On Some Radiative Heat Transfer Issues in Combustion Environments

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Abstract

This licentiate of Engineering focuses on radiative property models. Versions of the statistical narrow band model (SNB) are the subject of investigation. A non-correlated approach for solving the radiative transfer along a radiation path with a SNB model was evaluated, with soot present. A so-called fast narrow band model was extended to environments with high CO concentration. The importance of CO radiation was studied in the high CO concentration environment.

Modelling radiation can become very demanding computationally. It is therefore important to choose a property model that offers a good compromise between accuracy and computational demand. The non-correlated SNB can offer a significant decrease in the computational demand. The assumptions made in the non-correlated SNB can unfortunately lead to large errors in both the radiative heat source term and the wall heat flux. It is claimed that the non-correlated SNB performs better in the presence of soot. This work shows that the non-correlated SNB errors are decreased when soot is present. However simpler models, e.g., the weighted sum of gray gas model, can offer better accuracy to a much smaller computational cost.

The fast narrow band model also speeds up the SNB by acquiring the important structure parameters from a look-up-table. This method speeds up the model close to 30 times, compared to the original method in acquiring the parameters, with less than 1 percent error compared to the original SNB. The fast narrow band model has been extended with a CO look-up-table. The CO contribution to the total radiation can be significant in environments with high CO concentration and at low pressure. With increasing pressure the overlapping from CO$_2$ and H$_2$O bands quickly diminishes the CO contribution to the overall radiation.
Acknowledgements

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Finally I would like to express special thanks to my family for their patience when focus has been solely on work.
List of publications

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Nomenclature

1. Symbols

a  Weighting factor  [-]
2. Greek symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
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<td>Band overlap parameter</td>
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<td>( \varepsilon )</td>
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<td>( \kappa )</td>
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<td>[m]</td>
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<tr>
<td>( \mu )</td>
<td>Dynamic viscosity</td>
<td>[kg/s.m]</td>
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<td>( \mu )</td>
<td>Direction cosine</td>
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<tr>
<td>( \rho )</td>
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<td>Stefan-Boltzmann’s constant</td>
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<td>( \sigma_s )</td>
<td>Scattering coefficient</td>
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<td>( \omega )</td>
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3. Subscript

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<td>Black body</td>
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Chapter 1

Introduction

1.1 Background
The major part of the energy consumption in the world comes from carbon based fuels such as oil, coal, gas and bio fuels. Industry uses most of the energy, second comes transportation and third is residential use. Converting the bound energy in the carbon based fuels into usable energy is almost entirely by some form of combustion. Combustion, such as all other energy conversion processes, suffers from energy loss. From large losses in vehicle engines, where only a small part goes to propulsion, to minor losses in state of the art combined heat and power plants. Decreasing the losses is attempted in any combustion process, leading to less fuel consumption and a smaller environmental impact. The search for more efficient combustion implies new combustion processes and devices.

When the design of a combustion process or combustion device changes it changes the flow pattern, temperature, pressure and chemical reactions within the combustor. Understanding how the different physical processes are influenced by existing conditions is a key to create new designs and improving existing ones. Modelling the combustion processes is a way to gain better understanding and developing new designs. CFD (computational fluid dynamics) modelling of combustion is one modelling technique. The CFD modelling relies on physical models that are accurate and fast. For combustion the flow and chemical reactions are the processes normally considered in the model. Thermal radiation is a third physical process that is always present in combustion but not always considered. The importance of the thermal radiation in a model depends on the combustion conditions. For many combustion cases radiation only has a slight effect on the combustion process and can be disregarded but in other cases a crude simplification of the physics is enough. Radiation can also play a major role in the overall heat transfer, ignoring it then can lead to large errors in the results. The radiation model can be as computationally demanding as the flow and chemical reaction models. The reason for the computational demand is the nature of radiation, travelling from all positions in all direction. When radiation travels it can pass through the medium or become attenuated and augmented. The attenuation and augmentation depend on the radiative properties of the medium. The radiative properties change with temperature, pressure and wavelength etc. All these things put together can make the transport of radiation very complex.

1.2 Motivation
The radiation can in many combustion processes be the major source of heat transfer. The modelling of radiation transport in combustion environments can be performed with several different transport and property models. Depending on the choice of models the computational demand and accuracy change. Many of the models that are developed within the academic research society can be too heavy for engineering applications. Therefore the attempt must be to find fast, accurate and general radiation models suitable for the engineering society.
1.3 Work carried out in this thesis

The focus in this thesis is the radiation property models for gases and soot. First a short introduction to radiation is given then a description of the radiative transport equation follows. This equation describes how radiative energy is transported. The physical processes related to the radiation properties are described. A comprehensive description of the radiation property models follows. Then a short chapter on the radiation properties of soot are presented followed by the solution method used for the radiative transfer equation.

From this part the attention is focused on results, discussions and conclusions. This chapter is divided into two parts based on the two papers, first the 2012 paper followed by the older one from 2010. Suggestions for future work complete the thesis.
Chapter 2

Introduction to thermal radiation

Thermal radiation is the part of the radiation spectrum that is considered in heat transfer. The thermal radiation is defined as the radiation energy emitted by a medium solely due to the temperature of the medium [1] and it covers a part of the ultraviolet, the visible spectra and a part of the infrared spectrum, see Fig. 1. The thermal radiation spectrum varies between 0.1 μm and 100 μm. Radiation can travel without any medium present, such as in vacuum. When an object emits thermal radiation it can release no more than its black body radiation.

![Diagram of electromagnetic spectrum](image)

Figure 1. Part of the electromagnetic wave spectrum [2].

2.1 Black body radiation

The concept of black body radiation comes from the visible range of the electromagnetic spectrum. An object appears black to the human eye because it does not reflect any light. When an object does not reflect any radiation it is a perfect absorber, absorbing all radiation. This way of describing the black body has been adopted to the entire thermal spectrum. A black body is an object that is a perfect absorber at all wavelengths. When an object is a perfect absorber it can be shown by Kirchoff's law that it also is a perfect emitter. An object that is close to being a black body is the sun, at a black body temperature of 5777 K. Many researchers tried to describe the black body intensity distribution over the spectrum with the aid of the sun. But it was Max Planck in 1901 who first published work
on the black body spectral distribution from quantum mechanics. His work is now known as Planck’s law which tells how emissive power depends on wavelength and temperature, namely

\[
E_{\lambda}(T, \lambda) = \frac{2\pi h c_0^2}{n^2 \lambda^5 \left(e^{h c_0 / n k T} - 1\right)}, \quad (n = constant) \tag{1}
\]

where \( h, c_0, n, k \) is the Planck constant, speed of light, refractive index and Boltzmann’s constant, respectively. The higher the temperature of the black body is, the higher the emissive power, as illustrated in Fig. 2 for a number of temperatures.

\[
E_{\lambda}(T) = n^2 \sigma T^4 \tag{2}
\]

Figure 2. The blackbody emissive power at four temperatures.

The total black body emissive power is found by integrating eq. (1) over the whole spectrum, given in eq. (2), where \( \sigma \) is the Stefan Boltzmann’s constant. This is the well known expression for radiative energy and shows that of the emissive power depends on temperature to the power four.

