m the temperature was about 130 K higher than for the thermocouple measurements. Regarding the partial pressure of $\text{H}_2\text{O}$, the measurements for $\lambda = 3.049$ $\mu$m are used as reference measurements, to create a reliable database for the absorption coefficient $k$. For $\lambda = 2.877$ $\mu$m the database was created using the measurements with the gas tube. For the IREAT measurements this resulted in partial pressures that differed not more than 0.01 atm from the calculations, where the partial pressure of $\text{H}_2\text{O}$ was approximately 0.15 atm.

The main interest was in the measurements performed in the piloted jet diffusion flame. The mean temperature determined with the thermocouple and corrected for both radiation and conduction was not significantly different from the CARS measurements, considering the accuracy of respectively 40 and 50 K for both measurements techniques. The two techniques were comparable both in magnitude and shape of the profile. The temperature was also comparable with numerical calculations based on assumed PDF simulations or Monte Carlo simulations, for traverses where the flame
width and flame length of the simulations was predicted correct. This good comparison of the mean temperature showed that the thermocouple did not suffer from catalytic effects in the piloted jet diffusion flame. The axial traverses in flame A showed two temperature profiles, with a maximum temperature difference of about 500 K. When the temperature is below 1500 K and there is not sufficient oxidiser, for small axial positions near the centreline, soot will stick to the thermocouple resulting in the measured lower temperature.

Except for small axial positions near the centreline, where the time scales in the flame are the smallest, the rms value of the temperature fluctuations determined with the thermocouple was comparable with the values calculated from the Monte Carlo simulations. Compared with the values from the CARS measurements and from the simulations with assumed PDF, the latter values were about 150 K higher.

Simulations revealed that the turbulence level influenced the temperature determined with IREAT. The temperature error proved to be wavelength and radial position dependent. For \( \lambda = 1.624 \, \mu m \) and locations near the centreline, between the locations with maximum temperature, the minimal temperature difference was calculated to be 50-200 K. For the other two wavelengths this minimal temperature difference was between 0 and 100 K. In the, less interesting, exterior of the flame this temperature difference was much higher, with a maximum of respectively 700 and 400 K.

For \( \lambda = 1.624 \, \mu m \) the temperature measured with IREAT was at least 100 K higher than the thermocouple temperatures. In the exterior of the flame, peak temperatures were measured, more than 1000 K higher than the thermocouple temperatures. This was due to the fact that turbulence influences the width of the emission profile, but did not affect the width of the absorption profile. The measured soot volume fraction was comparable with the soot volume fraction determined with the suction probe. Due to ineffective quenching, the axial position with the maximum soot volume fraction was about 100 mm smaller for the suction probe measurement compared to the IREAT measurement. The maximum soot volume fraction in flame C was about \( 2 \cdot 10^{-8} \) for \( x \approx 600 \, \text{mm} \). With decreasing turbulence level the soot volume fraction increased, with a maximum of \( 10 \cdot 10^{-8} \) in flame A.

The temperature regarding the other two wavelengths was equivalent and the temperature difference with the thermocouple measurements was somewhat smaller than for \( \lambda = 1.624 \, \mu m \). Near the centreline the minimum temperature difference was about 100 K and in the exterior the largest temperature difference was about 500 K. The partial pressure of \( \text{H}_2\text{O} \) was about the same for all three flames and comparable with the values calculated by the assumed PDF simulations. The maximum measured partial pressure was about 0.15 atm. The partial pressure of \( \text{C}_2\text{H}_2 \) was about 0.08 atm, which is about 8 times the value calculated with the Monte Carlo simulations. The partial pressures of \( \text{C}_2\text{H}_2 \) for flame A and C were about the same. Since the soot volume fraction differed a lot for these two flames, it was concluded that \( \text{C}_2\text{H}_2 \) is a precursor of soot, but also the temperature and the amount of oxidiser are important parameters for the formation and oxidation of soot.

Regarding the extension of the database regarding the Delft piloted jet diffusion flame, the following can be concluded. We now have reliable mean temperatures for this flame. Also we have the rms value of the temperature fluctuations for the larger
axial positions, which are an extension to the CARS measurements. Completely new are the soot, $H_2O$ and $C_2H_2$ data for this flame.
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### Principal symbols

