Radiative and collisional processes in Argon-Mercury plasmas: application to the Philips QL-lamp: modeling and experiments

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RADIATIVE AND COLLISIONAL PROCESSES IN ARGON-MERCURY PLASMAS

Application to the Philips QL-lamp
Modeling and experiments

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Abstract

In the group Equilibrium and Transport in Plasmas at the Eindhoven University of Technology the plasma simulation program "PLASIMO" has been developed.

One of the weak points of PLASIMO used to be the treatment of radiative transfer, which is especially important in light-sources. A better description of radiative transport in the modeling of the Philips QL-lamp is the main topic of this study.

The collisional radiative model for mercury has been extended to six independent levels in order to treat the important radiative transition within PLASIMO. A more implicit treatment of the particle source terms proved to have large influence on the stability of the calculations.

Radiation transport can be dealt with in two different ways: it can be treated as a transport term by expressing the radiation transport in term of diffusion of the resonance state. The problem in using diffusion models is to obtain an accurate diffusion coefficient or mean free path length of the photons. The approach used in this work solves the radiation transport by the introduction of an escape factor. The source term of the excited state from which the radiation occurs can then be expressed as a net emission.

The escape factor can now be calculated numerically in PLASIMO. The calculation of the escape factor for a QL simulation consumes a lot of simulation time, but simulations on simplified lamp geometries reveal the importance of the escape factor calculation.

Some measurements on the QL-lamp have been carried out to verify the modeling results. From Laser Induced Fluorescence measurements the density profile of the metastable $6^3P_2$ state of mercury in the QL-lamp has been determined. The measured profiles have a similar shape as the profiles obtained by QL simulations with PLASIMO. The quantitative differences may be due to the assumptions made in both the numerical model and the interpretation of the measurements.
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Chapter 1

Introduction

1.1 Preface

In the group "Equilibrium and Transport in Plasmas" at the Eindhoven University of Technology PLASIMO, a plasma simulation program has been developed. This program is capable of calculating the temperatures, densities, velocities and other plasma quantities. The plasma is considered to be a multicomponent chemically reacting flowing fluidum. At the simplest level it consists of neutrals, ions and electrons. This model was designed by Denny Benoy, and was used to describe two-dimensional argon ICP’s at atmospheric pressure. Recently Marnix Tas, Ger Janssen and Jan van Dijk modified the code in order to simulate more complex mixtures as well. An example of such a plasma is the mercury/noble gas mixture in the Philips QL lamp.

One of the weak points of PLASIMO used to be the treatment of radiative transfer, which is especially important in light-sources. A better description of radiative transport will be the main topic of this study.

1.2 The system under study

The QL-lamp is depicted schematically in fig (1.1). It produces light in the same way the TL-lamp does, so that we can use the experience with TL-models to gain information about the QL-lamp. However, there are two major differences between the lamps.

The main difference between the TL-lamp and the QL-lamp is the energy incoupling. The TL-lamp is a DC-discharge where the electrodes are in direct contact with the plasma. The QL-lamp is an inductively coupled electodeless system, as a result of which the lifetime of the lamp is considerably longer, typically of 60,000 hours. This is due to the fact that the lifetime is no longer determined by the electrodes, but by the electronics. Other advantages are the more continuous efficacy during the lifetime.
The QL-lamp consists of three components: the induction coil with a ferrite core, the discharge vessel and the electronics. The inductive coil is located at the center of the bulb to avoid blocking of the light. This is positioned within a glass cavity in the discharge vessel see fig (1.1). The inside walls of the vessel are coated with a protective coating on which a fluorescent powder mix has been applied. PLASIMO does not model this coating which converts the ultra violet radiation into visual light. If the PLASIMO model has to be verified this can be done by spectral measurements on an uncoated QL-lamp. The electronics supply an alternating current of 1 A at a frequency of 2.65 MHz to the induction coil, which induces an alternating magnetic field. The system of induction coil and plasma can be interpreted as a transformer, with the induction coil as the primary coil (15 turns) and the electron current in the plasma ($\approx 10$A) as the secondary coil (1 turn).

Another difference between the TL- and QL-lamps is the current through the lamp. The TL-lamp has typically a current of 400 mA, whereas the QL-lamp has a typical plasma current of about 10 A. As a result the electron density is higher and therefore electron production via indirect processes is more likely. In order to compare the modeling results for the TL-lamp with those for the QL-lamp, the TL model was modified to handle these high currents. It must be noted that in the modeling of the TL-lamp only the positive column is considered by PLASIMO.
1.3 Technology assessment

In the world about 25% of all produced energy is electrical energy. About 25% of all electrical energy is used for lighting purposes. This means that it is very important to create lamps with a high efficacy (the intensity of the light coming out of the lamp as compared to the input power [lm/W]). If highly efficient lamps can be created less energy is needed to produce the same amount of light. This can be done by making and testing different lamps. Because this is a time and money consuming task, other methods to construct more efficient lamps are under investigation. This is the main reason a simulation model for the Philips QL-lamp is being developed within the PLASIMO project at the Eindhoven University of Technology. With this model it will be possible to calculate the effect of several parameters, such as the mercury and buffer gas pressure and design, and to create a more efficient lamp without having to build and test dozens of different lamps. An additional effect is the better understanding of the plasma in the lamp.

The advantage of the QL-lamp is the high lifetime of the lamp. Because there are no electrodes in the plasma, the lifetime of the lamp is limited by the electronics only. This means a lifetime of 60,000 hours continuous use, and this also means that the relative costs of maintenance and replacements can be greatly reduced. Furthermore the environment benefits form the fact that now less lamps have to be produced.
Chapter 2

Particle Source terms

2.1 Introduction

In this chapter the continuity equation is discussed. In 2.2 the particle continuity equation in a stationary system is expressed in terms of flux density and a source term. It is shown how the particle source term can be expressed in terms of effective rate-coefficients (J-coefficients) from which the destruction and production term of a level can be obtained. It will be demonstrated that collisional radiative models can be used to obtain the J-coefficients. We conclude this chapter by giving an application of the J-coefficients in case of a multilevel mercury plasma.

2.2 Continuity Equations

In this section we will discuss the general form of the particle and mass densities conservation law. Assume that $\phi$ is the number density of particles of a certain kind in a volume $V$. The accumulation of $\phi$ in $V$ is equal to the difference between the production of $\phi$ in $V$ and the efflux of $\phi$ through its boundary surface.

Let $\Gamma_\phi$ denote the flux density of $\phi$. If the normal is directed outward, the efflux through the surface element $d^2A$ is $(\Gamma_\phi, n)d^2A$. Further let $S_\phi$ denote the source intensity, so the source contribution of the volume element $d^3V$ is $S_\phi d^3V$. Integration then yields the general conservation law:

$$\frac{d}{dt} \int_V \phi d^3V = \int_V S_\phi d^3V - \int_A (\Gamma_\phi, n)d^2A. \quad (2.1)$$

We may express this equation in a different form by applying Gauß' theorem and realizing that the equation holds for any arbitrary volume $V$, viz.

$$\frac{\partial \phi}{\partial t} + (\nabla, \Gamma_\phi) = S_\phi. \quad (2.2)$$
CHAPTER 2. PARTICLE SOURCE TERMS

For particles the flux $\Gamma_\phi$ is given by $\Gamma_\phi = n_\phi \mathbf{V}_\phi$, yielding the general species continuity equation for species $\alpha$:

$$\frac{\partial n_\alpha}{\partial t} + (\nabla, n_\alpha \mathbf{V}_\alpha) = S_\alpha.$$  \hspace{1cm} (2.3)

Here $\mathbf{V}_\alpha$ denotes the mean $\alpha$-velocity and $n_\alpha$ the particle density of species $\alpha$. If we multiply equation (2.3) with $m_\alpha$ and sum over all species we obtain

$$\frac{\partial \rho}{\partial t} + (\nabla, \rho \mathbf{V}) = 0,$$ \hspace{1cm} (2.4)

because mass sources do not exist. This is the mass continuity equation.

In a stationary state the accumulation term in (2.1) vanishes by definition. Then the efflux of $\phi$ must equal the total production and so from (2.2) we obtain

$$(\nabla, \Gamma_\phi) = S_\phi.$$ \hspace{1cm} (2.5)

Our task will now be to determine the source term $S_\phi$. This will be discussed in the next sections.

2.3 J-coefficients

For stationary levels $j$ the continuity equation reads :

$$(\nabla, n_j \mathbf{V}_j) = S_j.$$ \hspace{1cm} \text{(2.6)}

The source term $S_j$ is the net number of particles of species $j$ which is produced per unit of volume and time. If the plasma is in LTE the production is equal to the destruction of a level and the source term vanishes. In non-LTE systems the source terms will not be zero in general. However for some excited states we may apply the Quasi Steady State (QSS) principle (J.A.M. VAN DER MULLEN [1]), which states that for most excited states the population and depopulation processes are much faster than the transport times, as a result of which the source term can be assumed zero. The levels for which the QSS assumption is made will be called dependent states. For the levels for which the QSS assumption is not valid we still have to calculate the source terms, these levels will be referred to as independent levels.

In the case of a two-state model (two independent levels) for atomic plasmas such as in an argon plasma where only $Ar$ and $Ar^+$ are considered, the source terms are commonly expressed in terms of the net coefficients of ionization and recombination $S_{cr}$ and $\alpha_{cr}$, respectively. The sources for the two species then take the form

$$S_+ = -S_1 = n_1 n_e S_{cr} - n_+ n_e \alpha_{cr}.$$ \hspace{1cm} (2.6)
2.4. **THE J-MATRIX**

The next section will deal with the question how this concept can be generalized to atomic systems in which more than two independent levels are considered; in this discussion equation 2.6 shall serve as starting point.

To do this first the *generalized net rate coefficients*, which shall be referred to as *J-coefficients*, will be introduced, by writing the previous equation in the form

\[
S_+ = n_1 n_e J_{1+} - n_+ n_e J_{+1},
\]

\[
S_1 = n_+ n_e J_{+1} - n_1 n_e J_{1+},
\]

(2.7) (2.8)

with the definitions \( J_{1+} = S_{cr}, \) \( J_{+1} = \alpha_{cr}. \) From inspection of these equations we adopt a general format for the reaction rates in electron-collision dominated plasmas.

\[
S_{ij} = n_i n_e J_{ij} - n_j n_e J_{ji},
\]

(2.9)

In the next section we shall elaborate this concept of a general \( J \)-matrix.

### 2.4 The \( J \)-matrix

In this section we introduce the general \( J \)-matrix, whose elements \( J_{ij} \) have been introduced already in the previous section. The net source of species \( j \) is given by adding the net rates of all reactions leading to species \( j \) and is denoted by \( S_j \),

\[
S_j = \sum_{i \neq j} S_{ij} = \sum_{i \neq j} n_i n_e J_{ij} - n_j \sum_{i \neq j} n_e J_{ji}.
\]

(2.10)

As reactions from \( i \) to \( i \) have no effect we may assume \( J_{ii} = 0 \) to obtain

\[
J = \begin{bmatrix}
0 & J_{12} & J_{13} & \ldots \\
J_{21} & 0 & J_{23} & \ldots \\
J_{31} & J_{32} & 0 & \ldots \\
\ldots & \ldots & \ldots & \ldots
\end{bmatrix}.
\]

(2.11)

The source vector \( S \) can be written as a matrix-vector product \( S = Mn \), with the matrix \( M \) closely related to the \( J^T \). The off-diagonal elements are the same as can easily be verified, these are the production terms of state \( j \). The destruction terms correspond to the diagonal elements, which are equal to \( M_{jj} = -\sum_{i \neq j} J_{ji} \).

It is convenient to write \( M = J^T + Id \), where \( I \) is the unity matrix, and \( d \) the vector whose elements are the diagonal elements of \( M \). The source term can be described by a *production term* \( P(j) \) and an *destruction factor* \( D(j) \) of the level \( j \) according to

\[
S_j = P(j) - n_j D(j),
\]

(2.12)

where the production term and destruction factor can now be given by respectively,

\[
P(j) = n_e (J^T n)_j,
\]

(2.13)

\[
D(j) = n_e (d)_j.
\]

(2.14)
The next objective is to obtain the J-coefficients which is the task of a collisional radiative model. This will be the topic of the following section. We finish this section with the observation that the J-coefficients provide uniformity in the modeling of reactions involving the various atomic transitions.

2.5 Collisional Radiative Model

2.5.1 Introduction

In this section we will show how the J-coefficients can be calculated. The problem is that we have to know the Atomic State Distribution Function (ASDF) if we want to calculate these coefficients. The ASDF describes how atoms and ions are distributed over the various excited states. The ASDF is related to basic plasma parameters, i.e. the electron density $n_e$, electron temperature $T_e$ and the state densities of the independent levels, in a two-level model $n_1$ and $n_+$. Determining the ASDF would not be difficult if the plasma is in Local Thermodynamic Equilibrium (LTE). In this case the information about the plasma can be obtained from the laws of statistical mechanics. The distribution of the electrons over the excited states is given by the laws of Boltzmann and Saha, which all depend on one single temperature. However if the plasma were in LTE no source terms have to be determined, these terms are zero. Unfortunately the plasma at hand is not in LTE. Because of this we have to use another method to calculate the ASDF.

2.5.2 Collisional Radiative Models

A Collisional Radiative Model (CRM) relate the densities of dependent levels to the densities of the independent levels. In these models we will consider atomic plasmas without heavy-heavy interactions. The models are based upon the mass balances for all the particle states:

$$\frac{\partial n_p}{\partial t} + (\nabla, n_p V_p) = \left( \frac{\partial n_p}{\partial t} \right)_{CR}.$$  \hspace{1cm} (2.15)

According to this equation, the increase in time of the density of a level is related to the decrease by divergence of the flow and the net result of populating and depopulating processes.

We showed that the particle source terms can be expressed in terms of a production term $P(p)$ and a destruction factor $D(p)$ of the level $p$ according to

$$S(p) = P(p) - n_p D(p).$$ \hspace{1cm} (2.16)

The contributions to the production term $P(p)$ are:

$$n_e \sum_{q \neq p} n_q K_{qp}.$$ \hspace{1cm} (a)
2.5. **COLLISIONAL RADIATIVE MODEL**

\[
+ \sum_{q>p} n_q A_{qp} \Lambda_{qp} \quad (b)
\]

\[
+ n_e n_e [n_e K_{+p} + A_{+p}] \quad (c)
\]

The contributions to the destruction factor \( D(p) \) are given by:

\[
- \sum_{q<p} A_{pq} \Lambda_{pq} \quad (d)
\]

\[
- n_e \sum_{q \neq p} K_{pq} \quad (e)
\]

\[-n_e S_p = 0. \quad (f)\]

(2.17)

where (a) represents population of \( p \) caused by (de)excitation of other levels, (b) the cascade radiation, i.e. the population of the level \( p \) by effective radiative decay of the higher levels \( q \), (c) three particle recombination, (d) depopulation by the effective radiative decay of \( p \) to \( q < p \). (e) depopulation by collisional transitions, and (f) ionization.