2.2 Radiation from surfaces and in participating media

The radiation from real surfaces is never black. Many surfaces are behaving close to a black surface and can in that sense be approximated as a black surface. The radiation leaving a non-black surface is less than that of a black surface. Emissivity, \( \varepsilon \), which is the fraction of emitted radiation of the surface to the emitted power by a black surface at the same temperature, is introduced. The emissivity has a value between zero and unity. A non-black surface can be either gray, then the emissivity is constant throughout the entire spectrum, or it can be non-gray, having a spectral dependence of the emissivity, \( \varepsilon_\lambda \). Real surfaces can also reflect radiation, either in a specular or diffusive way, and transmit radiation. For a ray hitting a surface it can be reflected, transmitted or absorbed. These
properties can, as emissivity, also be spectrally dependent. A similar description of the interaction between radiation and surfaces can be made to participating media. Participating media are gases and small particles. The emissivity of the participating media can be both gray or non-gray. In contrast to surfaces they are more non-gray than gray. Instead of emissivity one often uses absorptivity or transmissivity to handle participating media. For pure gases the attenuation by absorption follows an exponential decay relating the transmissivity to the absorption coefficient as,

\[ \tau_\eta = e^{-\kappa_\eta s} \]  

(3)

where \( \tau_\eta \) is the spectral transmissivity, \( \kappa_\eta \) is the spectral absorption coefficient and \( s \) is the travelled distance within the gas. Eq. (3) is known as Beer’s law. Scattering for gases and particles is used in place of reflection, for surfaces. Scattering includes a collection of interactions between the photon (electromagnetic wave) and the particle or molecule. These are diffraction, refraction and reflection, as illustrated in Fig. 3. The properties describing the participating media are the absorption coefficient, scattering coefficient and scattering phase function. These properties are essential to describe the transport of radiation in participating media. The transport of radiation through participating media is mathematically described in the next section. Also a short introduction is given to the relation between the energy equation and the radiative transfer.

Figure 3. Illustration of possible means of scattering from a particle.
Chapter 3

The radiative transport equation

Before presenting the radiative transport equation a short introduction is given to the relation between the radiative transport and the total energy transport. Radiation travels in all directions, while being absorbed, emitted, scattered or transmitted. If one considers a volume element in an enclosure and looks for the local contribution of radiation, then one calculates the radiative source term, $\nabla \cdot q_R$, in the energy equation, (or temperature based energy equation), eq. (4). Here $\rho$ is density, $c_p$ is the specific heat, $t$ is time, $\mathbf{v}$ is the velocity vector, $k$ is the thermal conductivity, $p$ is pressure, $\mu$ is viscosity, $\Phi$ is the dissipation function and $\dot{Q}''''$ is the generated heat. To find the local radiative heat flux one must consider all radiation entering and exiting the volume element. The transport of radiative energy within the enclosure is found by solving the radiative intensity field, a function depending on location, direction and wavenumber.

$$\rho c_v \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = \nabla \cdot (k \nabla T) - p \nabla \cdot \mathbf{v} + \mu \Phi + \dot{Q}'''' - \nabla \cdot q_R \quad (4)$$

3.1 Formulation

The transport of radiative energy in the enclosure is governed by the radiative transport equation (RTE). To understand the RTE it is appropriate to start of with a more generic and illustrative description. Looking at a pencil of rays travelling from a point $s'$ to $s$ in the direction $\mathbf{s}$ in a participating medium, the incident radiation at the point $s'$ is attenuated due to absorption and scattering out from the direction and augmented by emission and in scattering, graphically presented in Fig. 4. The common formulation of the RTE, independent of time, having constant index of refraction, one-dimensional, is

$$\frac{\partial I_\eta}{\partial s} = \kappa_\eta I_\eta - \kappa I_\eta - \sigma_{s\eta} I_\eta + \frac{\sigma_{s\eta}}{4\pi} \int I_\eta(\hat{s}_i) \Phi_\eta(\hat{s}, \hat{s}_i) d\Omega_i, \quad (5)$$

where $I_\eta$ is the spectral intensity, $\sigma_{s\eta}$ spectral scattering coefficient, $\hat{s}_i$ is the in scattered direction, $\hat{s}$ radiation direction, $\Phi_\eta$ is the spectral scattering phase function and $\Omega_i$ is the solid angle. The first term on the right hand side of eq. (5) is the emitted intensity, the second term is the absorbed intensity, the third term is the out scattering and the last term is the in scattering.
3.2 Solution

Solution to the RTE in complex cases, such as in a combustor, is found by radiation models. Direct solutions of the RTE are only possible in very simple and ideal cases. Cases that are often one dimensional involving only absorption and emittance. If scattering is present then this is commonly assumed as isotropic scattering. The participating media will most likely be isothermal and homogeneous. This type of simple and ideal cases are almost never representative for applications of real heat transfer cases. Therefore approximate solutions, models, are used in solving the RTE in real heat transfer cases. Simpler approximations originally developed for one-dimensional cases are the \textit{optically thin}, \textit{optically thick approximation} or the \textit{Schuster-Schwarzschild approximation} [3]. For more elaborate, multi-dimensional, cases, such as a combustor, the RTE is preferably solved in such way that it can be coupled to the energy equation. For this coupling the divergence of the radiant heat flux is of interest, see the energy eq. (4). From the RTE one can for a volume element express the divergence of the heat flux as, see Modest [2],

\[
\nabla \cdot \mathbf{q}_r = \int_0^\infty \kappa_\eta \left( 4\pi I_{\eta\eta} - G_\eta \right) d\eta,
\]

where \( G_\eta \) is the incident spectral radiation to the volume element. Several models exist that have a sound coupling with the energy equation. A selection of the more common ones being, the \textit{spherical harmonics method} (\( P_N \)-approximation), the \textit{discrete ordinates method} (DOM), or \( S_N \)-method, developed originally by Chandrasekhar [4], the discrete transfer method (DTM) by Lockwood and Shah [5], the finite volume method (FVM) by Raithby and Chui [6], the Monte Carlo method (MC) by Howell [7]. In chapter 6, \textit{Radiation transport models (solutions to RTE)}, the DOM model, used in this work, is described. Before the solution method is described the radiation properties of gases and soot are considered in chapter 4 and 5, respectively.
Chapter 4

Radiation properties in gases

This chapter concerns the radiation properties of gases. The first section follows the description in Modest [2] and the fundamental physical phenomena behind the interaction between radiation and molecules are given. From this explanation a description is given of the distribution of the properties for a molecule throughout the radiative spectrum. The second section deals with the calculation and modelling of the properties, from very exact and computationally heavy benchmark calculations to simpler global models. The property models cover the ones used in this work and a few other common ones.

4.1 Introduction to radiative properties of molecular gases

When radiation travels through molecular gases it can either be scattered, absorbed or transmitted. The molecule itself can contribute to the total radiative flux by emitting radiation. Scattering of radiation from molecules, small molecules, is not important in heat transfer applications and not be treated further. The radiation consists of photons (or electromagnetic waves), which have certain energies inversely proportional to their wavelengths. For a photon to interact with a molecule the energy level of the photon must match the energy level of the molecule. The energy levels of molecules, relevant for thermal radiation, are predominantly associated with the vibration and rotation of atoms within the molecule and electrons spinning around the nucleus within the molecule. From quantum mechanics it is known that these energies are quantised, related to discrete wavelengths. These quantised energy levels are not discrete but exist in a small interval. Translated to the energy of photons the energy levels of the molecule can be interpreted as positions in the radiative spectrum, as lines, with a broadening from those positions, the line centres. The broadening of the lines out from the line centre occurs because of so called natural, collision and/or Doppler broadening. These phenomena are explained in a later section. From the above given description of energy levels within a molecule a collection of photons travelling through a gaseous layer is now considered. The photons may be absorbed or emitted if the wavelength of the specific photon falls inside one of the broadened spectral lines. The energy transitions associated with vibration, rotation and electron excitation or relaxation within the molecules are known as the bound-bound transitions. Out of three existing transitions, bound-bound is the important one for combustion applications. In next subsection the bound-bound transitions are described leaving the reader to find out more about the other two types of transitions, bound-free and free-free transitions, in works on molecular spectroscopy and quantum mechanics.