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<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>$a$</td>
<td>thermal diffusivity</td>
<td>($m^2 s^{-1}$)</td>
</tr>
<tr>
<td>$A$</td>
<td>area</td>
<td>($m^2$)</td>
</tr>
<tr>
<td>$B$</td>
<td>Planck’s function</td>
<td>($W m^{-2}$)</td>
</tr>
<tr>
<td>$C_p$</td>
<td>specific heat at constant pressure</td>
<td>($J kg^{-1} K^{-1}$)</td>
</tr>
<tr>
<td>$d$</td>
<td>distance between location with maximum value</td>
<td>(mm)</td>
</tr>
<tr>
<td>$D$</td>
<td>diameter</td>
<td>($\mu m$)</td>
</tr>
<tr>
<td>$e$</td>
<td>electron charge</td>
<td>(C)</td>
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<tr>
<td>$f$</td>
<td>object function</td>
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</tr>
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<td>$F$</td>
<td>Fourier coefficient</td>
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</tr>
<tr>
<td>$g$</td>
<td>damping constant</td>
<td>($s^{-1}$)</td>
</tr>
<tr>
<td>$h$</td>
<td>convective heat transfer coefficient</td>
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</tr>
<tr>
<td>$i, j$</td>
<td>index</td>
<td>(-)</td>
</tr>
<tr>
<td>$I$</td>
<td>intensity</td>
<td>(a.u.)</td>
</tr>
<tr>
<td>$I_{BB}$</td>
<td>intensity radiation source</td>
<td>($W m^{-2}$)</td>
</tr>
<tr>
<td>$I_e$</td>
<td>local emitted intensity</td>
<td>($W m^{-2} m^{-1}$)</td>
</tr>
<tr>
<td>$I_t$</td>
<td>emitted flame intensity</td>
<td>($W m^{-2}$)</td>
</tr>
<tr>
<td>$I_{BB}$</td>
<td>intensity radiation source and flame</td>
<td>($W m^{-2}$)</td>
</tr>
<tr>
<td>$k$</td>
<td>absorption coefficient</td>
<td>($m^{-1} atm^{-1}$)</td>
</tr>
<tr>
<td>$k$</td>
<td>integer number</td>
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<tr>
<td>$k$</td>
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<td>path length</td>
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<td>$m$</td>
<td>mass</td>
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<tr>
<td>$m_0$</td>
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<td>number of volumes at one side</td>
<td>(-)</td>
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<td>$n$</td>
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<td>$N$</td>
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<tr>
<td>$[OH]$</td>
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<tr>
<td>$p$</td>
<td>partial pressure</td>
<td>(atm)</td>
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<tr>
<td>$P$</td>
<td>projection profile</td>
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<tr>
<td>$P^*$</td>
<td>filtered projection profile</td>
<td>(a.u.)</td>
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<tr>
<td>$P_T$</td>
<td>temperature PDF</td>
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### Principal symbols

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>$q$</td>
<td>ramp filter function in spatial domain</td>
<td>(−)</td>
</tr>
<tr>
<td>$\bar{q}$</td>
<td>improved ramp filter function in spatial domain</td>
<td>(−)</td>
</tr>
<tr>
<td>$Q$</td>
<td>Fourier transformed projection</td>
<td>(−)</td>
</tr>
<tr>
<td>$Q_{\text{rad}}$</td>
<td>radiation source term</td>
<td>(W m(^{-3}))</td>
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<td>$r_i$</td>
<td>pseudo projection</td>
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<td>$s$</td>
<td>line-of-sight position</td>
<td>(m)</td>
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<td>$s_i^k$</td>
<td>ART3 function</td>
<td>(a.u.)</td>
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<tr>
<td>$S_F$</td>
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<tr>
<td>$T$</td>
<td>time</td>
<td>(s)</td>
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<td>$u, v$</td>
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<tr>
<td>$u$</td>
<td>velocity</td>
<td>(m s(^{-1}))</td>
</tr>
<tr>
<td>$V$</td>
<td>variance</td>
<td>(−)</td>
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<tr>
<td>$V$</td>
<td>volume</td>
<td>(m(^{3}))</td>
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<tr>
<td>$W$</td>
<td>maximum frequency</td>
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<td>$x_{ij}$</td>
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<td>$x, y$</td>
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<td>$x$</td>
<td>axial position</td>
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<td>$x$</td>
<td>direction along thermocouple</td>
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<td>$X_1, X_2$</td>
<td>limit</td>
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<tr>
<td>$y$</td>
<td>radial position</td>
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### Greek symbols