Now we have two unknown variables, \( S(p) \) and \( n_p \), for each equation. All these equations are linear in \( n_p \) because we did not include the effects of heavy-heavy collisions. It is impossible to take all levels into account, because there are infinitely many of them. If too many levels are neglected, stepwise ionization will be underestimated. How to reduce the number of levels by the use of a cut-off procedure is described by Benoy [2] and J.A.M.Van der Mullen [1]. The source vector \( S \) can be written as

\[
S = M n,
\]

(2.19)

where \( n = [n_1, n_2, ..., n_N]^T \). In principle the vector components of \( n \) and \( S \) are unknown

\[
\begin{bmatrix}
M \\
\end{bmatrix}
\begin{bmatrix}
? \\
\end{bmatrix} = \begin{bmatrix}
? \\
\end{bmatrix}, \quad (2.20)
\]

To solve these balances, the Quasi Steady State Solution (QSSS) method is used. When the QSSS is applied the populating \( (P_p) \) and depopulating \( (n_p D_p) \) processes are assumed to be fast compared to the changes in time and by transport for all dependent levels. This leads to:

\[
\left( \frac{\partial n_q}{\partial t} \right)_{CR} = 0 \quad \text{and} \quad n_q D_q = P_q. \quad (2.21)
\]
CHAPTER 2. PARTICLE SOURCE TERMS

For the dependent levels the full mass balances still applies:

\[
\frac{\partial n_j}{\partial t} + (\nabla, n_j \mathbf{v}_j) = \left( \frac{\partial n_j}{\partial t} \right)_{CR}.
\]  

By using the QSS we assume that for the dependent level \( S_p = 0 \) and for the independent levels we can treat \( n_q \) as input. Then the set of equations takes the following form:

\[
\begin{bmatrix}
M
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix}
S_1 \\
S_2 \\
\vdots \\
S_+ 
\end{bmatrix}
\end{bmatrix}
= \begin{bmatrix}
\begin{bmatrix}
\begin{bmatrix}
1 \\
n_1 \\
\vdots \\
n_{\rho - 1} \\
n_+ 
\end{bmatrix}
\end{bmatrix}
\end{bmatrix} = 0.
\]  

First we will derive a subset of equations for the unknown components \( n' \) of \( \mathbf{n} \), here we do not consider the rows for which \( S_p \neq 0 \).

\[
\begin{bmatrix}
M_1 \\
M_2 \\
\vdots \\
M_+ 
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix}
\begin{bmatrix}
1 \\
n_1 \\
\vdots \\
n_{\rho - 1} \\
n_+ 
\end{bmatrix}
\end{bmatrix}
\end{bmatrix} = \begin{bmatrix}
\begin{bmatrix}
\begin{bmatrix}
1 \\
x \\
\vdots \\
x 
\end{bmatrix}
\end{bmatrix}
\end{bmatrix}.
\]  

The subset of equations of \( n' \) can be recast as

\[
M' n' = -n_1 M_1 - n_2 M_2 - n_+ M_+ = \sum_j n_j \Pi_j.
\]

The solution of this equation yields the ASDF:

\[
n_\rho = \sum_j n_j \left( M' \right)^{-1} \Pi_j
\]

As a result the density of a dependent level is a superposition of contributions from the independent levels \( j \),

\[
n_q = \sum_j n^j_q
\]

where \( n^j_q \) is the contribution from independent level \( j \) to dependent level \( q \). Now all densities are known, the remaining rows yield us \( S_1, S_2, \ldots, S_+ \) which are also linear combinations of \( n_j \).
We can rewrite (2.26) and (2.27) by relating \( n_q \) to the equilibrium contribution \( r_q^j n_q^{eq}(n_j) \) from the independent level. This is done to get information about the influence of the non-LTE effects on the ASDF. Then equation (2.27) is written as

\[
 n_q = \sum_j n_q^j n_q^{eq}(n_j) = \sum_j r_q^j n_q^{eq}(n_j) \tag{2.28}
\]

In which \( n_q^{eq}(n_j) \) is the density level \( q \) has when it is in equilibrium with the independent level \( j \), and the coefficients \( r_q^j \) relate the contributions from the independent levels to the equilibrium densities. The equilibrium density due to an independent ion level is given by the Saha density \( n_p^S \), the equilibrium density related to the independent atomic states are given by the Boltzmann density \( n_p^B \), where \( n_q^B \) and \( n_q^S \) are defined by:

\[
 \frac{n_q^B}{g_q} = \frac{n_j}{g_j} \exp(-E_{jq}/kT_e), \tag{2.29}
\]

\[
 \frac{n_q^S}{g_q} = \frac{n_e n_e^+}{2g_+} \left[ \frac{\hbar^2}{2\pi m_e kT_e} \right]^{\frac{3}{2}} \exp(-E_{q+}/kT_e). \tag{2.30}
\]

In these formulae, \( E_{jq} \) is the energy difference between independent level \( j \) and dependent level \( q \), \( E_{q+} \) the ionization energy of level \( q \) and \( g_q \) the statistical weight of level \( q \). The coefficients \( r_q^j \) express the contributions from \( n_q^S(n_+) \) or \( n_q^B(n_j) \).

If we know the the coefficients \( r_q^j \) we can calculate the J-coefficients \([m^3s^{-1}]\). This J-coefficient is the population of an independent level \( j \) from an other independent level \( i \), these transitions from \( i \) to \( j \) can happen in a direct way or via the dependent levels. The independent columns of (2.23) yield

\[
 J_{ij} = \frac{1}{n_e} (n_e K_{ij} + \Lambda_{ij}) + \frac{1}{n_e n_i} \left( \sum_{q>j} n_q^i n_e K_{qj} + \sum_{q>j} n_q^i \Lambda_{qj} \right) \quad \text{for } j < i,
\]

and

\[
 J_{ij} = K_{ij} + \frac{1}{n_i n_e} \left( \sum_{q>i} n_q^i n_e K_{qj} + \sum_{q>i} n_q^i \Lambda_{qj} \right) \quad \text{for } j > i, \tag{2.31}
\]

the first term on the RHS describes the direct processes, whereas the second term describes the indirect processes (via the dependent levels), with \( n_q^i \) the contribution from \( n_i \) to \( n_q \).

For a certain value of the electron temperature and electron density the CRM can calculate the J-coefficients, from (2.29) and (2.30) we see that \( n_q^j \) is proportional to \( n_i \) and independent of the other independent level densities. As a result \( n_q^j/n_i \) is independent of \( n_i \) and so the J-coefficients are not dependent on the
density of the independent levels as can be concluded from (2.5.2). As a result the J-coefficients are true coefficients.

The contributions from the direct processes to the J-coefficient do not depend on \( n_e \) and need in principle not to be calculated within the CRM but can be calculated by an external program and added later.

A. HARTGERS [5] developed a C++ program, which was later modified by J. van Dijk and H. v.d Heijden, to obtain the CR-coefficients for different input parameters of \( n_e \) and \( T_e \). These values will be used within PLASIMO as source terms. As we see from (2.18) the effective radiative decay of the upper lying level \( q \) can be given by the spontaneous decay rate \( A_{qp} \) corrected for self-absorption, resulting in an effective decay \( A_{qp} \Lambda_{qp} \). An accurate determination of the so called escape-factor \( \Lambda_{qp} \) will prove to be important, as will be shown in the next chapters.

### 2.6 The Six Level Mercury Model

In this section we will demonstrate a six-level mercury model which serves as an alternative for the two-level model developed by R. MASSAFRA [7]. In a two-level model the densities of the excited states are determined by the ground state and the ion state. This will prove to be a too simple representation. In fig (2.1) a simplified energy scheme of mercury is depicted, the most important levels are of course the ground state \( (6^1S_0) \) and the ion state, but also the metastable states.
(6^3P_0) and (6^3P_2), and resonant states (6^3P_1) and (6^1P_1) are important because in a QL or TL-lamp the light comes mostly from the transitions of the resonant states to the ground state. In the old CRM the reabsorption is dealt with by the introduction of an escape factor which expresses the emission and reabsorption in terms of a net emission. Of course absorption is a non-local process, and as a result the escape factor depends on the geometry and density profiles of the plasma, as will be shown in chapter (3).

Because we want the only input parameters of the CRM to be \( T_e \) and \( n_e \) only, the escape factor values in the CRM used to be fixed values. However if the resonance levels are independent levels the radiative transition from these levels to the ground state can be excluded from the CRM, so an accurate escape factor can be calculated and added to the involved J-coefficient as shown in chapter (3). In the previous section it was stated that the heavy-heavy collisions are not included in the CR-model. For the independent levels these processes can also be added to the J-coefficients obtained by the CRM if they do not disturb the ASDF too much.

That is way we will use a six level model to describe mercury. A CRM will be used in which the densities of the dependent levels \( q \) are determined by six independent levels, namely the ground state and ion ground state and four 6\( P \) levels: the metastable levels 6^3P_0 and 6^3P_2 and the resonant levels 6^3P_1 and 6^1P_1. When the radiative transition from the resonant level 6^3P_1 to the groundstate is left out of the CRM according to (2.31) the \( J' \)-coefficient will be given by:

\[
J'_{31} = \frac{1}{n_3n_e} \left( n_3[n_eK_{31}] + \sum q n_q^3n_eK_{q1} + \sum q n_q^3A_{q1}\Lambda_{q1} \right),
\]

PLASIMO will uses the J-coefficients as input values. In order to make these values of J available to PLASIMO for different values of \( n_e \) and \( T_e \), the following approach is used.

The results from the CRM are fitted to \( T_e \) for several possible values of \( n_e \) (\( n_e = 10^{18,19,\ldots} m^{-3} \)) using 5th-order logarithmic polynomial fit-functions. From the fit-coefficients PLASIMO can calculate the required J-coefficients. Because there are only fit-coefficients for discrete values of \( 10^\log[n_e m^{-3}] \), the J-coefficients are obtained for the two nearest discrete values of \( n_e \). The final J-coefficients are obtained by interpolating to the value of \( n_e \). Fig (2.2) shows the J-coefficients from five independent mercury levels (1 = 6S_0 2 = 6^3P_0 3 = 6^3P_1 4 = 6^3P_3 5 = 6^1P1) to the ion state. Fig (2.3) show the J-coefficients from five independent mercury levels to the resonant 6^3P_1 state.
Figure 2.2: Some $J$-coefficient for different values of $T_e$ and $n_e$. (a) $J_{1+}$, (b) $J_{2+}$, (c) $J_{3+}$, (d) $J_{4+}$ and (e) $J_{5+}$.
2.6. THE SIX LEVEL MERCURY MODEL

Figure 2.3: Some J-coefficient for different values of $T_e$ and $n_e$. (a) $J_{13}$, (b) $J_{23}$, (c) $J_{43}$, (d) $J_{53}$ and (e) $J_{+3}$. 
CHAPTER 2. PARTICLE SOURCE TERMS

From fig (2.2) it can be seen that the $n_e$ dependence of the J-coefficients will increase for higher departure levels. The J-coefficients to the ion level can be expressed by

$$J_{i+} = K_{i+} + \frac{1}{n_i n_e} \sum n_q^i n_e K_{q+}. \quad (2.33)$$

Because $K_{i+}$, the first term on the right hand side of the equation, does not depend on $n_e$ we conclude that the ionization via the dependent levels will become easier if the independent level is closer the ion-level. It can be observed that indeed $J_{i+} \approx K_{i+}$ for the lowest levels.

For the transition rates to the resonance state $6^3P_1$ the J-coefficients can be given by (for $i < 3$)

$$J_{i3} = K_{i3} + \left( \frac{1}{n_i n_e} \sum n_q^i n_e K_{q3} + \sum n_q^i A_{q3} \Lambda_{q3} \right) \quad \text{for } i < 3. \quad (2.34)$$

For these levels the second term on the right hand side seems not to be important, there are no dependent levels between the independent levels and apparently there is no direct contribution from the higher dependent levels due to independent level $i$. For $i > 3$ the J-coefficient is given by

$$J_{i3} = K_{i3} + \frac{1}{n_e} A_{i3} \Lambda_{i3} + \left( \frac{1}{n_i n_e} \sum n_q^i n_e K_{q3} + \sum n_q^i A_{q3} \Lambda_{q3} \right) \quad \text{for } i > 3. \quad (2.35)$$

Again for the transitions from the higher levels the $n_e$ dependence becomes more important as can be seen from fig (2.3), recombination via the dependent levels will become more important if there are more dependent levels between the independent levels. Further we see that $J_{i+3}$ depends linearly on $n_e$. This is an indication that 3-particle recombination is the dominant process. The rate of this process is given by $J_{i3} = n_e n_i n_e K_{i3} \Lambda_{i3}$, yielding a contribution to $J_{i3}$ of

$$J_{i3} = n_e K_{i+3}.$$
Chapter 3

Transport of Radiation

3.1 Introduction

The kind of radiation transport we will investigate is that of resonance radiation transport. The term "resonance" is applied to radiation emitted by an atom in an optical transition from an excited state to the ground state. A photon emitted by an individual atom, after traveling a short distance, is absorbed by an other atom. The result of this process of emission and re-absorption is merely the transfer of excitation energy from atom to atom. The most important transition in the QL lamp is that of the mercury resonance state $6^3P_1$ to the ground state, from which the well know 254nm line originates.

The transport of radiation can be expressed by a diffusion equation. E.A. MILNE [14], showed that the differential equations giving the concentration of excited atoms and the intensity of resonance radiation as a function of distance and time were similar to the ordinary diffusion equation except for a third order term that arose from the finite lifetime of the excited state. Milne's theory is of value in considering the one-dimensional flow of resonance radiation of very narrow spectral width, but leads to mathematical difficulties when applied to the more complicated conditions that are present in connection with an actual lamp. C. KENTY [15] gave a better mathematical description from which he calculated a diffusion coefficient when spectral broadening was involved. An other way of describing the transport of radiation was introduced by T. HOLSTEIN [12] who described a method where he treated the radiation transport by means of net local emission with the introduction of a so-called escape factor. In this chapter we will discuss these different ways of describing radiation transport.
3.2 Emission and Absorption: the transmission factor

A photon emitted in a dense plasma, will after traveling a distance be absorbed by an other atom. After a certain time this excited atom will decay and the emitted photon will again travel through the plasma. The process of (re)emission and absorption can be seen as a random walk process.

We will now determine the probability, \( T(\rho) \) that a photon travels a distance \( \rho \) before being absorbed. For monochromatic radiation of frequency \( \nu \) the transmission factor \( T \) can be expressed in terms of an absorption coefficient \( k(\nu) \),

\[
T_{\nu}(\rho) = e^{-k(\nu)\rho}. \tag{3.1}
\]

When line broadening mechanisms are present the monochromatic transmission factor has to be averaged over the frequency spectrum of the line \( P(\nu) \) because \( k(\nu) \) is a function of the frequency, the transmission factor is then given by:

\[
T(\rho) = \int P(\nu)e^{-k(\nu)\rho}d\nu, \tag{3.2}
\]

where the frequency spectrum \( P(\nu) \) is normalized according to

\[
\int P(\nu)d\nu = 1. \tag{3.3}
\]

In the special case \( P(\nu) = \delta(\nu - \nu_0) \) we again obtain the monochromatic transmission factor (3.1)

\[
T(\rho) = \int \delta(\nu - \nu_0)e^{-k(\nu)\rho}d\nu = e^{-\rho k(\nu_0)}. \tag{3.4}
\]

In the case of Doppler-broadened absorption one obtains:

\[
k(\nu) = k_0 \exp\left[-\frac{(\nu - \nu_0)^2}{c^2(v_0)^2}\right], \tag{3.5}\]

where \( c \) is the speed of light, \( \nu_0 = (2RT/M)^{1/2} \), \( \nu_0 \) the frequency at which \( k(\nu) \) reaches its maximum and

\[
k_0 = \frac{\lambda_0^3n_qg_pA_{21}}{8\pi g_q^{1/2}v_0}, \tag{3.6}\]

with \( n_q \) the density of the ground state and \( \lambda_0 = c/v_0 \) the central wave length.

Holstein [12] showed that, in the case of Doppler broadening, if the temperature differences in the plasma are not too large, we may assume that the absorption profile is proportional to the emission profile,

\[
P(\nu) \equiv \frac{k(\nu)}{\kappa}. \tag{3.7}\]
We will use (3.7) in the evaluation of $T(\rho)$. For the transmission $T(\rho)$ we then obtain the expression

$$T(\rho) = \int P(\nu)e^{-\kappa \rho P(\nu)}d\nu.$$  

(3.8)

In case of Doppler broadening the normalization of $P(x)$ yields

$$P(x) = \frac{1}{\pi^{1/2}} \exp(-x^2)$$  

(3.9)

in which $x$ is defined as

$$x = \left[ (\nu - \nu_0)/\nu_0 \right] (c/\nu_0).$$  

(3.10)

We also obtain

$$k(x) = \kappa P(x) = k_0 \exp(-x^2),$$  

(3.11)

where $k_0$ is given by (3.6). By inserting (3.9) and (3.11) into (3.8) we finally obtain

$$T(\rho) = \int_{-\infty}^{\infty} \frac{1}{\pi^{1/2}} \exp x^2 \exp \left[ -k_0 \rho \exp(-x^2) \right] dx.$$  

(3.12)

If we now substitute $x = (\ln k_0\rho/y)^{1/2}$ we obtain the next equation

$$T(\rho) = \frac{1}{k_0\rho^{1/2}} \int_{0}^{k_0 \rho} \frac{e^{-y}dy}{(\ln k_0\rho - \ln y)^{1/2}}.$$  

(3.13)

To obtain $T(\rho)$ a numerical integration is needed in principal. However if we are interested in values for large $k_0\rho$ we can approximate $(\ln k_0\rho - \ln y)^{1/2}$ by $\ln k_0\rho$ and extend the upper limit of integration to infinity, yielding.

$$T(\rho) \approx 1/k_0\rho(\pi \ln k_0\rho)^{1/2}.$$  

(3.14)

For small values this equation does not hold, this can easily be seen because the transmission factor has to be $T = 1$ for $\rho = 0$: the probability that a photon travels at least a distance zero is unity.