4.1.1 Rotation and vibration of molecules

The two important bound-bound transitions in heat transfer are the rotational and vibrational transitions. If one starts by considering a single atom it can move in three dimensions. If more atoms are added and a molecule is created the atoms can together also move in three dimensions and more than that they can move relative to each other. These types of extra moments are recognised as
vibration and rotation of the molecule. The more number of atoms in a molecule the more relative
degrees of freedom exist. For N number of atoms in a molecule 3N-3 degrees of freedom exist.

The rotational motions of a molecule can in most cases be accurately predicted by the *Schrödinger wave equation* for a rigid rotator model. From the solution of this equation the possible energy levels of the molecules can be detained. There are three possible energy transitions related to rotation; increasing one energy level which corresponds to absorption, decreasing one energy level which corresponds to emission and a zero level transition which is related to a simultaneous vibration transition. Every transition corresponds to a wavenumber, a spectral line. Not all molecules exhibit rotational lines such as O₂ and N₂ as these are lacking the electrical dipole moment.

The vibrational movements of a molecule can also be predicted by the *Schrödinger wave equations* in this case for a harmonic oscillator. This prediction, where the molecules are assumed to be connected by a perfectly elastic massless spring, does not give an entirely accurate result. The harmonic oscillator predicts a single spectral line, wavenumber, where the vibrational transitions take place. Instead an assumption of a rigid rotator with a more advanced string constant then the linear constant of a harmonic oscillator gives a better result. More than the single spectral line of the harmonic oscillator known as the fundamental transition the rigid rotator also predicts several weaker lines known as overtones.

The vibrational transitions are almost exclusively accompanied by rotational transitions. These two transitions are together known as the combined transitions. The energy needed for a vibrational transition is much larger than for a rotational transition. As the transitions occur together they build up closely packed lines centred around the vibrational wavenumbers. These packed lines are known as the vibration-rotation bands of a molecule. In combustion applications, in the thermal region of the spectrum, the important vibration-rotation bands for H₂O are at 6.3, 2.7, 1.87 and 1.38 μm, for CO₂ at 15.0, 4.3 and 2.7 μm and for CO at 4.7 μm.

### 4.1.2 Line radiation

Moving on from the knowledge of how the spectral lines arise in the spectrum for a molecule, this section will explain the different effects that broaden the lines and give rise to different line shapes. The three different ways of broadening the lines are the natural, collision and Doppler broadening, see Fig. 5. In combustion applications the collision broadening is the most dominant broadening effect.

The collision broadening comes from the collision of molecules, the more collisions the more effect on collision broadening. The collisions between molecules introduce or remove a small portion of the energy during transitions. The line shape of collision broadening follows the *Lorentz* line shape as

\[
\kappa_\eta = \frac{S}{\pi \left( \eta - \eta_0 \right)^2 + b_C^2}, \quad S \equiv \int_{-\Delta \eta}^{\Delta \eta} \kappa_\eta \, d\eta
\]

where \(S\) is the line strength, \(b_C\) is the line half-width and \(\eta_0\) is the wavenumber at the line center. The line half-width is in units of wavenumber and is found at half the maximum absorption coefficient. The line half-width is defined as
The broadening increases from the reference state, noted "0", as pressure increases and as temperature decreases. The natural broadening has the same Lorentz shape as the collision broadening. Natural broadening comes from the relaxation of excited molecules with the release of a photon as a consequence of the relaxation. The broadening comes from the fact that the photon energy cannot be exactly determined, governed by the Heisenberg uncertainty relation. The relaxation of molecules occurs much more seldom than collision of molecules within the thermal part of the spectrum. The small contribution to the broadening of the lines from natural broadening, \( b_N \), can be added to the collision broadening, \( b_C \). Together these establish the Lorentz broadening, \( b_L \).

The Doppler broadening comes from the compression of the electromagnetic wave as the emitter is also travelling towards the observer. The Doppler line shape is defined as

\[
\kappa_\eta = \frac{\ln 2}{\pi} \left( \frac{S}{b_D} \right) e^{-\ln 2 \left( \frac{\eta - \eta_0}{b_D} \right)^2}
\]

where \( b_D \) is the line half-width for Doppler broadening. The Doppler line half-width is defined as

\[
b_D = \frac{\eta_0}{c_0} \sqrt{\frac{2kT}{m \ln 2}}
\]

where \( c_0 \) is the velocity of light in vacuum, \( m \) is mass of the radiating molecule. Unlike natural and collision broadening the Doppler broadening depends on the wavenumber. Combined effects of all three broadening effects can be described by using a Voigt profile which has a much more advanced definition,

\[
\kappa_\eta = \frac{S b_L}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{e^{-x^2} dx}{\left( \eta - \eta_0 - \frac{x b_D}{\sqrt{\ln 2}} \right)^2 + b_L^2}, \quad x = v \sqrt{\frac{m}{2kT}}
\]

where \( v \) is the probability of a relative velocity from the Doppler broadening. For normal combustion cases the Lorentz profile is the dominant profile. As the temperature reaches very high value, above 2000 K, the Doppler broadening starts to dominate but even then the lines take the Lorentz shape in the important line-wings.
4.2 Calculation and modelling radiative properties of gases

The radiative properties of gases are very erratic as has been explained in the previous chapter. The absorption coefficient, being the property of interest for thermal radiation, is found at a vast number of spectral positions which can have very sharp gradients over small increments of the spectrum. Research of the spectral properties of molecules is constantly contributing to an increasing spectral database. For the most accurate calculations of the absorption coefficient the spectral database is used directly. These types of calculations are known as line-by-line calculations. A large part of the methods for calculating or modelling the radiative properties of the gases are based on spectral data, some uses molecular models and other correlations from experimental data. Three spectral models are demonstrated in Fig. 6. The difference in spectral resolution between the models is illustrated. This section will give an introduction to the line-by-line calculations, a more in depth description of a selection of narrow band models and finally a brief description of wide band models, i.e. three spectral models, and finally short on some global models. Depending on the problem at hand one or several models can be used to find the radiation properties. The choice of model depends on several factors such as accuracy needed, the different species and their concentrations in the gas, the level of inhomogeneity etc. Very often the problem lies in a trade off between computational demand and accuracy. When a problem exists at "standard" conditions, such as in the post flame zone of a methane flame, where species distribution and other properties are known, correlations for the simpler models are often found. For such a case there is no point in choosing a more advanced model for calculating the properties. As a problem moves away from being "standard" one must turn to more advanced models if accuracy is to be maintained. Knowledge of the problem and the model limitations beforehand can serve well in choosing the appropriate model.
4.2.1 Line by line calculations

The method of line-by-line calculations is the most accurate method in finding the absorption coefficient. With the use of high resolution spectral data it predicts the absorption coefficient for an increment of the radiative spectrum as small as 0.001 cm$^{-1}$, less the thickness of a single line. With such a high resolution of the radiative spectrum these types of calculations demand substantial computational resources. Therefore most of the line-by-line calculations are for benchmarking of simpler gas radiation models. Using line-by-line calculations for radiation properties in combustion environments is still considered prohibitive because of the high computational load. The accuracy of the calculations is dependent on the accuracy of the spectral data. Calculating the spectral absorption coefficient from the spectral data the line by line calculations use the line intensity, $S$, the air and self broadened parameter, $b_{air}$ and $b_{self}$, temperature dependence parameter, $n$, and the lower state energy, $E_l$. The well known spectral database of HITRAN [9] supplies these spectral data for 42 different molecules. The HITRAN data base is a very important source for calculating radiation around normal pressure and temperature (NPT) but as temperature increases the accuracy of HITRAN data base for line by line calculations is diminished. The reason for this is the lack of hot lines in the HITRAN spectral data. The hot lines originate from high vibrational levels of molecules. At low
temperatures, close to NPT, the contribution of hot lines to the absorption is negligible and is therefore not included in the HITRAN. For higher temperatures the HITEMP [10] spectral database is recommended. This is a further development of the HITRAN with many more bands and transitions. Early line-by-line calculations for combustion environments, inhomogeneous and non-isothermal environments, have been performed by Taine [11].