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<tr>
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<tr>
<td>$\Delta$</td>
<td>width</td>
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<td>$\epsilon$</td>
<td>error tolerance</td>
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<tr>
<td>$\epsilon$</td>
<td>permittivity</td>
<td>(C(^{2}) N(^{-1}) m(^{-2}))</td>
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<tr>
<td>$\epsilon$</td>
<td>absolute uncertainty</td>
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<td>emissivity</td>
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<td>$\phi$</td>
<td>polar angle</td>
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<td>$\phi$</td>
<td>flow rate</td>
<td>(g s(^{-1}))</td>
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<td>$\phi_V$</td>
<td>volumetric flow</td>
<td>(m(^{3}) s(^{-1}))</td>
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<tr>
<td>$\kappa$</td>
<td>local absorption coefficient</td>
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<tr>
<td>$\lambda$</td>
<td>wavelength</td>
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<td>$\lambda_g$</td>
<td>thermal conductivity of the gas</td>
<td>(W m(^{-1}) K(^{-1}))</td>
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<tr>
<td>$\lambda_k$</td>
<td>relaxation factor</td>
<td>(−)</td>
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<td>thermal conductivity of the thermocouple</td>
<td>(W m(^{-1}) K(^{-1}))</td>
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<tr>
<td>$\nu$</td>
<td>kinematic viscosity</td>
<td>(m(^{2}) s(^{-1}))</td>
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<tr>
<td>$\rho$</td>
<td>density</td>
<td>(kg m(^{-3}))</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stefan-Boltzmann constant (5.67 \cdot 10(^{-8}))</td>
<td>(W m(^{-2}) K(^{-4}))</td>
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<tr>
<td>$\tau$</td>
<td>spatial resolution</td>
<td>(mm)</td>
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### Principal symbols

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<td>(s)</td>
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<tr>
<td>$\omega$</td>
<td>polar frequency</td>
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<tr>
<td>$\omega$</td>
<td>radiation frequency</td>
<td>(s$^{-1}$)</td>
</tr>
<tr>
<td>$\omega_{k,j}$</td>
<td>natural frequency of bound electrons</td>
<td>(s$^{-1}$)</td>
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<tr>
<td>$\xi$</td>
<td>mixture fraction</td>
<td>(-)</td>
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### Calligraphic symbols

- $B$: Back projection
- $\mathcal{F}$: Fourier transform
- $\mathcal{R}$: Radon transform

### Subscripts

- air: property of air flow
- ann: property of annulus flow
- $\alpha$: based on absorption profile
- BB: radiation source
- c: centre
- co: property of coflow
- $C_2H_2$: property of acetylene
- e: emitted
- e, w: east, west
- E, W: East, West neighbouring point
- f: flame
- f: free electron
- gas: property of gas flow
- g: property of gas
- i: ray index
- j: pixel index
- j: bound electron index
- jet: property of jet flow
- H$_2$O: property of water (vapour)
- NO: based on NO profile
- OH: based on OH profile
- P: grid point
- rms: root mean square value
- soot: property of soot
- t: total
- t: property of thermocouple
- tc: thermocouple volume
- T: based on $T$ profile
Superscripts

-1  inverse
0   initial value
\(\bar{\cdot}\)  average
\(\hat{\cdot}\)  estimator
\(\cdot')\)  fluctuating value
\(\cdot')\)  ratio for \(\lambda = 2.877 \, \mu m\) and \(\lambda = 1.624 \, \mu m\)
\(\cdot'')\)  ratio for \(\lambda = 3.049 \, \mu m\) and \(\lambda = 1.624 \, \mu m\)
k    iteration number
Summary: IR Emission/Absorption Tomography in Flames

To improve the efficiency of combustion processes, with less emission of noxious gases a lot of research is done for a better fundamental understanding of those combustion processes, in particularly in turbulent diffusion flames. The main aim of the work described in this thesis was the extension of the database regarding the Delft piloted jet diffusion flame. For an improvement of the modelling of the radiative heat transfer, the soot volume fraction had to be determined with an optical technique. The technique employed is Infra-Red Emission/Absorption Tomography (IREAT). Because most soot is expected in the region with axial positions between 300 and 700 mm, most experiments are concentrated on this region. These data are a supplement to other studies, where a lot of effort was made to validate the initial conditions of the complete process and the experiments covered the lower axial positions. These other studies include the work of De Vries (1994), Stroomer (1995), Peeters (1995) and Mantzaras and Van der Meer (1997). In these studies, the Delft piloted jet diffusion flame was described with LIF measurements regarding OH and NO, LDA measurements regarding the velocity, thermocouple and CARS measurements regarding the temperature and with assumed PDF modelling for numerical simulation.

Varying the wavelength in IREAT, it is possible to determine the species concentration of other species than soot. The used wavelength regions correspond with the absorption by water vapour and by acetylene. The first is an end product of combustion and the latter an intermediate product, which is believed to be a precursor of soot. For comparison the soot volume fraction is also measured with a suction probe. Besides the species concentration, IREAT simultaneously determines the local temperature. These temperature data are validated with thermocouple measurements. To improve the conduction correction, the thermocouple measurements are not done with a conventional thermocouple, but with a triple thermocouple. With the relatively small thermocouple it is possible to determine not only the mean temperature, but also the rms value of the temperature fluctuations.