### 3.3 Diffusion Equation

In this section we will show how radiation transport can be treated by means of a diffusion equation for the excited state. It will turn out that the problem, in using a diffusion equation, is the determination of an accurate diffusion coefficient.

K.T. Compton [13] obtained a diffusion-type equation for the density of excited atoms which was later modified by E.A. Milne [14],

$$(S_p)_{Rad} = -D \nabla^2 n_p,$$  

(3.15)
in which $D$ is the diffusion coefficient;

$$D = \frac{\bar{I}^2}{3\tau} = \frac{\bar{I}v}{3} \quad (3.16)$$

Here $\bar{I}$ is the mean free path of the photon, $\tau$ the lifetime of the individual atom and $v = (\bar{I}/\tau)$, which is not the velocity of light. This reveals an important difference between the motion of resonance quanta and that of material particles: in the case of quanta the time between collisions is much smaller than the time of a collision in contrary with material particles.

The probability of a quantum penetrating a distance $\rho$ in the gas before being absorbed is given by an exponential law $e^{-\rho/\bar{I}}$. One way of defining the mean free path is via the introduction of the probability, $K(\rho)d\rho$,

$$K(\rho)d\rho = T(\rho) - T(\rho + d\rho) = -d\rho \frac{\partial T}{\partial \rho} \quad (3.17)$$

that the quantum is captured in the interval between $\rho$ and $\rho + d\rho$ from its emission point. The mean free path, $\bar{I}$, may then be defined as

$$\bar{I} = \int_0^\infty \rho K(\rho)d\rho = -\int_0^\infty \rho \frac{\partial T}{\partial \rho} d\rho. \quad (3.18)$$

If we insert the exponential form of (3.4) into (3.18) we obtain $\bar{I} = 1/k(\nu_0)$. If on the other hand we insert (3.14) the integral does not converge. It can be shown that in case of an arbitrary spectral distribution $P(\nu)$ which is related to the absorption coefficient $k(\nu)$ of the medium by relation (3.7) the mean free path cannot be defined. From (3.18) and (3.2) we obtain the general form

$$\bar{I} = \int_0^\infty \int_0^\infty \rho P(\nu) \frac{\partial e^{-\kappa \rho P(\nu)}}{\partial \rho} d\nu d\rho, \quad (3.19)$$

by first integrating over $\rho$ one obtains

$$\bar{I} = \int_0^\infty \int_0^\infty P(\nu) e^{-\kappa \rho P(\nu)} d\rho d\nu = \frac{1}{\kappa} \int d\nu, \quad (3.20)$$

which diverges. We can explain this in an other way: the absorption in the wings of the spectral line will gradually decrease to zero for increasing $|\nu - \nu_0|$. As a result the free path for these frequencies will go to infinity, so the mean free path length will go to infinity for a non-monochromatic spectral line.

The statement that a mean free path can not be determined, is only partially true. What we actually showed was that in an infinite volume the mean free path will be infinite when broadening mechanisms are involved. C. Kenty [15] showed that earlier diffusion models [13] can only be used to gas of infinite volume, in which case both the diffusion coefficient and the mean free path of the radiation
are found to be infinite. However Kenty introduced a method which is valid for a finite layer of gas. He showed that the diffusion coefficient of Doppler broadened line in a gas can be given by

\[ D = \frac{1}{3\pi k_0^2} \int_0^{\infty} R f_1(R) dR \]  

(3.21)

where \( k_0 \) is the absorption coefficient of the gas for the center of the line, \( \tau \) the lifetime of the excited state and \( f_1(R) \) is the fraction of all emitted photons which travel at least a distance \( R \) times the free path length, \( 1/k_0 \) of the center of the line. It is given by

\[ f_1(R) = \frac{4}{\pi^{1/2}} \int_0^\infty \int_0^y y e^{-y^2} e^{-\tau e^{-x^2}} dx dy. \]  

(3.22)

Substituting (3.22) in (3.21) and integrating \( R f_1(R) \) from 0 to \( \infty \), we obtain

\[ D = \frac{2\sqrt{2}}{3\pi^{1/2} \tau k_0^2} \int_0^{\infty} ye^{-y^2} dy \int_0^{\sqrt{2}y} e^{x^2} dx. \]  

(3.23)

The integration over \( y \) is an integration over the velocities of the emitting atoms. If all velocities are taken into account \( D \) becomes infinite. Kenty's approximate method of handling a practical situation is to integrate \( y \) from 0 to an upper limit \( y_1 \), where \( y_1 \) is given by the formula

\[ k_0 e^{-y_1^2} = 1/l, \]  

(3.24)

\( l \) being the thickness of the layer of gas. Equation (3.23) then becomes

\[ D = \frac{\sqrt{2}}{3\pi^{1/2} \tau k_0^2} \int_0^{y_1} ye^{y^2} F(\sqrt{2}y) dy \]  

(3.25)

where

\[ F(t) = e^{-t^2} \int_0^t e^{x^2} dx \]  

(3.26)

The integral (3.23) can be expressed in terms of the \( F \) function defined by (3.26) by integrating by parts. We have

\[ \int_0^{y_1} ye^{y^2} F(\sqrt{2}y) dy = ey_1^2 \left[ F(y_1) - F(\sqrt{2}y_1) \right], \]  

(3.27)

the final diffusion coefficient is found to be

\[ D = \left[ \frac{\sqrt{2}l}{3\pi^{1/2} \tau k_0} \right] \left[ F^{1/2}(\ln k_0 l) - F^{1/2}(2\ln k_0 l) \right]. \]  

(3.28)

MILNE [14] showed that radiation of infinitesimal spectral width diffused through a gas with a diffusion coefficient equal to

\[ D' = \frac{1}{4\alpha^2 \tau} \]  

(3.29)
where \( \alpha \) stands for the absorption coefficient of the gas for the radiation in question. If the radiation is not of infinitesimal spectral width we may define an equivalent absorption coefficient as a quantity \( \bar{k} \) which, when substituted for \( \alpha \), will give the correct diffusion coefficient to be used when the diffusing radiation is not of infinitesimal spectral width. Kenty's expression for the diffusion coefficient enables us to compute \( \bar{k} \) when the Doppler effect is present.

\[
\bar{k}l = \left[ \frac{3}{4} \left( \frac{\pi}{2} \right) \right]^{1/2} \left[ \frac{k_0l}{\sqrt{2}F^{1/2}(\ln k_0l) - F^{1/2}(2 \ln k_0l)} \right]^{1/2}
\]

(3.30)

As a final result the diffusion coefficient for a layer of gas can be given by

\[
D = \frac{1}{4\bar{k}^2\tau} = \frac{l^2}{3\tau}.
\]

(3.31)

For (3.30) we see that \( \bar{k} \) and so the diffusion coefficient is a function of the thickness of the layer. By using (3.16) we obtain the mean free path. This \( l \) can not simply be obtained by limiting the integration over the distance in (3.19) to \( l \), instead of infinite, for a finite volume also the integration over the frequency will be limited. Because the derivation of an accurate diffusion coefficient proves to be such a difficult concept, we will look for a different treatment of describing radiation transport.

### 3.4 Holstein's Method, the escape factor

We consider a two-level system and express the transport of radiation in terms of transport of the excitation. In doing this we will look at the net radiation source for the excited state,

\[
(S_p)_\text{Rad} = P(p) - D(p)n_p.
\]

(3.32)

Here \( P(p) \) represents the increase in the number density of excited atoms due to absorption of radiation, whereas \( D(p)n_p \) is related to the decrease due to spontaneous emission, no stimulated emission is assumed. For \( D(p)n_p \) we have

\[
D(p)n_p = A_{pq}n_p
\]

(3.33)

in which \( A_{pq} \) is the transition probability of spontaneous emission to the ground-state.

In order to derive \( P(p) \) we introduce the probability \( G(r', r) \) that a photon emitted at \( r' \) is absorbed in a volume element around the point \( r \). \( P(p) \) is obtained by summing over the contributions of all other volume elements. Integration over these volume elements gives

\[
P(p) = A_{qp} \int n(r')G(r', r)d^3r'.
\]

(3.34)
3.4. **HOLSTEIN'S METHOD, THE ESCAPE FACTOR**

By inserting (3.33) and (3.34) into (3.32) we arrive at the integral equation of HOLSTEIN [12]:

\[(S_p)_{Rad} = -A_{pq} n(r) + A_{pq} \int n(r') G(r', r) d^3r'. \]  \hspace{1cm} (3.35)

We will now specify \(G(r', r)\) in terms of the transmission \(T(p)\).

---

**Figure 3.1:** The volume element \(d^3r\) is defined by the solid angle \(d\omega\) and the spheres of radius \(\rho\) and \(\rho + dp\) from the emission point.

The probability that a photon is absorbed in a volume element defined by the solid angle \(d\omega\) and by spheres of radius \(\rho\) and \(\rho + dp\) from the emission point is:

\[\frac{1}{4\pi} K(\rho) d\omega dp. \]  \hspace{1cm} (3.36)

We see that, with \(\rho = |r - r'|\), \(d^3r = \rho^2 dp d\omega\) as shown in fig (3.1), \(G(\rho) dp = (1/4\pi \rho^2) K(\rho) dp\), or from (3.17),

\[G(r', r) = -\frac{1}{4\pi \rho^2} \frac{\partial T}{\partial \rho}. \]  \hspace{1cm} (3.37)

As a result the source term can now be written as

\[(S_p)_{Rad} = -A_{pq} n(r) - A_{pq} \int n(r') \frac{1}{4\pi \rho^2} \frac{\partial T}{\partial \rho} d^3r'. \]  \hspace{1cm} (3.38)

The probability that a photon which is emitted is absorbed in \(r\) depends on the distance between emitter and absorber \(\rho\), and the derivative of the transmission \(T\) with respect to \(\rho\). The net radiation source is often written in terms of the effective transition probability

\[(S_p)_{Rad} = -A_{eff} n_p(r) \equiv -A_{pq} \Lambda(r) n_p(r). \]  \hspace{1cm} (3.39)
Here the *escape factor* $\Lambda$ has been introduced. From (3.35) and (3.39) we have

$$\Lambda(r) = 1 - \frac{\int G(r, r')n_p(r')dr'}{n_p(r)}. \quad (3.40)$$

Summarizing, the effect of absorption is taken into account by considering the effective transition probability $A_{eff} = A_{pq}\Lambda$.

Analytical solutions can only be obtained in special cases. Holstein was able to calculate the escape factor at the axis of an infinite cylinder, under the assumption of a uniform radial absorption coefficient, a parabolic excited state distribution and Doppler-broadening. The escape factor is then given by

$$\Lambda = \frac{1.60}{k_0R\sqrt{\pi \ln k_0R}}, \quad (3.41)$$

in which $R$ is the radius of the cylinder and $k_0$ is given by

$$k_0 = \frac{\lambda_0^3 n_g g_p A_{ap}}{8\pi g_q \sqrt{\pi v_0}}, \quad (3.42)$$

with $v_0 = \sqrt{2kT/M_{atom}}$. The equation for $\Lambda$ only holds for large values of $k_0R$ because use has been made of the asymptotic form of the *transmission* factor given by (3.14).

### 3.5 Application to Mercury

In the previous chapter we showed how the escape-factor was used in the CR-model and how we obtained the particle source terms from this model. The escape-factor within the old CR-model cannot be adjusted to different geometries if we want $T_e$ and $n_e$ to be the only input parameters for the CRM.

In the six-level model the $6^3P_1$ level is one of the independent levels. The radiative transition of this level to and from the ground state is a very important process because about 80 percent of the light from a QL-lamp originates from this transition, the well known 254 nm line. If we leave this transition out of the CR-model it will only affect the J-coefficients of the $6^3P_1$ level to the groundstate ($J_{31}$). If we are now able to calculate the escape-factor in PLASIMO we can add the radiative transition to the J-coefficients to obtain

$$J_{31} = (J_{31})_{CRM} + \frac{A_{31}\Lambda_{31}}{n_e}. \quad (3.43)$$

The $J_{13}$ coefficient does not change because absorption is treated as effective emission within $J_{31}$. This is one of the reasons we will decide to use an escape factor to treat radiation transport.
3.6 Flux vs Production

3.6.1 Introduction

In this section we will derive an expression for the radiation flux and show how the escape factor can be derived from this expression. In the case of the QL lamp the flux density on the ferrite core is also an interesting quantity, because a flux on the ferrite core causes heat which is unwanted. The total net photon production in a lamp is shown to be equal to the total photon flux through the surface of the lamp.

3.6.2 Definition of the Flux

First the flux density at position \( r \) due to radiation occurring from a volume element around position \( r' \) is defined as

\[
f(\rho) = n_p(r') A_{pq} T(\rho) \frac{\rho}{4\pi \rho^3}
\]

with \( \rho = r - r' \), \( \rho = |r - r'| \) and \( T(\rho) \) the transmission, the probability that a photon travels a distance \( \rho \) without being captured, under the assumption of a uniform absorption coefficient \( k_0 \).

In obtaining the total flux at \( r \) we have to integrate over all volume elements \( r' \). The total flux density at position \( r \) then equals

\[
\Gamma(r) = \int_V f(\rho) d^3r'
\]

We are interested in the net flux density through a surface element. The flux through a surface element \( dA \) at \( r \) is now given by

\[
F_A(r)dA = \int_V (f(\rho), n) dAd^3r'.
\]

From this equation the flux density on the plasma walls can be calculated.

3.6.3 Derivation of \( \Lambda \) from the Flux

We will show how the escape factor can be derived from the definition of the flux, by making use of the photon continuity equation,

\[
(\nabla, \Gamma) = S
\]

in which the flux \( \Gamma \) given by (3.44) and (3.45)

\[
\Gamma(r) = \int_V n_p(r') A_{pq} T(\rho) \frac{\rho}{4\pi \rho^3} d^3r'
\]
The left hand side of equation (3.47) can be written as

\[ \nabla \cdot \Gamma = A_{pq} \int_{V'} n_p(r') (\nabla \cdot T(\rho) \frac{\rho}{4\pi \rho^3}) d^3 r' \]  (3.49)

where we used \((\nabla \cdot f, v) = f (\nabla \cdot v) + (\nabla f, v)\). In appendix (A) it is shown that this can be cast as

\[ \nabla \cdot \Gamma = -A_{pq} \int_{V'} n_p(r') \{-T(\rho) \delta(r - r') + \frac{(\nabla T(\rho), \rho^{-1})}{4\pi}\} d^3 r'. \]  (3.50)

If we use \(T(0) = 1\) and \((\nabla T(\rho), \epsilon_P) = dT(\rho)/d\rho = -dT(\rho)/d\rho\) we obtain

\[ \nabla \cdot \Gamma = A_{pq} n_P(r) - A_{pq} \int_{V'} n_p(r') \frac{\partial T(\rho)}{\partial \rho} \frac{1}{4\pi \rho^2} d^3 r'. \]  (3.51)

From (3.47) and (3.39) we see that \((\nabla \cdot \Gamma)\) equals the net local production \(\Lambda(r) n_p(r) A_{pq}\) from which we again obtain the escape factor definition:

\[ \Lambda(r) = 1 - \frac{\int_{V'} n_p(r') \frac{\partial T(\rho)}{\partial \rho} \frac{1}{4\pi \rho^2} d^3 r'}{n_p(r)} \]  (3.52)

which is a nice way of validating Holstein's derivation.

### 3.6.4 The Integrated Flux

If we want to determine the total photon production we have to integrate (3.47) over the whole volume. The total photon production equals

\[ P = \int_V (\nabla \cdot \Gamma) d^3 r = \int_V n_p(r) \Lambda(r) A_{pq} d^3 r \]  (3.53)

The lhs of this equation can be rewritten by using Gauß' theorem:

\[ P = \int_V (\nabla \cdot \Gamma) d^3 r = \int_A (\Gamma, n) d^2 r \]  (3.54)

where A is the surface surrounding the volume V. As a result we see that the total flux through the surface equals the total production within the enclosure,

\[ \int_A (\Gamma, n) d^2 r = \int_V n_p(r) \Lambda(r) A_{pq} d^3 r \]  (3.55)

If we calculate both the escape factor and the flux then the previous equation can serve as a check for the accuracy of the calculated values.
3.7 Interpretation of $\Lambda$ as escape probability

The escape factor as we will use it is defined by (3.35) and $nA_{pq}\Lambda$ can be seen as local emission minus local absorption from all other regions. Often the escape factor is referred to as the chance that a photon escapes from the plasma (F.E. IRONS [17]). We shall investigate this interpretation.