4.2.2 Narrow band model

Narrow band models have been used in this work. It is one of the most exact models for calculating the absorption coefficient is the narrow band model. The narrow band model divides the vibration-rotation bands into parts in the order of 10 wavenumbers and averages the properties within these parts, narrow bands. The averaging of the properties is possible as a consequence of the smallness of the narrow bands and that the Planck function can be considered as constant within the bands. Depending on how well the averaging of the properties within the bands is done, a narrow band model can be as accurate as the line-by-line calculations. The traditional narrow band models are much faster than the line-by-line models. Though being much faster than the line-by-line it is still considered as prohibited to use in combustion modelling. There exist narrow band models which have potential in being of interest for combustion applications. These are versions of the fast narrow band model and versions of the k-distribution method. Both of these methods will be addressed in later sub sections. The accuracy is as stated dependent on the accuracy of the averaging of the absorption coefficient within the narrow band. Two commonly known models used to acquire the band properties is the Elsasser and the statistical models. The statistical models are used in this work. They are better in capturing the properties of combustion gases than the earlier Elsasser model. For both these types of narrow band models, the average emissivity of the narrow band is often expressed. The averaged spectral emissivity is

$$\bar{\varepsilon}(\eta) = \frac{1}{\Delta \eta} \int_{\eta-\Delta \eta/2}^{\eta+\Delta \eta/2} \left[ 1 - e^{-\int_{\eta-\Delta \eta/2}^{\eta+\Delta \eta/2} \kappa(\eta)d\eta} \right] d\eta$$

(12)

where $X$ is the optical path length.

4.2.2.1 The Elsasser model

The Elsasser model is applicable for gases containing simple molecules, such as diatomic and linear polyatomic molecules. The model assumes an equal strength and distance of lines within the band. This assumption is consistent with the simpler type of molecules mentioned earlier, with equal line distribution and small intensity changes inside the band. The absorption coefficient was described by Elsasser [12] and was later written for lines with Lorentz profiles as

$$\kappa(\eta) = \frac{S}{d} \sinh(2\beta), \quad \beta = \frac{\pi b_0}{d}, \quad z = \frac{2\pi\eta}{d}$$

(13)

where $d$ is the line distance, $\beta$ is the line overlap parameter and $z$ is just a letter of convenience. The emissivity is often presented as depending on the level of overlap between lines and how strong these are. For no overlap, $\beta<<1$, and strong overlap, $\beta>>1$. The strength of the lines are given by the strength parameter for the Lorentz lines as
\[ x = \frac{SX}{2\pi b_L} \]  

(14)

also known as the non-dimensional optical path length. Weak lines are \( x << 1 \) and strong lines are \( x >> 1 \). A third non-dimensional parameter, other than \( \beta \) and \( x \), is the narrow band optical thickness given by \( \tau = \kappa X \). The emissivities for the Elsasser model in the different regimes are presented in table 1.

4.2.2.2 The statistical models

The statistical models are based on the hypothesis of Goody [13] stating that the line within a narrow band are randomly distributed. The intensity is not equal as for the Elsasser model but follows a probability distribution. For more complex molecules this hypothesis coincides much better than the Elsasser model. The emissivity for the statistical models can be expressed as

\[ \bar{\epsilon}_\eta = 1 - e^{-\frac{W}{\sigma}} \]  

(15)

where \( \bar{W} \) is the average equivalent line strength and \( d \) is in this case the average line distance. A probability distribution for the line intensity was suggested by Goody as

\[ p(S) = \frac{1}{S} e^{-\frac{S}{S}}, \quad 0 \leq S \leq \infty \]  

(16)

which is an exponential tailed line intensity distribution. Later Malkmus [14] suggested an inverse exponentially tailed line intensity distribution

\[ p(S) = \frac{1}{S} e^{-\frac{S}{S}}, \quad 0 \leq S \leq \infty \]  

(17)

The average equivalent line strength can now be expressed with a probability function for the line intensity distribution as (including the definition of the equivalent line strength and when the number of lines within the narrow band approaches infinity),

\[ \bar{W} = \int_{0}^{\infty} W(S, X)p(S)dS = \int_{0}^{\infty} p(S) \int_{-\infty}^{+\infty} (1 - e^{-\kappa \eta(S)X})d\eta dS. \]  

(18)

The ratio between the average equivalent line strength and the line distance can now be found by solving the above equation for a line profile. The spectrally averaged emissivity and the ratio \( \bar{W}/d \) are presented in table 1 in the different regimes for the statistical models of Goody and Malkmus and the Elsasser model for Lorentz lines.
Table 1. $\bar{W}/d$ and spectrally averaged emissivity for narrow band models in different regimes for Lorentz lines [2].

<table>
<thead>
<tr>
<th></th>
<th>Weak line</th>
<th>Strong line</th>
<th>No overlap</th>
<th>All regimes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$X&lt;&lt;1$</td>
<td>$X&gt;&gt;1$</td>
<td>$&lt;&lt;1$</td>
<td>All regimes</td>
</tr>
</tbody>
</table>

### Elsasser model

\[
\frac{W}{d} = \tau, \quad 2\sqrt{\tau/\beta/\pi}, \quad 2\beta L(\tau/2\beta) \\
\bar{\varepsilon}_\eta = 1 - e^{-\tau}, \quad \text{erf} \left( \sqrt{\tau/\beta} \right), \quad \frac{W}{d}, \quad \text{erf} \left( \frac{\sqrt{\pi} W}{2d} \right)
\]

### Statistical models

#### Goody

\[
\frac{\bar{W}}{d} (\text{Goody}) = \tau, \quad \sqrt{\tau/\beta}, \quad \frac{\tau}{\sqrt{1 + \tau/\beta}}
\]

#### Malkmus

\[
\frac{\bar{W}}{d} (\text{Malkmus}) = \tau, \quad \sqrt{\tau/\beta}, \quad \frac{\bar{W}}{d}, \quad \frac{\beta}{2} \left[ \sqrt{1 + 4\tau/\beta} - 1 \right]
\]

\[
\bar{\varepsilon}_\eta = 1 - e^{-\tau}, \quad 1 - e^{-\bar{W}/d}, \quad 1 - e^{-\bar{W}/d}
\]

The parameters needed to find the band properties are $S/d$, $1/d$ and the line half width, for Lorentz lines $b_l$. The parameters are dependent on the wavelength, temperature and for the line half width also the pressure. The structure parameters of $S/d$ and $1/d$ can be found from molecular models such as the ones developed by Malkmus [15, 16], by interpolating experimental data which was done in Grosshandlers [17] RADCAL or developed from a spectral database, done by Soufiani and Taine [18]. The line half width is found from kinetic theory, also found in the work of Soufiani and Taine. The calculation or interpolation of the structure parameters consumes a large portion of the computational time. The fast narrow band model, explained in an upcoming subsection, speeds up the narrow band models by predetermining these parameters and reusing them.

The Malkmus and the Goody models have been compared in several works, among them Soufiani et al. and Marakis [19, 20]. Soufiani et al. investigated for combustion like environments while Marakis considered inhomogeneous and non-isothermal paths of $H_2O/N_2$ mixtures. Marakis came to the same conclusion as Soufiani et al. already made, namely that the Malkmus model gives better accuracy than the Goody model. Marakis also investigated the effect of the database for the structure parameters on the Goody model, comparing the two databases which he named LMRT (Ludwig, Malkmus, Reardon, Thomson), [21], and HL$^2$ST (Hartmann, Levi Di Leon, Soufiani, Taine), [19, 22]. The later HL$^2$ST gave more accurate results than the earlier LMRT, showing the importance of the database choice. Marakis concluded that though the Malkmus model is more accurate than the Goody model the latter is still interesting because of the simpler mathematics associated with it. Both
these models have been used in this work. The Goody model is a part of the fast narrow band model used in Hofgren et al. [23] and the Malkmus model is used in the work of Hofgren and Sundén [24].