There are two flame types used in this work. Our main interest is in the Delft piloted jet diffusion flame. The setup consists of a fuel pipe with inner diameter of 6 mm, inside two air streams. The fuel used is Groningen natural gas. The primary air is supplied by an annulus with inner diameter of 35 mm and outer diameter of 45 mm. The whole is placed in a throat with burner chamber on top for the secondary coflow. This burner configuration is used to produce three different flames, with the same fuel to air ratio, but with increasing velocities and thus Reynolds number and turbulence level. The other flame type used is a flat flame produced by a McKenna burner. This burner consists of a porous disk of about 61 mm, where the fuel air mixture is supplied. In this case the fuel is methane (99.5%). The flame is shielded with nitrogen issuing from a ring with inner diameter of 63 mm and outer diameter of 73 mm. Because this flame is very well known from literature, it is used to validate and calibrate (parts of) the experimental techniques.

IREAT uses both an emission and an absorption measurement to determine the temperature as well as the species concentration. The measurements are line-of-sight.
Our interest is in local values, so a tomographic reconstruction technique has to be applied. A tomographic reconstruction technique is either based on a transform method, like BackProjection, Filtered BackProjection or Convolution BackProjection, or on a iterative method like the Algebraic Reconstruction Technique. From an evaluation of these techniques it followed that a FBP technique with a carefully chosen cutoff leads to satisfactory results. To improve the reconstruction it is convenient when some a-priori knowledge is known about the emission and/or absorption profile.

To calculate the species concentration from the absorption measurement, the absorption coefficient \( k \) has to be known for the different species. In the literature, several models are found with data for the various species under investigation. These data are compared with each other and with calibration measurements performed with a gas tube and in the flat flame. This comparison leads to the conclusion that one has to be very careful when applying most of these absorption models, because there is a wide spread between the various models and experimental data, especially for high temperatures.

When the wavelength region of interest has a certain bandwidth, it is very hard to find a region where all the absorption and emission can be attributed to just one species. Therefore it is normally necessary to correct the IREAT measurements for the absorption and/or emission of other species than the one under investigation. For the measurements regarding H\(_2\)O the correction for CO\(_2\) is done by assuming a constant ratio between the two species. All the other corrections are done by calculating the absorption or emission at that wavelength by the other species, using the species concentration from other IREAT measurements.

To validate the temperature measurements also a thermocouple is employed. Instead of a conventional thermocouple, a triple thermocouple is used. The conventional thermocouple consists of two thin wires supported by two thicker wires of the same material. This thermocouple has one hot junction, where the two different materials are welded. The triple thermocouple consist of two thin wires, each supported by two different thicker wires. This way the thermocouple has three hot junctions. Not only the temperature between the two thin wires is known, but also the temperature at the boundary of the thin wires, where they are connected to the thicker wires. To calculate the gas temperature out of the measured thermocouple temperature, the latter is corrected for radiation losses, as is done by most investigators. To improve the correction, the thermocouple temperature is also corrected for conduction losses. For this, three different methods are applied. For method a the second derivative of the thermocouple temperature is determined using the second derivative of the measured hot junction temperatures. For method b the second derivative is calculated assuming a parabolic fit through the measured hot junction and boundary junction temperatures. For method c the temperature profile in the thermocouple is calculated iteratively, using both the measured hot junction temperature and the temperature of the boundary junctions. Method c is believed to be the most reliable. The conduction of an extremely long thermocouple is fully determined by the temperature gradient in the flame. The axial traverse in the flat flame showed that it is also possible to use method b with a correction to get the same results as with method c.

To get an indication about the soot volume fraction at the centreline, it is also
measured with a suction probe. This setup is very simple and no precautions were
made to measure isokinetic or prevent ineffective quenching in the probe tube. The
setup did contain a water reservoir and a furnace to extract all the water from the
sample. All together this resulted in an accuracy of about 25%.

First measurements are done in the non-sooting flat flame. From the thermocouple
measurements it is seen that the new conduction correction leads to good results. Even
in a flat flame the conduction correction is significant. With the assumption that the
difference between method b and c is constant, it is even possible to correct an axial
traverse. This axial traverse reveals that the thermocouple measurements suffer from
catalysis near the reaction zone. All these measurements in the flat flame are used to
tune the parameters in the calculation of the corrections. Compared with the initial
values, the difference with the tuned values is small. The flat flame is non-sooting and
acetylene is only present near the reaction zone. Therefore the tomography measure-
ments, all done above the reaction zone, only determined the partial pressure of H₂O
and the temperature. With the adapted tuned databases the results regarding the partial
pressure of H₂O are comparable with numerical simulations. For λ = 3.049 μm the
temperature is in agreement with the CARS measurements and the numerical simu-
lations. For λ = 2.877 μm the temperature is about 130 K higher. Therefore, the
correct temperature is used to calculate the partial pressure of H₂O . Assuming a flat
radial profile for the properties in the flame and with the determination of the flame
width from several radial traverses, it is possible to do an axial traverse and calculate
the local partial pressure and the temperature. This leads to the same results as for the
radial traverses.