A photon emitted at a point $r$ has a probability $T(|r-r'|)$ of traveling directly to the surface point $r'$ and escaping without being captured. This probability, when averaged over all surface points, gives the escape probability $\Theta(r)$,

$$\Theta(r) = \int_A T(\rho)(\frac{\rho}{4\pi|\rho|^3},n)d^3r'.\quad (3.56)$$

We will now show that this definition of $\Theta$ only equals the escape factor $\Lambda$ if we assume a uniform excitation profile. We will start again from (3.47)

$$n_p\Lambda A_{pq} = (\nabla, \Gamma).\quad (3.57)$$

With (3.44) this can be written as

$$n_p\Lambda A_{pq} = A_{pq} \int_A (\nabla, n_p(r')T(\rho)\frac{\rho}{4\pi|\rho|^3})d^3r'.\quad (3.58)$$

We may use the theorem of Gauss to obtain:

$$n_p\Lambda A_{pq} = A_{pq} \int_A n_p(\rho)\frac{\rho}{4\pi|\rho|^3}(\rho) d^3r'.\quad (3.59)$$

If $n_p$ is uniform it can be taken outside the integral and as a result we get back the expression (3.40) for the escape probability $\Theta$. Division by $A_{pq} n_p$ yields

$$\Lambda = \int_A (T(\rho)\frac{\rho}{4\pi|\rho|^3},n)d^3r' \equiv \Theta.\quad (3.60)$$

Summarizing if we want to use the escape factor to express net emission we can only use (3.56) in the case of a uniform excitation profile throughout the plasma. In all other cases we must use (3.35).
CHAPTER 3. TRANSPORT OF RADIATION
Chapter 4

Numerical Implementation

In this chapter we will discuss how the particle source terms have been implemented in PLASIMO, and how we can gain stability by linearization of the source terms. The numerical implementation of the escape factor calculating will be described and finally the numerical calculation of the radiation flux density will be discussed.

4.1 Solution Procedure

In this section we will discuss how the particle equations are solved within PLASIMO. PLASIMO is a control volume element method. A description of this plasma simulation program can be found in BENOY [2]. We will briefly discuss the geometrical setup and the importance of source term linearization. Further it is assumed that the physical system under study is stationary and axisymmetric so that we have in fact a two-dimensional problem.

4.1.1 Geometrical Setup

Let the coordinates \((\xi_1, \xi_2, \xi_3)\) be functions of \((x, y, z)\), which are assumed to be single-valued and to have continuous derivatives. The corresponding geometrical scale factors \(l_i, i = 1, 2, 3\) are defined in terms of an elementary arc length \((ds)^2\):

\[
(ds)^2 = g_{ij} d\xi^i d\xi^j \quad \text{orthogonal} \quad l_1^2(\xi_1)^2 + l_2^2(\xi_2)^2 + l_3^2(\xi_3)^2
\]

(4.1)

If a TL-tube is modeled, cylindrical coordinates will be used. For such coordinates we have

\[
ds^2 = (dz)^2 + (dr)^2 + r^2(d\phi)^2\]

(4.2)

In this case the scale factors \((l_z, l_r, l_\phi) = (1, 1, r)\). All further references to coordinates will be to these (not necessarily cylindrical) computational grid coordinates.
4.1.2 Numerical Solution Procedure

Writing the transport equation (2.5)
\[(\nabla, \Gamma_\phi) = S_\phi \quad \text{with} \quad \Gamma_\phi = \rho v \phi - \mu_\phi \nabla^2 \phi, \] (4.3)

where \(\rho v \phi\) represents convection and \(\mu_\phi \nabla^2 \phi\) diffusion. In physical components we obtain
\[
\frac{\partial}{\partial \xi_1} (l_2 l_3 (\rho v_1 \phi - \frac{\mu_\phi}{l_1} \frac{\partial \phi}{\partial \xi_1})) + \frac{\partial}{\partial \xi_2} (l_1 l_3 (\rho v_2 \phi - \frac{\mu_\phi}{l_2} \frac{\partial \phi}{\partial \xi_2})) S_\phi l_1 l_2 l_3. \] (4.4)

Integrating over a finite volume and using Gauß' theorem we get for a typical control volume
\[
\Gamma_e A_e - \Gamma_w A_w + \Gamma_n A_n - \Gamma_s A_s = SV_p. \] (4.5)

where the lower indices of the fluxes refer to the boundary points "east", "west", "north" and "south" as depicted in Fig. (4.1).

There is an essential difference between the boundary points of a control volume denoted by small letters and the grid points denoted by capitals. The former \(e, w, n, s\), serve as intermediates to get via (4.5) a relation between the qualities \(\phi\) at \(P\) and at the neighboring grid points \(E, W, N, S\).

\[
ap_p \phi_P = a_E \phi_E + a_S \phi_S + a_W \phi_W + a_N \phi_N + S_p l_1 l_2 l_3 \Delta \xi_1 \Delta \xi_2 \] (4.6)

This relationship in the computational domain will be found by using an appropriate discretization procedure [10] to get \(\phi_e\) from \(\phi_E\) ad \(\phi_P\) etc., and is described by the discretization coefficients \(a_{E,S,W,N}\). Due to the non-linearity of the transport equations (4.3), the discretization coefficients \(a_{E,S,W,N}\) are functions of \(\phi\), so that an iterative solution method will be used. The source term \(S_\phi\) can be treated explicitly, which means that in a new iteration the old value of \(\phi\) is used to compute \(S_\phi\). The convergence can be increased by linearizing the source term according to \(S_\phi = \hat{S}_p \phi_p + \hat{S}_c\) (in which \(\hat{S}_p\) has to be negative [10]) so that the source term is treated more implicitly. Equation (4.6) is then written as:

\[
(a_P (\phi^n) - \hat{S}_p (\phi^n)) \phi_P^{n+1} = \sum_{NB} a_{NB} (\phi^n) \phi_{NB}^{n+1} + \alpha \hat{S}_C + (1 - \alpha) a_P (\phi^n) \phi_P^n \] (4.7)
in which an *under-relaxation* factor \(0 < \alpha < 1\) is introduced and \(NB\) stands for neighbor grid points. The superscript \(n\) means that the quantity \(\phi^n\) is calculated in the \(n\)-th iteration cycle.

### 4.2 Implicit Treatment of the Source Term

As stated in the previous section linearization of the source term \(S_\phi = \hat{S}_c + \hat{S}_r \phi\) will improve convergence; we will demonstrate this by means of a general example. Let's start from the next differential equation:

\[
\frac{d\phi}{dx} = A\phi + B. \tag{4.8}
\]

If we use the most simple discretization scheme we can write (4.8) as

\[
\frac{\phi(x + h) - \phi(x)}{h} = A\phi(x) + B, \tag{4.9}
\]

from which we obtain the explicit form

\[
\phi^h_{t+1} = \phi^h_t + hA\phi^h_t + hB = \Psi(\phi^h_t). \tag{4.10}
\]

where \(\phi^h_t\) denotes the numerical approximated value of the exact \(\phi(x)\) value. For reasons of numerical stability we demand that \(\left|\frac{\partial \phi}{\partial \phi}\right| \leq 1\) ([9]) which results in

\[
|1 + hA| \leq 1 \quad \text{and so} \quad h \leq -2/A. \tag{4.11}
\]

As a result we see that \(A\) has to be negative. This treatment can cause instabilities because for large values of \(|A|\) the step factor \(h\) has to be very small.

Equation (4.8) can also be approximated by

\[
\frac{\phi(x + h) - \phi(x)}{h} = A\phi(x + h) + B, \tag{4.12}
\]

from which we obtain the implicit form

\[
\phi^h_{t+1} = \phi^h_t + hA\phi^h_{t+1} + hB \tag{4.13}
\]

\[
\phi^h_{t+1} = \frac{1}{1 - hA} \left[\phi^h_t + hB\right] = \Psi(\phi^h_t) \tag{4.14}
\]

Again for reasons of numerical stability \(\left|\frac{\partial \phi}{\partial \phi}\right| \leq 1\) ([9]) which results in

\[
\left|\frac{1}{1 - hA}\right| \leq 1. \tag{4.15}
\]

As a result we see that if \(A < 0\) this method is stable for every step factor \(h\).
We will now assume the rhs of (4.8) as our source term $S_\phi$. If we do not linearize the source term it will be determined by the value of $\phi$ of the previous iteration $\phi_t$. However if we do linearize the source term we are able the use the new value of $\phi$, $\phi_{t+1}$ in solving (4.8). We then obtain $|\frac{1}{1-hS_p}| < 1$ which is valid for all values of $h$ when $\hat{S}_p$ is negative.

We showed that the particle density source term can be described by a production term $P(j)$ and an destruction factor $D(j)$ of the level $j$.

$$S_j = P(j) - n_jD(j), \quad (4.16)$$

now the linear source term coefficients $\hat{S}_c$ and $\hat{S}_p$ can be given by respectively,

$$\hat{S}_c = P(j), \quad (4.17)$$
$$\hat{S}_p = -D(j). \quad (4.18)$$

Previously this linearization was not implemented in PLASIMO. The source term $S_\phi$ was artificially split-up in $S_c$ and $S_p$ according to

$$S_\phi = S_c + S_p\phi, \quad (4.19)$$
$$S_c = 0, \quad S_p = \frac{S_\phi}{\phi} \text{ if } S_\phi < 0, \quad (4.20)$$
$$S_c = S_\phi, \quad S_p = 0 \text{ if } S_\phi > 0. \quad (4.21)$$

For convergence reasons $S_p$ has to be negative [10], that is why $S_p$ was set zero if the total source term was positive, so $S_c = S_\phi$, if the source term was negative $S_c$ is assumed zero and $S_p$ is derived by dividing $S_\phi$ by $\phi$.

By using the J-coefficients now it is easy to calculate $\hat{S}_c$ and $\hat{S}_p$ as described before. From (2.10) we obtain:

$$S_j = \hat{S}_c + \hat{S}_p n_j \quad (4.22)$$
$$\hat{S}_c = \sum_{i \neq j} n_i n_e J_{ij} \quad (4.23)$$
$$\hat{S}_p = - \sum_{i \neq j} n_e J_{ji}. \quad (4.24)$$

As an example we consider the two level Ar model, for which we have

$$J_{Ar} = \begin{bmatrix} 0 & S_{cr} \\ \alpha_{cr} & 0 \end{bmatrix}. \quad (4.25)$$

For the ion level the source term $\hat{S}_p$ will be $\alpha_{cr}$ and $\hat{S}_c$ will be $n_1 S_{cr}$, in the source term for the groundstate $S_p$ will be $S_{cr}$ and $S_c$ will be $n_+ \alpha_{cr}$. 
4.3 Calculation of the Escape Factor

In this section it will be explained how the escape factor will be calculated numerically for cylindrical geometries and Doppler broadened spectral profiles. A numerical treatment is interesting because analytical calculations are restricted to limiting situations. In order to validate the numerically obtained values the escape-factor are compared to the results of known analytical solutions which can only be found for central axial positions. If we want to calculate escape factors for different radial positions in the cylinder the only way to obtain valid escape factors is by numerical integration.

In order to obtain an escape factor we have to compute the integral of equation (4.26).

\[ \Lambda(r) = 1 - \frac{1}{4\pi\rho} \int_{\rho}^{\infty} n_q(r') \frac{\partial T}{\partial \rho} dr' n_q(r), \tag{4.26} \]

which will be done numerically by summing the contributions \( \frac{1}{4\pi\rho} n_q(r') \frac{\partial T}{\partial \rho} d^3r' \) of all volume elements. The contribution of a volume element around \( r' \) to the escape factor in \( r \) depends on:

1. the density of the excited atoms \( n_q(r') \)
2. the distances \( \rho = |r - r'| \) and
3. the derivative of the transmission with respect to the distance, \( \frac{\partial T}{\partial \rho} \).

For Doppler broadening the latter is a function of the distance and the absorption at line center \( k_0 \), which depends on the ground-state density and the heavy-particle temperature.

In a first approximation we will assume a uniform \( k_0 \) according to (3.6), that is, we assume a uniform groundstate density and a uniform plasma temperature.

In obtaining accurate values for \( T(\rho) \) and \( \frac{\partial T(\rho)}{\partial \rho} \) we can not use the approximation given by (3.14) since these are not valid for small values of \( k_0\rho \) (for contribution from nearby volumes). We have to start from the next equation:

\[ T(\rho) = \int_{-\infty}^{\infty} \frac{1}{\pi^2} \exp x^2 \exp [-k_0\rho \exp -x^2]dx \tag{4.27} \]

so

\[ \frac{\partial T(\rho)}{\partial \rho} = -k_0 \int_{-\infty}^{\infty} \frac{1}{\pi^2} \exp [-k_0\rho \exp -x^2]dx = -k_0 f(k_0\rho) \tag{4.28} \]

We will solve \( \frac{\partial T}{\partial \rho} \) numerically by using the Gauss-Laguerre quadrature method. The numerical calculation of \( \frac{\partial T}{\partial \rho} \) is a very time consuming process. That's why we decided to generate a fit-function for \( f(k_0\rho) \). The result is given in fig (4.2).
The fit-coefficients can now be obtained from a look-up table so that \( f(k_0\rho) \) and \( \frac{\partial f}{\partial p} \) can be calculated without using the slow numerical calculation every time \( \frac{\partial f}{\partial p} \) is needed.

From Fig(4.2) we see that for small values of \( k_0\rho \), \( \frac{\partial f}{\partial p} \) will change rapidly with \( k_0 \). This means that for a given relatively large \( k_0 \) values small steps in \( \rho \) must be considered so that a fine grid is needed.

In the case where we want to calculate the escape factor on the axis of an "infinite" cylinder we only need to sum over \( z \) and \( r \) directions. The integration over all possible \( \phi \) values simply means a multiplication with a factor \( 2\pi \). This means that the contribution from a volume element denoted by \( r \) and \( z \) can be given by

\[
\delta(1 - \Lambda) = \frac{2\pi}{n_q(0)} \delta z n_q(r) A_{pq} k_0 f(k_0\rho) \frac{1}{4\pi \rho^2} \delta r
\]  

(4.29)

By summing over all grid point we obtain \( (1 - \Lambda) \)

\[
(1 - \Lambda) = \frac{2\pi}{n_q(0)} 2 \sum_0^Z \delta z \sum_0^R n_q(r) A_{pq} k_0 f(k_0\rho) \frac{1}{4\pi \rho^2} \delta r
\]  

(4.30)

where in principle we need to take \( Z \to \infty \). However in practice this means that \( Z \) has to be sufficiently large. The distance \( \rho \) is represented by \( \rho = \sqrt{r^2 + z^2} \) and \( n_q(0) \) is the density of the excited state on the axis of the cylinder. The layout of the grid is shown in Fig(4.3). Because of the high grid density which is needed for calculating the escape factor we cannot use plasimo's grid-generation (defining a grid will consume too much memory). The grid we will use to calculate

Figure 4.2: The function \( f(k_0\rho) \) for different values of \( k_0\rho \).
4.4 Calculation of the escape factor for different radial positions

So far we only calculated the escape factor on the axis of the cylinder. If we want to calculate it for different radial positions we have to design a special grid in which the integration in the $\phi$ direction will still result in a multiplication factor between 0 and $2\pi$ in order to save calculation time. The radial position where the escape-factor is calculated will be denoted by $r = r_a$. The new grid is based upon circles or circle segments with different radii, that originate at $-r_a$ in the previous grid. The radius of the circles will equal $r + r_a$. This is depicted in fig(4.4).

In the new grid we redefine $r$ as $r_{old} + r_a$ ($r = 0$ at $r_a$), so $\rho$ is still defined by $\rho = \sqrt{r^2 + z^2}$. Note that the axis of the cylinder is no longer the symmetry axis. The grid used to evaluate the escape factor on the axis of an (infinite) cylinder.

Figure 4.3: The grid which is used to evaluate the escape factor on the axis of an (infinite) cylinder.
of the coordinate system.

![Diagram of coordinate system](image)

Figure 4.4: Treatment of the $\phi$-integration.