4.2.2.3 k-distribution method
The k-distribution method reorders the absorption coefficient over an increment of the spectral range. This reordering was first explained by Arking and Grossman [25] showing that when determining the transmissivity the order of the absorption coefficient is not important just the distribution within the small spectral increment. In this way the frequency dependence of the absorption coefficient is dropped and integration is instead over the k-space. The use of the k-distribution for an inhomogeneous path is carried out by a correlated-k method. This method is applied on inhomogeneous radiation paths which will be presented in the next section together with methods for the other narrow band models.

4.2.2.4 Inhomogeneous and non-isothermal paths of gas mixture
So far radiation for a homogeneous path of a single species has been considered. Reality is that the combustion environment radiation paths are far from homogeneous and consist of several species. This section deal with the theory in adopting the narrow band models to inhomogeneous radiation paths and how mixtures are treated. It has been shown that the transmissivity of a mixture of gases is the product of the individual gas transmissivities as,

\[ \tau_{\eta, \text{mixture}} = \prod \tau_{\eta, \text{species}} \quad (19) \]

For the Elsasser and statistical models the method normally adopt approximation of the transmissivity and the line overlap parameter along the path. The commonly used method is the Curtis-Godson approximation [26] which is described together with its more accurate follower, Curtis-Godson two parameter scaling approximation, by Young [27]. First the definition of the transmissivity in the limits of weak and strong lines with the traditional formulation of the Curtis Godson approximation for a band is

\[ \tau = \frac{\bar{\nu}(s)}{d} = \frac{u(s)\bar{k}_e(s)}{d}, \quad x_e(s) \ll 1 \quad (20) \]

\[ \tau = \frac{1}{\beta_e(s)} \frac{\bar{\nu}(s)}{d} = \frac{2}{\beta_e(s)} \frac{u(s)\bar{k}_e(s)\bar{b}_L}{d} x_e(s) \gg 1 \quad (21) \]

where \( u(s) = cps \) is the optical depth expressed by the sum of concentration, pressure and path length, \( \bar{k}_e \) is the effective band absorption coefficient and \( x_e(s) \) is the effective non-dimensional optical strength expressed as

\[ x_e(s) = \frac{u(s)\bar{k}_e(s)}{\beta_e(s)} \quad (22) \]

where \( \beta_e \) is the effective line overlap parameter. The two effective parameters are written in terms of the path averaged parameters of line strength, \( S_e(i,s) \) and half width \( b_L(i,s) \). All the steps can be
found in the work of Young [27]. Finally the effective parameters end up being defined by the average value of $\bar{k}$ and $\bar{\beta}$ over the inhomogeneous path as

$$\bar{k}_e(s) = \frac{1}{u(s)} \int_0^s c(\hat{s}) P(\hat{s}) \bar{k}(\hat{s}) d\hat{s}$$

$$\bar{\beta}_e(s) = \frac{1}{u(s) \bar{k}_e(s)} \int_0^s c(\hat{s}) P(\hat{s}) \bar{k}(\hat{s}) \bar{\beta}(\hat{s}) d\hat{s}$$

where $c$ is species mole fraction and $P$ is total pressure. This general way of defining the narrow band properties makes it applicable to any inhomogeneous path. However, there is no guarantee that the method is accurate for any path. The Curtis-Godson approximation is sensitive to large pressure gradients. Another approximation for inhomogeneous paths is the Lindquist-Simmons approximation, also described in Young [27].

The use of the k-distribution for a non-homogeneous path is not straight forward as the spectral data has been scrambled. Goody et al. [28] investigated the non-homogeneous path with focus on the overlapping bands. They suggested a multiplication property directly into the correlated-k (CK) method to consider the overlapping bands. These type of CK methods have proven to be accurate for atmospheric applications having small temperature gradients and high pressure gradients. With higher temperature gradients the accuracy of the model is decreased, which is the case in combustion environments. A research group around Taine at the EM2C laboratory has performed a lot of work on the CK model. From this group Riviere et al. [29] suggested a correlated-k fictitious gas method (CKFG) for high temperature gradients. They tested their model for the 2.7 μm H2O band between 300-1500 K and for pressures in the range of 0.2-3 atm. They continued their work and Soufiani and Taine [18] produced CK parameters for CO2 and H2O between 300-2500 K.

4.2.2.5 Fast narrow band model
Applying the traditional narrow band models to engineering applications for modeling combustion is still considered prohibitive. This section will describe the fast narrow band model developed by Yan and Holmstedt [30]. The model is developed for the Elsasser and statistical narrow band models. It speeds up the narrow band models by avoiding to repetitively acquire the structure parameters, S/d and 1/d, from molecular models or interpolation of experimental values. Instead the method pre-evaluates the structure parameters and store them in a look-up table. The evaluation of the structure parameters is a large part of the computational load of the narrow band models. The look-up table speeds up the well known RADCAL program of Grosshandler [17] close to 30 times compared to its original form. The fast narrow band model has been proven for water, carbon dioxide and soot in original work of Yan and Holmstedt and in a later work of Hofgren et al. [23] it has been further verified with the inclusion of carbon monoxide. Hofgren et al. also investigated the effect of CO radiation in combustion environments when having large CO concentrations.

4.2.2.6 The correlated and non-correlated SNB
The statistical narrow band model is an accurate but computationally demanding model. One of the reasons is that it uses a large number of narrow bands, each band connecting to a solution of the
RTE. The second part that makes it computationally demanding is the spectral correlation between the transmissivity and the intensity. When solving the RTE, eq. (5), based on the transmissivity, and discretising it along a path of cells one finds the correlated form of the SNB, for a non scattering case,

\[
\bar{I}_{\Delta \eta, n} = \bar{I}_{b, \Delta \eta, 0} \bar{r}_{\Delta \eta, 0 \rightarrow n} + \sum_{j=0}^{n-1} \left( \bar{r}_{\Delta \eta, j+1 \rightarrow n} - \bar{r}_{\Delta \eta, j \rightarrow n} \right) \bar{I}_{b, \Delta \eta, j+1/2} \tag{25}
\]

starting from a wall, point 0, and moving into a domain to the point \( n \). The intensity at the point \( n \) receives radiation from all prior cells along the radiation path. This is mentioned as the historical effects. The non-correlated SNB drops the spectral relation between the transmissivity and the intensity and by this it avoids the summation term of eq. (25). The non-correlated form becomes,

\[
\bar{I}_{\Delta \eta, j} = \bar{I}_{\Delta \eta, j-1} \bar{r}_{\Delta \eta, j-1 \rightarrow j} + (1 - \bar{r}_{\Delta \eta, j-1 \rightarrow j}) \bar{I}_{b, \Delta \eta, j-1/2}. \tag{26}
\]

This reduces the total number of spectral transmissivity evaluations, which is for a standard narrow band model proportional to \( N^2 \) elements, to be proportional to \( N \). The added approximation results in a speed up proportional to the number of elements in the radiation path. The model has been investigated by Zhang et al. [31] and Marakis [20] both not recommending it to be used as it can cause large errors both in the radiative flux and source term. Yan [32] further developed the earlier FASTNB model, calling it a fast spectral approximation of a narrow band model. The model uses the non-correlated approach to the SNB. Yan suggests that this model is a true candidate to the correlated SNB, especially in sooting environments.

### 4.2.3 Wide band models

A wide band model divides the spectrum into bands where each band can cover an entire vibration-rotation band. The simplest of wide band models assumes a constant absorption coefficient over the wide band. This is the box model first developed by Penner et al. [33]. The most accepted and used wide band model is the exponential model first developed by Edwards and Menard [34]. The approximate average error of the band absorption compared to experimental data is about 20% but can reach as high as 50-80 %, see Modest [2].