After tuning the parameters in the experimental setups with the measurements in
the flat flame, the techniques are employed to the Delft piloted jet diffusion flame.
Firstly measurements are done with the thermocouple regarding the mean temperature.
These are compared with CARS measurements, numerical simulations with assumed
PDF and Monte Carlo simulations. The comparison is good. However, the simulations
predict a flame that is smaller and longer than seen in the experiments. The thermo-
couple measurements also reveal that the measurements in the turbulent flame do not
suffer from catalytic effects. An axial traverse demonstrated that soot deposition on
the thermocouple influences the measurement, since the difference between two tem-
perature readings at the same position are proportional to the soot volume fraction
determined with the suction probe. Besides the mean temperature, also time-resolved
measurements are done in the Delft piloted jet diffusion flame. This resulted in the rms
value of the temperature fluctuations and a PDF for the temperature. The comparison
with the CARS measurements and the two simulations is reasonable.

Before the tomography measurements are done, first the influence of turbulence on
the results is studied. From this it is seen that the absorption measurement is hardly
influenced. The influence on the emission is considerable and wavelength dependent,
where the greatest temperature difference occurs for the smallest wavelengths.

The temperature determined with the tomography measurements regarding soot is
indeed much higher than the temperature from the thermocouple measurements. The
temperature profile is also strongly peaked at the exterior of the flame. The latter is a
consequence of the turbulence. The temperature fluctuations influence the width of the
emission profile, but the absorption profile is hardly affected. The soot volume fraction is highest in the low velocity flame A and lowest in the most turbulent flame C, with a maximum, at the centreline, of about $1.0 \cdot 10^{-7}$ and $2.3 \cdot 10^{-8}$ respectively. Compared with the measurements at the centreline with the suction probe, the absolute values are comparable, but the axial position where the maximum occurs is lower for the suction probe measurements.

The temperature determined with the tomography measurement regarding water vapour is also higher than the temperature from the thermocouple measurements. This difference is smaller than for the soot measurements, indicating that the influence of turbulence is indeed wavelength dependent. The correction for the absorption by soot, to calculate the partial pressure of H$_2$O seems to be negligible. Comparing this partial pressure with the numerical predictions from the assumed PDF simulations shows that the magnitude is about the same, but the flame width and flame length from the simulations is not correct.

The temperature determined from the measurements regarding acetylene is comparable with the temperature determined from the measurements regarding water vapour. This is expected, since the difference in wavelength is small. Calculating the partial pressure of C$_2$H$_2$, the correction for absorption by soot is again negligible, but the correction for absorption by H$_2$O is considerable. Comparing the partial pressure of C$_2$H$_2$ with the results from Monte Carlo simulations reveals that the latter are about a factor of ten smaller. Qualitatively the comparison between the radial profiles is reasonable. For the C$_2$H$_2$ concentration profile at the centreline, there is hardly any difference between flame A and C. This shows that more parameters are involved to start the soot formation than just the partial pressure of C$_2$H$_2$.

From the width of the radial profiles, the reaction zone and the shear layer are located. For axial positions smaller than 300 mm the inner shear layer is located at the fuel rich side of the reaction zone. This is also the location where H$_2$O and C$_2$H$_2$ are formed. The profiles with the width of the various radial profiles also reveal that the diffusion of H$_2$O is greater than the diffusion of heat in the Delft piloted jet diffusion flame. Qualitatively the width of the various profiles and their mutual differences are comparable with the results from the simulations with assumed PDF.
Samenvatting: IR Emissie/Absorptie Tomografie in Vlammen

Om de efficiëntie van verbrandings-processen te verbeteren, met minder uitstoot van giftige gassen, wordt er een heleboel onderzoek gedaan om een beter fundamenteel begrip van die verbrandings-processen te krijgen, vooral met betrekking tot turbulente diffusie-vlammen. Het belangrijkste doel van het werk, beschreven in dit proefschrift, was het uitbreiden van de database betreffende de Delftse diffusie-vlam met stabilisatie-vlammetjes. Voor een verbetering van de modellerings van de stralingswarmte-overdracht, moest de roet-volumefractie bepaald worden met een optische techniek. De toegepaste techniek is Infra-Rood Emissie/Absorptie Tomografie, IREAT. Omdat het meeste roet verwacht wordt in het gebied met axiale posities tussen 300 en 700 mm, zijn ook de meeste experimenten geconcentreerd op dit gebied. Deze data zijn een uitbreiding op andere studies, waar veel moeite gedaan is om de begincondities van het complete proces te valideren en waar de experimenten de lagere axiale posities bestreken. Deze andere studies bevatten het werk van De Vries (1994), Stroomer (1995), Peeters (1995) en Mantzaras en Van der Meer (1997). In deze studies is de Delftse diffusie-vlam met stabilisatie-vlammetjes beschreven met behulp van LIF-metingen betreffende OH en NO, LDA-metingen betreffende de snelheid, thermokoppel- en CARS-metingen betreffende de temperatuur en met veronderstelde PDF-modellering voor numerieke simulaties.