The integration in $\phi$ direction will only take place for the part of the circles, with radius $r$, within the cylinder. So the integration will result in a factor between 0 and $2\pi$ (fig 4.4) according to:

$$\phi(r) = 2 \arccos \frac{R^2 - r_a^2 - r^2}{-2rr_a}$$

as we can see $\phi$ only depends on $r$ $\Lambda$ can still be calculated by summing over $r$ and $z$ directions by first summing over $r$ direction we can gain some speed because $n_q$ and $\phi$ only depend on $r$ and not on $z$ (or $\rho$).

$$1 - \Lambda = A_{pq} \frac{2\pi}{n_q(r)} \sum_{0}^{R} \phi(r)n_q(r)\delta r \sum_{0}^{Z} \frac{\partial T(\rho)}{\partial \rho} \frac{1}{4\pi \rho^2} \delta z,$$
4.4. CALCULATION OF THE ESCAPE FACTOR FOR...

where \(n_q(r)\) is the density of the excited state at the radial position where the escape factor is calculated.

### 4.4.1 Calculation of the escape factor for a QL geometry

In an "infinite" cylinder we assumed that the density of the excited state only depends on the radial position in the lamp, if we are modeling a TL-tube this assumption is still valid. However in the QL-lamp the densities do depend on the axial \(z\) position. The calculation of \(\Lambda\) can now be represented by

\[
1 - \Lambda = A_{pq} \frac{2\pi}{n_q(r)} \sum_{Z} \Delta z \int_0^{R(z)} \frac{\partial T(\rho)}{\partial \rho} \frac{1}{4\pi \rho^2} \phi(r) n_q(z,r) \Delta r,
\]

where \(R(z)\) defines the boundary of the lamp. This calculation is much slower because now we have to obtain the density for every grid point. In obtaining the density \(n(r, z)\) from PLASIMO we again have to exchange information from the PLASIMO grid to the grid used for these escape factor calculations (see Appendix C.1). Another difficulty in obtaining escape factors in the QL-lamp is the ferrite core in the lamp which blocks the radiation emitted at opposite sides. This is shown in fig(4.6). We can account for this by changing the integration factor \(\phi\).

![Figure 4.6: The ferrite will block part of the radiation this can be dealt with by limiting the \(\phi\) integration boundaries.](image)

\[
\phi(r) = \phi_{\text{max}}(r) - \phi_{\text{min}}(r) \quad \phi(r) \leq 0,
\]

where \(\phi_{\text{max}}\) represents the maximum integration angle before reaching the boundary of the lamp and \(\phi_{\text{min}}\) the minimum angle due to the ferrite core.
4.5 Calculation of the flux density

We want to calculate the flux through the surface and check if it equals the production within the enclosure. In evaluating (3.55) we first need to determine the flux through the surface,

$$\int_S \int_{V'} n(r') A^p \frac{T(\rho)}{4 \pi |\rho|^3} (\hat{n}, n) d^3r' d^2r. \quad (4.35)$$

This will be done by determining the net flux through the surface of an "infinite" cylinder fig(4.7). A coordinate system in which (0,0,0) is a point at the surface at half the height of the cylinder will be used. The net flux through (0,0,0) perpendicular to the surface will be calculated. The dot product $(\hat{n}, n)$ has to be determined, from fig(4.8) we see that the n vector is given by $n(x, y, z) = -(1, 0, 0)$ and the vector $\rho$ by $\rho = (r \cos \phi, r \sin \phi, z)$ so that

$$(\hat{n}, n) = \frac{r \cos \phi}{\sqrt{r^2 + z^2}} \quad (4.36)$$

where $r$ is a value between 0 and $2R$ and $r = (0, 2R)$ with $R$ the radii of the cylinder fig(4.8).

For the calculation of the flux density the same grid as in the escape factor calculation for different radial positions will be used (see section 4.4). The radial position will correspond to the borders of the lamp. The $\phi$ integration will be dealt with in a similar way, but the inner product is also $\phi$ dependent. The integration boundaries are still determined by the relation

$$\phi_{max}(r) = \arccos \left( \frac{R^2 - r \cdot a^2 - r^2}{-2rr \cdot a} \right). \quad (4.37)$$
4.5. CALCULATION OF THE FLUX DENSITY

The integral over the volume \( V' \) equals

\[
2 \int_0^Z \frac{dz}{2} \int_0^{\phi_{\text{max}}} d\phi \int_0^{2R} n(r') \frac{A_{pq} T(\rho) r \cos(\phi)}{4\pi \rho^2} r dr
\]

(4.38)

Where \( \rho(r) = \rho(r, z), n(r) = n(r) \) and \( \phi_{\text{max}} = \arccos(r/2R) \) For this special coordinate system the \( \phi \) integration can be performed analytically.

\[
\int_0^Z dz \int_0^{2R} n(r') \frac{A_{pq} T(\rho) r \sin(\phi_{\text{max}})}{\pi \rho^2} r dr
\]

(4.39)

If we want to perform this integral numerically we first have to determine the transmission \( T(\rho) \),

\[
T(\rho) = \int_{-\infty}^{\infty} \frac{1}{\pi^{\frac{3}{2}}} \exp x^2 \exp [\quad k_0 \rho \exp x^2] dx.
\]

(4.40)

We will solve this equation numerically by using the Gauss-Laguerre quadrature method. The numerical calculation of \( T(\rho) \) is a very time consuming process, thats why we decided to fit \( T(\rho) \) for different values of \( k_0 \rho \), just like we did to evaluate \( \frac{\partial T}{\partial \rho} \) in section 4.4. The result is shown in fig (4.9).

Because of the rapid changes in \( T(\rho) \) for small values of \( k_0 \rho \) we have to define a very fine grid near \( \rho = 0 \), just like we did to evaluate \( \frac{\partial T}{\partial \rho} \) in section 4.4. The result is shown in fig(4.10).

Now the flux density perpendicular to the surface can be calculated by summing over the contributions \( \delta^2 F(0) \)

\[
\delta^2 F(0)_{\perp} = \delta z n(r) A_{pq} \frac{T(\rho)}{\pi \rho^3} r^2 \sin(\phi_{\text{max}}) \delta r,
\]

(4.41)
Figure 4.9: *The transmission* \( T(k_0 \rho) \) *as function of* \( k_0 \rho \).

of all grid points shown in fig(4.10) as shown by

\[
F(0)_\perp = \sum_{0}^{Z} \Delta z \sum_{0}^{2R} n(r) A_{pq} \frac{T(\rho)}{\rho^2} r^2 \sin(\arccos(r/2R)) \Delta r. \tag{4.42}
\]

From this equation we can calculate the flux density at the plasma wall. In the case of an infinite cylinder it is now easy to determine the total flux through the entire surface. We will assume a cylinder sector as shown in fig(4.7) where the net flux through the top and bottom of the cylinder sector are assumed zero. The total flux through the entire surface is then given by

\[
S = 2\pi R F(0)_\perp h, \tag{4.43}
\]

in which \( h \) is the height of the cylinder. The total photon production can be expressed as

\[
P = \int_{0}^{h} dz \int_{0}^{R} \Lambda(r) n(r) A_{pq} dr, \tag{4.44}
\]

which can easily be calculated numerically, the result is

\[
P = h \sum_{0}^{R} \Lambda(r) n(r) A_{pq} \delta r \tag{4.45}
\]

because \( \Lambda \) does not depend on \( z \).

If we want to calculate the flux density at the boundaries of the QL-lamp there are a few differences with respect to the previous approach:

1. The \( n \)-vector perpendicular to the surface will in general no longer be perpendicular to \( z \);
2. We have to take the ferrite core into account, this will again affect to integration in $\phi$ direction;

3. If we want to calculate the flux on the ferrite core, the origin of the grid will be on the boundary of the ferrite core.

How this has been dealt with can be seen in Appendix C.2. Here we end the discussion of the numerical implementation. Results from the numerical calculations are shown in the next chapter.
Chapter 5

Numerical results

In this chapter we will discuss the numerical results. First the benefits of the implicit treatment of the source terms are discussed for various models with different numbers of independent levels. The numerical calculation of the escape factor will be compared to the known analytical ones. The effect of various uniform escape factors, as well as numerically calculated escape factors on the results from PLASIMO will be shown. The flux density on the plasma walls as well as the total photon production and total radiated power are calculated.

5.1 Implicit treatment of the particle source terms

The implicit treatment of source terms is now implemented in PLASIMO. For simulating the TL and QL-lamps we can choose what kind of mixture we will use and how many independent levels are taken into account. We can use a pure "Ar2" model consisting of two independent levels, or a mixture of Argon and Mercury in which there is a choice between two "Ar2Hg2" or six "Ar2Hg6" independent Mercury levels.

Some PLASIMO simulations for TL- and QL lamps with different numbers of independent levels have been performed. The results, of what we will now call implicit calculation as opposed to the explicit treatment of the source terms is examined. From the work of P. HERBEN [8] it followed that the six level model does not converge to a solution when using the explicit calculation method. In using the implicit treatment where the source term is linearized in order to treat the $\phi$ dependent part of the source term implicitly (see section 4.2), the instabilities are solved: the six level model can now be used.

From the results in table (5.1) and (5.2) we notice that implicit calculation does not improve the speed (the number of iterations needed to reach an accurate solution) for the two level model, for which the source is given by (2.6). For the simulated plasmas the ionization is much larger than the recombination, so $S_p n_+ / S_e << 1$. As a result $S \approx S_e$, in which case the new treatment of the source
terms will almost be as explicit as the old treatment. In the six level model the population and depopulation rates are much more balanced, especially for the excited states which can be assumed to be (almost) in QSS. Further we notice that implicit calculations are so stable that relaxation is hardly needed, which will improve convergence speed.

<table>
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<th>relaxation-factor</th>
<th># iterations</th>
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</tbody>
</table>

Table 5.1: Simulations for a TL-lamp with diameter=19.5 mm, Argon-pressure 205 Pa at current 3A.

<table>
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<th>mixture</th>
<th>model</th>
<th>method</th>
<th>convergence</th>
<th>relaxation-factor</th>
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<td>4300</td>
</tr>
</tbody>
</table>

Table 5.2: Simulations for the QL-lamp with Argon-pressure of 133 Pa.

Because of the implicit calculation method the Hg-6 model can now be used for both TL and QL simulations. This is important, because in the six level model radiation transport can be treated within PLASIMO, as in this model also the resonance and metastable levels are independent, as has been discussed in Chapter (2).

5.2 Numerical Solution of the Escape Factor vs Analytical Results

Holstein derived a model for the escape factor which is valid on the axis of an infinite cylinder under the assumption of uniform radial absorption, a parabolic radial distribution of the excited state density and Doppler-broadening of the resonance line. Under these conditions \( \Lambda \) was found to be

\[
\Lambda(0) = \frac{1.60}{k_0 R \sqrt{\pi \ln k_0 R}}; \tag{5.1}
\]

in which \( R \) is the radius of the infinite cylinder (see section 3.4). Now we will check our numerical model with the help of this analytical solution. For this purpose
we will not use plasma parameters from PLASIMO but just assume a parabolical excitation profile as Holstein did. For an assumed $k_0$ value we will change $R$, so we will calculate numerical and analytical solutions for infinite cylinders of different diameters. Figure (5.1) shows both the analytical and the numerical solution for the escape factor as a function of the optical depth $k_0 R$ of the plasma. We see how Holstein's derivation, which is based upon the assumption of large optical depth, fails for small tube radii $R$ or absorption coefficients $k_0$.

![Figure 5.1: Escape factor as a function of absorption depth, derived from numerical and analytical calculations.](image)

The numerical calculation is also valid for small optical depths. For an infinitely small optical depth the escape factor will be unity because there is no absorption. As a result the local emission is equal to the net local emission.

### 5.3 Escape Factor Calculations for Different Radial Positions

In this section results from the numerical escape factor calculation for different radial positions will be shown. A uniform excitation profile, $n_p = 10^{18} \, m^{-3}$, will be assumed, so that the escape factor can be interpreted as the probability that a photon escapes the plasma (see section 3.7). In fig (5.2) the escape factor is depicted for $k_0 = 5000 \, m^{-1}$, a ground density of $n_q = 10^{20} \, m^{-3}$ and a heavy particle temperature of $T_g \approx 400K$.

Because of the uniform plasma parameters we can conclude that the higher escape factor near the plasma wall has a purely geometrical background. Near
the plasma wall there are less neighbors from which radiation can be captured. Alternatively follows the second definition, the chance of a photon reaching the plasma wall will be higher if it is emitted closer to the wall as can be seen form the transmission factor (4.27).

Next we will assume a (ferrite) core with a radius of half a centimeter at the center of the cylinder. In this case the escape factor will behave as shown in fig (5.3). Here we see the effect of a core in the middle of the system. The average escape factor in the plasma is higher than in the plasma without core, because the core blocks part of the radiation so the local absorption will be limited by the presence of the core, as a result the net relative local emission will be large. Of course also this uniform plasma the chance of a photon escaping from the plasma by reaching the core will increase if the photon is emitted closer to the core resulting in a higher escape factor.

5.3.1 Total Production vs Flux

For the two configurations that have been described above the flux on the walls has been calculated.

From the results in table (5.4) we see that the total production is about equal to the total radiated power, as was expected from (3.55). This indicates that the numerical models used to calculate the escape factor and the flux are sufficiently accurate.

Figure 5.2: Escape factor for different radial position for $k_0 = 5000\text{m}^{-1}$ for a cylinder of radius $R=2.5 \text{ cm}$.
5.3. CALCULATION OF THE ESCAPE FACTOR FOR ...

Figure 5.3: Escape factor for different radial position for $k_0 = 5000$ for a cylinder of radius $R=2.5$ cm with a core radius of 0.5 cm.

<table>
<thead>
<tr>
<th>Radius (cm)</th>
<th>Flux ($W/m^2$)</th>
<th>Lamp</th>
<th>Core</th>
<th>Wall</th>
<th>Core</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>$8.56 \times 10^3$</td>
<td>0</td>
<td>8.63 $10^3$</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>$8.36 \times 10^3$</td>
<td>0.5</td>
<td>7.61 $10^3$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.3: Radiative energy flux density on the walls.

<table>
<thead>
<tr>
<th>Radius (cm)</th>
<th>Power ($W/m$)</th>
<th>Lamp</th>
<th>Core</th>
<th>Wall</th>
<th>Core</th>
<th>Total</th>
<th>Total Production</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5 cm</td>
<td>$1.35 \times 10^2$</td>
<td>0</td>
<td>$1.32 \times 10^2$</td>
<td>-</td>
<td>$1.35 \times 10^2$</td>
<td>$1.33 \times 10^2$</td>
<td></td>
</tr>
<tr>
<td>2.5 cm</td>
<td>$1.35 \times 10^2$</td>
<td>0.5</td>
<td>$0.24 \times 10^2$</td>
<td>$1.56 \times 10^2$</td>
<td>$1.58 \times 10^2$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.4: Total radiated power and total volumetric production per unit of tube length.
5.4 Results from PLASIMO

In this section we will discuss the full simulations done with PLASIMO for both uniform and non-uniform (calculated) escape factors. The simulation of the TL-lamp will be compared with measurements done by P. HERBEN [8]. As PLASIMO is a self-consistent simulation program the escape factor is recalculated every iteration to obtain accurate values for the next iteration. In modeling the TL and QL lamp the six level mercury model has been used, for which the escape factor involving the transition from the resonance state $6^3P_1$ to the groundstate can be calculated separately. The escape factor involving the transition from the resonance state $6^1P_1$ to the groundstate is assumed uniform and equals $10^{-3}$ in all simulations.

5.4.1 TL simulations

The calculation of the escape factor has been incorporated in the PLASIMO simulation program. This allows a calculation which is self-consistent with the computed fluid dynamics data (densities, temperatures). The escape factor depends on the density profile of the excited state, and because the escape factor influences the local particle densities it has to be recalculated every iteration. The calculation which will be presented in this section have been obtained for a high-current TL with cylindrical geometry. This TL lamp has an argon filling pressure of 205 Pa, a cold spot mercury pressure of 0.6 Pa and an internal diameter of 19.5 mm. In the simulation a current of 3A has been taken.

Fig (5.4) shows the calculated value of the escape factor. Here $k_0$ is determined by the average groundstate density and heavy particle temperature, the final $k_0 = 5100$. Fig (5.5) shows the converged excited state density profile.

The simulated value of the escape factor on the axis is $\Lambda(0) = 7.6 \times 10^{-4}$. The escape factor on the axis can be calculated by the analytical solution of Holstein (see section 3.4) the escape factor $\Lambda_H(0) = 9.2 \times 10^{-3}$ where a parabolical excitation profile is assumed according to $n(r) = (1 - R^2)n(0)$. 
5.4. RESULTS FROM PLASIMO

Figure 5.4: The Escape factor as a function of radial position in a high-current tube lamp $R = 9.75$ mm, $k_0 = 5100$.