### 4.2.4 Global models

The global models are also known as full spectrum models. They use a method in describing the properties over the whole spectrum, most often the absorption coefficient. A commonly known global model is the total emissivity based weighted sum of gray gas model (WSGGM) first developed by Hottel and Sarofim [35]. This model has been used in this work and will first be described. The WSGG model will be followed by an extension of the WSGGM made by Denison and Webb [36] called the single line weighted sum of gray gas model (SLW). Finally the full spectrum correlated k-distribution model (FSCK) of Modest and Zhang [37] will be briefly described. Other global models, not described below, are the cumulative wavenumber method (CV) Solovjov and Webb [38] and the ADF method, Riviere [39].

In the WSGG model the total emissivity is expressed by the weighted gray gases as
\( \varepsilon = \sum_{i=1}^{l} a_i(T) \left( 1 - e^{-\kappa_i x} \right) \) (27)

where \( a_i(T) \) is the weighting factor of the black body radiation and \( \kappa_i \) is the absorption coefficient for every \( i \)-th gray gas. Modest [40] showed that the RTE can be written for every gray gas as

\[
\frac{dl_i}{ds} = \kappa_i (a_i l_b - I_i)
\]

which is similar to the traditional non-scattering RTE. The method in finding the weighting factor and absorption coefficient is by fitting the parameters to emissivity data. For combustion application it is important to have emissivity data for both high temperature and sometimes high pressure. Bahador and Sundén [41] produced this kind of data for the parameters by fitting them to emissivity data produced by LBL calculations of HITEMP1995 [42] database with a polynomial function of the weighting factor as

\[
a_i = \sum_{j=1}^{4} b_{i,j} T^{j-1},
\]

where \( b \) are the polynomial coefficients. The parameters were produced for three gray gases, \( i=3 \), and polynomials of third order, \( j=4 \). The temperature range was from 500 K to 2500 K. The parameters were presented for two mixtures of water and carbon dioxide, one with equal amount and one with twice the amount of water, for total pressures from 1 to 20 atm. Soufiani and Djavdan [43] had prior to the work of Bahador and Sundén made WSGG coefficients correlated to the emissivity from the SNB model with the HL2ST database. The LBL and SNB calculations of Chu et al. [44] on planar enclosures show that the accuracy of the HITEMP1995 is not as good as the SNB based on the HL2ST database when comparison is done with the HITEMP2010. Several other published works on the WSGG model are treated in the work of Lallemant et al. [8].

With the SLW, the weighting factors and absorption coefficients found in eq. (28) are still used. Compared to the WSGG model the weighting factors are not depending on the local temperature alone but also on the local concentration. To add this new feature Denison and Webb [45] introduced an absorption line blackbody distribution function to describe the weighting factor. This distribution function is based on local gray gas absorption cross section, temperature, pressure and concentration. An expansion of the SLW model for non-isothermal and non-homogeneous mixtures can be found in the continued work by Denison and Webb [46, 47]. According to Modest the WSSG model and SLW model are the crudest possible implementation of the FCSK model.

The FCSK model is developed from the correlated-\( k \) distribution model with an inclusion of a weighting of the Planck function to cover the entire spectrum. The weighting is done by defining a fractional Planck function as
\[
\begin{align*}
i(T, \eta) &= \frac{1}{I_b(T)} \int_0^\eta I_b \eta \, d\eta, \\
\end{align*}
\]  

(30)

where \(0 \leq i(T, \eta) \leq 1\). From eq. (30) one can arrive to a gray, non-scattering RTE, see Modest et al. [37] for derivation,

\[
\begin{align*}
\frac{dI_g}{ds} &= k(g)u(s)(aI_b - I_g), \quad 0 \leq g \leq 1.
\end{align*}
\]  

(31)

where \(g\) is an equivalent fractional Planck function. For the absorption coefficient in eq. (31) a scaling approximation can also be used, postulating that the spatial and spectral dependence of the absorption coefficient are separable. The global model with the scaling is known as the full spectrum scaled \(k\)-distribution (FSSK). The correlated method works better for large pressure changes and small temperature changes, as in atmospheric modelling. Modest [48] has shown that for combustion applications the FSSK outperforms the FSCK.
Chapter 5

Radiation properties of soot

Char, ash and soot are the particles that are more or less relevant for radiation in combustion systems. What kind of particles being present depends on the type of combustion device, fuel and conditions in the combustor. Already a small volume fraction of particles in a combustion device can dominate the radiation making gas radiation less important. This section will focus on the soot in combustion devices. Soot is usually formed in fuel rich regions of a combustor. Soot are very small, normally spherical, carbon particles which can agglomerate to larger ones. The size of the particles normally range between 5 nm to 80 nm [2]. For flames, with soot, relevant volume fractions can be found in the range of $10^{-8}$ to $10^{-5}$ [49],[2].

5.1 Radiation from soot

The small size of the soot particles ensures that the particles have the same temperature as the surroundings. The size also enables that Rayleigh’s theory can be applied, at least it is a good approximation. For some large particles and the shortest wavelength Rayleigh’s theory is not valid, therefore it only makes a good approximation. When Rayleigh’s theory is valid scattering can be neglected and only absorption and emission are of interest. The soot absorption continues over the entire spectrum, being proportional to the volume fraction, $f_v$, and inversely proportional to the wavelength as

$$\kappa_\lambda = \frac{c f_v}{\lambda} \quad (32)$$

where the constant $c$ can be found in the range 3.7-7.5 [49] depending on the refractive and absorptive indices. For a simple radiation analysis a mean absorption coefficient is normally used such as the Planck-mean, eq. (33), and the Rosseland-mean absorption coefficient. In the Rosseland-mean the value of Planck-mean, 3.83, changes to 3.60.

$$\kappa_p = 3.83 f_v C_0 T / C_2 \quad (33)$$

In eq. (33) the first constant, $C_0$, is the same as the constant $c$ for the spectral absorption coefficient of soot, eq. (32). The second constant is $C_2 = 1.4388$ cm K. Truelove [50] has produced parameters for the WSGG for various mixture fractions of water and carbon dioxide and soot. Felske et al. [51] has done similar work such as Truelove but only the gray gases for soot. Both works are used in this work.
Several models have been developed over the years to solve the RTE. An optimal model does not exist for every case instead a certain model can be the best for the problem at hand. Conditions such as the type of geometry, temperature field and radiative properties affect the choice of an appropriate model. In this work the discrete ordinates method (DOM) has been used, as it has been most frequently used in solving the RTE in combustion applications.

### 6.1 The discrete ordinates method (DOM)

The DOM, also known as the $S_N$-method, is one of the most common solution methods in solving the RTE for combustion applications. The method is regarded to offer a good compromise between accuracy and computational demand. It was developed by Chandrasekhar and it divides the total solid angle, $4\pi$, into a number of discrete smaller angles, ordinates. The RTE is then, eq. (5), approximated as,

\[
\frac{\partial I(\hat{s}, s_i)}{\partial s} = \kappa I_{bn} - \kappa I(\hat{s}, s_i) + \frac{\sigma_{sn}}{4\pi} \sum_{j=1}^{n} w_j l_{\eta,-}(s_j) \Phi_{\eta}(s_i, s_j),
\]

where the $w_j$ are the quadrature weights that relate to the directions $s_j$. The boundary conditions, from a non-gray wall, of the DOM are,

\[
I_{\eta,w}(\hat{s}_w, s_i) = \varepsilon_{\eta} I_{bn,w} - \frac{1 - \varepsilon_{\eta}(\hat{s}_w)}{\pi} \sum_{j=1}^{n} w_j l_{\eta,-}(s_j)|\vec{n} \cdot \vec{s_j}|.
\]