Door de golflengte te variëren in IREAT, is het mogelijk om de concentratie van andere stoffen dan roet te bepalen. De gebruikte golflengte-gebieden komen overeen met de absorptie van waterdamp en acetylen. De eerste is een eind-product van verbranding en de laatste is een tussen-product, waarvan aangenomen wordt dat het een voorloper van roet is. Ter vergelijking wordt de roet-volumefractie ook gemeten met een afzuig-probe. Naast de stofconcentratie, bepaalt IREAT simultaan de temperatuur. Deze temperatuur-data worden gevalideerd met behulp van thermokoppel-metingen. Om de geleidingscorrectie te verbeteren, worden deze thermokoppel-metingen niet met een conventioneel thermokoppel gedaan, maar met een drievoudig thermokoppel. Met het relatief kleine thermokoppel is het mogelijk om niet alleen de gemiddelde temperatuur te bepalen, maar ook de rms-vaarde van de temperatuurfluctuaties.

Er zijn twee vlamtypen gebruikt in dit werk. Onze grootste interesse gaat uit naar de Delftse diffusie-vlam met stabilisatie-vlammetjes. De opstelling bestaat uit een brandstofpijp met binnendiameter van 6 mm, in twee luchtstromingen. De brandstof die gebruikt wordt, is Gronings aardgas. De primaire lucht wordt aangeleverd via een annulus met een binnendiameter van 35 mm en een buitendiameter van 45 mm. Het geheel is geplaatst in een tunnel voor de secundaire coflow, met daar bovenop een branderkaas. Deze branderconfiguratie wordt gebruikt om drie verschillende vlammen te produceren, met dezelfde brandstof/lucht verhouding maar met toenemende snelheden en dus ook toenemend Reynolds getal en turbulentie-niveau. Het andere vlamtype dat gebruikt is, is een vlakke vlam geproduceerd door een McKenna-brander. Deze brander bestaat uit een poreuze disk van 61 mm, waar het brandstof/lucht mengsel aangeleverd wordt. Nu is de brandstof methaan (99,5%). De vlam wordt afgeschermd door stikstof, die komt uit een ring met binnendiameter 63 mm en een buitendiameter
van 73 mm. Omdat deze vlam erg bekend is uit de literatuur, wordt hij gebruikt ter validatie en calibratie van (delen van) de experimentele opstellingen.

IREAT gebruikt zowel een emissie- als een absorptie-meting om de temperatuur en de stofconcentratie te bepalen. De metingen zijn pad geïntegreerd. Onze interesse gaat uit naar lokale waarden, zodat het dus nodig is een tomografische reconstructietechniek toe te passen. Een tomografische reconstructietechniek is gebaseerd op een transformatiemethode, zoals BackProjection, Filtered BackProjection of Convolution BackProjection, of op een iteratieve methode zoals de Algebraic Reconstruction Technique. De conclusie van een evaluatie van deze technieken was dat een FBP-techniek met een zorgvuldig gekozen cutoff tot bevredigende resultaten leidt. Om de reconstructie te verbeteren is het handig wanneer a-priori kennis voor handen is betreffende het emissie- en/of absorptie-profiel.

Om de stofconcentratie te kunnen berekenen uit een absorptie-meting, moet de absorptie-coëfficiënt $k$ voor de verschillende stoffen bekend zijn. In de literatuur zijn verschillende modellen gevonden met data voor de verschillende stoffen die gebruikt worden in dit onderzoek. Deze data zijn met elkaar vergeleken en met calibratietellingen met de gas-houder en de vlakke vlam. Deze vergelijking leidt tot de conclusie dat je gelijk voorzichtig moet zijn met de toepassing van deze absorptie-modellen, aangezien er een grote spreiding is tussen de verschillende modellen en experimentele data, vooral voor hoge temperaturen.

Wanneer het golflengte-gebied een bepaalde bandbreedte heeft, is het erg moeilijk om een gebied te vinden waar alle absorptie en emissie toegeschenven kan worden aan slechts één stof. Daarom is het normaal gesproken nodig om de IREAT-metingen te corigeren voor absorptie en/of emissie van andere stoffen dan die waar de interesse naar uit gaat. Voor de metingen betreffende $H_2O$ wordt de correctie voor $CO_2$ be-werkstelligd door middel van de aannemer dat er een constante verhouding is tussen de twee stofconcentraties. Alle andere correcties zijn gedaan door de absorptie en/of emissie van de andere stof bij die golflengte te berekenen, gebruik makend van de stofconcentraties van andere IREAT-metingen.