Figure 5.5: The excited density profile of a TL simulation resulting from a radially dependent escape factor.
CHAPTER 5. NUMERICAL RESULTS

From section 3.4 we see that the escape factor definition is based upon a uniform \( k_0 \). However if we look at the escape factor definition

\[
\Lambda(r) = 1 - \frac{1}{n(r)} \int n(r') \frac{1}{4\pi \rho^2} \frac{\partial T(k_0 \rho)}{\partial \rho} d^3r',
\]

(5.2)

where \( \frac{\partial T(k_0 \rho)}{\partial \rho} \) depends on \( k_0 \) and \( \rho \) it is tempting to use an average value of \( k_0 \) for each pair of absorber \( (r) \) and emitter \( (r') \) and not one \( k_0 \) value throughout the entire plasma. Fig (5.6) shows the result of this treatment. One first observes a decreasing escape factor with increasing radial position caused by the higher absorption coefficient closer the wall, near the wall the escape factor again starts to increase, this is because the geometrical effect on the escape factor becomes larger than the increasing absorption coefficient. A picture of \( k_0 \) versus the radius \( r \) is shown in fig (5.7).

The same simulation has also been done with a uniform escape factor of \( \Lambda = 10^{-2} \); the excited state density profile then obtained is shown in fig (5.8). If we look at these excitation profiles we see that the escape factor has a large influence on the excitation profile. If we start with a uniform excited state density the net excitation near the plasma wall will be higher than at the center of the lamp, leading to a decreasing density near the plasma wall, and this will itself influence the escape factor.

Also for this lamp the total production and total radiation are calculated; the results are shown in table (5.5). The total production is obtained by summing

Figure 5.6: The Escape factor as a function of radial position in a high-current tube lamp \( R = 9.75 \) mm, with non-uniform \( k_0 \) values.
5.4. RESULTS FROM PLASIMO

Figure 5.7: \( k_0 \) as function of radial position in a high-current tube lamp \( R = 9.75 \) mm.

the local production contributions \( n_p (r) \Lambda (r) A_{pq} \) over the whole volume, where \( \Lambda (r) \) is the calculated escape factor.

<table>
<thead>
<tr>
<th>Radius (mm)</th>
<th>Radiative Energy (W/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.75</td>
<td>2.7 ( 10^2 )</td>
</tr>
<tr>
<td></td>
<td>3.0 ( 10^2 )</td>
</tr>
</tbody>
</table>

Table 5.5: Total radiated power and total UV production per unit of tube length.

From (3.55) it can be seen that the total radiated power must equal the total production, the measured results show a small difference. This indicates that there are small inaccuracies in the model which can for instance be dealt with by using more grid points, or a higher-order interpolation scheme.

We will now examine the influence of the escape factor on other plasma parameters, therefore the voltage fall over the positive column of a high-current TL-lamp has been calculated with the PLASIMO model. Various models for the escape factor have been tested fig (5.9). The results have been compared with the measurements of P.HERBEN [8] and B.JACOBS. One observes that for higher escape factors the voltages increase, as there is a larger 'leak' in the ionization channel. For higher currents the assumption of uniform absorption becomes dubious and the results should be interpreted with care. It can be seen that the escape factor has no influence on the qualitative behavior of the V-I characteristic. When using the calculated values of the escape factor the discrepancies are
Figure 5.8: The excited state density profile from a TL simulation. A radially independent escape factor of $10^{-2}$ has been used.

still quite high. This may be due to other flows in the PLASIMO model, like the poor treatment of diffusion.
Figure 5.9: The influence of the escape factor on the VI-characteristic for a tube lamp.
5.4.2 QL simulations

In this section some results from simulations of the QL lamp will be shown. We will model a QL-lamp with an argon filling pressure of 66 Pa and a mercury cold spot pressure of 0.6 Pa. The lamp is operated at 1 A coil current. In a QL-lamp the escape factor has to be calculated not only for different radial positions but also for different axial positions because in the QL lamp we have a non-uniform axial density profile and the shape of the lamp varies with the axial position. The escape factor calculation for a non uniform axial density profile itself is about 10 times slower than in the case of a uniform profile. If in the case of QL the full escape factor calculation will be about 300 times slower than the same calculation for a TL-lamp. A full TL simulation, with calculated escape factors, takes about one day on a pentium-II 233 MHz processor running Linux. As a result a QL simulation which makes use of calculated escape factors at every QL PLASIMO grid position can not be included in this work. That is why we decided to model a TL shaped lamp with a ferrite core in order to study the effects of the escape factor calculations. But first some results from a QL-simulation with a uniform escape factor of $10^{-2}$ for the $6^3P_1$ state will be shown.

5.4.3 QL Simulation with a Uniform Escape Factor

Results for a QL simulation with a uniform escape factor of $10^{-2}$ for the $6^3P_1$ state are presented. As stated before we are not able to perform a simulation using calculated (non-uniform) escape factors. But we can calculate the flux density on the ferrite core and on the wall. This flux calculation is also much slower than the calculation in the case of a TL lamp but the flux density calculation has only to be performed once, at the end of the simulation: it is merely a diagnostic number.

Fig (5.10) shows the density of the resonance level $6^3P_1$ of mercury. The z-axis is the symmetrical axis of the QL-lamp. The ferrite core is situated along the z-axis from $z = 0.04$ m to $z = 0.16$ m. At $z = 0.08$ m and $r = 0.08$ m we observe a maximum in the excited state densities. The maximum in the density coincides with the maximum of dissipated power density induced by the current through the core-coil system. Fig (5.11) shows the density of the metastable state $6^3P_2$ of mercury.

For the axial position $z = 0.06$ m a radial profile of the density of the metastable state $6^3P_2$ is shown in fig (5.12). In the next chapter on the Laser Induced Fluorescence measurements we will present the experimental density profile of this metastable state.

The maximum flux density on the ferrite core appears at $z = 8.0$ cm, as is shown in table (5.6).

The flux on the core does not contribute to the efficacy (the experienced intensity of the light coming out of the lamp as compared to the input power
5.4. RESULTS FROM PLASIMO

Figure 5.10: Calculated density of the resonance state $6^3P_1$ with a uniform $\Lambda = 10^{-2}$.

Table 5.6: Radiative energy flux density on the core.

<table>
<thead>
<tr>
<th>Axial position z (cm)</th>
<th>Flux ($W/m^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Core</td>
</tr>
<tr>
<td>7.5</td>
<td>$1.3 \times 10^3$</td>
</tr>
<tr>
<td>8.0</td>
<td>$1.8 \times 10^3$</td>
</tr>
<tr>
<td>8.5</td>
<td>$1.2 \times 10^3$</td>
</tr>
</tbody>
</table>

[lm/W]) of the lamp. Instead it will heat the core which is unwanted because it can damage the lamp and shorten its lifetime.

5.4.4 Cylindrical QL Simulation

Now we will present results on a cylindrical geometry representing the QL lamp, the sector is assumed to have a constant outer radius of 5 cm and contains a ferrite core with a radius of 1 cm. This is an approximation of the QL lamp shape at $z = 0.06$ m. In this simulation we used calculated escape factors. The simulation took about 24 hours of simulation time on a P2-233 MHz running Linux.

The final values of the escape factor is shown in fig (5.13). Fig (5.14) shows the density profiles of the resonance state $6^3P_1$. In order to visualize the effect of
CHAPTER 5. NUMERICAL RESULTS

Figure 5.11: Calculated density of the metastable state $6^3P_2$ with a uniform $\Lambda = 10^{-2}$.

the escape factor on the density profile of the state the same simulation has been carried out with a uniform escape factor. The results are depicted in fig (5.15). If we want to compare these profiles with the profiles of the QL simulation of the previous section we must be careful, because in the cylindrical QL simulation there is a less obvious maximum in dissipated energy. From these two figures we can see that the escape factor has a significant effect on the density profile. Finally we will examine the influence of the escape factor on the metastable state $6^3P_2$. Fig (5.16) and (5.17) show the density of the metastable state $6^3P_2$ with a calculated and uniform escape factor respectively.

We conclude that the influence of the escape factor calculations on the metastable state is less important. The result of the simulations with the cylindrical QL can be used to gain some insight in the behavior of the escape factor in the actual QL lamp, an assumed radial dependent escape factor can be used in simulating the QL lamp.
5.4. RESULTS FROM PLASIMO

Figure 5.12: Radial density profile of the metastable state $^6P_2$ at $z = 0.06$ m.

Figure 5.13: The calculated escape factor for a cylinder sector of radius 5 cm with a ferrite core of radius 1 cm.
Figure 5.14: Calculated density of the $6^3P_1$ state.

Figure 5.15: Calculated density of the $6^3P_1$ state, under the assumption of a uniform escape factor.
5.4. RESULTS FROM PLASIMO

Figure 5.16: Calculated density of the $6^3P_2$ state with a non uniform escape factor.

Figure 5.17: Calculated density of the $6^3P_2$ state with a uniform escape factor of $10^{-2}$. 
Chapter 6

Laser Induced Fluorescence Measurements

6.1 Introduction

In this chapter experiments on the QL-lamp are discussed in order to verify the modeling results presented in the previous chapter. We will discuss both laser induced fluorescence and absorption measurements.

Laser Induced Fluorescence (LIF) is a well established technique to measure atomic or molecular densities. In the next section some principles of LIF are treated and a relation between the intensity of the fluorescent light and the state density will be derived.

LIF spectroscopy is one of the basic diagnostic techniques for detecting very low densities of non-radiative species such as metastables or studying internal state distributions of molecules. It essentially consists of exciting an atom or molecule in a specific initial quantum state to a selected excited state, after which the fluorescence to a third state is detected. The intensity of the LIF signal depends on the density of the atoms in the initial state.

Especially for mercury LIF is a well suited technique because the transitions are in the visible regions of the electromagnetic spectrum which can be easily generated with dye lasers.

6.2 Principles of LIF

The technique of Laser Induced Fluorescence consists of exciting an atom in state \( p \) with laser light that matches the optical frequency of the transition from state \( p \) to \( q \), and observing the spontaneously emitted light originating from the laser excited atoms.

A laser photon of frequency \( \nu \) is absorbed by an atom in state \( p \) which then makes a transition to state \( q \) (see figure 6.1). The effect of the laser intensity \( I_L \)
The rate equation can now be given by:

\[
\frac{dn_x}{dt} = \sum_i A_{x_i} n_i - \delta_x n_x
\]

in which \( \delta_x \) is the statistical weight of level \( x \). If the laser is used in pulsed mode, the stimulated emission will not be an important depopulation factor after the end of the laser pulse. In this case the main depopulation mechanisms are spontaneous emission (fluorescence) and collisions with electrons or heavy particles (quenching).

The first term on the right-hand side describes the increase due to absorption of photons by atoms in state \( p \) while the second term describes the decrease due to spontaneous emission and stimulated emission. \( \sigma_p \) and \( \sigma_q \) are the cross sections for laser-induced excitation and stimulated emission and \( \epsilon_p \) and \( \epsilon_q \) are proportional to the Einstein coefficients \( B_{pq} \) and \( B_{qp} \) for absorption and stimulated emission, respectively. Because both Einstein coefficients are related via:

\[
B_{pq} = \frac{\epsilon_p}{\epsilon_q} = \frac{\epsilon_q}{\epsilon_p}
\]

equation (6.1) can be written as:

\[
\frac{dn_q}{dt} = \frac{\sigma_p}{\hbar \nu_p} n_p (n_q - g_q) - \frac{\sigma_q}{\hbar \nu_q} n_q = \frac{\sigma_p}{\hbar \nu_p} n_p (n_q - g_q)
\]

in which \( g_q \) is the statistical weight of level \( q \). If the laser is used in pulsed mode, the stimulated emission will not be an important depopulation factor after the end of the laser pulse. In this case the main depopulation mechanisms are spontaneous emission (fluorescence) and collisions with electrons or heavy particles (quenching). The rate equation can now be given by:

\[
\frac{dn_q}{dt} = -c_q (A_q n_q + Q n_q)
\]

on the population \( n_q \) of level \( q \) is given by the next differential equation [6]:

\[
\frac{dn_q}{dt} = -c_q (A_q n_q + Q n_q)
\]
6.3. EXPERIMENTAL SETUP FOR QL LIF MEASUREMENTS

where $\sum_{i \leq q} A_{qi}$ is the total rate of transitions to all levels with lower energy than $q$ due to spontaneous emission and $Q$ is the quenching rate. The total number of photons produced in a time interval $[t, t+dt]$ during the decay of $n_q$ is proportional to $\sum_{i \leq q} A_{qi} n_q(t)$.

### 6.2.1 Obtaining the density of the lower state

Again the number of photons produced due to the spontaneous transition from $q$ to $r$ is proportional to $A_{qr} n_q(t)$. From (6.1) we see that the population of $n_q$ after the laser pulse will be proportional to $n_p$ and according to (6.3), the observed fluorescence signal $S$ will be proportional to $n_q$. As a result the measured fluorescence (LIF signal) is proportional to

$$S \propto n_p. \quad (6.4)$$

If the LIF signal is measured at different positions a relative density profile can be determined.

### 6.3 Experimental Setup for QL LIF Measurements

In this section we will discuss the setup used to perform LIF measurements on the Philips QL-lamp. We will determine the density profile of the $6^3P_2$ state of mercury. Figure (6.2) gives a schematic view of the photon excitation from state $6^3P_2$ to state $7^3S_1$. In the experiments we will use an uncoated QL lamp in order to obtain the direct LIF signal, which is not influenced by a coating on the lamp.

A schematic view of the setup used for measuring LIF is shown in fig (6.3). First we need a laser system to produce photons of the right frequency (546.1 nm). Therefore we pump a tunable Dye laser with a YAG laser at 532 nm at 10Hz, the pump energy is 100 mJ per pulse of 7ns. The Dye laser is operated with fluoricine and is tuned to 546.1 nm.

By using two prisms the laser beam enters the QL-lamp as shown in more detail in fig(6.4). The detection of the LIF signal takes place at a 90° angle with the laser beam. The LIF signal is focused on the entrance slit (10µ) of a monochromator which selects the 404.7nm LIF signal from the light on the entrance slit (also containing the 435.8nm LIF signal and background light from the QL-lamp). By using a photo-multiplier (PMT) the LIF signal is made visible on a digital oscilloscope.

The QL-lamp is placed on a movable table. The table (and so the lamp) can be moved up and down which corresponds to the r-direction in fig(6.3) and fig(6.4) to change the position where the laser beam enters the lamp. The lamp can be moved in axial ($z$) direction along the laser beam, so that with fixed detection
6.4 Experimental results of LIF

The LIF signal obtained by the measurements is shown in appendix (B.1). Fig (6.5) shows the positions where the measurements took place. The LIF signal ($-V_{peak}$ PMT) represents the relative density profile of the $6^3P_2$ state of mercury as concluded from (6.4).

The LIF signals are obtained by scanning over all radial positions for certain values of $z$. The cold spot temperature of the lamp is $60^\circ C$. Because we want to link these data sets to each other, one axial scan is measured at radial position $r = 14$ mm it is shown in fig (6.6). The results of the radial scans are shown in fig (6.7 and 6.8).

The same experiments are done with a cold spot temperature of $80^\circ C$. The results are shown in appendix (B.1). Again we made one axial scan to link the radial scans to each another; it shown in fig (6.9). The results of the radial scans are shown in fig (6.10 and 6.11)
6.4. EXPERIMENTAL RESULTS OF LIF

Figure 6.3: Outline of the setup used for LIF.

Figure 6.4: Outline of the positioning of the laser beam and the detection position of the LIF signal, at a 90° angle of the laser beam. In the figure the laser beam is positioned in front of the ferrite core.
Figure 6.5: Outline of the positioning of the experiments.

Figure 6.6: Axial profile of the relative density of the $6^3P_2$ state at $r=14$ mm with cold spot temperature of $60^\circ C$. 
6.4. EXPERIMENTAL RESULTS OF LIF

Figure 6.7: Radial density profile of the $6^3P_2$ state of mercury for a cold spot temperature of $60^\circ C$ at two axial positions: (a) $z = 3\, \text{cm}$, (b) $z = 5\, \text{cm}$.