The directions $s_j = \xi \hat{i} + \eta \hat{j} + \mu \hat{k}$ and weights are in this work the ones developed by Fiveland [52]. Eight ordinate sets were used, $S_8$. The ordinate sets are related to the number of directions by, $n = N(N + 2)$. In this work one-dimensional non-scattering cases have been considered. The angular discretised version of eq. (34), for one dimension, without scattering, dropping spectral dependence, is then,

\[
\mu_i \frac{dI_i}{dx} = \kappa I_b - \kappa I_i \quad i = 1, 2, \ldots, n.
\]

with the direction cosine, $\mu_i = \cos \theta_i$. A spatial discretisation is performed along each direction, over homogeneous and isothermal volume elements. Using the finite difference method, leaving out a few of the steps, to discretise eq. (36) the intensity in each cell becomes,
using a step difference scheme to relate cell edges intensity to the central intensity. When all intensities are found the radiative source term is found from

\[ \nabla \cdot q = 4 \pi \kappa I_b - \kappa \sum_{i=1}^{n} w_i I_i(\hat{s}, s_i). \]  

For non-absorption coefficient based models, such as the SNB model, a different spatial discretisation is used. The calculations and expression for the SNB are somewhat more cumbersome than the ones used for the absorption coefficient based models, see Kim et al. [53].

There are two major problems with the DOM and one of them can be the ray effects. The ray effect is a product of the angular discretisation. The ray effects decrease with the number of directions but can never disappear. Lee et al. [54] gave a good description of ray effects with the help of Fig. 7. Consider a small hot plate surrounded by cold walls, Fig. 7. The radiation coming from the small hot plate is discretised into six directions. In reality the cold walls receive a continuous radiation from the hot plate. With the discretisation of the directions the wall instead experience step wise changes of the heat flux and some parts experience no flux at all. The second major problem can be false scattering. As a radiation beam is traced through an enclosure a type of broadening takes place of the beam because of the way the DOM functions. This is an unphysical behaviour and can be decreased with an increased number of cells, refined mesh.

Figure 7. Illustration of ray effects. [54]
Chapter 7

Results, discussions and conclusions

This chapter is divided into two parts. The first part is based on the paper submitted for the NHT conference 2012 in Poland, the second part is from the paper presented at the RAD-10 conferences of 2010 in Turkey [23].

7.1 Radiation property models in sooting environments

7.1.1 Results and discussion

Sooting environments change the conditions of the radiative transfer in such a way that the radiation can become totally dominated by soot, making the gas property model much less important. The reason for this is the continuous spectral distribution of the soot absorption coefficient, see eq. (32). The soot absorption coefficient increases with volume fraction and decreases with wave number, making the radiative property spectra much more gray. Several investigations exist on how different property models perform in sooting environments [49, 55-57]. So far the performance of the nc-SNB has yet not been thoroughly investigated regarding the effects of soot. Yan compared his version of the nc-SNB to a narrow band model for a few sooting cases. This work is a more comprehensive investigation on the effects of soot on the nc-SNB. Three test cases compares nc-SNB with the much simpler WSGG model and the correlated SNB. Both the SNB and nc-SNB use the database of HLST for the structure parameters. Three versions of the WSGG model are compared with the nc-SNB. The difference between the WSGG models is the way soot is included in the model. The simplest is named the WSGG-P. It uses the Planck average absorption coefficient for the soot, see eq. (33). The WSGG coefficients for the gases are the ones developed by Babador and Sundén. The other two include soot by representing it as extra gray gases. The first of these two is named WSGG-F. The gray gases of soot are taken from the work of Felske and WSGG coefficients for gases are from Babador and Sundén. The third one is named WSGG-T with all coefficients from the work of Truelove. The test cases have been solved with the same solver, the DOM, and with the same angular and spatial discretisation. The quadrature points and weights are taken from Fiveland.

All test cases considered are for plane parallel cases with conditions representative for combustion environments. In the first test case, case 1, a homogeneous hot gas with soot at 1 atm. and 1000 K between cold walls separated by a distance of 1 meter was considered. The participating gases were 20 percent H\textsubscript{2}O and 10 percent CO\textsubscript{2}. Three volume fractions for soot were used, 10\textsuperscript{-8}, 10\textsuperscript{-7} and 10\textsuperscript{-6}, representing low, moderate and high soot loads. The contribution by the low, moderate and high soot loads to the total intensity of the gas column in case 1 is illustrated in Fig. 8, produced by the SNB model. At small soot loads the contribution of soot is minor to the overall intensity, i.e. the gases dominate. At high soot loads it is the other way around, soot dominates and the gas contribution is minor to the overall intensity.
Figure 8. Fraction of blackbody intensity of only soot and soot together with gases for case 1 with the three soot loads, $10^{-8}$, $10^{-7}$ and $10^{-6}$.

In Fig. 9a, the radiative source term is presented for the SNB of case 1. In Figs. 9b-d the deviation is presented for the nc-SNB and the three WSGG models to the SNB, again for the three soot loads. It is clear from Fig. 9 that the overall performance of the nc-SNB is worse than the WSGG models. Large errors occur close to the wall. In this region the absolute values of the source term are highest and gradients are large. The gas layers in the outer part of the domain are most affected by the cold walls. The relatively high deviation for the low soot load was expected as the effects of soot are almost negligible. The performance of the other models for moderate and high soot loads are better even though the nc-SNB and the SNB use the same constants for the soot absorption coefficient eq. (32). The assumption of omitting the spectral dependence between the transmissivity and the intensity has evidently also a relatively large effect on the accuracy, compared to the other models, in high sooting environments.
The second and third test cases, cases 2 and 3, relate more to the combustion environment inside a combustor. Both cases are non-homogeneous, non-isothermal environments with varying soot load.
Case 2 represents a high soot loading and case 3 a moderate soot loading. The temperature, species mole fraction and soot volume fraction distributions for the two cases are presented in table 2, all having a parabolic distribution with the highest value in the center of the domain. The results from the two test cases are presented in Fig. 10. Included in this figure is the reference case by Demarco et al. [55] using the same SNB model with a ray tracing method. The absolute value of the source term is overpredicted by all models in the middle of the domain both in cases 2 and 3. The difference in performance compared to the SNB is not easily distinguished from Fig. 10. Table 3 presents the average absolute deviation and the maximum absolute deviation of the models compared to the SNB model, to aid the comparison between the models. Table 3 also gives the deviation of the flux compared to the SNB, for case 2 having $-197$ kW/m², case 3 having $-167$ kW/m². Like the homogeneous case, case 1, the nc-SNB performs best for the high soot load, case 2. Also, as in case 1, the maximum errors are found close to the wall for all models. Here one can find deviations of the source term as high as 86 percent for the nc-SNB compared to the SNB. The WSGG-P performs best regarding both maximum deviation and average deviation of the radiative source term. WSGG-P has also the highest error when it comes to the heat flux. The WSGG-F performs better on some points compared to nc-SNB and worse on others. The WSGG-T performs worse then nc-SNB on all points. The flux is very well captured by the nc-SNB model, which is in conflict with the results found by Zhang and Soufiani. They presented a 30 percent overprediction by the nc-SNB, for a parabolic temperature case with pure water as the participating gas. By removing the soot from cases 2 and 3 one finds similar results to those of Zhang and Soufiani. The wall flux from the SNB becomes $-75$ kW/m² and wall the flux for nc-SNB becomes $-90$ kW/m², a 20 percent overprediction by the nc-SNB. The flux to the walls is dominated by emission from soot in cases 2 and 3, having 62 and 55 percent of the flux, respectively, coming from soot. Regarding the heat flux to the wall soot has an improving effect on the accuracy of the nc-SNB compared to cases without soot.