Ter validatie van de temperatuur-metingen zijn er ook thermokoppel-metingen uitgevoerd. In plaats van een conventioneel thermokoppel is er gebruik gemaakt van een drieduivoudig thermokoppel. Het conventionele thermokoppel bestaat uit twee dunne draadjes ondersteund door twee dikkere draden van hetzelfde materiaal. Dit thermokoppel heeft één warme las, daar waar de twee verschillende materialen aan elkaar ge- last zijn. Het drieduivoudige thermokoppel bestaat uit twee dunne draden, elk ondersteund door twee verschillende dikke draden. Op deze manier heeft het thermokoppel drie warme lassen. Niet alleen de temperatuur tussen de twee dunne draden is nu bekend, maar ook de temperatuur aan het uiteinde van de dunne draden, waar ze aan de dikkere draden vast zitten. Om de gas-temperatuur te bepalen uit de gemeten thermokoppel-temperatuur, wordt de laatste gecorrigeerd voor stralings-verlies, zoals door vele onderzoekers gedaan wordt. Om de correctie te verbeteren, wordt de thermokoppel-temperatuur ook gecorrigeerd voor geleidingsverlies. Hiervoor worden drie methoden toegepast. Voor methode a wordt de tweede afgeleide van de thermokoppel-temperatuur bepaald als de tweede afgeleide van de warme las-temperatuur. Voor methode b is de tweede afgeleide berekend met behulp van de aannemer dat er een para-
bolisch profiel fit door de warme las- en de uiteinde las-temperaturen. Voor methode c is het temperatuur-profiel in het thermokoppelp iteratief berekend, gebruik makend van de temperatuur van de warme las en de beide uiteinde lassen. Methode c wordt als het meest betrouwbaar beschouwd. De geleiding van een extreem lang thermokoppel wordt volledig bepaald door de temperatuurgradiënt in de vlam. De axiale traverse in de vlakke vlam toonde aan dat het ook mogelijk is om methode b te gebruiken met een correctie, om dezelfde resultaten te verkrijgen als was methode c toegepast.

Ter indicatie van de roet-volumefractie op de as, is deze ook gemeten met een afzuig-probe. Deze opstelling is erg simpel en er zijn geen voorzieningen getroffen om isokinetisch te meten of om niet effectieve doving in de probe te voorkomen. De opstelling bevatte een water-reservoir en een overtje om al het water uit het sample te verwijderen. In totaal resulteerde dit in een onnauwkeurigheid van ongeveer 25%.

De eerste metingen zijn gedaan in de niet-roetende vlakke vlam. De thermokoppel-metingen tonen aan dat de nieuwe geleidingscorrectie naar goede resultaten leidt. Zelfs in de vlakke vlam is de geleidingscorrectie significant. Met de aannamer dat het verschil tussen methode b en c constant is, is het zelfs mogelijk om een axiale traverse te corrigeren. Deze axiale traverse toont aan dat de thermokoppel-metingen in de reactiezone last hebben van katalyse. Al deze metingen in de vlakke vlam zijn gebruikt om de parameters in de correctie-methode af te regelen. Vergeleken met de oorspronkelijke waarden zijn de verschillen klein. De vlakke vlam is niet-roetend en acetylen is alleen aanwezig in de reactiezone. Daarom bepalen de tomografische metingen, allen gedaan boven de reactiezone, alleen de partiële druk van H₂O en de temperatuur. Met de toegepaste, geoptimaliseerde database, zijn de resultaten betreffende de partiële druk van H₂O vergelijkbaar met numerieke simulaties. Voor λ = 3.049 μm is de temperatuur vergelijkbaar met de CARS-metingen en de numerieke simulaties. Voor λ = 2.877 μm is de temperatuur 130 K hoger. Daarom is de werkelijke temperatuur gebruikt om de partiële druk van H₂O te berekenen. Met de aannamer van een vlak radiëel profiel voor de grootheden in de vlam en door de bepaling van de breedte van de vlam uit verschillende radiële traversen, is het mogelijk om een axiale traverse te doen en de locale partiële druk en temperatuur te berekenen. Dit geeft dezelfde resultaten als de radiële traversen.