Figure 6.8: Radial density profile of the $6^3P_2$ state of mercury for a cold spot temperature of $60^\circ C$ at two axial positions: (a) $z = 7\, \text{cm}$, (b) $z = 9\, \text{cm}$.
CHAPTER 6. LASER INDUCED FLUORESCENCE MEASUREMENTS

Figure 6.9: Axial profile of the relative density of the $6^3P_2$ state at $r=14$ mm with cold spot temperature of $80^\circ C$.

Figure 6.10: Radial density profile of the $6^3P_2$ state of mercury for a cold spot temperature of $80^\circ C$ at two axial positions: (a) $z = 3$ cm, (b) $z = 5$ cm.
Figure 6.11: Radial density profile of the $^6P_2$ state of mercury for a cold spot temperature of 80°C at two axial positions: (a) $z = 7\text{cm}$, (b) $z = 9\text{cm}$.
6.5 Absorption of Radiation

In this section we will evaluate the radiation absorbed in a particular transition, from which we will try to determine the density of the absorbing state.

6.5.1 Absorption coefficient along a line-of-sight

When light passes through an absorbing medium, the energy absorbed in a distance $\delta x$ is proportional to both $\delta x$ and the incident flux. The equation

$$-\delta I_\nu(x) = k_\nu I_\nu(x) \delta x \quad (6.5)$$

defines the absorption coefficient $k_\nu$, expressed in $m^{-1}$. For a thickness $l$ of absorbing medium as shown in fig(6.12), the relation between incident and emerging intensities is found by integrating (6.5):

$$I_\nu(l) = I_\nu(0) \exp \left[- \int_0^l k_\nu dx \right], \quad (6.6)$$
in which the integral expresses the optical depth of the medium. If this is homogeneous, so the $k_\nu$ is independent of $x$, the optical depth is $k_\nu l$ and we have

$$I_\nu(l) = I_\nu(0) \exp \left[-k_\nu l \right]. \quad (6.7)$$
The absorption from an isolated spectral line is spread over a finite frequency range by the various broadening mechanisms. In most cases the optical depth is small, $k_{\nu}l << 1$. As a result (6.7) can be written as

$$I_{\nu}(l) = I_{\nu}(0)(1 - k_{\nu}l).$$

(6.8)

In this case $I_{\nu}(l)$ is proportional to $k_{\nu}$.

We will now derive the spectral integrated form. If $k_{\nu}$ is assumed much broader than $I_{\nu}$ we have

$$I(l) = I(0)[1 - lk_0],$$

(6.9)

in which

$$I(l) = \int_{0}^{\infty} I_{\nu}(l) d\nu,$$

and $k_0$ the absorption coefficient at the center of the line. In case of Doppler broadening $k_0$ is defined by

$$k_0 = \frac{\lambda_0^2 g_1 g_2 A_{21}}{8\pi g_1 \pi^{1/2} v_0},$$

(6.11)

If we now measure $I(0)$ and $I(l)$ the density of the absorbing state along the line of sight can be determined.

### 6.6 Absorption Measurements

For the absorption measurements we will use the same laser setup as for the LIF measurements. But now the laser beam will enter the QL-lamp from one side and leaves it from the other side of the lamp at $r = 0.8$ cm above the ferrite core of the lamp and at axial position $z = 5$ cm. As a result the laser beam travels through the assumed position of the maximum of density of the absorbing state in the lamp.

An outline of the setup is given by fig (6.13). After the beam travels through the lamp it will be detected by a photodiode. We will measure both the signal on the photodiode when the lamp is operational and when its off. This will be done for cold spot temperatures of 60°C and 80°C respectively. In order to measure any absorption the laser intensity has to be very weak, saturation should be avoided. The intensity should be weakened until the absorption reaches a constant factor, $I(l)/I(0)$ must be independent of $I(0)$. Further we assume a purely Doppler broadened line which is (much) broader than the laser line.
6.7 **Determination of the Density of the Hg $^6P_2$ state**

From the absorption measurements discussed in the previous section we will now try to derive the density of the $^6P_2$ state of mercury.

From the LIF measurements we notice the highest density at $r = 0.8$ cm above the core. In a first approximation most of the absorption will take place near the core over a length of approximately 1 cm ($l = 1$ cm). The result of the experiments can be seen in table (6.1): $I$ is the intensity of the laser beam measured by the photodiode, $I_0$ is the intensity measured when the QL lamp is not operational, $I(l)$ is the intensity of the laser beam after traveling through the operational QL-lamp.

<table>
<thead>
<tr>
<th>Cold-spot $T$ (°C)</th>
<th>$I_0$</th>
<th>$I(l)$</th>
<th>$I$ (cm)</th>
<th>$\lambda$ (nm)</th>
<th>$A_{pq} \times 10^8$ (s$^{-1}$)</th>
<th>$T_p$ (K)</th>
<th>$g_1$</th>
<th>$g_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>4.7</td>
<td>3.8</td>
<td>1</td>
<td>546.1</td>
<td>0.418</td>
<td>800</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>80</td>
<td>8.1</td>
<td>6.1</td>
<td>1</td>
<td>546.1</td>
<td>0.418</td>
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</table>

Table 6.1: Results of the absorption measurements for cold spot temperatures of 60°C and 80°C.

From equations (6.9), (6.11) and the data from table (6.1) we obtain the densities of the absorbing state $^6P_2$ which are represented in table (6.2).
6.8 Comparing QL-simulations with Measurements

Now we will compare the values for the $6^3P_2$ state obtained by LIF and the absorption measurements with the QL simulation described in section (5.4.2).

The density obtained by absorption measurements seems a bit too low in comparison with the simulation results. The simulated density of the metastable state is about $10^{18} \text{ m}^{-3}$ as can be seen from fig (5.12). Of course the modeling result can be too high but we must also take into account the assumptions made in the absorption measurements. At first it is assumed that the width of the laser beam is smaller than the Doppler broadening of the line. The experiments show that absorption can be measured however further experiments are needed. The method described by J. Jonkers [4] where a diode laser is used to scan the absorption at wavelength should be considered.

Both the relative density profiles measured with LIF and those obtained by the simulation are depicted in fig (6.14). The picture shows the radial profiles at the axial position where the density reaches its top value. Both profiles show a maximum near the core. Compared to the measurements, the maximum in density of the simulation is situated closer to the core and is higher. In the QL simulation a uniform escape factor has been used, from the cylindrical QL simulation we know that the escape factor near the core will be much higher than the the assumed $10^{-2}$. A higher escape factor near the core will cause the density to drop so that the maximum in density will occur at greater distance of the core, as is predicted by the experiments. This simulation should be performed in the future to check this explanation.
Figure 6.14: Radial profile of the relative density of the $6^3 P_2$ state. Measured and simulated values.
Chapter 7

Conclusions

The collisional radiative model for mercury is extended to six independent levels in order to treat the important radiative transition within PLASIMO. The particle source term can be expressed in a production term and a destruction factor, which makes an implicit treatment of the source term possible. By using J-coefficients it is easy to obtain these terms from the collisional radiative model. Before the implicit treatment of the particle source terms the six level CRM could not be used for TL and QL simulation in PLASIMO. Because of the implicit treatment the six level model can now be used. The new treatment is so stable that relaxation is hardly needed which highly improves convergence speed.

Radiation transport can be dealt with in two different ways: it can be treated as a transport term by expressing the radiation transport in term of diffusion of the resonance state. In this diffusion model the time between emission and (re)absorption of a photon is mostly determined by the duration of the interaction and not by the time between collisions, as is the case with material particles. The problem in using diffusion models is to obtain an accurate diffusion coefficient or mean free path length of the photons.

An other approach solves the radiation transport by the introduction of an escape factor. The source term of the excited state from which the radiation occurs can then be expressed by a net emission.

The escape factor can now be calculated numerically in PLASIMO. The result of the calculation of the escape factor on the axis of an infinite cylinder agrees with Holstein's analytical solution for large optical depths. The numerical calculation of the escape factor can also be done for off-axis positions. The effect on TL simulations can especially be seen in the density profile of the excited state from which the radiation occurs.

The calculation of the escape factor for a QL simulation consumes a lot of simulation time, but simulations on simplified QL geometries reveal the importance of the escape factor calculation. The radiative flux density on the core of the QL-lamp can also be calculated.

From Laser Induced Fluorescence measurements the density profile of the
metastable $6^3P_2$ state of mercury in the QL-lamp is measured. The measured profiles show a similar shape as the profiles obtained by QL simulations with PLASIMO. The absolute values are too low by a factor of two. This may be due to uncertainties in the assumptions made to interpret the measurements. In the simulations the position of the maximum in intensity is closer to the core than follows from the LIF measurements.
Appendix A

Flux density

A.1 Determining the Escape Factor from the Flux definition

We will show how the escape factor can be derived from the definition of the flux, by making use of the photon continuity equation,

\[(\nabla, \Gamma) = S\]  \hspace{1cm} (A.1)

in which the flux \(\Gamma\) given by (3.44) and (3.45)

\[\Gamma(r) = \int_{V'} n_p(r') A_{pq} T(\rho) \frac{\rho}{4\pi \rho^3} d^3 r'\]  \hspace{1cm} (A.2)

The left hand side of equation (A.1) can now be write as follows:

\[(\nabla, \Gamma) = A_{pq} \int_{V'} n_p(r') (\nabla, T(\rho) \frac{\rho}{4\pi |\rho|^3}) d^3 r'\]  \hspace{1cm} (A.3)

where we used \((\nabla, f \nu) = f(\nabla, \nu) + (\nabla f, \nu)\). Then further we have,

\[(\nabla, \Gamma) = -A_{pq} \int_{V'} n_p(r') (\nabla, T(\rho) \frac{\nabla \rho^{-1}}{4\pi}) d^3 r'\]  \hspace{1cm} (A.4)

By using a theorem of Green

\[\nabla^2 \frac{1}{4\pi |\rho|} = -\delta(\rho)\]  \hspace{1cm} (A.5)

one obtains

\[(\nabla, \Gamma) = -A_{pq} \int_{V'} n_p(r') \{-T(\rho) \delta(\rho) + (\nabla T(\rho), \rho^{-1})\} d^3 r'\]  \hspace{1cm} (A.6)
when we use $T(0) = 1$ and $(\nabla T(\rho), e_\rho) = dT(\rho)/dr = -dT/d\rho$

$$S = A_{pq} n(r) - A_{pq} \int_{V'} n_p(r') \frac{\partial T(\rho)}{\partial \rho} \frac{1}{4\pi \rho^2} d^3r'.$$  \hspace{1cm} (A.7)

From (A.1) and (3.39) we see that $(\nabla, \Gamma)$ equals local production $\Lambda(r)n_p(r)A_{pq}$ from which we again obtain the escape factor definition:

$$\Lambda(r) = 1 - \frac{\int_{V'} n_p(r') \frac{\partial T(\rho)}{\partial \rho} \frac{1}{4\pi \rho^2} d^3r'}{n_p(r)}$$  \hspace{1cm} (A.8)

which is a nice way of validating the previous definitions.
Appendix B

Results of LIF measurements

B.1 The measured LIF signal at different positions

In table (B.1) the signal (-$V_{peak}$ PMT) represents the relative density profile of the $6^3P_2$ state of mercury as concluded from (6.4).

The same experiments are done with a cold spot temperature of 80°C the results are shown in table (B.2)
## APPENDIX B. RESULTS OF LIF MEASUREMENTS

### Table B.1: The LIF measurements for cold spot temperature 60°C, the signal is represented in arbitrary units.

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### Table B.2: The LIF measurements for cold spot temperature 80°C, the signal is represented in arbitrary units.

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Appendix C

Code documentation

C.1 Numerical Escape Factor Calculation

The function \texttt{real calc\_dT(real k\_0,real r)} returns the value of \( \frac{\partial T}{\partial \rho} \) for particular values of \( k_0\rho \). A fit \( f(k_0\rho) \) is performed with a fourth-order polynomial and split-up in domains because of the rapid changes in \( \frac{\partial T}{\partial \rho} \) for increasing \( k_0\rho \). Fig (C.1) shows the fit function \( f(k_0\rho) \) which can be obtained from the fit-coefficients in \texttt{real calc\_dT(real k\_0,real r)}

\[
\frac{\partial T(\rho)}{\partial \rho} = -k_0 \int_{-\infty}^{\infty} \frac{1}{\pi^{1/2}} \exp \left[-k_0\rho \exp -x^2\right] dx = -k_0 f(k_0\rho) \quad \text{(C.1)}
\]

![Figure C.1: The function f(k_0\rho) for different values of k_0\rho](image_url)
#include "plasimo.h"

real calc_dT(real k_0, real r)
{
    int order = 0;
    real a[7];
    real t = k_0 * sqrt(r);

    if (t <= 3.0) {
        a[0] = 3531.33876;
        a[1] = -2833.18608;
        a[2] = 1114.0265;
        a[3] = -238.17204;
        order = 4;
    }
    else if (t <= 8) {
        a[0] = 2126.96773;
        a[1] = -1073.06922;
        a[3] = -20.91634;
        a[4] = 0.76319;
        order = 4;
    }
    else if (t <= 15) {
        a[0] = 441.68382;
        a[1] = -116.51188;
        a[2] = 12.33435;
        a[3] = -0.60036;
        a[4] = 0.01117;
        order = 4;
    }
    else if (t <= 40) {
        a[0] = 48.87063;
        a[1] = -5.23591;
        a[2] = 0.23425;
        a[3] = -0.00486;
        a[4] = 3.83362e-5;
        order = 4;
    }
    else if (t <= 80) {
        a[0] = 12.146;
        a[1] = -0.58135;
        a[2] = 0.01099;
        a[4] = 3.20228e-7;
        order = 4;
    }
}
The following short function returns the density of the excited state at position \( r' \) divided by the local density of the excited state at position \( r \). As a result 
\[
\text{dens}_p = \frac{n_{a(r')}}{n_p(r)}.
\]
The integers \( j \) and \( j_a \) denote the closest grid-point (Plasimo Grid) to position \( r' \) and \( r \), respectively.

```c
real get_dens(State *upper_state, int i, int j, int j_a)
{
    return upper_state->dens[i][j_a] / upper_state->dens[i][j];
}
```