<table>
<thead>
<tr>
<th>Case 2, case 3</th>
<th>Temperature (K)</th>
<th>$4000x(L-x)+800$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 2, case 3</td>
<td>CO₂ mole fraction (-)</td>
<td>$0.4x(L-x)+0.06$</td>
</tr>
<tr>
<td>Case 2, case 3</td>
<td>H₂O mole fraction (-)</td>
<td>$0.8x(L-x)+0.12$</td>
</tr>
<tr>
<td>Case 2</td>
<td>Soot volume fraction (-)</td>
<td>$[40x(L-x)+6]·10^{-7}$</td>
</tr>
<tr>
<td>Case 3</td>
<td>Soot volume fraction (-)</td>
<td>$[40x(L-x)+6]·10^{-8}$</td>
</tr>
</tbody>
</table>
Figure 10. Source term for case 2 and case 3 by the SNB, nc-SNB, WSGG-F, WSGG-P and the WSGG-T. Reference case from Demarco et al. is included in case 3.

Table 3. Average absolute deviation, maximum deviation for the source term and heat flux deviation in percent in case 2 and case 3, respectively, between the SNB and the nc-SNB, WSGG-F, WSGG-P and the WSGG-T.

<table>
<thead>
<tr>
<th>Model</th>
<th>nc-SNB</th>
<th>WSGG-F</th>
<th>WSGG-P</th>
<th>WSGG-T</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avg. abs. deviation</td>
<td>17, 22</td>
<td>32, 13</td>
<td>15, 7</td>
<td>41, 78</td>
</tr>
<tr>
<td>Max deviation</td>
<td>70, 86</td>
<td>214, 78</td>
<td>27, 19</td>
<td>313, 453</td>
</tr>
<tr>
<td>Flux deviation</td>
<td>1,5</td>
<td>5,-1</td>
<td>29,7</td>
<td>-18,11</td>
</tr>
</tbody>
</table>

One reason for using the nc-SNB model instead of the SNB model is the decreased computational demand, i.e., the time to solve a problem. The computational time for the nc-SNB and the SNB is proportional to $N^2$ and $N$, respectively, where $N$ is the number of cells in a domain. Between the nc-SNB model and the WSGG models the computational time is proportional to the number of narrow bands and gray gases, where each extra narrow band and gray gas means an extra RTE to solve. The four models were compared using case 3. The WSGG-T and WSGG-F offered a 47 times speedup, in line with the fraction of 367 narrow bands to 8 gray gases. The WSGG-P offered a speedup of 67 times, somewhat less than the fraction of 367 narrow bands to 4 gray gases.

7.1.2 Conclusions
The non-correlated SNB is an attempt to speed up the calculation of the correlated SNB model, a well recognised model. The simpler implementation into CFD environments, using a cell to cell calculation without historical effects, also makes it interesting. The assumption used in the model, by
omitting the spectral dependence between the transmissivity and the intensity, has no physical ground. With this fact and the fact that it has been proven before in non-sooting environments and proven now also in sooting environments to predict the radiation sometimes fairly bad, it is recommended that the model should not be used in combustion environments. Instead could a much simpler model, like the WSGG-P could be used for sooting environments. Although care has to be taken as the WSGG-P can give rather large error in the wall heat flux.

### 7.2 Extension of a NB model for high CO combustion environments

#### 7.2.1 Result and Discussion

In combustion environments there exists several molecular species that contribute to the radiation. In a normal combustion environment most of the molecular species have a very small, negligible, contribution to the overall radiation compared to the two major species of water and carbon dioxide. Carbon monoxide is one of the species that normally is neglected in combustion environments. CO is a weaker radiator than the H$_2$O and CO$_2$ and it exists in small volume fractions in normal combustion. There exists combustion environments where CO is the major species, in terms of its volume fraction. One such environment is the gasification environment. In such an environment the CO volume fractions can reach values around 50 percent. To estimate the contribution of CO in this type of environments a narrow band model has been used. The narrow band model, described in chapter 4.2.2.3, that has been used is the so-called FASTNB model developed by Yan and Holmstedt.

The model has been extended with a look-up-table for the CO. The look-up-table stores the structure parameters of the narrow band model, avoiding the original way of acquiring them from molecular models or by interpolating experimental values. Yan and Holmstedt state that the method offers a speed up by 20 times with less than 1 percent loss in accuracy, compared to the original narrow band model, Grosshandlers RADCAL.

The extension of the FASTNB model was verified against a homogeneous radiation path of pure carbon taken from experimental work on the absorptivity of the fundamental band of CO. The comparison showed good agreement between the experimental results and the FASTNB model. Also a comparison was done against measured intensity along a natural gas flame, by Komornicki and Tomerczek [58], containing a mixture of water, carbon dioxide, methane and carbon monoxide. The distributions of gases and temperature from Komornicki and Tomerczek are shown in Fig. 11, followed by the spatial intensity in Fig. 12. The results of the FASTNB model captured the intensity from the experimental work well. Unfortunately the CO mole fraction was very low leading to a very small contribution to the overall radiation, as seen in Fig. 12. A reference with a high CO content would be preferable but such a reference was not found. The verification with the two cases was anyhow considered to be sufficient.
The investigation of radiation from CO in high CO environments continued by using the molecular species and temperature distribution of Wen and Chaung [59] on a Texaco entrainment plant gasifier. This gasifier was a high pressure gasifier, at 24 atmospheres. The CO contribution to the radial directional heat flux was evaluated by considering three positions along the gasifier. The contribution from CO to the total radial directional heat flux was at its highest 0.5 percent out of the three positions. Gasifiers operate in a pressure range from atmospheric pressure to above 30 atmospheres. To investigate the effect of pressure on the CO radiation, the radiation path with the highest CO, out of the three, was used for further evaluation, see Fig. 13. The pressure has a large
effect on the CO contribution. At atmospheric pressure the contribution from CO to the total directional heat flux is close to 15 percent, not at negligible.

![Graph](image)

Figure 13. Contribution of CO to the total radial directional heat flux for different pressures from a homogeneous mixture of CO, H₂O and CO₂ in a gasifier [23].

The reason for decreased CO contribution with increased pressure is that the line overlapping between the species increase. CO, CO₂ and H₂O have important vibration-rotation bands close to each other. When pressure increases the bands spread out over the spectrum and starts to overlap each other. As illustrated in Fig. 14, the spectral emissivity for the mixture of gases and for the three individual gases together with the relative black body radiance are shown. The case in Fig. 13 is the high CO contribution path of the Texaco gasifier. From the figure it is clear that the CO band does not singly occupy a large part of the spectrum, instead the same spectral part is also occupied by CO₂ and H₂O. For the Texaco case with highest CO contribution at 24 atmospheres, CO contributes to more than 16 percent of the total directional heat flux, disregarding the overlap from CO₂ and H₂O. This means that the overlap from CO₂ and H₂O results in a decrease of CO contribution to the total directional heat flux down to 0.5 percent. This occurs when CO₂ and H₂O mole fractions are only a few percent.

### 7.2.2 Conclusions

An extension of the FASTNB model was made and verified for radiation in environments with CO. Investigation of an gasifying environment showed that the CO contribution to the total directional heat flux can be significant at low pressures but negligible at high pressure. Already small portions of CO₂ and H₂O are sufficient to overlap the CO important rotation-vibration band at higher pressure.
Figure 14. Spectral emissivity of CO, H$_2$O and CO$_2$ and mixture of the gases along with relative black body radiance at the high CO position in the Texaco gasifier [23].
Chapter 8

Future work

The radiation heat transfer has in this work been evaluated with a selection of transfer and property models for plane parallel combustion like cases. The radiation has been the only part that has been considered, no relation to other modes of heat transfer or other physical phenomena has been outlined. The natural step forward is applying the current models to 2-D and possibly 3-D environments together with other physical models. So far rather general combustion cases have been considered, no direct application has been the sole focus.
Chapter 9

References


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