Na het afregelen van de parameters in de experimentele opstellingen met behulp van de metingen in de vlakke vlam, worden de technieken toegepast op de Delftse diffusie-vlam met stabilisatie-vlammetjes. Als eerste zijn metingen met het thermokoppel gedaan, betreffende de gemiddelde temperatuur. Deze zijn vergeleken met CARS-metingen, numerieke simulaties met aangenoemde PDF en Monte Carlo-simulaties. De vergelijking is goed. Echter, de simulaties voorspellen een vlam, die smaller en langer is, dan volgt uit de experimenten. De thermokoppel-metingen tonen ook aan dat de metingen in de turbulente vlam geen last hebben van katalytische effecten. Een axiale traverse laat zien dat roet-neerslag op het thermokoppel de meting beïnvloedt, omdat het verschil tussen twee temperatuurwaarden voor dezelfde positie proportioneel is met de roet-volumefractie gemeten met de afzuig-probe. Naast de gemiddelde temperatuur zijn er ook tijdafhankelijke metingen gedaan in de Delftse diffusie-vlam met stabilisatie-vlammetjes. Dit resulteerde in de rms-waarde van de temperatuurfluctuaties en een PDF voor de temperatuur. De vergelijking met de CARS-metingen
en de twee simulaties is redelijk.

Voordat de tomografische metingen gedaan zijn, is eerst de invloed van turbulentie op de resultaten bestudeerd. Hieruit blijkt dat de absorptie-meting amper beïnvloed wordt. De invloed op de emissie-meting is aanzienlijk en golflengte-afhankelijk, waar het grootste temperatuurverschil optreedt voor de kleinste golflengte.

De temperatuur, bepaald uit de tomografische metingen betreffende roet is inderdaad veel hoger dan de temperatuur volgens de thermokoppel-metingen. Het temperatuur-profiel is bovendien sterk gepiekt aan de buitenkant van de vlam. Dit laatste is een consequentie van de turbulentie. De temperatuur-fluctuaties beïnvloeden de breedte van het emissie-profiel, maar het absorptie-profiel wordt nauwelijks beïnvloed. De roet-volumefractie is het hoogste in de lage snelheid vlam A en het laagste in de meest turbulent vlam C, met een maximum op de as van respectievelijk ongeveer $1.0 \cdot 10^{-7}$ en $2.3 \cdot 10^{-8}$. Vergelijken met de metingen op de as met de afzuig-probe, zijn de waarden vergelijkbaar, maar de axiale positie waar het maximum optreedt is lager voor de afzuig-probe metingen.

De temperatuur, bepaald met de tomografische metingen betreffende waterdamp, is ook hoger dan de temperatuur volgens de thermokoppel-metingen. Dit verschil is kleiner dan voor de roet-metingen, wat aantoont dat de invloed van turbulentie inderdaad golflengte afhankelijk is. De correctie voor de absorptie door roet, om de partiële druk van $\text{H}_2\text{O}$ te bepalen, blijkt verwaarloosbaar. Vergelijking van deze partiële druk met de numerieke voorspellingen van de simulaties met de aangenomen PDF laten zien dat de grootte-orde ongeveer gelijk is, maar dat de vlam-breedte en -lengte volgens de simulaties niet goed is.

De temperatuur, bepaald met de tomografische metingen betreffende acetylen, is vergelijkbaar met de temperatuur bepaald uit de metingen betreffende waterdamp. Dit werd ook verwacht, aangezien het verschil in golflengte ook klein is. Voor de berekening van de partiële druk van $\text{C}_2\text{H}_2$ is de absorptie door roet weer te verwaarlozen, maar de correctie voor absorptie door $\text{H}_2\text{O}$ is aanzienlijk. Vergeleken met de resultaten van Monte Carlo-simulaties is de partiële druk van $\text{C}_2\text{H}_2$ voor deze laatste ongeveer een factor tien kleiner. Kwalitatief is de vergelijking voor de radiële profielen redelijk. Voor het $\text{C}_2\text{H}_2$-concentratie-profiel op de as is er bijna geen verschil tussen vlam A en C. Dit toont aan dat er meer parameters betrokken zijn bij het begin van de roetvorming dan alleen de partiële druk van $\text{C}_2\text{H}_2$.

Uit de breedte van de radiële profielen is de locatie van de reactie-zone en de menglaag bepaald. Voor axiale posities kleiner dan 300 mm bevindt de binnenste menglaag zich aan de brandstofrijke kant van de reactie-zone. Dit is ook de locatie waar $\text{H}_2\text{O}$ en $\text{C}_2\text{H}_2$ gevormd worden. De profielen met de breedte van de verschillende radiële profielen toont ook aan dat, in de Delftse diffusie-vlam met stabilisatievlammetjes, de diffusie van $\text{H}_2\text{O}$ groter is dan de diffusie van warmte. Kwalitatief zijn de breedte van de verschillende profielen en hun onderlinge verschillen vergelijkbaar met de resultaten van de simulaties met de aangenomen PDF.
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