Here the actual procedure for calculating the escape-factor starts. We will use cylindrical-coordinates. With the code below we will calculate the escape factor for different radial positions in an infinite cylinder. In the procedure \( r \) will be the radial coordinate, \( z \) is the axial coordinate,
\( R,Z \) define the boundaries of the grid.
\( dr,dz \) denote the (equidistant) grid-spacing.

```cpp
order=4;}
else if (t<=120) {
    a[0] = 3.61534;
    a[1] = -0.12076;
    a[2] = 0.00156;
    a[4] = 2.01305e-8;
}
else if (t<=350) {
    a[0] = 0.11647;
    a[1] = -0.0012;
    a[3] = -1.66872e-8;
}
else {
    a[0] = 0.05264;
    a[1] = -1.61049e-4;
    a[2] = 2.10162e-7;
    a[3] = -1.35051e-10;
    a[4] = 3.50737e-14;
}
return k_0*polynomial( a, order, t)*0.0002;
}```
Because of rapid changes in $\frac{\partial t}{\partial \rho}$ for small values of $\rho$ we will need a fine grid near $r = 0$ and $z = 0$:

$r_{\text{o}}, z_{\text{o}}$: the boundary of the narrow grid.

$\Delta r, \Delta z$: the grid-spacing.

$k_0$ is the absorption at line-center.

$E$ will be the rhs of (4.26), which has to be calculated.

$j_a$ determines the position of $r$ on the plasma grid.

If we want to calculate the escape factor for different radial positions we have to design a special grid in which the integration in $\phi$ direction will result in a factor. This grid is based upon circles or parts of circles with different radii, which originate at $r_a$ from the axis of the cylinder. The radius of the circles will equal $r$. $r$ will be limited between 0 and $R + r_a$ where $R$ is the radius of the cylinder and $r_a$ the radial position where the escape factor as to be calculated.

The grid used is shown in fig(C.3).

![Grid Diagram](image)

**Figure C.2:** This is not a computational grid, the figure shows how the $\phi$ integration is handled.

In this grid $\rho$ is still defined by $Q_{\rho \phi} = \text{SQR}(r) + \text{SQR}(z)$. Beware that the axis of the cylinder is no longer the symmetric axis of the coordinate system. The integration in $\phi$ direction will only take place for the part of the circle within the cylinder. This is depicted in fig(C.2) So the integration will result in a factor between 0 and $2\pi$ derived by:

\[
\phi = \arccos \left( \frac{R^2 - r_a^2 - r^2}{-2rr_a} \right) \quad \text{(C.2)}
\]
Figure C.3: *Grid used to calculate the escape-factor for different radial positions*
void calc_escape(Geometry dim, Rmat Lambda, State *lower_state,
State *upper_state, real wavelength, real A_pq, real M_mol, int g_upper, Rmat at, int i)
{
    int k, l, p, q, m, n, j, a, j;
    real rhoQ, E, k_0, s;
    real dT;
    real Z, R, z, r, dz, dr, ddz, ddr, z_0, r_0, r_a;
    int i_0, i_b, h, h1;
    real phi, phi_0, alpha, alpha_a, c;
    real dens_p;
    real E_temp1, E_temp2;
    Rvec E_temp0;
    FILE *fp;

    printf("Start calculating escape-factor \n");

    R = dim.x2max;
    Z = 2*R;
    wavelength* = 1.0e-9;
    M_mol* = 1.0e-3;

    z_0 = 1.0e-5; r_0 = 2.0e-5;
    dz = z_0; dr = r_0/2.0;
    q_max = ceil((r*R)/dr);
    Temp_0 = dvector(0, q_max);

    The escape factor will be calculated at every PLASIMO grid point \( j \), that
    represents the radial coordinate \( \) in the plasimo grid.
    for (j=0; j<= dim.nj; j++)
    {
        r_a = dim.y[i][j];
        c = dim.y[i][0];

        c \ is \ the \ radius \ of \ the \ ferrite \ core \ if \ there \ is \ one. \n
        if (r_a < 1.0e-6) r_a = 0.0;
        E = 0.0;

        m = 250; n = 250;

        \( n \) \ and \( m \) \ give \ the \ number \ of \ grid \ points \ of \ the \ fine \ grid \ near \( r_a \) \ in \ respectively \( r \)
C.1. NUMERICAL ESCAPE FACTOR CALCULATION

and z direction.
\[ p = \text{ceil}(Z/dz); \quad q = \text{ceil}((R+r_a)/dr); \]
\[
r_a = (dr*q) - R;
\]
\[ \text{if} \ (r_a < 1.0e-6) \ r_a = 0.0; \]
\[ h = \text{dim}.x2\text{max}; \]
\[ s = \text{SQR}(R) + \text{SQR}(r_a); \]
\[ i_0 = \text{ceil}(z_0/dz); \]
\[ ddz = z_0/m; \quad ddr = r_0/n; \]

OK now we are going to calculate the amount or radiation captured within a volume element denoted by \( r_a \) and \( z = 0 \) from within its direct neighborhood, using grid spacing \( ddz \) and \( ddr \). So \( E \) will be the rhs of (4.26) for the part of the volume were we need a fine grid.

```plaintext
/*--------fine grid near \( r_a \)--------*/
```

Here we determine \( k_0 \) in the case of Doppler broadening (3.5) assuming \( k_0 \) equals \( k_0 \) local.

\[ k_0 = 0.00549g_{\text{upper}}\text{power(wavelength,3)} * A_{pq} \text{sqrt(M}_{\text{mol}}; \]
\[ k_0 = ( ( \text{lower state} \rightarrow \text{dens[i][j]}/\text{sqrt(at[i][j])} ) ) ; \]

```plaintext
for (l=0; l<n; l++) {
    r = (l+0.5)*ddr;
    if (r <= (R-r_a)) phi = PI;
    else
        phi = acos((s+SQR(r))/(2*r*r_a));
    for (k=0; k<m; k++) {
        z = (k+0.5)*ddz;
        rhoQ = SQR(r) + SQR(z);
        dT = calc_dT(k,0,rhoQ);
        E += dT/rhoQ*r*ddz*ddr*(phi)/PI;
    }
}
```

And now we are going to calculate the amount or radiation capture at a volume element denoted by \( r_a \) and \( z = 0 \) form within the total volume excluding the direct neighborhood, using grid spacing \( dz \), and \( dr \). Then \( E \) will be the rhs of (4.26) for the total volume!

```plaintext
/*--------normal grid--------*/
```
Here $k_0$ in the average $k_0$ in case of Doppler broadening (3.5). $k_0$ is determined by the gas temperature and groundstate density at center of the plasma and the boundary of the plasma. First the summation over the $r$ direction is done because the density and $\phi$ calculations are not dependent on $Z$. As a result they are only calculated $q$ times instead of $q \times p$ times, where $q$ and $p$ are the number of grid point in respectively $r$ and $z$ direction. 

$$k_0 = 0.00549 \times g_{upper}\times power(\text{wavelength}, 3) \times A_{pq} \times \sqrt{M_{mol}};$$

$$k_0^* = 0.5 \times \left( \frac{(\text{lower}_{\text{state}} \rightarrow \text{dens}[i][0]/\sqrt{a_{i}[0]}) + (\text{lower}_{\text{state}} \rightarrow \text{dens}[i][\text{dim.nj}]/\sqrt{a_{i}[\text{dim.nj}])}}{} \right);$$

```plaintext
for (l=0; l<q; l++) {
    r=(l+0.5)*dr;
    if ((r<=(r_a-c)) || (c==0.0)) phi_0=0.0;
    else if (r<sqrt(SQR(c)+SQR(r_a)))
        phi_0=acos((-SQR(c)+SQR(r_a)+SQR(r))/(2*r*r_a));
    else
        phi_0=asin(c/r_a);

    if (r<=(R-r_a)) phi=PI;
    else phi=acos((s+SQR(r))/(2*r*r_a));

    if (phi>phi_0)
        The only problem occurring due to the new grid is the determination of the position on the plasimo grid. For every point with coordinate $r$ we need to know the matching radius $a_{fig}$ (C.2) which originates at the radius of the cylinder. First we will define the $\phi$ integration in $h$ parts at which we will assume an uniform excited density. For each value of those parts defined by $\alpha$ the matching radius $a$ can be defined by

$$a = \sqrt{r^2 + r_a^2 - 2rr_a \cos(\alpha)} \quad (C.3)$$

in which $\alpha$ is $\frac{h}{h} \times h1$ and $h1 = 0..h$; Now we know the matching radius $a$ the next task is to obtain the matching PLASIMO grid point index number, which will be denoted by $j_a$. If we determined $j_a$, get_dens() can be called to obtain the relative density of the excited state.

```
while ((a>((y[i][j_a]+(sns[j_a]*l2[j][j_a]*0.5)))
&& (j_a<dim.nj)) j_a++;
    dens_p+=get_dens(upper_state,j,j_a)/h;
}
E_temp1=dens_p*r*dr*(phi-phi_0)/PI;
E_temp2=0.0;

The next part of the calculation uses the escape factor calculation on the axis of the cylinder as input in the calculation of a non axial escape factor this is done to speed up the calculation, in the case that the escape factor has to be calculated at every PLASIMO grid point denoted by j.

if ((j==0) || (r>(R+dim.y[i][j-1]))) {
    E_temp0[i]=0.0;
    if (r<r_0) Lb=i_0; else i_0=0;
    for (k=Lb; k<p; k++) {
        z=(k+0.5)*dz;
        rhoQ=SQR(r)+SQR(z);
        dT=calc_dT(k_0,rhoQ);
        E_temp0[i]+=(dT/rhoQ)*dz;
    }
    E+=E_temp1+E_temp0[i];
}

/* ------- Now 1-E is the escape factor ------- */

fp=fopen("escape.txt","a");
if (1-E<=0.0) E=1;
fprintf(fp," %1.5e ",r_a);
fprintf(fp," %e 
",1-E);
fclose(fp);

printf(" r' , Lambda %e %e \n",r_a,1-E);
Lambda[i][j]=1-E;
}
free_dvector(E_temp0,0,q_max);
C.2 Numerical Calculation of the Flux

The function `real calc_T(real k_0, real r)` returns the value of $T$, the transmission, for particular values of $k_0\rho$.

```c
#include "plasimo.h"

real calc_T(real k_0, real r)
{
    int order = 0;
    real a[7];
    real t=k_0*sqrt(r);
    real log_coef;

    if (t<=4.0) {
        a[0] =-6.47562e-6;
        a[1] =-0.307;
        a[2] =0.0165;
        a[3] =0.00159;
        a[4] =-2.02469e-4;
        order=4;
    }
    else if (t<=10.0) {
        a[0] =0.05348;
        a[1] =-0.36176;
        a[2] =0.03785;
        a[3] =-0.00218;
        a[4] =5.18453e-5;
        order=4;
    }
    else if (t<=20.0) {
        a[0] =-0.39676;
        a[1] =-0.18728;
        a[2] =0.0118;
        a[3] =-4.02682e-4;
        a[4] =5.36997e-6;
        order=4;
    }
    else if (t<=40.0) {
        a[0] =-1.10385;
        a[1] =-0.04387;
        a[2] =6.47331e-4;
    }
    return log_coef;
}
```
C.2. NUMERICAL CALCULATION OF THE FLUX

\[ a[4] = 8.10911 \times 10^{-8}; \]
order=4;

else if (t<=100.0) {
    a[0] = -0.94143;
    a[1] = -0.05128;
    a[2] = 5.88971 \times 10^{-4};
    order=4;
}

else {
    a[0] = -2.44993;
    a[1] = -0.00204;
    a[2] = 3.16325 \times 10^{-6};
    order=4;
}

log_coef polynomial( a, order, t);
return \exp(\log10*\log_coef);
}

void calc_jlux(Geometry dim, Rmat Lambda, State *lower_state,
State *upper_state, real wavelength, real A_pq, real M_mol, int g_upper,
int i, Rmat at)
{

    int k,j,p,q,m,n,j,a,j;
    real rhoQ,E,k,s;
    real T;
    real Z,R,z,r,dz,dr,ddz,ddr,z_0,r_0;
    int i_0,i,b,h,h1,i,a;
    real r,a;
    real phi,phi_0,alpha,dalpha,a,c;
    real dens_p;
    FILE *fp;
    real P,S,V,PV,Z_s,Z_min,A,B,AB;
    int m_min;

    printf(" %d ",dim.nj);
printf("Start calculating flux \n");

R=dim.y[i][dim.nj];
Z=dim.x1max;
Z_min=dim.x[ dim.begin][dim.begin];
Z_s=dim.x[i][dim.begin];

wavelength* =1.0e-9;
M_mol* =1.0e-3;

c =dim.y[i][0];
r_a=R;

when \( r_a = c \) the flux on the ferrite core can be calculated.

if \((r_a < 1.0e-6) r_a = 0.0;\)
E=0.0; V=0.0;
m=250; n=250;
h=dim.nj;

z_0=1.0e-5; r_0=2.0e-5;

dz=z_0; dr=r_0/2.0;

p=ceil((Z-Z_min)/dz); q=ceil((R+r_a)/dr);

r_a=(dr*q)-R;
if \((r_a < 1.0e-6) r_a = 0.0;\)
s=SQR(R)-SQR(r_a);
i_0=ceil(r_0/dr);
ddz=z_0/m; ddr=r_0/n;

The next part will determine the \( n \) vector.
if \((r_a == R) \&\& (i!=0)) \{
A=dim.x[i][dim.nj]-dim.x[i-1][dim.nj];
B=dim.y[i][dim.nj]-dim.y[i-1][dim.nj];
AB=SQR(A)+SQR(B);
A*=1/sqrt(AB); B*=1/sqrt(AB); \}
else if \((r_a == R)) \{
A=-dim.x[i][dim.nj]+dim.x[i+1][dim.nj];
B=-dim.y[i][dim.nj]+dim.y[i+1][dim.nj];
AB=SQR(A)+SQR(B);
For a cylinder the \( \mathbf{n} \) vector will be \((-1, 0, 0)\). The inner product \((\mathbf{p}, \mathbf{n})\) is defined by

\[
(\mathbf{p}, \mathbf{n}) = \frac{A r \cos \phi + B z}{\sqrt{r^2 + z^2}}
\]

where \( \sqrt{r^2 + z^2} = |\mathbf{p}|\).

\[
\text{C.2. NUMERICAL CALCULATION OF THE FLUX}
\]

\[
A^* = \frac{1}{\sqrt{AB}}; \quad B^* = \frac{1}{\sqrt{AB}}; \\
\text{else} \\
\{ A=1; \quad B=0; \}
\]

\[
\text{For a cylinder the } \mathbf{n} \text{ vector will be } (-1, 0, 0). \text{ The inner product } (\mathbf{p}, \mathbf{n}) \text{ is defined by}
\]

\[
(\mathbf{p}, \mathbf{n}) = \frac{A r \cos \phi + B z}{\sqrt{r^2 + z^2}}
\]

where \( \sqrt{r^2 + z^2} = |\mathbf{p}| \).
E+=dens_p*A_pq*(T/(rhoQ*sqrt(rhoQ)*PI))*
    r*ddz*ddr*(A*r*(sin(phi)-sin(phi_0))+B*z*(phi-phi_0))/2;

V+=r*ddr*ddz*2*phi;
}
}

/* --------normal grid---------*/

k_0=0.00549*g_upper*power(wavelength,3)*A_pq*sqrt(M_mol);
k_0* =0.5*( (lower_state->dens[i][0]/sqrt(at[i][0]))+
    (lower_state->dens[i][dim.nj]/sqrt(at[i][dim.nj])) )

for (k=0; k<p; k++) {
    z=(k+0.5)*dz;
    z-=Z_s;

    i_a=0;
    while ((z>(dim.x[i_a][dim.nj]-Z_s)) && (i_a<dim.nn)) i_a++;
    R=dim.y[i_a][dim.nj];
    q=ceil((R+r_a)/dr);

    if (((z<Z_0) && (z>-Z_0)) i_b=i_0; else i_b=0;
    for (l=i_b; l<q; l++) {

        r=(l+0.5)*dr;
        if ((r<=(r_a-c)) || (c==0.0)) phi_0=0.0;
        else if (r<sqrt(-SQR(c)+SQR(r_a)))
            phi_0=acos((-SQR(c)+SQR(r_a)+SQR(r))/(2*r*r_a));
        else
            phi_0=asin(c/r_a);

        if (r<(R-r_a)) phi=PI;
        else phi=acos((SQR(r)-s)/(2*R*r));

        if (phi>phi_0)
        {
            dalpha=(phi-phi_0)/h;
            dens_p=0.0;
            for (h1=0; h1<h; h1++) {

                ...
            }
        }
    }
}

if (k==0) {

    ...
}
C.2. NUMERICAL CALCULATION OF THE FLUX

\[ j_{a}=0; \]
\[ \alpha=(h1+0.5)\times d\alpha+\phi_0; \]
\[ a=\sqrt{SQR(r)+SQR(r_a)-2*r_a*r*\cos(\alpha)}; \]
\[ \text{while} \ ((a>(dim.y[i_a][j_a]+(dim.sns[j_a]*dim.l2[i_a][j_a]*0.5))) \ \&\& \ (j_a<dim.nj)) \ j_a++; \]
\[ \text{dens}_{p}+=\text{upper.state} \to \text{dens}[i_a][j_a]/h; \]
\[ \text{rhoQ}=SQR(r)+SQR(z); \]
\[ T=\text{calc}_T(k_0,\text{rhoQ}); \]
\[ E+=\text{dens}_{p}A_{pq}*(T/(\pi*\text{rhoQ}^{\sqrt{\text{rhoQ}}}))\times r \]
\[ \times dr \times dz \times (A_{pq}(\sin(\phi)-\sin(\phi_0))+B_{z}(\phi_0))/2; \]
\[ V+=r*dr*dz*2*\phi; \]

\[ \text{This will finish the flux calculation.} \]
\[ \text{Now the total photon production} \ P \ \text{will be calculated.} \]

\[ P=0.0; \]
\[ PV=0.0; \]
\[ m=\text{dim.nj}; \]
\[ /* \text{now valid for non-equidistant \ PLASIMO grid}! */ \]
\[ \text{for} \ (j=0; j<=m; j++) \ \{ \]
\[ dr=\text{dim.sns}[j]\times \text{dim.l2}[2][j]; \]
\[ r=\text{dim.y}[2][j]; \]
\[ \text{printf("r %e \n",r);} \]
\[ P+=r*2*\pi*A_{pq}*\text{upper.state} \to \text{dens}[2][j]*dr*\text{Lambda}[2][j]; \]
\[ \}
\[ PV+=r*2*\pi*dr*Z; \]
\[ \} \]

\[ \text{At last the total flux through the suffice defined at} \ r_a \ \text{will be calculated.} \]
\[ S=0; \]
\[ S=E*2*\pi*r_a; \]
\[ \} \]
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